

固体理论, Homework 03

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1 教材习题 7.2

Calculate explicitly the $\varepsilon_{n\sigma}$ s in the Hartree-Fock approximation to the Anderson model.

Solution: From textbook, we have

$$\varepsilon_{n\sigma} \langle \mathbf{k}\sigma | n\sigma \rangle = \varepsilon_{\mathbf{k}} \langle \mathbf{k}\sigma | n\sigma \rangle + V_{\mathbf{k}d} \langle d\sigma | n\sigma \rangle \quad (1.1)$$

$$\varepsilon_{n\sigma} \langle d\sigma | n\sigma \rangle = E_{d\sigma} \langle d\sigma | n\sigma \rangle + \sum_{\mathbf{k}} V_{\mathbf{k}d} \langle \mathbf{k}\sigma | n\sigma \rangle \quad (1.2)$$

with (1.1), we get

$$\langle \mathbf{k}\sigma | n\sigma \rangle = \frac{V_{\mathbf{k}d}}{\varepsilon_{n\sigma} - \varepsilon_{\mathbf{k}}} \langle d\sigma | n\sigma \rangle \quad (1.3)$$

plug it into (1.2),

$$(\varepsilon_{n\sigma} - E_{d\sigma}) \langle d\sigma | n\sigma \rangle = \sum_{\mathbf{k}} \frac{V_{\mathbf{k}d}^2}{\varepsilon_{n\sigma} - \varepsilon_{\mathbf{k}}} \langle d\sigma | n\sigma \rangle \quad (1.4)$$

thus

$$\varepsilon_{n\sigma} = E_{d\sigma} + \frac{V_{\mathbf{k}d}^2}{\varepsilon_{n\sigma} - \varepsilon_{\mathbf{k}}} \quad (1.5)$$

2 教材习题 7.4

Show that when $\varepsilon_d = U/2$ the impurity terms in the Anderson model, $\sum_{\sigma} (\varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow})$, are invariant under the transformation $a_d^{\dagger} \leftrightarrow a_d$.

Solution:

$$\begin{aligned} \sum_{\sigma} (\varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}) &= \varepsilon_d (a_{d\uparrow}^{\dagger} a_{d\uparrow} + a_{d\downarrow}^{\dagger} a_{d\downarrow}) + U a_{d\uparrow}^{\dagger} a_{d\uparrow} a_{d\downarrow}^{\dagger} a_{d\downarrow} \\ &= -\frac{U}{2} (a_{d\uparrow}^{\dagger} a_{d\uparrow} + a_{d\downarrow}^{\dagger} a_{d\downarrow}) + U a_{d\uparrow}^{\dagger} a_{d\uparrow} a_{d\downarrow}^{\dagger} a_{d\downarrow} \\ &= U \left(-\frac{1}{2} a_{d\uparrow}^{\dagger} a_{d\uparrow} - \frac{1}{2} a_{d\downarrow}^{\dagger} a_{d\downarrow} + a_{d\uparrow}^{\dagger} a_{d\uparrow} a_{d\downarrow}^{\dagger} a_{d\downarrow} \right) \end{aligned} \quad (2.1)$$

after the transformation $a_d^{\dagger} \leftrightarrow a_d$,

$$\begin{aligned} \sum_{\sigma} (\varepsilon_d n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}) &= -\frac{U}{2} (a_{d\uparrow} a_{d\uparrow}^{\dagger} + a_{d\downarrow} a_{d\downarrow}^{\dagger}) + U a_{d\uparrow} a_{d\uparrow}^{\dagger} a_{d\downarrow} a_{d\downarrow}^{\dagger} \\ &= -\frac{U}{2} (1 - a_{d\uparrow}^{\dagger} a_{d\uparrow} + 1 - a_{d\downarrow}^{\dagger} a_{d\downarrow}) + U (1 - a_{d\uparrow}^{\dagger} a_{d\uparrow}) (1 - a_{d\downarrow}^{\dagger} a_{d\downarrow}) \\ &= U \left(-1 + \frac{1}{2} a_{d\uparrow}^{\dagger} a_{d\uparrow} + \frac{1}{2} a_{d\downarrow}^{\dagger} a_{d\downarrow} + 1 - a_{d\uparrow}^{\dagger} a_{d\uparrow} - a_{d\downarrow}^{\dagger} a_{d\downarrow} + a_{d\uparrow}^{\dagger} a_{d\uparrow} a_{d\downarrow}^{\dagger} a_{d\downarrow} \right) \\ &= U \left(-\frac{1}{2} a_{d\uparrow}^{\dagger} a_{d\uparrow} - \frac{1}{2} a_{d\downarrow}^{\dagger} a_{d\downarrow} + a_{d\uparrow}^{\dagger} a_{d\uparrow} a_{d\downarrow}^{\dagger} a_{d\downarrow} \right) \end{aligned} \quad (2.2)$$

\therefore the impurity terms are invariant under the transformation $a_d^{\dagger} \leftrightarrow a_d$ when $\varepsilon_d = U/2$