Quantum Theory of Many-Body systems in Condensed Matter (4302112) 2020

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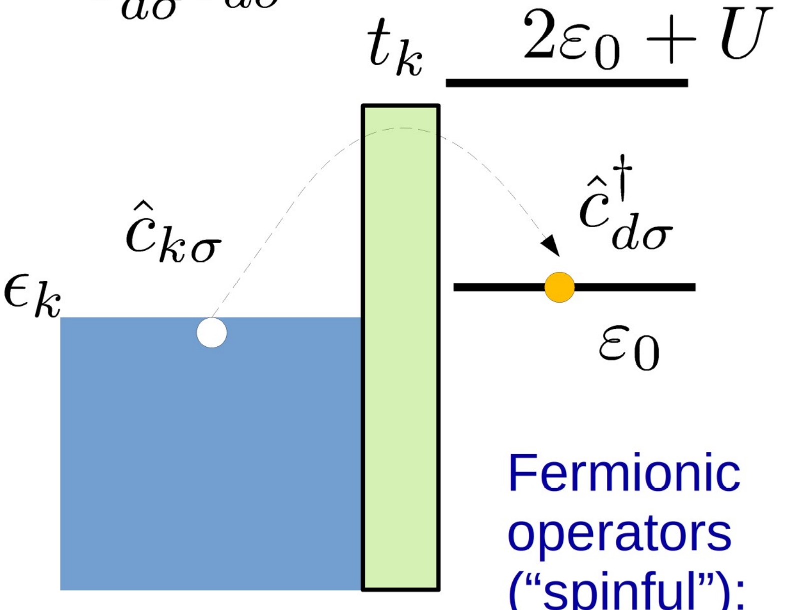
Today's class: *Schrieffer-Wolff transformation (Kondo model)*

- Anderson model: projection into the n_d=1 subspace.
- Schrieffer-Wolff transformation.
- Kondo model.

Anderson impurity model

$$\hat{H} = \hat{H}_{\text{imp}} + \hat{H}_{\text{coup}} + \hat{H}_{\text{band}} \qquad \hat{n}_{d\sigma} \equiv \hat{c}^\dagger_{d\sigma}\hat{c}_{d\sigma}$$

$$\begin{cases} \hat{H}_{\text{imp}} = \sum_{\sigma=\uparrow,\downarrow} \varepsilon_0 \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow}\hat{n}_{d\downarrow} \\ \hat{H}_{\text{coup}} = \sum_{k,\sigma} t_k \hat{c}^\dagger_{d\sigma}\hat{c}_{k\sigma} + t_k^* \hat{c}^\dagger_{k\sigma}\hat{c}_{d\sigma} \\ \hat{H}_{\text{band}} = \sum_{k,\sigma} \epsilon_k \hat{c}^\dagger_{k\sigma}\hat{c}_{k\sigma} \end{cases}$$



Fermionic operators (“spinful”):

Anderson impurity states

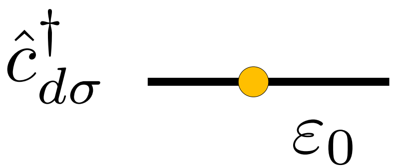
$$\hat{H}_{\text{imp}} = \sum_{\sigma=\uparrow,\downarrow} \varepsilon_0 \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$$

$$E_0 = 0$$

$$\langle 0 | \sum_\sigma \hat{n}_{d\sigma} | 0 \rangle = 0$$

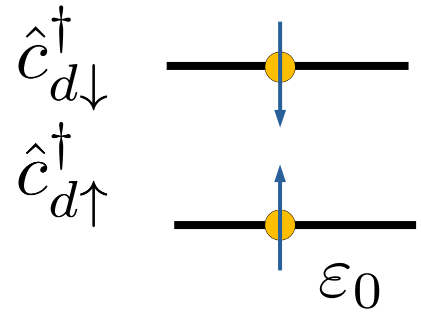
$$E_1 = \varepsilon_0$$

2x degenerate!



$$\langle 1 | \sum_\sigma \hat{n}_{d\sigma} | 1 \rangle = 1$$

$$E_2 = 2\varepsilon_0 + U$$



$$\langle 2 | \sum_\sigma \hat{n}_{d\sigma} | 2 \rangle = 2$$

Particle-hole symmetry point: $\varepsilon_0 = -U/2 \Rightarrow E_0 = E_2$

Schrieffer-Wolff transformation

$$\hat{H} = \hat{H}_{\rm imp} + \hat{H}_{\rm coup} + \hat{H}_{\rm band}$$

The goal: suppress charge transfer and project in $\langle 1 | \sum_\sigma \hat{n}_{d\sigma} | 1 \rangle = 1$ subspace.

Canonical transformation: $\hat{H}_S = e^{i\hat{S}} \hat{H} e^{-i\hat{S}} = \hat{H}_{\rm imp} + \hat{H}_{\rm band} + \mathcal{O}((t_k)^2)$

As it turns out, choosing $\hat{S} = \hat{S}_+ + \hat{S}_- = \left(\hat{S}_-\right)^\dagger + \hat{S}_-$

with:

$$i\hat{S}_- = \sum_{k\sigma} t_k^* \left(\frac{\hat{n}_{d\bar{\sigma}}}{\epsilon_k - E_2 + E_1} + \frac{(1 - \hat{n}_{d\bar{\sigma}})}{\epsilon_k - E_0 + E_1} \right) \hat{c}^\dagger_{k\sigma} \hat{c}_{d\sigma}$$

leads to $\hat{H}_S = \hat{H}_{\rm imp} + \hat{H}_{\rm band} + \hat{H}_S^{(2)}$

Schrieffer, J.R. and Wolff, P.A.
Phys. Rev. **149** 491 (1966)

Schrieffer-Wolff transformation

Result: $$\hat{H}_S^{(2)} = \sum_{kk'} J_{kk'} \mathbf{S}_d \cdot \mathbf{s}_{kk'} + \sum_{kk',\sigma} W_{kk'} \hat{c}^\dagger_{k\sigma} \hat{c}_{k'\sigma}$$

Spin-scattering (Kondo) | Charge scattering

$$\mathbf{S}_d \cdot \mathbf{s}_{kk'} = \frac{1}{4} \sum_i \sum_{\substack{\sigma\sigma' \\ \sigma_1\sigma_1'}} \left(\hat{c}^\dagger_{d\sigma} (\tau^i)_{\sigma\sigma'} \hat{c}_{d\sigma'} \right) \left(\hat{c}^\dagger_{k\sigma} (\tau^i)_{\sigma_1\sigma_1'} \hat{c}_{k\sigma_1'} \right)$$

$$J_{kk'} = 2 \left(\frac{t_k t^*_{k'}}{E_2 - E_1} + \frac{t_k t^*_{k'}}{E_0 - E_1} \right) = \frac{2U t_k t^*_{k'}}{(\varepsilon_0 + U)(-\varepsilon_0)}$$

$$W_{kk'} = -\frac{1}{2} \left(\frac{t_k t^*_{k'}}{E_2 - E_1} + \frac{t_k t^*_{k'}}{E_1 - E_0} \right) = \frac{(2\varepsilon_0 + U) t_k t^*_{k'}}{2(\varepsilon_0 + U)(-\varepsilon_0)}$$