固体理论, Homework 03

王石嵘 20110220098

March 30, 2021

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

$$\varepsilon_{n\sigma} \langle \mathbf{k}\sigma \,|\, n\sigma \rangle = \varepsilon_{\mathbf{k}} \langle \mathbf{k}\sigma \,|\, n\sigma \rangle + V_{\mathbf{k}d} \langle d\sigma \,|\, n\sigma \rangle \tag{1.1}$$

$$\varepsilon_{n\sigma} \langle d\sigma \,|\, n\sigma \rangle = E_{d\sigma} \langle d\sigma \,|\, n\sigma \rangle + \sum_{\mathbf{k}} V_{\mathbf{k}d} \langle \mathbf{k}\sigma \,|\, n\sigma \rangle \tag{1.2}$$

with (1.1), we get

$$\langle \mathbf{k}\sigma \,|\, n\sigma \rangle = \frac{V_{\mathbf{k}d}}{\varepsilon_{n\sigma} - \varepsilon_{\mathbf{k}}} \langle d\sigma \,|\, n\sigma \rangle \tag{1.3}$$

plug it into (1.2),

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

thus

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

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:

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

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

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

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