# Schrieffer-Wolff Transformation: Relation of Anderson and Kondo Models

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## Contents



## 1 Schrieffer-Wolff transformation

Here, we first give a general derivation of the Schrieffer-Wolff transformation [1–3]. We will focus on the derivation of the transformation from a Green's function approach, which is analogous to the $T$-matrix method.

Consider two subspaces $A$ and $B$ described by the following Hamiltonian,

$$H = H_0 + \Sigma. \tag{1.1}$$

Here,

$$H_0 = \begin{pmatrix} H_A & \\ & H_B \end{pmatrix} \tag{1.2}$$

represents the two *uncoupled* subspaces $A$ and $B$ and is thus block-diagonal. The hybridization of the two subspaces is off-diagonal and given by

$$\Sigma = \begin{pmatrix} & V_{AB} \\ V_{BA} & \end{pmatrix}. \tag{1.3}$$

The main goal of the Schrieffer-Wolff transformation is to find an effective Hamiltonian which is block-diagonal by performing a perturbative expansion in $\Sigma$, *i.e.*

$$H = \begin{pmatrix} H_A & V_{AB} \\ V_{BA} & H_B \end{pmatrix} \mapsto \tilde{H} = \begin{pmatrix} \tilde{H}_A & 0 \\ 0 & \tilde{H}_B \end{pmatrix}, \tag{1.4}$$

in which $\tilde{H}_A$ and $\tilde{H}_B$ are effective Hamiltonians for subspaces $A$ and $B$. One then projects to a single subspace, with the effective Hamiltonian now containing contributions from fluctuations from the other subspace, which enter via the off-diagonal coupling $\Sigma$.

We now want to use this $T$-matrix expansion to derive an effective Hamiltonian for a given subspace. Let us derive the effective Hamiltonian $\tilde{H}_A$ without loss of generality. Consider the Green's function

$$\mathcal{G}(i\omega) = (i\omega - H)^{-1} \equiv \begin{pmatrix} \tilde{\mathcal{G}}_A(i\omega) & \mathcal{F}(i\omega) \\ \mathcal{F}^\dagger(i\omega) & \tilde{\mathcal{G}}_B(i\omega) \end{pmatrix}. \tag{1.5}$$

We are interested in projecting to an effective Hamiltonian $\tilde{H}_A$ for subspace $A$. We define an effective Hamiltonian for the $A$ subspace by

$$\tilde{\mathcal{G}}_A(i\omega) \equiv (i\omega - \tilde{H}_A(i\omega))^{-1}. \tag{1.6}$$

As shown in Appendix A, it follows that

$$\tilde{\mathcal{G}}_A(i\omega) = (i\omega - H_A - V_{AB}\mathcal{G}_B(i\omega)V_{BA})^{-1} \tag{1.7}$$

in which

$$\mathcal{G}_B(i\omega) = (i\omega - H_B)^{-1} \tag{1.8}$$

is the free Green's function for subsystem $B$. It follows that the effective Hamiltonian is given by

$$\boxed{\tilde{H}_A(i\omega) = H_A + \underbrace{V_{AB}\mathcal{G}_B(i\omega)V_{BA}}_{\equiv \Delta H_A}.} \tag{1.9}$$

This is a generalized second-order perturbation theory which contains the effects of the fluctuations in subsystem $B$ in subsystem $A$. This is in fact equivalent to the Schrieffer-Wolff transformation, which instead derives the effective Hamiltonian using a canonical transformation and then projects to subspace $A$[1]. For higher-order corrections, one can consider corrections to $\mathcal{G}_B(i\omega)$ coming from the self-energy terms. An important note here is that $i\omega = E + i\eta$ refers to the energy of the *entire* system (both $A$ and $B$ subsystems).

### 1.1 Example: Diagonal subspaces

Suppose that the two subspaces are diagonal, satisfying $(H_A)_{aa'} = E_a^A \delta_{a,a'}$ and $(H_B)_{bb'} = E_b^B \delta_{b,b'}$. For clarity, we use subscripts $a$ and $b$ to denote the degrees for subsystems $A$ and $B$ respectively. It follows that

$$[\mathcal{G}_B(i\omega)]_{b,b'} = \frac{\delta_{b,b'}}{i\omega - E_b^B}. \tag{1.10}$$

As such, the effective Hamiltonian for subsystem $A$ is given by

$$[\tilde{H}_A]_{a,a'} = [H_A]_{a,a'} + \sum_b \frac{[V_{AB}]_{a,b}[V_{BA}]_{b,a'}}{i\omega - E_b^B}, \tag{1.11}$$

which contains the summation over intermediate states with energy $E_b^B$. This may also be rewritten as

$$\langle a|\tilde{H}_A|a'\rangle = \langle a|H_A|a'\rangle + \sum_b \frac{\langle a|V_{AB}|b\rangle\langle b|V_{BA}|a'\rangle}{i\omega - E_b^B}. \tag{1.12}$$

Here, we see that we are projecting to intermediate states $\{|b\rangle\}$ of subsystem $B$.

## 2 Application: Relation of Anderson and Kondo Hamiltonians

Using the effective Hamiltonian in Eq. (1.9), we derive the Kondo model from the Anderson model. Consider the Anderson model,

$$H_{\text{Anderson}} = H_{\text{itinerant}} + H_{\text{local}} + H_{\text{hybridization}}. \tag{2.1}$$

Here, $H_{\text{itinerant}}$ describes itinerant electrons, $H_{\text{local}}$ localized states, and $H_{\text{hybridization}}$ the hybridization between the two. These correspond to $H_A$, $H_B$, and $\Sigma$ respectively in Eq. (1.1). We consider the simplest case: spin-degenerate itinerant bands and localized $f$-electrons,

$$H_{\text{itinerant}} = \sum_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c_{\mathbf{k},\sigma} \tag{2.2a}$$

$$H_{\text{local}} = \xi_f \sum_{\mathbf{r},\sigma} f^\dagger_{\mathbf{r},\sigma} f_{\mathbf{r},\sigma} + U \sum_{\mathbf{r}} n_{f,\uparrow} n_{f,\downarrow} \tag{2.2b}$$

For a given orbital of $f$-electrons, the state can be unoccupied ($E_{\text{local}} = 0$), singly-occupied ($E_{\text{local}} = \xi_f$), or doubly occupied ($E_{\text{local}} = 2\xi_f + U$). The hybridization of itinerant and local electron moments is given by

$$H_{\text{hybridization}} = V + V^\dagger \tag{2.3}$$

in which

$$V = \sum_{\mathbf{k},\mathbf{r},\sigma} \left( v_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} f_{\mathbf{r},\sigma} + v^*_{\mathbf{k}} f^\dagger_{\mathbf{r},\sigma} c_{\mathbf{k},\sigma} \right) \tag{2.4}$$

is the spin-independent off-diagonal coupling. Here, we keep both parts such that $V$ is Hermitian. We assume weak coupling, treating $H_{\text{hybridization}}$ perturbatively.

From Eq. (1.11), the effective Hamiltonian for itinerant electrons is given by

$$[\tilde{H}_{\text{itinerant}}]_{a,a'} = [H_{\text{itinerant}}]_{a,a'} + \sum_{b=0,1,2} \frac{[V]_{a,b}[V^\dagger]_{b,a'}}{i\omega - E^f_b} \tag{2.5}$$

We note that subscripts $a$ and $a'$ refer to many-body states of subsystem $A$. Using the form of the coupling, we have

$$\begin{aligned}
[\Delta H_{\text{itinerant}}]_{a,a'} &= \langle a| \sum_b \sum_{\mathbf{k},\mathbf{r},\sigma;\mathbf{k}',\mathbf{r}',\sigma'} \frac{\left( v_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} f_{\mathbf{r},\sigma} + v^*_{\mathbf{k}} f^\dagger_{\mathbf{r},\sigma} c_{\mathbf{k},\sigma} \right) P_b \left( v_{\mathbf{k}'} c^\dagger_{\mathbf{k}',\sigma'} f_{\mathbf{r}',\sigma'} + v^*_{\mathbf{k}'} f^\dagger_{\mathbf{r}',\sigma'} c_{\mathbf{k}',\sigma'} \right)}{i\omega - E^f_b} |a'\rangle \\
&= \langle a| \sum_b \sum_{\mathbf{k},\mathbf{r},\sigma;\mathbf{k}',\mathbf{r}',\sigma'} \left( \frac{v_{\mathbf{k}} v^*_{\mathbf{k}'} \left( c^\dagger_{\mathbf{k},\sigma} f_{\mathbf{r},\sigma} \right) P_b \left( f^\dagger_{\mathbf{r}',\sigma'} c_{\mathbf{k}',\sigma'} \right) + v^*_{\mathbf{k}} v_{\mathbf{k}'} \left( f^\dagger_{\mathbf{r},\sigma} c_{\mathbf{k},\sigma} \right) P_b \left( c^\dagger_{\mathbf{k}',\sigma'} f_{\mathbf{r}',\sigma'} \right)}{i\omega - E^f_b} \right) |a'\rangle \\
&\quad + \langle a| \sum_b \sum_{\mathbf{k},\mathbf{r},\sigma;\mathbf{k}',\mathbf{r}',\sigma'} \left( \frac{v_{\mathbf{k}} v_{\mathbf{k}'} \left( c^\dagger_{\mathbf{k},\sigma} f_{\mathbf{r},\sigma} \right) P_b \left( c^\dagger_{\mathbf{k}',\sigma'} f_{\mathbf{r}',\sigma'} \right) + v^*_{\mathbf{k}} v^*_{\mathbf{k}'} \left( f^\dagger_{\mathbf{r},\sigma} c_{\mathbf{k},\sigma} \right) P_b \left( f^\dagger_{\mathbf{r}',\sigma'} c_{\mathbf{k}',\sigma'} \right)}{i\omega - E^f_b} \right) |a'\rangle
\end{aligned} \tag{2.6}$$

Above, $P_b = |b\rangle\langle b|$ projects to state $|b\rangle$ of subsystem $B$. We will disregard the latter contribution, which involves changing the particle number in both subsystems. Under assumption that the systems do not conserve particle number (*e.g.* a superconducting system), this term can be nonvanishing.

We next use the following identity,

$$\delta_{\alpha\gamma}\delta_{\beta\eta} = \frac{1}{2}\left( \delta_{\alpha\beta}\delta_{\gamma\eta} + \boldsymbol{\sigma}_{\alpha\beta} \cdot \boldsymbol{\sigma}_{\eta\gamma} \right). \tag{2.7}$$

This can be seen from decomposing a $2 \times 2$ matrix as

$$\begin{aligned}
M_{\alpha\beta} &= \frac{1}{2}\text{Tr}(M)\delta_{\alpha\beta} + \frac{1}{2}\text{Tr}(M\boldsymbol{\sigma}) \cdot \boldsymbol{\sigma}_{\alpha\beta} \\
\implies M_{\gamma\eta}\delta_{\alpha\gamma}\delta_{\beta\eta} &= \frac{1}{2} M_{\gamma\eta} \left( \delta_{\gamma\eta}\delta_{\alpha\beta} + \boldsymbol{\sigma}_{\eta\gamma} \cdot \boldsymbol{\sigma}_{\alpha\beta} \right).
\end{aligned} \tag{2.8}$$

We additionally use the anticommutativity, *e.g.* $\{f_{\mathbf{r},\sigma}, f^\dagger_{\mathbf{r}',\sigma'}\} = \delta_{\mathbf{r},\mathbf{r}'}\delta_{\sigma,\sigma'}$. The interaction terms can be reexpressed as follows:

**Term I:**

$$\begin{aligned}
&\left(c^\dagger_{\mathbf{k},\alpha} f_{\mathbf{r},\alpha}\right)\left(f^\dagger_{\mathbf{r}',\beta} c_{\mathbf{k}',\beta}\right) = \sum_{\gamma\eta}\left(c^\dagger_{\mathbf{k},\alpha} f_{\mathbf{r},\gamma}\right)\left(f^\dagger_{\mathbf{r}',\eta} c_{\mathbf{k}',\beta}\right)\delta_{\alpha\gamma}\delta_{\beta\eta} \\
&= \sum_{\gamma\eta}\Big(c^\dagger_{\mathbf{k},\alpha} c_{\mathbf{k}',\beta} \underbrace{f_{\mathbf{r},\gamma} f^\dagger_{\mathbf{r}',\eta}}_{\delta_{\gamma\eta}\delta_{\mathbf{r}\mathbf{r}'} - f^\dagger_{\mathbf{r}',\eta} f_{\mathbf{r},\gamma}}\Big)\delta_{\alpha\gamma}\delta_{\beta\eta} \\
&= c^\dagger_{\mathbf{k},\alpha} c_{\mathbf{k}',\beta}\delta_{\alpha\beta}\delta_{\mathbf{r},\mathbf{r}'} - \sum_{\gamma\eta}\left\{\left(c^\dagger_{\mathbf{k},\alpha} c_{\mathbf{k}',\beta} f^\dagger_{\mathbf{r}',\eta} f_{\mathbf{r},\gamma}\right)\underbrace{\delta_{\alpha\gamma}\delta_{\beta\eta}}_{\text{Eq. (2.7)}}\right\} \\
&= c^\dagger_{\mathbf{k},\alpha} c_{\mathbf{k}',\beta}\delta_{\alpha\beta}\delta_{\mathbf{r},\mathbf{r}'} - \frac{1}{2}\sum_{\eta}\left(c^\dagger_{\mathbf{k},\alpha} c_{\mathbf{k}',\alpha}\right)\left(f^\dagger_{\mathbf{r}',\eta} f_{\mathbf{r},\eta}\right)\delta_{\alpha\beta} - \frac{1}{2}\sum_{\gamma\eta}\left(c^\dagger_{\mathbf{k},\alpha}\boldsymbol{\sigma}_{\alpha\beta} c_{\mathbf{k}',\beta}\right)\cdot\left(f^\dagger_{\mathbf{r}',\eta}\boldsymbol{\sigma}_{\eta\gamma} f_{\mathbf{r},\gamma}\right)
\end{aligned} \tag{2.9}$$

**Term II:**

$$\begin{aligned}
&\left(f^\dagger_{\mathbf{r},\alpha} c_{\mathbf{k},\alpha}\right)\left(c^\dagger_{\mathbf{k}',\beta} f_{\mathbf{r}',\beta}\right) = f^\dagger_{\mathbf{r},\alpha} f_{\mathbf{r}',\beta}\delta_{\alpha\beta}\delta_{\mathbf{k},\mathbf{k}'} - \left(c^\dagger_{\mathbf{k}',\beta} c_{\mathbf{k},\alpha} f^\dagger_{\mathbf{r},\alpha} f_{\mathbf{r}',\beta}\right) \\
&= f^\dagger_{\mathbf{r},\alpha} f_{\mathbf{r}',\alpha}\delta_{\alpha\beta}\delta_{\mathbf{k},\mathbf{k}'} - \left(c^\dagger_{\mathbf{k}',\beta} c_{\mathbf{k},\alpha} f^\dagger_{\mathbf{r},\gamma} f_{\mathbf{r}',\eta}\right)\underbrace{\delta_{\alpha\gamma}\delta_{\beta\eta}}_{\text{Eq. (2.7)}} \\
&= f^\dagger_{\mathbf{r},\alpha} f_{\mathbf{r}',\alpha}\delta_{\alpha\beta}\delta_{\mathbf{k},\mathbf{k}'} - \frac{1}{2}\sum_{\gamma}\left(c^\dagger_{\mathbf{k}',\alpha} c_{\mathbf{k},\alpha}\right)\left(f^\dagger_{\mathbf{r},\gamma} f_{\mathbf{r}',\gamma}\right)\delta_{\alpha\beta} - \frac{1}{2}\sum_{\gamma,\eta}\left(c^\dagger_{\mathbf{k}',\beta}\boldsymbol{\sigma}_{\alpha\beta} c_{\mathbf{k},\alpha}\right)\cdot\left(f^\dagger_{\mathbf{r},\gamma}\boldsymbol{\sigma}_{\eta\gamma} f_{\mathbf{r}',\gamma}\right)\Big\} \\
&= f^\dagger_{\mathbf{r},\alpha} f_{\mathbf{r}',\alpha}\delta_{\alpha\beta}\delta_{\mathbf{k},\mathbf{k}'} - \frac{1}{2}\sum_{\gamma}\left(c^\dagger_{\mathbf{k}',\alpha} c_{\mathbf{k},\alpha}\right)\left(f^\dagger_{\mathbf{r},\gamma} f_{\mathbf{r}',\gamma}\right)\delta_{\alpha\beta} - \frac{1}{2}\sum_{\gamma,\eta}\left(c^\dagger_{\mathbf{k}',\beta}\boldsymbol{\sigma}_{\beta\alpha} c_{\mathbf{k},\alpha}\right)\cdot\left(f^\dagger_{\mathbf{r},\gamma}\boldsymbol{\sigma}_{\gamma\eta} f_{\mathbf{r}',\gamma}\right)\Big\}
\end{aligned} \tag{2.10}$$

In the last equality, we have used the fact that $\boldsymbol{\sigma}^{\mathrm{T}} = (\sigma_x, -\sigma_y, \sigma_z)$, and $\boldsymbol{\sigma}_{\alpha\beta}\boldsymbol{\sigma}_{\gamma\eta} = \boldsymbol{\sigma}_{\beta\alpha}\cdot\boldsymbol{\sigma}_{\eta\gamma}$. We define the spin of the local $f$ electron as

$$\sum_{\alpha\beta} f^\dagger_{\mathbf{r},\alpha}\frac{\boldsymbol{\sigma}_{\alpha\beta}}{2} f_{\mathbf{r}',\beta} = \mathbf{S}_f(\mathbf{r})\delta_{\mathbf{r},\mathbf{r}'}. \tag{2.11}$$

## 2.1 System at half-filling

To simplify, we consider a system in which $f$-electrons are at half-filling in the strong $U$ limit ($U > 0$), such that all sites are singly-occupied by $f$-electrons. We take $f^\dagger_{\mathbf{r},\alpha} f_{\mathbf{r}',\beta} = \delta_{\mathbf{r}\mathbf{r}'}\delta_{\alpha\beta}$ for simplicity. As such, the two terms reduce to

$$\left(c^\dagger_{\mathbf{k},\alpha} f_{\mathbf{r},\alpha}\right)\left(f^\dagger_{\mathbf{r}',\beta} c_{\mathbf{k}',\beta}\right) \to \frac{1}{2} c^\dagger_{\mathbf{k},\alpha} c_{\mathbf{k}',\alpha}\delta_{\mathbf{r}\mathbf{r}'}\delta_{\alpha\beta} - \frac{1}{2}\sum_{\gamma,\eta}\left(c^\dagger_{\mathbf{k},\alpha}\boldsymbol{\sigma}_{\alpha\beta} c_{\mathbf{k}',\beta}\right)\cdot\left(f^\dagger_{\mathbf{r}',\eta}\boldsymbol{\sigma}_{\eta\gamma} f_{\mathbf{r},\gamma}\right) \tag{2.12a}$$

$$\left(f^\dagger_{\mathbf{r},\alpha} c_{\mathbf{k},\alpha}\right)\left(c^\dagger_{\mathbf{k}',\beta} f_{\mathbf{r}',\beta}\right) \to -\frac{1}{2} c^\dagger_{\mathbf{k}',\alpha} c_{\mathbf{k},\alpha}\delta_{\mathbf{r}\mathbf{r}'}\delta_{\alpha\beta} - \frac{1}{2}\sum_{\gamma,\eta}\left(c^\dagger_{\mathbf{k}',\beta}\boldsymbol{\sigma}_{\beta\alpha} c_{\mathbf{k},\alpha}\right)\cdot\left(f^\dagger_{\mathbf{r},\gamma}\boldsymbol{\sigma}_{\gamma\eta} f_{\mathbf{r}',\gamma}\right) + \delta_{\mathbf{r},\mathbf{r}'}\delta_{\alpha\beta}\delta_{\mathbf{k},\mathbf{k}'} \tag{2.12b}$$

It is important to note the difference in the overall sign of the first term. Above, we see that the hybridization includes a residual scattering term and also a Kondo-like coupling between $c$ and $f$ electrons.

Now, we determine the coefficients in the couplings. There are three intermediate states for subsystem $b$, which we label below:

$$\begin{aligned}
|f^0\rangle &\to E_{\text{local}} = 0 && \text{(unoccupied)} \\
|f^1\rangle &\to E_{\text{local}} = \xi_f && \text{(singly occupied)} \\
|f^2\rangle &\to E_{\text{local}} = 2\xi_f + U && \text{(doubly occupied).}
\end{aligned} \tag{2.13}$$

Under our simplification, subsystem $B$ starts in state $|f^1\rangle$, and intermediate states are $|f^0\rangle$ and $|f^2\rangle$. This leads to

$$\begin{aligned} i\omega - E_b^f &= \Big(\xi_{\mathbf{k}} + \xi_f + i\eta\Big) - \begin{cases} 0 & (b=0) \\ 2\xi_f + U & (b=2) \end{cases} \\ &= \begin{cases} \xi_{\mathbf{k}} + \xi_f + i\eta & (b=0) \\ \xi_{\mathbf{k}} - \xi_f - U + i\eta & (b=2) \end{cases} \end{aligned} \tag{2.14}$$

We make the assumption that $\xi_f \gg \xi_{\mathbf{k}}$ and can disregard $\xi_{\mathbf{k}}$ to leading order. From Eq. (2.6), we have (only keeping the particle-number-preserving contribution)

$$\begin{aligned} [\Delta H_{\text{itinerant}}]_{a,a'} &= \langle a| \sum_{b=0,2} \sum_{\mathbf{k},\mathbf{r},\sigma;\mathbf{k}',\mathbf{r}',\sigma'} \left( \frac{v_{\mathbf{k}} v_{\mathbf{k}'}^* \Big(c_{\mathbf{k},\sigma}^\dagger f_{\mathbf{r},\sigma}\Big) P_{f^2} \Big(f_{\mathbf{r}',\sigma'}^\dagger c_{\mathbf{k}',\sigma'}\Big) + v_{\mathbf{k}}^* v_{\mathbf{k}'} \Big(f_{\mathbf{r},\sigma}^\dagger c_{\mathbf{k},\sigma}\Big) P_{f^2} \Big(c_{\mathbf{k}',\sigma'}^\dagger f_{\mathbf{r}',\sigma'}\Big)}{i\omega - E_b^f} \right) |a'\rangle \\ &\approx \langle a| \sum_{\mathbf{k},\mathbf{r},\sigma;\mathbf{k}',\mathbf{r}',\sigma'} \left( \frac{v_{\mathbf{k}} v_{\mathbf{k}'}^* \Big(c_{\mathbf{k},\sigma}^\dagger f_{\mathbf{r},\sigma}\Big) P_{f^0} \Big(f_{\mathbf{r}',\sigma'}^\dagger c_{\mathbf{k}',\sigma'}\Big)}{-\xi_f - U} + \frac{v_{\mathbf{k}}^* v_{\mathbf{k}'} \Big(f_{\mathbf{r},\sigma}^\dagger c_{\mathbf{k},\sigma}\Big) P_{f^0} \Big(c_{\mathbf{k}',\sigma'}^\dagger f_{\mathbf{r}',\sigma'}\Big)}{\xi_f} \right) |a'\rangle \end{aligned} \tag{2.15}$$

We see above that the first contribution involves double occupancy of $f$-orbitals as an intermediate state, whereas the second term involves unoccupied $f$-orbitals as its intermediate state. From Eq. (2.12), we have

$$\boxed{\begin{aligned} [\Delta H_{\text{itinerant}}]_{a,a'} \approx \langle a| \sum_{\mathbf{k},\alpha;\mathbf{k}',\beta} \sum_{\mathbf{r}} \Big( J(\mathbf{k},\mathbf{k}') \Big(c_{\mathbf{k},\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{\mathbf{k}',\beta}\Big) \cdot \mathbf{S}_f(\mathbf{r}) \Big) |a'\rangle \\ + \langle a| \sum_{\mathbf{k},\mathbf{k}',\alpha} \sum_{\mathbf{r}} \left( \frac{1}{2} K(\mathbf{k},\mathbf{k}') c_{\mathbf{k},\alpha}^\dagger c_{\mathbf{k}',\alpha} \right) |a'\rangle + \text{const.} \end{aligned}} \tag{2.16}$$

in which

$$J(\mathbf{k},\mathbf{k}') \approx -v_{\mathbf{k}} v_{\mathbf{k}'}^* \left( \frac{1}{-\xi_f - U} + \frac{1}{\xi_f} \right) \tag{2.17}$$

and

$$K(\mathbf{k},\mathbf{k}') = v_{\mathbf{k}} v_{\mathbf{k}'}^* \left( \frac{1}{-\xi_f - U} - \frac{1}{\xi_f} \right). \tag{2.18}$$

The first contribution is exactly that of the Kondo model, whereas the second term is remnant spin-independent scattering off of localized $f$ states.

For a system with $U > |\xi_f|$, in which $\xi_f < 0$, it follows that $J(\mathbf{k},\mathbf{k}') > 0$ indicating antiferromagnetic coupling. Secondly, when the $f$-electrons have a particle-hole symmetric spectrum, with two bands $|\xi_f|$ and $-|\xi_f|$ and $U = 2|\xi_f|$, the second term vanishes.

Typically, one only considers the Kondo-like term, and we can drop the $k$-dependence of the coupling constant. We also suppose that the Kondo coupling is local. Fourier transforming and disregarding the momentum dependence of the Kondo coupling gives the familiar form,

$$H_{\text{Kondo}} = \sum_{\mathbf{k}\alpha} \xi_{\mathbf{k}} c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k},\alpha} + J \sum_{\mathbf{r}} \sum_{\alpha,\beta} c_{\mathbf{r}\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} c_{\mathbf{r},\beta} \cdot \mathbf{S}_f(\mathbf{r}). \tag{2.19}$$

# A Refresher: Inverse of block matrix and Schur complement

We present a quick math refresher to find the inverse of a square matrix. Consider the matrix

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{A.1}$$

where $A$, $B$, $C$, and $D$ are matrices. We compute the inverse by Gauss-Jordan elimination

$$\begin{aligned}
M &= \mathbb{1}M \\
\begin{pmatrix} A & B \\ C & D \end{pmatrix} &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} M \\
\begin{pmatrix} 1 & A^{-1}B \\ C & D \end{pmatrix} &= \begin{pmatrix} A^{-1} & 0 \\ 0 & 1 \end{pmatrix} M \\
\begin{pmatrix} 1 & A^{-1}B \\ 0 & D - CA^{-1}B \end{pmatrix} &= \begin{pmatrix} A^{-1} & 0 \\ -CA^{-1} & 1 \end{pmatrix} M \\
\begin{pmatrix} 1 & A^{-1}B \\ 0 & 1 \end{pmatrix} &= \begin{pmatrix} A^{-1} & 0 \\ -[D - CA^{-1}B]^{-1}CA^{-1} & [D - CA^{-1}B]^{-1} \end{pmatrix} M \\
\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} &= \begin{pmatrix} A^{-1} + A^{-1}B[D - CA^{-1}B]^{-1}CA^{-1} & -A^{-1}B[D - CA^{-1}B]^{-1} \\ -[D - CA^{-1}B]^{-1}CA^{-1} & [D - CA^{-1}B]^{-1} \end{pmatrix} M
\end{aligned} \tag{A.2}$$

If one were to instead start with the bottom row, then the top left matrix element would read $M_{11}^{-1} = [A - BD^{-1}C]^{-1}$. We show this equality below:

$$\begin{aligned}
M_{11}^{-1} &= A^{-1} + A^{-1}B[D - CA^{-1}B]^{-1}CA^{-1} \\
&= A^{-1}\Big(1 + B[D - CA^{-1}B]^{-1}CA^{-1}\Big) \\
&= A^{-1}\Big(1 + B\Big\{D[1 - D^{-1}CA^{-1}B]\Big\}^{-1}CA^{-1}\Big) \\
&= A^{-1}\Big(1 + B\Big[1 - \underbrace{D^{-1}CA^{-1}B}_{\equiv\Delta}\Big]^{-1}D^{-1}CA^{-1}\Big) \\
&= A^{-1}\Big(1 + B\Big[1 + \Delta + \Delta^2 + \Delta^3 + \cdots\Big]D^{-1}CA^{-1}\Big) \\
&= A^{-1}\Big(1 + \underbrace{BD^{-1}CA^{-1}}_{\equiv\Delta'} - BD^{-1}CA^{-1}BD^{-1}CA^{-1} + \cdots\Big) \\
&= A^{-1}\Big(1 + \Delta' + \Delta'^2 + \Delta'^3 + \cdots\Big) = A^{-1}(1 - \Delta')^{-1} \\
&= A^{-1}\Big(1 - BD^{-1}CA^{-1}\Big)^{-1} \\
&= \Big[\Big(1 - BD^{-1}CA^{-1}\Big)A\Big]^{-1} \\
&= \Big(A - BD^{-1}C\Big)^{-1}.
\end{aligned} \tag{A.3}$$

This element is defined as the Schur complement of $D$.

# B Refresher: Dyson's Equation

Consider the Green's functions

$$\mathcal{G}(i\omega) = (i\omega - H)^{-1} = (i\omega - H_0 - \Sigma)^{-1} \tag{B.1}$$

Consider the following expansion (taking $\mathcal{G}(i\omega) \to \mathcal{G}$ for simplicity),

$$\begin{aligned}
\mathcal{G}(i\omega) &= (\underbrace{i\omega - H_0}_{\mathcal{G}_0^{-1}} - \Sigma)^{-1} \\
&= (1 - \mathcal{G}_0\Sigma)^{-1}\mathcal{G}_0 \\
&= \Big(1 + (\mathcal{G}_0\Sigma) + (\mathcal{G}_0\Sigma)^2 + \cdots\Big)\mathcal{G}_0 \\
&= \mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G}_0 \underbrace{\Big(1 + (\Sigma\mathcal{G}_0) + (\Sigma\mathcal{G}_0)^2 + \cdots\Big)}_{=(1-\Sigma\mathcal{G}_0)^{-1}} \\
&= \mathcal{G}_0 + \mathcal{G}_0\Sigma \underbrace{(\mathcal{G}_0^{-1} - \Sigma)^{-1}}_{=\mathcal{G}}
\end{aligned} \tag{B.2}$$

This yields Dyson's equation,

$$\mathcal{G}(i\omega) = \mathcal{G}_0(i\omega) + \mathcal{G}_0(i\omega)\Sigma\mathcal{G}(i\omega) \tag{B.3}$$

which can equivalently be expressed as

$$\mathcal{G}(i\omega) = \mathcal{G}_0(i\omega) + \mathcal{G}_0(i\omega)\tilde{\Sigma}(i\omega)\mathcal{G}_0(i\omega), \tag{B.4}$$

with

$$\tilde{\Sigma}(i\omega) = \Sigma\mathcal{G}(i\omega)\mathcal{G}_0^{-1}(i\omega) = \Sigma + \Sigma\mathcal{G}_0(i\omega)\tilde{\Sigma}(i\omega) \tag{B.5}$$

serving as the $T$-matrix. Here, the bare Green's function (in absence of subspace coupling) is given by

$$\mathcal{G}_0(i\omega) = (i\omega - H_0)^{-1} = \begin{pmatrix} \mathcal{G}_A(i\omega) & \\ & \mathcal{G}_B(i\omega) \end{pmatrix}, \tag{B.6}$$

in which $\mathcal{G}_A(i\omega) = (i\omega - H_A)^{-1}$ and $\mathcal{G}_B(i\omega) = (i\omega - H_B)^{-1}$.

## References


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