The Kondo problem

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Abstract

The goal of this note is to discuss the physics of the Kondo problem. To this end, I will first introduce the so-called effective Hamiltonian method which I find quite handy. The method is then applied to the introduction of the effective propagator, non-degenerate and degenerate perturbation theory, as well as superexchange in the Hubbard model. It is then used to show that the form of the Kondo Hamiltonian can be motivated by considering the limit of single occupancy of the Anderson impurity model. Finally, Anderson's poor man's scaling is carried out using the effective Hamiltonian method.

1 The effective Hamiltonian method

The stationary state Schrodinger equation

$$H\psi = E\psi$$

can be written as, for example,

$$\begin{aligned} H_{11}\psi_1 + H_{12}\psi_2 &= E\psi_1 \\ H_{21}\psi_1 + H_{22}\psi_2 &= E\psi_2 \end{aligned}$$

The second equation can be used to solve for ψ_2, at least formally:

$$\psi_2 = \frac{1}{E - H_{22}} H_{21}\psi_1$$

which gives us a self-consistent equation

$$\left(H_{11} + H_{12}\frac{1}{E - H_{22}} H_{21}\right)\psi_1 = E\psi_1$$

2 The effective propagator

We have seen that the effective Hamiltonian is

$$H_{\text{eff}}(\omega) = H_{11} + H_{12}\,\frac{1}{\omega - H_{22}}\,H_{21}$$

and one can verify that the effective propagator is simply

$$\mathcal{P}_1\,\frac{1}{\omega - H}\,\mathcal{P}_1 = \frac{1}{\omega - H_{\text{eff}}(\omega)}$$

3 The Brillouin-Wigner perturbation theory

The effective Hamiltonian is

$$\begin{aligned}
H_{\text{eff}} &= H_{11} + H_{12}\,\frac{1}{E - H_{22}}\,H_{21} \\
&= (H_0)_{11} + V_{11} + V_{12}\,\frac{1}{E - (H_0)_{22} - V_{22}}\,V_{21} \\
&= (H_0)_{11} + V_{11} + V_{12}\,\frac{1}{E - (H_0)_{22}}\,V_{21} + V_{12}\,\frac{1}{E - (H_0)_{22}}\,V_{22}\,\frac{1}{E - (H_0)_{22}}\,V_{21} + \cdots
\end{aligned}$$

and the eigenstates are

$$\begin{aligned}
\psi_2 &= \frac{1}{E - H_{22}}\,H_{21}\psi_1 \\
&= \frac{1}{E - (H_0)_{22} - V_{22}}\,V_{21}\psi_1 \\
&= \frac{1}{E - (H_0)_{22}}\,V_{21}\psi_1 + \frac{1}{E - (H_0)_{22}}\,V_{22}\,\frac{1}{E - (H_0)_{22}}\,V_{21}\psi_1 + \cdots
\end{aligned}$$

4 Applications to degenerate perturbation theory

To second order in the perturbation,

$$\begin{aligned}
H_{\text{eff}} &= E_1 1 + V_{11} + V_{12}\,\frac{1}{E - (H_0)_{22} - V_{22}}\,V_{21} \\
&\approx E_1 1 + V_{11} + V_{12}\,\frac{1}{E_1 - (H_0)_{22}}\,V_{21}
\end{aligned}$$

5 AFM coupling in the Hubbard model

Consider the Hubbard model with only two sites

$$H = -t \sum_{i \neq j} (a_{is})^\dagger a_{js} + U \sum_i n_{i+} n_{i-}$$

The effective Hamiltonian is

$$\begin{aligned} H_{\text{eff}} &= \frac{t^2}{E-U} \sum_{i \neq j} \sum_{k \neq l} (a_{is})^\dagger a_{js} (a_{kr})^\dagger a_{lr} \\ &= \frac{t^2}{E-U} \sum_{i \neq j} (a_{is})^\dagger a_{js} (a_{jr})^\dagger a_{ir} \end{aligned}$$

Notice that

$$\begin{aligned} \sum_{i \neq j} S_i \cdot S_j &= \frac{1}{2} \sum_{i \neq j} (a_{is})^\dagger a_{ir} (a_{jr})^\dagger a_{js} - \frac{1}{4} \sum_{i \neq j} (a_{is})^\dagger a_{is} (a_{jr})^\dagger a_{jr} \\ &= \frac{1}{2} \sum_{i \neq j} (a_{is})^\dagger a_{is} - \frac{1}{2} \sum_{i \neq j} (a_{is})^\dagger a_{ir} a_{js} (a_{jr})^\dagger \\ &= \frac{1}{2} - \frac{1}{2} \sum_{i \neq j} (a_{is})^\dagger a_{js} (a_{jr})^\dagger a_{ir} \end{aligned}$$

and thus the effective Hamiltonian contains an anti-ferromagnetic interaction

$$H_{\text{eff}} \approx \frac{2t^2}{U} \sum_{i \neq j} S_i \cdot S_j - \frac{t^2}{U}$$

6 The Anderson impurity model

The Hamiltonian of the Anderson model is

$$H = \sum_{ks} \varepsilon_k n_{ks} + \sum_{ks} V_k (a_{ks})^\dagger A_s + \text{h.c.} + \sum_s \mathcal{E} N_s + U N_+ N_-$$

Notice that we have

$$H_{02} = H_{20} = 0$$

7 The low-energy effective Hamiltonian

In the **low-energy** subspace, we have

$$
\begin{aligned}
H_{10}\,\frac{1}{E-H_{00}}\,H_{01} &= \sum_{ks}\sum_{lr} V_{k*}\,V_l\,(A_s)^\dagger a_{ks}\,\frac{1}{E-H_{00}}\,(a_{lr})^\dagger A_r \\
&= \sum_{ks}\sum_{lr} V_{k*}\,V_l\,(A_s)^\dagger a_{ks}\,(a_{lr})^\dagger A_r\,\frac{1}{E-H_{00}-\varepsilon_l} \\
&\approx \sum_{ks}\sum_{lr} V_{k*}\,V_l\,(A_s)^\dagger a_{ks}\,(a_{lr})^\dagger A_r\,\frac{1}{\mathcal{E}-\varepsilon_l}
\end{aligned}
$$

as well as

$$
\begin{aligned}
H_{12}\,\frac{1}{E-H_{22}}\,H_{21} &= \sum_{ks}\sum_{lr} V_k V_{l*}\,(a_{ks})^\dagger A_s\,\frac{1}{E-H_{22}}\,(A_r)^\dagger a_{lr} \\
&= \sum_{ks}\sum_{lr} V_k V_{l*}\,(a_{ks})^\dagger A_s\,(A_r)^\dagger a_{lr}\,\frac{1}{E-H_{22}+\varepsilon_l} \\
&\approx \sum_{ks}\sum_{lr} V_k V_{l*}\,(a_{ks})^\dagger A_s\,(A_r)^\dagger a_{lr}\,\frac{1}{-\mathcal{E}-U+\varepsilon_l}
\end{aligned}
$$

The low-energy effective Hamiltonian

$$
H_{\text{l-e}} \approx H_{11} - \sum_{ks}\sum_{lr} V_{k*}\,V_l \left[\frac{(A_s)^\dagger a_{ks}\,(a_{lr})^\dagger A_r}{-\mathcal{E}+\varepsilon_l} + \frac{(a_{lr})^\dagger A_r\,(A_s)^\dagger a_{ks}}{\mathcal{E}+U-\varepsilon_k}\right]
$$

Notice that

$$
\begin{aligned}
s_{lk}\cdot S &= \frac{1}{2}\sum_{sr}(a_{lr})^\dagger a_{ks}\,(A_s)^\dagger A_r - \frac{1}{4}\sum_{sr}(a_{lr})^\dagger a_{kr}\,(A_s)^\dagger A_s \\
&= \frac{1}{2}\sum_{sr}(a_{lr})^\dagger a_{ks}\,(A_s)^\dagger A_r - \frac{1}{4}\sum_{r}(a_{lr})^\dagger a_{kr}
\end{aligned}
$$

We see that the low-energy effective Hamiltonian contains an interaction

$$
2\sum_{kl} V_{k*}\,V_l \left[\frac{1}{-\mathcal{E}+\varepsilon_l} + \frac{1}{\mathcal{E}+U-\varepsilon_k}\right] s_{lk}\cdot S
$$

which is **anti-ferromagnetic** at low energy, i.e., near the **Fermi surface**.

8 Anderson: poor man's scaling

The Hamiltonian of the Kondo model is

$$H = \sum_{ks} \varepsilon_k n_{ks} + \sum_{kl} \left[J_z S_z (s_{kl})_z + \tfrac{1}{2} J_+ S_+ (s_{kl})_- + \tfrac{1}{2} J_- S_- (s_{kl})_+ \right]$$

where for example,

$$\begin{aligned} (s_{kl})_+ &= (a_{k+})^\dagger a_{l-} \\ (s_{kl})_- &= (a_{k-})^\dagger a_{l+} \end{aligned}$$