Schrieffer-Wolff transformation

The Schrieffer-Wolff transformation is a version of degenerate perturbation theory in which the low-energy effective Hamiltonian is obtained from the exact one by a unitary transformation decoupling the low-energy and high-energy sectors. In this session we will apply this method to relate the Anderson model of a localized impurity to the Kondo model. We follow the paper by Schrieffer and Wolff:


I. Single impurity Anderson model (SIAM)

The Anderson model describes a single localized orbital of type $d$ coupled to a single conduction band. The impurity has a local Hamiltonian

$$H_{\text{imp}} = \epsilon_d (n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow$$

(a) Rewrite this Hamiltonian in terms of creation and annihilation operators $d_\sigma, d_\sigma^\dagger$, were $\sigma \in \{\uparrow, \downarrow\}$. What are the commutation relations of the operators $d_\sigma, d_\sigma^\dagger$? What are the commutation relations of the occupation numbers $n_\sigma$ with $d_\sigma, d_\sigma^\dagger$?

(b) Give the four eigenstates of $H_{\text{imp}}$ in second quantization. What is the physical interpretation of $\epsilon_d$ and $U$?

This impurity is coupled to electrons in the conduction band of a metal, whose Hamiltonian is

$$H_{\text{band}} = \sum_{k, \sigma} \epsilon_k c_{k, \sigma}^\dagger c_{k, \sigma}$$

via an interaction of the generic form

$$V = \sum_{k, \sigma} (v_k c_{k, \sigma}^\dagger d_\sigma + \text{h.c.}) , \quad v_k \in \mathbb{C}$$

(c) What are the commutation relations of operators of $d$ and $c$ type? Give the explicit expression of the term ”h.c.”.

(d) Derive formula (1) for free electrons in a box of size $L^3$ (with p.b.c.). What is then $\epsilon_k$? ** Same question for 1d electrons in a 1d lattice (with tight-binding Hamiltonian $H = -t \sum_{n \in \mathbb{Z}} (|\phi_n\rangle \langle \phi_{n+1}| + \text{h.c.})$, with $\langle \phi_n| \phi_m \rangle = \delta_{n,m}$).

(e) Compute $v_k$ in formula (2) for an ultra-local coupling of the form $V = \Psi_\sigma^\dagger(0)d_\sigma + \text{h.c.}$. Same question for $V = \int d^3r \left( f(r)\Psi_\sigma^\dagger(r)d_\sigma + \text{h.c.} \right)$ with $f(r) \propto e^{-r^2/2\sigma^2}$.
(f) In the following we will choose $v_k$ to be real numbers. Is this a loss of generality?

II. Schrieffer-Wolff transformation

The single-impurity Anderson model (SIAM) is defined by the Hamiltonian

$$H = H_0 + \lambda V, \quad H_0 = H_{\text{imp}} + H_{\text{band}}$$

We are concerned with the regime $\epsilon_d \ll 0$ and $\epsilon_d + U \gg 0$, so that the energy of the singly occupied orbital $\epsilon_d$ is much lower than the energy of the empty and doubly occupied states $|0\rangle$ and $|2\rangle$. Accordingly we split the Fock space of the orbital into a low energy sector, in which the orbital contains a single electron, and a high energy sector spanned by the empty and doubly occupied states $|0\rangle$ and $|2\rangle$. The objective is to obtain an effective, simpler Hamiltonian capturing the low energy physics of the SIAM. To do so one must project out the high energy subspace and obtain an effective Hamiltonian in which a single electron occupies the localized orbital. In the limit of weak interaction $\lambda \to 0$, the ground state will be given by a Fermi sea and a single electron occupying the localized orbital. Since the states $|\uparrow\rangle$ and $|\downarrow\rangle$ are degenerate, a localized spin $1/2$ moment occurs. Virtual exchange of electrons with the conduction band lead to spin-flip processes.

(a) Write down the projectors to the low and high energy subspaces $P_l$ and $P_h$ in terms of the occupation numbers $n_\sigma$.

(b) The SIAM hamiltonian $H$ can be split into 2 parts : a diagonal part $P_l H P_l + P_h H P_h$ and an off-diagonal part $P_h H P_l + P_l H P_h$. Identify these two parts. Why is it difficult to project out the high energy subspace?

In order to go around this problem, Schrieffer and Wolf proposed to perform a well-chosen unitary transformation before doing the projection. They considered a unitary transformation $U = e^{\lambda S}$ defined by the requirement of eliminating the linear term in $\lambda$

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

(c) Should $S$ be chosen hermitian?

(d) Recall the formal series expansion of $e^{\lambda S} H e^{-\lambda S}$ in terms of commutators.

(e) What does the requirement of eliminating the linear term in $\lambda$ implies for the commutator $[H_0, S]$?

(f) Using this condition, simplify the formal expression of the question II (d). In particular, what is the dominant interaction term as $\lambda \to 0$?

(g) From the constraint obtained in (e), explain why $S$ can be chosen off-diagonal, i.e. $S = P_h S P_l + P_l S P_h$. Why is the new Hamiltonian $H_0 + \lambda^2 [S, V]$ better suited for a projection to the low energy sector?
III. The operator $S$ in the absence of Coulomb repulsion

At this stage it is not clear whether an operator $S$ obeying the constraint II.(c) exists. The point of this section is to find one.

In the absence of Coulomb repulsion in the localized orbital, the Hamiltonian $H$ is quadratic, and it is sensible to look for a quadratic $S = S_0$ (why?). We adopt the following ansatz

$$S_0 = \sum_{k,\sigma} s_k \left( c_{k,\sigma}^\dagger d_\sigma + c_{k,\sigma} d_\sigma^\dagger \right)$$

(a) Calculate $[S, d_\sigma], [S, c_{k,\sigma}]$ and their hermitian conjugates.

(b) What is $[S, H_0]$? What should we choose for $s_k$?

(c) What is $[S, V]$?

IV. The operator $S$ in the generic case

(a) Calculate $[S_0, n_\uparrow n_\downarrow]$. What is $[S_0, H_0]$ when $U \neq 0$?

To get rid of the unwanted quartic term, we improve our ansatz for $S$ by adding a quartic term $T$ such that $[T, H_0] = -U \sum_{k,\sigma} s_k \left( c_{k,\sigma}^\dagger d_\sigma + d_\sigma^\dagger c_{k,\sigma} \right) n_{-\sigma}$. For this we use the following ansatz

$$S = S_0 + T, \quad T = \sum_{k,\sigma} t_k \left( c_{k,\sigma}^\dagger d_\sigma + c_{k,\sigma} d_\sigma^\dagger \right) n_{-\sigma}$$

(b) Calculate $[T, H_0]$. Does this ansatz work?

(c) Show that

$$[T, V] = -4 \left( \sum_k t_k v_k \right) n_\uparrow n_\downarrow + \sum_{k', k,\sigma} t_{k'} v_k \left( c_{k',\sigma}^\dagger c_{k,\sigma}^\dagger d_\sigma + h.c. \right)$$

$$+ \sum_{k', k,\sigma} t_{k'} v_k \left( c_{k',\sigma} c_{k,\sigma} n_{-\sigma} - c_{k',\sigma}^\dagger c_{k,\sigma} d_{-\sigma} + h.c. \right)$$

(d) Using the compact notations

$$\Psi_k = \begin{pmatrix} c_{k,\uparrow} \\ c_{k,\downarrow} \end{pmatrix}, \quad \Psi_d = \begin{pmatrix} d_\uparrow \\ d_\downarrow \end{pmatrix}$$

show that the interaction $\frac{1}{2}[S, V]$ is of the form $H_{ex} + H_{dir} + H_0' + H_{ch}$, where we have

- an $s - d$ exchange interaction

$$H_{ex} = \sum_{k, k'} J_{k', k} \left( \Psi_k^\dagger \vec{\sigma} \Psi_{k'} \right) \cdot \vec{s}_d, \quad \vec{s}_d = \begin{pmatrix} \vec{\sigma} \Psi_d \end{pmatrix}$$
• a direct (spin-independent) interaction

\[ H_{\text{dir}} = \sum_{k,k'} \left( W_{k',k} + \frac{1}{4} J_{k',k} \left( \Psi_{d}^\dagger \Psi_{d} \right) \right) \left( \Psi_{k'}^\dagger \Psi_{k} \right) \]

• a mere shift of the energy level \((i.e.\) that can be absorbed in \(H_0\) by shifting \(\epsilon_{d}\) and \(U)\)

\[ H'_0 = \alpha (n^+_\uparrow + n^+_\downarrow) + \beta n^+_\uparrow n^+_\downarrow \]

• a pair tunneling term

\[ H_{\text{ch}} = - \sum_{k,k'} J_{k',k} \left( c_{k',\uparrow}^\dagger c_{k,\downarrow}^\dagger d_{\uparrow} d_{\downarrow} + \text{h.c.} \right) \]

(e) Which of these terms are left in the low energy effective Hamiltonian? Conclude that the Schrieffer-Wolff transformation generates an effective Kondo Hamiltonian for the low energy sector of the SIAM in second order in the hybridization. We recall the Kondo interaction

\[ H_{K} = \sum_{k,k'} J_{k',k} \left( \Psi_{k'}^\dagger \frac{\vec{\sigma}}{2} \Psi_{k} \right) \cdot \vec{S}_{d} \]