Schrieffer-Wolff Transformation of the SIA

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Prelude: I will show the step-by-step calculations of the Schrieffer-Wolff transformation to the single impurity Anderson model, following very closely a tutorial provided by the Master's program of the International Centre for Fundamental Theory at the ENS university of Paris [2]. Fun fact: I did all of these calculations on a road trip from Ohio to Yellowstone National Park!

1 Model

The single impurity Anderson model has the following form,

$$\begin{aligned} H &= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \sum_{\mathbf{k},\sigma} \left(v_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} f_{\sigma} + \text{h.c.} \right) + \epsilon_f (n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow \\ &\equiv H_{\text{band}} + V + H_{\text{atom}}. \end{aligned} \tag{1}$$

This model combines two essential ideas [1],

- Sufficiently strong Coulomb repulsion in atomic orbitals would restrict the movement of conduction electrons, converting a metal into a Mott insulator.
- Conduction electrons scattering off of transition metals atoms can form virtual bound state resonances. This is realized via a physical tunneling process between localized d or f orbitals and the conduction sea.

The impurity term V consists of a single localized orbital of type f. The dispersion $v_{\mathbf{k}}$ is complex in general, but is usually manifest as an overall phase that can be absorbed into the definitions of the c-operators, which are defined up to an overall phase. So we can take $v_{\mathbf{k}}$ (and $\epsilon_{\mathbf{k}}$) to be purely real. The conduction band term H_{band} needs no explanation. The atomic (impurity) term is constructed in such a way that singly-occupied states $|\sigma\rangle = f^{\dagger}_{\sigma} |0\rangle$ have energy ϵ_f, and doubly occupied states $|\uparrow\downarrow\rangle = f^{\dagger}_{\uparrow} f^{\dagger}_{\downarrow} |0\rangle$ have energy $2\epsilon_f + U$, where U is an on-site Coulomb interaction.

Commutation Relations

The c-electrons satisfy the usual commutation relations,

$$\{c, c\} = \{c^{\dagger}, c^{\dagger}\} = 0, \qquad \{c_a, c^{\dagger}_b\} = \delta_{a,b}, \tag{2}$$

and all possible combinations of c, f operators anti-commute since they're distinguishable. The f-electron operators satisfy the same relations, but also obey

$$[n_\sigma, f_{\sigma'}] = -\delta_{\sigma,\sigma'} f_{\sigma'}, \qquad [n_\sigma, f^{\dagger}_{\sigma'}] = \delta_{\sigma,\sigma'} f^{\dagger}_{\sigma'}, \tag{3}$$

where $n_\sigma = f^{\dagger}_{\sigma} f_{\sigma}$. To save a lot of time, I will also compute various commutations relations beforehand. $\forall$ electronic operators $A \in \{c, f\}$:

$$[A_a, A_b] = \{A_a, A_b\} - 2A_b A_a = -2A_b A_a, \qquad [A^{\dagger}_a, A^{\dagger}_b] = -2A^{\dagger}_b A^{\dagger}_a, \qquad [A_a, A^{\dagger}_b] = \delta_{a,b} - 2A^{\dagger}_b A_a. \tag{4}$$

Also, since c, f always anti-commute for all possible combinations, the commutator $[c, f] = -2fc$ for all possible combinations. The rest of the commutators encountered are derivable from these relations.

2 Details

I wish to integrate out the empty and doubly occupied states, leaving only singly occupied states. This regime would have $\epsilon_f \ll 0$ and $\epsilon_f + U \gg 0$; I will separate the Hamiltonian into a low energy sector spanned by the singly occupied states, and a high energy sector spanned by the empty and doubly occupied states. The projectors that map to these spaces must sum to one, and have the following form:

$$P_h = n_\uparrow n_\downarrow + (1 - n_\uparrow)(1 - n_\downarrow), \qquad P_l = n_\uparrow + n_\downarrow - 2n_\uparrow n_\downarrow, \tag{5}$$

such that the Hamiltonian (1) can be written as

$$\begin{aligned} H &= (P_l H P_l + P_h H P_h) + (P_l H P_h + P_h H P_l) \\ &\equiv H_0 + \lambda V, \end{aligned} \tag{6}$$

where I have parameterized the off-diagonal elements by λ.

Before doing the projection, Schrieffer and Wolff first performed the following unitary transformation on the Hamiltonian,

$$e^{\lambda S} H e^{-\lambda S} = H_0 + \mathcal{O}(\lambda^2), \tag{7}$$

where off-diagonal elements are eliminated to leading order. This is because a straight-forward projection scheme yields a model where the impurity and conduction sea no longer react. S is some antihermitian quantity, $S^\dagger = -S$, and in order to determine S I first recall

$$e^A B e^{-A} = B + [A, B] + \frac{1}{2!}[A, [A, B]] + \cdots . \tag{8}$$

I'll use this to expand (7) and choose S such that the term linear in λ is eliminated,

$$\begin{aligned} e^{\lambda S} H e^{-\lambda S} &= H + \lambda[S, H] + \frac{\lambda^2}{2}[S, [S, H]] + \cdots \\ &= H_0 + \lambda V + [S, H_0 + \lambda V] + \frac{\lambda^2}{2}[S, [S, H_0 + \lambda V]] + \cdots \\ &= H_0 + \lambda V + \lambda[S, H_0] + \lambda^2[S, V] + \frac{\lambda^2}{2}[S, [S, H_0] + \lambda[S, V]] + \cdots . \end{aligned} \tag{9}$$

Clearly then, I require S be chosen such that

$$[S, H_0] = -V \tag{10}$$

is a true statement, eliminating the linear term in the process. With this choice, (9) simplifies to

$$e^S H e^{-S} \approx H_0 + \frac{1}{2}[S, V], \tag{11}$$

to second order, dropping the expansion parameter λ. Note that (10) implies that some unknown quantity S, when commuted with a diagonal quantity H_0, gives a purely off-diagonal quantity V. So, S can be chosen to be off-diagonal, as any diagonal elements would vanish in the Hamiltonian anyway. This choice implies that $[S, V]$ is diagonal.

2.1 Determining S – Without U

I will first determine S without the local Coulomb interaction. It is natural to assume the following ansatz,

$$S_0 = \sum_{\mathbf{k},\sigma} s_{\mathbf{k}} \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + c_{\mathbf{k},\sigma} f^\dagger_\sigma \right), \tag{12}$$

which is reminiscent of V. I require that $[S_0, H_0] = -V$ (10), which translates to

$$-\sum_{\mathbf{k},\sigma} \left(v_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} f_\sigma + \text{h.c.} \right) = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} \left[S_0, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \right] + [S_0, \epsilon_f (n_\uparrow + n_\downarrow)]. \tag{13}$$

I will evaluate the necessary commutators below.

For the commutators against the number operator, note first that

$$[S_0, f_\sigma] = \sum_{\mathbf{k},\sigma'} s_{\mathbf{k}} \left[\left(c^\dagger_{\mathbf{k},\sigma'} f_{\sigma'} + c_{\mathbf{k},\sigma'} f^\dagger_{\sigma'} \right), f_\sigma \right] = \sum_{\mathbf{k}} s_{\mathbf{k}} c_{\mathbf{k},\sigma} \iff [S_0, f^\dagger_\sigma] = \sum_{\mathbf{k}} s_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma}, \tag{14}$$

where I used the relations

$$\left[c^\dagger_{\mathbf{k},\sigma'} f_{\sigma'}, f_\sigma \right] = 0, \qquad \left[c_{\mathbf{k},\sigma'} f^\dagger_{\sigma'}, f_\sigma \right] = \delta_{\sigma,\sigma'} c_{\mathbf{k},\sigma'}, \tag{15}$$

and the implication follows because S is antihermitian. From the representation $n_\sigma = f^\dagger_\sigma f_\sigma$, this results in

$$[S_0, n_\sigma] = [S, f^\dagger_\sigma f_\sigma] = f^\dagger_\sigma [S, f_\sigma] + [S_0, f^\dagger_\sigma] f_\sigma = \sum_{\mathbf{k}} s_{\mathbf{k}} \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma - c_{\mathbf{k},\sigma} f^\dagger_\sigma \right), \tag{16}$$

and I find that

$$[S_0, \epsilon_f (n_\uparrow + n_\downarrow)] = \sum_{\mathbf{k},\sigma} s_{\mathbf{k}} \epsilon_f \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma - c_{\mathbf{k},\sigma} f^\dagger_\sigma \right) \tag{17}$$

for the atomic term. Now, for the kinetic term note that

$$[S_0, c_{\mathbf{k},\sigma}] = \sum_{\mathbf{k}',\sigma'} s_{\mathbf{k}'} \left[\left(c^\dagger_{\mathbf{k}',\sigma'} f_{\sigma'} + c_{\mathbf{k}',\sigma'} f^\dagger_{\sigma'} \right), c_{\mathbf{k},\sigma} \right] = -s_{\mathbf{k}} f_\sigma \iff [S_0, c^\dagger_{\mathbf{k},\sigma}] = -s_{\mathbf{k}} f^\dagger_\sigma, \tag{18}$$

where I used the relations

$$\left[c^\dagger_{\mathbf{k}',\sigma'} f_{\sigma'}, c_{\mathbf{k},\sigma} \right] = -\delta_{\mathbf{k},\mathbf{k}'} \delta_{\sigma,\sigma'} f_{\sigma'}, \qquad \left[c_{\mathbf{k}',\sigma'} f^\dagger_{\sigma'}, c^\dagger_{\mathbf{k},\sigma} \right] = -\delta_{\mathbf{k},\mathbf{k}'} \delta_{\sigma,\sigma'} f^\dagger_{\sigma'}. \tag{19}$$

This allows me to write

$$[S_0, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}] = c^\dagger_{\mathbf{k},\sigma} [S_0, c_{\mathbf{k},\sigma}] + [S_0, c^\dagger_{\mathbf{k},\sigma}] c_{\mathbf{k},\sigma} = -s_{\mathbf{k}} \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma - c_{\mathbf{k},\sigma} f^\dagger_\sigma \right), \tag{20}$$

such that the condition (13) translates to

$$-\sum_{\mathbf{k},\sigma} \left(v_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} f_\sigma + \text{h.c.} \right) = \sum_{\mathbf{k},\sigma} s_{\mathbf{k}} (\epsilon_f - \epsilon_{\mathbf{k}}) \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma - c_{\mathbf{k},\sigma} f^\dagger_\sigma \right) \iff s_{\mathbf{k}} = \frac{v_{\mathbf{k}}}{\epsilon_{\mathbf{k}} - \epsilon_f}. \tag{21}$$

2.2 Determining S – With U

Incorporating the U-term with H_0, the previous condition $[S_0, H_0] = -V$ gains the following correction,

$$\begin{aligned}
[S_0, H_0] &= -V + U[S_0, n_\uparrow n_\downarrow] \\
&= -V + U \left(n_\uparrow [S_0, n_\downarrow] + U[S_0, n_\uparrow] n_\downarrow \right) \\
&= -V + U \sum_{\mathbf{k}} s_{\mathbf{k}} \left(n_\uparrow c^\dagger_{\mathbf{k},\downarrow} f_\downarrow - n_\uparrow c_{\mathbf{k},\downarrow} f^\dagger_\downarrow + c^\dagger_{\mathbf{k},\uparrow} f_\uparrow n_\downarrow - c_{\mathbf{k},\uparrow} f^\dagger_\uparrow n_\downarrow \right) \\
&= -V + U \sum_{\mathbf{k}} s_{\mathbf{k}} \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma - c_{\mathbf{k},\sigma} f^\dagger_\sigma \right) n_{-\sigma},
\end{aligned} \tag{22}$$

where $-\sigma =\downarrow \iff \sigma =\uparrow$ and vice-versa. Clearly I need a better ansatz for S than S_0, so I'll add an additional term

$$S = S_0 + \sum_{\mathbf{k},\sigma} t_{\mathbf{k}} \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + c_{\mathbf{k},\sigma} f^\dagger_\sigma \right) n_{-\sigma} \equiv S_0 + T, \tag{23}$$

with T being chosen to cancel the correction in (22). How does T commute with things? I find first that

$$\begin{aligned}
[T, f_\sigma] &= \sum_{\mathbf{k},\sigma'} t_{\mathbf{k}} \left(\left[c^\dagger_{\mathbf{k},\sigma'} f_{\sigma'} n_{-\sigma'}, f_\sigma \right] + \left[c_{\mathbf{k},\sigma'} f^\dagger_{\sigma'} n_{-\sigma'}, f_\sigma \right] \right) \\
&= \sum_{\mathbf{k},\sigma'} t_{\mathbf{k}} \Big(c^\dagger_{\mathbf{k},\sigma'} f_{\sigma'} \left[n_{-\sigma'}, f_\sigma \right] + c^\dagger_{\mathbf{k},\sigma'} \left[f_{\sigma'}, f_\sigma \right] n_{-\sigma'} + \left[c^\dagger_{\mathbf{k},\sigma'}, f_\sigma \right] f_{\sigma'} n_{-\sigma'} \\
&\qquad + c_{\mathbf{k},\sigma'} f^\dagger_{\sigma'} \left[n_{-\sigma'}, f_\sigma \right] + c_{\mathbf{k},\sigma'} \left[f^\dagger_{\sigma'}, f_\sigma \right] n_{-\sigma'} + \left[c_{\mathbf{k},\sigma'}, f_\sigma \right] f^\dagger_{\sigma'} n_{-\sigma'} \Big) \\
&= \sum_{\mathbf{k},\sigma'} t_{\mathbf{k}} \Big(- c^\dagger_{\mathbf{k},\sigma'} f_{\sigma'} \delta_{-\sigma,\sigma'} f_\sigma - c_{\mathbf{k},\sigma'} f^\dagger_{\sigma'} \delta_{-\sigma',\sigma} f_\sigma - 2 c^\dagger_{\mathbf{k},\sigma'} f_\sigma f_{\sigma'} n_{-\sigma'} \\
&\qquad c_{\mathbf{k},\sigma'} \delta_{\sigma,\sigma'} n_{-\sigma'} - 2 c_{\mathbf{k},\sigma'} f_\sigma f^\dagger_{\sigma'} n_{-\sigma'} - 2 f_\sigma c^\dagger_{\mathbf{k},\sigma'} f_{\sigma'} n_{-\sigma'} - 2 f_\sigma c_{\mathbf{k},\sigma'} f^\dagger_{\sigma'} n_{-\sigma'} \\
&= \sum_{\mathbf{k}} t_{\mathbf{k}} c_{\mathbf{k},\sigma} n_{-\sigma} - \sum_{\mathbf{k}} t_{\mathbf{k}} \left(c^\dagger_{\mathbf{k},-\sigma} f_{-\sigma} + c_{\mathbf{k},-\sigma} f^\dagger_{-\sigma} \right) f_\sigma
\end{aligned} \tag{24}$$

$$\iff [T, f^\dagger_\sigma] = \sum_{\mathbf{k}} t_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} n_{-\sigma} + \sum_{\mathbf{k}} t_{\mathbf{k}} \left(c^\dagger_{\mathbf{k},-\sigma} f_{-\sigma} + c_{\mathbf{k},-\sigma} f^\dagger_{-\sigma} \right) f^\dagger_\sigma, \tag{25}$$

Continuing naturally, the commutator $[T, n_\sigma]$ is written

$$\begin{aligned}
[T, n_\sigma] &= f^\dagger_\sigma [T, f_\sigma] + [T, f^\dagger_\sigma] f_\sigma \\
&= \sum_{\mathbf{k}} t_{\mathbf{k}} f^\dagger_\sigma c_{\mathbf{k},\sigma} n_{-\sigma} - \sum_{\mathbf{k}} t_{\mathbf{k}} f^\dagger_\sigma \left(c^\dagger_{\mathbf{k},-\sigma} f_{-\sigma} + c_{\mathbf{k},-\sigma} f^\dagger_{-\sigma} \right) f_\sigma \\
&\qquad + \sum_{\mathbf{k}} t_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} n_{-\sigma} f_\sigma + \sum_{\mathbf{k}} t_{\mathbf{k}} \left(c^\dagger_{\mathbf{k},-\sigma} f_{-\sigma} + c_{\mathbf{k},-\sigma} f^\dagger_{-\sigma} \right) f^\dagger_\sigma f_\sigma \\
&= \sum_{\mathbf{k}} t_{\mathbf{k}} \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + f^\dagger_\sigma c_{\mathbf{k},\sigma} \right) n_{-\sigma}.
\end{aligned} \tag{26}$$

Last, I find that

$$\begin{aligned}
[T, c_{\mathbf{k},\sigma}] &= \sum_{\mathbf{k}',\sigma'} t_{\mathbf{k}'} \left(\left[c^\dagger_{\mathbf{k}',\sigma'} f_{\sigma'} n_{-\sigma'}, c_{\mathbf{k},\sigma} \right] + \left[c_{\mathbf{k}',\sigma'} f^\dagger_{\sigma'} n_{-\sigma'}, c_{\mathbf{k},\sigma} \right] \right) \\
&= \sum_{\mathbf{k}',\sigma'} t_{\mathbf{k}'} \Big(c^\dagger_{\mathbf{k}',\sigma'} f_{\sigma'} \left[n_{-\sigma'}, c_{\mathbf{k},\sigma} \right] + c^\dagger_{\mathbf{k}',\sigma'} \left[f_{\sigma'}, c_{\mathbf{k},\sigma} \right] n_{-\sigma'} + \left[c^\dagger_{\mathbf{k}',\sigma'}, c_{\mathbf{k},\sigma} \right] f_{\sigma'} n_{-\sigma'} \\
&\qquad + c_{\mathbf{k}',\sigma'} f^\dagger_{\sigma'} \left[n_{-\sigma'}, c_{\mathbf{k},\sigma} \right] + c_{\mathbf{k}',\sigma'} \left[f^\dagger_{\sigma'}, c_{\mathbf{k},\sigma} \right] n_{-\sigma'} + \left[c_{\mathbf{k}',\sigma'}, c_{\mathbf{k},\sigma} \right] f^\dagger_{\sigma'} n_{-\sigma'} \Big) \\
&= \sum_{\mathbf{k}',\sigma'} t_{\mathbf{k}'} \Big(- 2 c^\dagger_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma} f_{\sigma'} n_{-\sigma'} + 2 c^\dagger_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma} f_{\sigma'} n_{-\sigma'} - \delta_{\mathbf{k},\mathbf{k}'} \delta_{\sigma,\sigma'} f_{\sigma'} n_{-\sigma'} \\
&\qquad - 2 c_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma} f^\dagger_{\sigma'} n_{-\sigma'} - 2 c_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma'} f^\dagger_{\sigma'} n_{-\sigma'} \Big) \\
&= -t_{\mathbf{k}} f_\sigma n_{-\sigma}
\end{aligned} \tag{27}$$

$$\iff [T, c^\dagger_{\mathbf{k},\sigma}] = t_{\mathbf{k}} f^\dagger_\sigma n_{-\sigma}, \tag{28}$$

from which follows that

$$[T, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}] = c^\dagger_{\mathbf{k},\sigma} [T, c_{\mathbf{k},\sigma}] + [T, c^\dagger_{\mathbf{k},\sigma}] c_{\mathbf{k},\sigma} = -t_{\mathbf{k}} \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + f^\dagger_\sigma c_{\mathbf{k},\sigma} \right) n_{-\sigma}. \tag{29}$$

Putting everything together, I find

$$
\begin{aligned}
[T, H_0] &= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} [T, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}] + \epsilon_f [T, n_\uparrow] + \epsilon_f [T, n_\downarrow] + U[T, n_\uparrow n_\downarrow] \\
&= \sum_{\mathbf{k},\sigma} (-\epsilon_{\mathbf{k}} t_{\mathbf{k}}) \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + f^\dagger_\sigma c_{\mathbf{k},\sigma} \right) n_{-\sigma} + \sum_{\mathbf{k},\sigma} \epsilon_f t_{\mathbf{k}} \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + f^\dagger_\sigma c_{\mathbf{k},\sigma} \right) n_{-\sigma} + \sum_{\mathbf{k},\sigma} (U t_{\mathbf{k}}) \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + f^\dagger_\sigma c_{\mathbf{k},\sigma} \right) n_{-\sigma} \\
&= \sum_{\mathbf{k},\sigma} (U + \epsilon_f - \epsilon_{\mathbf{k}}) t_{\mathbf{k}} \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + f^\dagger_\sigma c_{\mathbf{k},\sigma} \right) n_{-\sigma},
\end{aligned}
\tag{30}
$$

which must cancel the correction in (22), giving the condition

$$
-U s_{\mathbf{k}} = (U + \epsilon_f - \epsilon_{\mathbf{k}}) t_{\mathbf{k}} \implies t_{\mathbf{k}} = \frac{U}{\epsilon_{\mathbf{k}} - \epsilon_f - U} s_{\mathbf{k}} = \frac{U}{(\epsilon_{\mathbf{k}} - \epsilon_f - U)(\epsilon_{\mathbf{k}} - \epsilon_f)} v_{\mathbf{k}}, \tag{31}
$$

where I used the result (21) to replace $s_{\mathbf{k}}$. Therefore, the full form of S is

$$
\boxed{S = \sum_{\mathbf{k},\sigma} \frac{v_{\mathbf{k}}}{\epsilon_{\mathbf{k}} - \epsilon_f} \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + c_{\mathbf{k},\sigma} f^\dagger_\sigma \right) + \sum_{\mathbf{k},\sigma} \frac{U v_{\mathbf{k}}}{(\epsilon_{\mathbf{k}} - \epsilon_f - U)(\epsilon_{\mathbf{k}} - \epsilon_f)} \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + c_{\mathbf{k},\sigma} f^\dagger_\sigma \right) n_{-\sigma}} \tag{32}
$$

which satisfies $[S, H_0] = -V$.

2.3 Finalizing the Unitary Transformation

Now that S is determined, I recall the unitary transformation (11),

$$e^S H e^{-S} \approx H_0 + \frac{1}{2}[S,V] \tag{33}$$

All that is left is to compute the quantity $[S,V]/2$, then project out the resulting low energy sector to have successively integrated out the empty and doubly occupied states. I find

$$\begin{aligned}
[S_0,V] &= \left[\sum_{\mathbf{k},\sigma} s_{\mathbf{k}}\left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + c_{\mathbf{k},\sigma} f^\dagger_\sigma\right), \sum_{\mathbf{k}',\sigma'} v_{\mathbf{k}'}\left(c^\dagger_{\mathbf{k}',\sigma'} f_{\sigma'} + f^\dagger_{\sigma'} c_{\mathbf{k}',\sigma'}\right)\right] \\
&= \sum_{\mathbf{k},\sigma}\sum_{\mathbf{k}',\sigma'} s_{\mathbf{k}} v_{\mathbf{k}'}\left(\cancel{[c^\dagger_{\mathbf{k},\sigma} f_\sigma, c^\dagger_{\mathbf{k}',\sigma'} f_{\sigma'}]} + [c^\dagger_{\mathbf{k},\sigma} f_\sigma, f^\dagger_{\sigma'} c_{\mathbf{k}',\sigma'}] + [c_{\mathbf{k},\sigma} f^\dagger_\sigma, c^\dagger_{\mathbf{k}',\sigma'} f_{\sigma'}] + \cancel{[c_{\mathbf{k},\sigma} f^\dagger_\sigma, f^\dagger_{\sigma'} c_{\mathbf{k}',\sigma'}]}\right) \\
&= \sum_{\mathbf{k},\sigma}\sum_{\mathbf{k}',\sigma'} s_{\mathbf{k}} v_{\mathbf{k}'}\Big(c^\dagger_{\mathbf{k},\sigma}[f_\sigma, f^\dagger_{\sigma'}]c_{\mathbf{k}',\sigma'} + c^\dagger_{\mathbf{k},\sigma} f^\dagger_{\sigma'}[f_\sigma, c_{\mathbf{k}',\sigma'}] + [c^\dagger_{\mathbf{k},\sigma}, f^\dagger_{\sigma'}]c_{\mathbf{k}',\sigma'} f_\sigma + f^\dagger_{\sigma'}[c^\dagger_{\mathbf{k},\sigma}, c_{\mathbf{k}',\sigma'}]f_\sigma \\
&\qquad + c_{\mathbf{k},\sigma}[f^\dagger_\sigma, c^\dagger_{\mathbf{k}',\sigma'}]f_{\sigma'} + c_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}',\sigma'}[f^\dagger_\sigma, f_{\sigma'}] + [c_{\mathbf{k},\sigma}, c^\dagger_{\mathbf{k}',\sigma'}]f_{\sigma'} f^\dagger_\sigma + c^\dagger_{\mathbf{k}',\sigma'}[c_{\mathbf{k},\sigma}, f_{\sigma'}]f^\dagger_\sigma\Big) \\
&= \sum_{\mathbf{k},\sigma}\sum_{\mathbf{k}',\sigma'} s_{\mathbf{k}} v_{\mathbf{k}'}\left(c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma'}\delta_{\sigma,\sigma'} - f^\dagger_{\sigma'} f_{\sigma'}\delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'} - c_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}',\sigma'}\delta_{\sigma,\sigma'} + f_{\sigma'} f^\dagger_\sigma \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'}\right).
\end{aligned} \tag{34}$$

When I normal order the last two terms, the two delta functions cancel each other out, leaving

$$\begin{aligned}
[S_0,V] &= -2\sum_{\mathbf{k},\sigma} s_{\mathbf{k}} v_{\mathbf{k}} n_\sigma + \sum_{\mathbf{k},\mathbf{k}',\sigma} s_{\mathbf{k}} v_{\mathbf{k}'}\left(c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma} + c^\dagger_{\mathbf{k}',\sigma} c_{\mathbf{k},\sigma}\right) \\
&= -2\sum_{\mathbf{k}} s_{\mathbf{k}} v_{\mathbf{k}}\left(n_\uparrow + n_\downarrow\right) + \sum_{\mathbf{k},\mathbf{k}',\sigma} s_{\mathbf{k}} v_{\mathbf{k}'}\left(c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma} + c^\dagger_{\mathbf{k}',\sigma} c_{\mathbf{k},\sigma}\right),
\end{aligned} \tag{35}$$

where $s_{\mathbf{k}}$ is defined in (21). Next,

$$\begin{aligned}
[T,V] = \left[\sum_{\mathbf{k},\sigma} t_{\mathbf{k}}\left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + c_{\mathbf{k},\sigma} f^\dagger_\sigma\right) n_{-\sigma}, V\right] &= \sum_{\mathbf{k},\sigma} t_{\mathbf{k}}\Big(c^\dagger_{\mathbf{k},\sigma} f_\sigma [n_{-\sigma}, V] + c^\dagger_{\mathbf{k},\sigma}[f_\sigma, V]n_{-\sigma} + [c^\dagger_{\mathbf{k},\sigma}, V]f_\sigma n_{-\sigma} \\
&\qquad + c_{\mathbf{k},\sigma} f^\dagger_\sigma [n_{-\sigma}, V] + c_{\mathbf{k},\sigma}[f^\dagger_\sigma, V]n_{-\sigma} + [c_{\mathbf{k},\sigma}, V]f^\dagger_\sigma n_{-\sigma}\Big).
\end{aligned} \tag{36}$$

I know that

$$[f_\sigma, V] = \sum_{\mathbf{k}',\sigma'} v_{\mathbf{k}'}\left([f_\sigma, c^\dagger_{k',\sigma'} f_{\sigma'}] + [f_\sigma, f^\dagger_{\sigma'} c_{\mathbf{k}',\sigma'}]\right) = \sum_{\mathbf{k}'} v_{\mathbf{k}'} c_{\mathbf{k}',\sigma} \iff [f^\dagger_\sigma, V] = -\sum_{\mathbf{k}'} v_{\mathbf{k}'} c^\dagger_{\mathbf{k}',\sigma}, \tag{37}$$

and one can do the same calculation and find

$$[c_{\mathbf{k},\sigma}, V] = v_{\mathbf{k}} f_\sigma, \qquad\qquad [c^\dagger_{\mathbf{k},\sigma}, V] = -v_{\mathbf{k}} f^\dagger_\sigma, \tag{38}$$

allowing me to write (36) as

$$\begin{aligned}
[T,V] &= \sum_{\mathbf{k},\mathbf{k}',\sigma} t_{\mathbf{k}} v_{\mathbf{k}'}\left(c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma} - c_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}',\sigma}\right) n_{-\sigma} + \sum_{\mathbf{k},\sigma} t_{\mathbf{k}} v_{\mathbf{k}}\left(f_\sigma f^\dagger_\sigma - f^\dagger_\sigma f_\sigma\right) n_{-\sigma} \\
&\qquad + \sum_{\mathbf{k},\sigma} t_{\mathbf{k}}\left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + c_{\mathbf{k},\sigma} f^\dagger_\sigma\right)[n_{-\sigma}, V].
\end{aligned} \tag{39}$$

Using the fact that $[f_\sigma, f^\dagger_\sigma] = 1 - 2n_\sigma$, and that the resulting term cancels the term gained when the c-electron operators are anti-commuted in the first term, gives

$$\begin{aligned}
[T,V] &= \sum_{\mathbf{k},\mathbf{k}',\sigma} t_{\mathbf{k}} v_{\mathbf{k}'}\left(c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma} + c^\dagger_{\mathbf{k}',\sigma} c_{\mathbf{k},\sigma}\right) n_{-\sigma} - 2\sum_{\mathbf{k},\sigma} t_{\mathbf{k}} v_{\mathbf{k}} n_\sigma n_{-\sigma} + \sum_{\mathbf{k},\sigma} t_{\mathbf{k}}\left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + c_{\mathbf{k},\sigma} f^\dagger_\sigma\right)[n_{-\sigma}, V] \\
&= \sum_{\mathbf{k},\mathbf{k}',\sigma} t_{\mathbf{k}} v_{\mathbf{k}'}\left(c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma} + c^\dagger_{\mathbf{k}',\sigma} c_{\mathbf{k},\sigma}\right) n_{-\sigma} - 4\sum_{\mathbf{k}} t_{\mathbf{k}} v_{\mathbf{k}} n_\uparrow n_\downarrow + \sum_{\mathbf{k},\sigma} t_{\mathbf{k}}\left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + c_{\mathbf{k},\sigma} f^\dagger_\sigma\right)[n_{-\sigma}, V],
\end{aligned} \tag{40}$$

where I used the fact that

$$\sum_{\sigma} n_\sigma n_{-\sigma} = n_\uparrow n_\downarrow + n_\downarrow n_\uparrow = 2 n_\uparrow n_\downarrow. \tag{41}$$

The last commutator I need to evaluate is

$$[n_{-\sigma}, V] = f^\dagger_{-\sigma}[f_{-\sigma}, V] + [f^\dagger_{-\sigma}, V] f_{-\sigma} = -\sum_{\mathbf{k}'} v_{\mathbf{k}'} \left(c^\dagger_{\mathbf{k}',-\sigma} f_{-\sigma} + c_{\mathbf{k}',-\sigma} f^\dagger_{-\sigma} \right), \tag{42}$$

giving

$$\begin{aligned}
[T, V] = &\sum_{\mathbf{k},\mathbf{k}',\sigma} t_{\mathbf{k}} v_{\mathbf{k}'} \left(c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma} + c^\dagger_{\mathbf{k}',\sigma} c_{\mathbf{k},\sigma} \right) n_{-\sigma} - 4 \sum_{\mathbf{k}} t_{\mathbf{k}} v_{\mathbf{k}} n_\uparrow n_\downarrow \\
&- \sum_{\mathbf{k},\mathbf{k}',\sigma} t_{\mathbf{k}} v_{\mathbf{k}'} \left(c^\dagger_{\mathbf{k},\sigma} f_\sigma + c_{\mathbf{k},\sigma} f^\dagger_\sigma \right) \left(c^\dagger_{\mathbf{k}',-\sigma} f_{-\sigma} + c_{\mathbf{k}',-\sigma} f^\dagger_{-\sigma} \right) \\
= &\sum_{\mathbf{k},\mathbf{k}',\sigma} t_{\mathbf{k}} v_{\mathbf{k}'} \left(c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma} + c^\dagger_{\mathbf{k}',\sigma} c_{\mathbf{k},\sigma} \right) n_{-\sigma} - 4 \sum_{\mathbf{k}} t_{\mathbf{k}} v_{\mathbf{k}} n_\uparrow n_\downarrow \\
&- \sum_{\mathbf{k},\mathbf{k}',\sigma} t_{\mathbf{k}} v_{\mathbf{k}'} \Big(c^\dagger_{\mathbf{k},\sigma} f_\sigma c^\dagger_{\mathbf{k}',-\sigma} f_{-\sigma} + c^\dagger_{\mathbf{k},\sigma} f_\sigma c_{\mathbf{k}',-\sigma} f^\dagger_{-\sigma} \\
&+ c_{\mathbf{k},\sigma} f^\dagger_\sigma c^\dagger_{\mathbf{k}',-\sigma} f_{-\sigma} + c_{\mathbf{k},\sigma} f^\dagger_\sigma c_{\mathbf{k}',-\sigma} f^\dagger_{-\sigma} \Big) \\
= &-4 \sum_{\mathbf{k}} t_{\mathbf{k}} v_{\mathbf{k}} n_\uparrow n_\downarrow + \sum_{\mathbf{k},\mathbf{k}',\sigma} t_{\mathbf{k}} v_{\mathbf{k}'} \left(c^\dagger_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}',-\sigma} f_\sigma f_{-\sigma} + \text{h.c.} \right) \\
&+ \sum_{\mathbf{k},\mathbf{k}',\sigma} t_{\mathbf{k}} v_{\mathbf{k}'} \left(c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma'} n_{-\sigma} - c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',-\sigma} d^\dagger_{-\sigma} d_\sigma + \text{h.c.} \right),
\end{aligned} \tag{43}$$

where the last step is simply a re-ordering. At long last, $[S, V]/2 = [S_0, V]/2 + [T, V]/2$ is nothing but

$$\begin{aligned}
\frac{1}{2}[S, V] = &-\sum_{\mathbf{k}} s_{\mathbf{k}} v_{\mathbf{k}} \left(n_\uparrow + n_\downarrow \right) + \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\sigma} s_{\mathbf{k}} v_{\mathbf{k}'} \left(c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma} + c^\dagger_{\mathbf{k}',\sigma} c_{\mathbf{k},\sigma} \right) \\
&- 2 \sum_{\mathbf{k}} t_{\mathbf{k}} v_{\mathbf{k}} n_\uparrow n_\downarrow + \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\sigma} t_{\mathbf{k}} v_{\mathbf{k}'} \left(c^\dagger_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}',-\sigma} f_\sigma f_{-\sigma} + \text{h.c.} \right) \\
&+ \frac{1}{2} \sum_{\mathbf{k},\mathbf{k}',\sigma} t_{\mathbf{k}} v_{\mathbf{k}'} \left(c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma'} n_{-\sigma} - c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',-\sigma} d^\dagger_{-\sigma} d_\sigma + \text{h.c.} \right),
\end{aligned} \tag{44}$$

which is the additional term obtained by the unitary transformation of H in (33).

To greater simplify things, I will use my divine intuition to define the following spinors

$$\Psi_k = \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c_{\mathbf{k},\downarrow} \end{pmatrix}, \qquad \Psi_f = \begin{pmatrix} f_\uparrow \\ f_\downarrow \end{pmatrix}. \tag{45}$$

The value of this representation can be seen by evaluating

$$\begin{aligned}
\left(\Psi^\dagger_{\mathbf{k}} \vec{\sigma} \Psi_{\mathbf{k}'} \right) \cdot \left(\Psi^\dagger_f \vec{\sigma} \Psi_f \right) = &\left(\Psi^\dagger_{\mathbf{k}} \sigma_x \Psi_{\mathbf{k}'} \right) \left(\Psi^\dagger_f \sigma_x \Psi_f \right) + \left(\Psi^\dagger_{\mathbf{k}} \sigma_y \Psi_{\mathbf{k}'} \right) \left(\Psi^\dagger_f \sigma_y \Psi_f \right) \\
&+ \left(\Psi^\dagger_{\mathbf{k}} \sigma_z \Psi_{\mathbf{k}'} \right) \left(\Psi^\dagger_f \sigma_z \Psi_f \right),
\end{aligned} \tag{46}$$

in which case

$$\begin{aligned}
\left(\Psi^\dagger_{\mathbf{k}} \sigma_x \Psi_{\mathbf{k}'} \right) \left(\Psi^\dagger_f \sigma_x \Psi_f \right) + \left(\Psi^\dagger_{\mathbf{k}} \sigma_y \Psi_{\mathbf{k}'} \right) \left(\Psi^\dagger_f \sigma_y \Psi_f \right) = &\left(c^\dagger_{\mathbf{k},\uparrow} c_{\mathbf{k}',\downarrow} + c^\dagger_{\mathbf{k},\downarrow} c_{\mathbf{k}',\uparrow} \right) \left(f^\dagger_\uparrow f_\downarrow + f^\dagger_\downarrow f_\uparrow \right) \\
&+ \left(c^\dagger_{\mathbf{k},\uparrow} c_{\mathbf{k}',\downarrow} - c^\dagger_{\mathbf{k},\downarrow} c_{\mathbf{k}',\uparrow} \right) \left(-f^\dagger_\uparrow f_\downarrow + f^\dagger_\downarrow f_\uparrow \right) \\
= &\, 2 c^\dagger_{\mathbf{k},\uparrow} c_{\mathbf{k}',\downarrow} f^\dagger_\uparrow f_\downarrow + 2 c^\dagger_{\mathbf{k},\downarrow} c_{\mathbf{k}',\uparrow} f^\dagger_\uparrow f_\downarrow \\
= &\, 2 \sum_{\sigma} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',-\sigma} f^\dagger_{-\sigma} f_\sigma,
\end{aligned} \tag{47}$$

$$\left(\Psi_{\mathbf{k}}^\dagger\sigma_z\Psi_{\mathbf{k}'}\right)\left(\Psi_f^\dagger\sigma_z\Psi_f\right) = \left(c_{\mathbf{k},\uparrow}^\dagger c_{\mathbf{k}',\uparrow} - c_{\mathbf{k},\downarrow}^\dagger c_{\mathbf{k}',\downarrow}\right)\left(f_\uparrow^\dagger f_\uparrow - f_\downarrow^\dagger f_\downarrow\right)$$
$$= c_{\mathbf{k},\uparrow}^\dagger c_{\mathbf{k}',\uparrow}\left(n_\uparrow + n_\downarrow\right) - 2c_{\mathbf{k},\uparrow}^\dagger c_{\mathbf{k}',\uparrow}n_\downarrow + c_{\mathbf{k},\downarrow}^\dagger c_{\mathbf{k}',\downarrow}\left(n_\uparrow + n_\downarrow\right) - 2c_{\mathbf{k},\downarrow}^\dagger c_{\mathbf{k}',\downarrow}n_\uparrow \tag{48}$$
$$= \sum_\sigma c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',\sigma}\left(n_\uparrow + n_\downarrow\right) - 2\sum_\sigma c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',\sigma}n_{-\sigma}.$$

resulting in

$$\left(\Psi_{\mathbf{k}}^\dagger\vec{\sigma}\Psi_{\mathbf{k}'}\right)\cdot\left(\Psi_f^\dagger\vec{\sigma}\Psi_f\right) = \sum_\sigma c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',\sigma}\left(n_\uparrow + n_\downarrow\right) - 2\sum_\sigma\left(c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',\sigma}n_{-\sigma} - c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',-\sigma}f_{-\sigma}^\dagger f_\sigma\right)$$
$$\iff \sum_\sigma\left(c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',\sigma}n_{-\sigma} - c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',-\sigma}f_{-\sigma}^\dagger f_\sigma\right) = \frac{1}{2}\sum_\sigma c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',\sigma}\left(n_\uparrow + n_\downarrow\right) - \vec{S}_f\cdot\left(\Psi_{\mathbf{k}}^\dagger\vec{\sigma}\Psi_{\mathbf{k}'}\right), \tag{49}$$

where I defined

$$\vec{S}_f \equiv \Psi_f^\dagger\frac{\vec{\sigma}}{2}\Psi_f \tag{50}$$

as the operator that measures the vector spin of the f-electron. The last term of (44) can be simplified using this relation. Since the hermitian conjugate simply swaps $\mathbf{k} \leftrightarrow \mathbf{k}'$, it can be written as

$$\frac{1}{2}\sum_{\mathbf{k},\mathbf{k}',\sigma} t_{\mathbf{k}}v_{\mathbf{k}'}\left(c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',\sigma'}n_{-\sigma} - c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',-\sigma}d_{-\sigma}^\dagger d_\sigma + \text{h.c.}\right)$$
$$= \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}',\sigma}\left(t_{\mathbf{k}}v_{\mathbf{k}'} + t_{\mathbf{k}'}v_{\mathbf{k}}\right)\left(c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',\sigma'}n_{-\sigma} - c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',-\sigma}d_{-\sigma}^\dagger d_\sigma\right)$$
$$= \sum_{\mathbf{k},\mathbf{k}'}\left(t_{\mathbf{k}}v_{\mathbf{k}'} + t_{\mathbf{k}'}v_{\mathbf{k}}\right)\left(\frac{1}{4}\sum_\sigma c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',\sigma}\left(n_\uparrow + n_\downarrow\right) - \vec{S}_f\cdot\left(\Psi_{\mathbf{k}}^\dagger\frac{\vec{\sigma}}{2}\Psi_{\mathbf{k}'}\right)\right) \tag{51}$$
$$= \sum_{\mathbf{k},\mathbf{k}'}\left(t_{\mathbf{k}}v_{\mathbf{k}'} + t_{\mathbf{k}'}v_{\mathbf{k}}\right)\left(\frac{1}{4}\left(\Psi_{\mathbf{k}}^\dagger\Psi_{\mathbf{k}'}\right)\left(\Psi_f^\dagger\Psi_f^\dagger\right) - \vec{S}_f\cdot\left(\Psi_{\mathbf{k}}^\dagger\frac{\vec{\sigma}}{2}\Psi_{\mathbf{k}'}\right)\right).$$

Therefore, (44) becomes

$$\frac{1}{2}[S,V] = -\sum_{\mathbf{k}} s_{\mathbf{k}}v_{\mathbf{k}}\left(n_\uparrow + n_\downarrow\right) - 2\sum_{\mathbf{k}} t_{\mathbf{k}}v_{\mathbf{k}}n_\uparrow n_\downarrow + \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'}\left(s_{\mathbf{k}}v_{\mathbf{k}'}\right)\left(\Psi_{\mathbf{k}}^\dagger\Psi_{\mathbf{k}'} + \text{h.c.}\right)$$
$$+ \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}',\sigma} t_{\mathbf{k}}v_{\mathbf{k}'}\left(c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',-\sigma}^\dagger f_\sigma f_{-\sigma} + \text{h.c.}\right)$$
$$+ \sum_{\mathbf{k},\mathbf{k}'}\left(t_{\mathbf{k}}v_{\mathbf{k}'} + t_{\mathbf{k}'}v_{\mathbf{k}}\right)\left(\frac{1}{4}\left(\Psi_k^\dagger\Psi_{k'}\right)\left(\Psi_f^\dagger\Psi_f\right) - \vec{S}_f\cdot\left(\Psi_{\mathbf{k}}^\dagger\frac{\vec{\sigma}}{2}\Psi_{\mathbf{k}'}\right)\right)$$
$$= -\sum_{\mathbf{k},\sigma}\left(s_{\mathbf{k}}v_{\mathbf{k}} + t_{\mathbf{k}}v_{\mathbf{k}}n_{-\sigma}\right)n_\sigma + \frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'}\left(s_{\mathbf{k}}v_{\mathbf{k}'} + s_{\mathbf{k}'}v_{\mathbf{k}}\right)\left(\Psi_{\mathbf{k}}^\dagger\Psi_{\mathbf{k}'}\right) \tag{52}$$
$$+ \frac{1}{4}\sum_{\mathbf{k},\mathbf{k}',\sigma}\left(t_{\mathbf{k}}v_{\mathbf{k}'} + t_{\mathbf{k}'}v_{\mathbf{k}}\right)\left(c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',-\sigma}^\dagger f_\sigma f_{-\sigma} + \text{h.c.}\right)$$
$$+ \sum_{\mathbf{k},\mathbf{k}'}\left(t_{\mathbf{k}}v_{\mathbf{k}'} + t_{\mathbf{k}'}v_{\mathbf{k}}\right)\left(\frac{1}{4}\left(\Psi_{\mathbf{k}}^\dagger\Psi_{\mathbf{k}'}\right)\left(\Psi_f^\dagger\Psi_f\right) - \vec{S}_f\cdot\left(\Psi_{\mathbf{k}}^\dagger\frac{\vec{\sigma}}{2}\Psi_{\mathbf{k}'}\right)\right).$$

By defining the couplings

$$W_{\mathbf{k},\mathbf{k}'} = \frac{1}{2}\left(s_{\mathbf{k}}v_{\mathbf{k}'} + s_{\mathbf{k}'}v_{\mathbf{k}}\right), \qquad J_{\mathbf{k},\mathbf{k}'} = \left(t_{\mathbf{k}}v_{\mathbf{k}'} + t_{\mathbf{k}'}v_{\mathbf{k}}\right), \tag{53}$$

then the unitary transformation of the SIAM (33) can be written succinctly as

$$
\begin{aligned}
e^{S}He^{-S} = H_0 &- \sum_{\mathbf{k},\sigma}\left(W_{\mathbf{k},\mathbf{k}} + \frac{1}{2}J_{\mathbf{k},\mathbf{k}}n_{-\sigma}\right)n_\sigma + \sum_{\mathbf{k},\mathbf{k}'}\left(W_{\mathbf{k},\mathbf{k}'} + \frac{1}{4}J_{\mathbf{k},\mathbf{k}'}\left(\Psi_f^\dagger\Psi_f\right)\right)\left(\Psi_{\mathbf{k}}^\dagger\Psi_{\mathbf{k}'}\right) \\
&+ \frac{1}{4}\sum_{\mathbf{k},\mathbf{k}',\sigma}J_{\mathbf{k},\mathbf{k}'}\left(c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',-\sigma}^\dagger f_\sigma f_{-\sigma} + \text{h.c.}\right) - \sum_{\mathbf{k},\mathbf{k}'}J_{\mathbf{k},\mathbf{k}'}\,\vec{S}_f\cdot\left(\Psi_{\mathbf{k}}^\dagger\frac{\vec{\sigma}}{2}\Psi_{\mathbf{k}'}\right),
\end{aligned} \tag{54}
$$

which is exactly the form derived by Schrieffer, Wolff [3].

3 Analysis of Resulting Hamiltonian

3.1 Energy Scaling

The first term,

$$
\tilde{H}_0 \equiv -\sum_{\mathbf{k},\sigma}\left(W_{\mathbf{k},\mathbf{k}} + \frac{1}{2}J_{\mathbf{k},\mathbf{k}}n_{-\sigma}\right)n_\sigma, \tag{55}
$$

is a shift of energy levels and can be absorbed into H_0 through a shift of U, ϵ_f. As such, it will be ignored.

3.2 Direct (Spin-Independent) s-f Interaction

The second term,

$$
H_{\text{dir}} \equiv \sum_{\mathbf{k},\mathbf{k}'}\left(W_{\mathbf{k},\mathbf{k}'} + \frac{1}{4}J_{\mathbf{k},\mathbf{k}'}\left(\Psi_f^\dagger\Psi_f\right)\right)\left(\Psi_{\mathbf{k}}^\dagger\Psi_{\mathbf{k}'}\right), \tag{56}
$$

is independent of spin and therefore acts as a direct s-f interaction. The low-energy sector consists of singly occupied f-electron states, in which case $\Psi_f^\dagger\Psi_f = 1$ and $H_{\text{dir.}}$ reduces to a one-body potential. This can be eliminated by transforming from the k-states to a set of 1-electron conduction states which includes this direct scattering term.

3.3 Pair Tunneling

The third term,

$$
H_{\text{tun.}} \equiv \frac{1}{4}\sum_{\mathbf{k},\mathbf{k}',\sigma}J_{\mathbf{k},\mathbf{k}'}\left(c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k}',-\sigma}^\dagger f_\sigma f_{-\sigma} + \text{h.c.}\right), \tag{57}
$$

does not conserve the number of f-electrons, and can be neglected in the low-energy regime since it doesn't connect the single f-electron subspace to the rest of the Hilbert space.

3.4 s-f Exchange Interaction

The last term,

$$
H_K \equiv -\sum_{\mathbf{k},\mathbf{k}'}J_{\mathbf{k},\mathbf{k}'}\,\vec{S}_f\cdot\left(\Psi_{\mathbf{k}}^\dagger\frac{\vec{\sigma}}{2}\Psi_{\mathbf{k}'}\right), \tag{58}
$$

is a spin-exchange interaction between the conduction sea and the local magnetic moment. This term is what gives rise to the Kondo effect, which describes the transition between local moment (free impurity) behavior and the low temperature physics where the c-electrons and f-electrons form a spin singlet.

Performing the Projection

I will now project out the low-energy sector, giving the low energy physics regime without empty and doubly occupied states. I find just the Kondo term (58), and the lower energy subspace of H_0 is simply the conduction band H_{band}, such that the transformed SIAM (54) in the lower energy (singly occupied f-electron) regime has the form

$$\boxed{H_{\text{Kondo}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} - \sum_{\mathbf{k},\mathbf{k}'} J_{\mathbf{k},\mathbf{k}'}\ \vec{S}_f \cdot \left(\Psi^\dagger_{\mathbf{k}} \frac{\vec{\sigma}}{2} \Psi_{\mathbf{k}'} \right)} \tag{59}$$

which is the Kondo Hamiltonian.

Is $J_{\mathbf{k},\mathbf{k}'}$ positive or negative? Well, if $k, k' \approx k_F$ then $\epsilon_{\mathbf{k}} \approx 0$ and

$$\begin{aligned} -J_{\mathbf{k},\mathbf{k}'} &\approx -2t_{\mathbf{k}} v_{\mathbf{k}} \\ &\approx -2v^2_{\mathbf{k}} \left(\frac{U}{\epsilon_f (U + \epsilon_f)} \right) > 0 \end{aligned} \tag{60}$$

which is because $\epsilon_f \ll 0$ and $U + \epsilon_f \gg 0$ in this regime. Therefore, the interaction between the local moment and the c-electron band is antiferromagnetic. In many cases, like in the mean-field approach, $J_{\mathbf{k},\mathbf{k}'}$ is momentum independent. This motivates

$$\boxed{H_{\text{Kondo}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + J \sum_{\mathbf{k},\mathbf{k}'} \vec{S}_f \cdot \left(\Psi^\dagger_{\mathbf{k}} \frac{\vec{\sigma}}{2} \Psi_{\mathbf{k}'} \right) \qquad (J \in \mathbb{R}^+)} \tag{61}$$

as the single impurity Kondo model.

References

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