Heisenberg model

- Effective spin models arise when electrons are localized

  → basic ingredients appear to be half-filled bands and strong onsite Coulomb repulsion

  → last class we looked at the $2$-site Hubbard model

\[
\hat{H} = -t \sum_{\alpha = \uparrow, \downarrow} (c_{1\alpha}^\dagger c_{2\alpha} + c_{2\alpha}^\dagger c_{1\alpha}) + U \sum_{j=1,2} n_{j\uparrow} n_{j\downarrow}
\]

- hopping between the two sites
- repulsion term that discourages double occupancy

- $4 + \int U$ separation of energy scales
at half-filling (exactly 2 electrons on the two sites) the number of vacancies ("holes") is exactly equal to the number of double occupancies

\[ \uparrow \downarrow \text{ and } \downarrow \uparrow \]

are connected by the hopping term to \(-\uparrow \uparrow\) and \(\downarrow \downarrow\)

At large $U$, the vacancies and double occupancies are "gapped away", and the model becomes ever closer to satisfying

\[ \hat{n}_{j} = \hat{n}_{j\uparrow} + \hat{n}_{j\downarrow} = 1 \text{ in the low-lying states} \]

\[ |1T_{2} \rangle - 10T_{2} \rangle \]
\[ |1T_{2} \rangle + 10T_{2} \rangle \]

$U/\epsilon$

spin triplet

spin singlet
The four lowest energy states seem to be described by an effective spin model:

\[
\hat{H}_{\text{eff}} = \frac{4t^2}{U} \sum_{\alpha \beta} \frac{1}{2} \sigma_\alpha \sigma_\beta \cdot \frac{1}{2} \sum_{\mu \nu} {C}_\mu \sigma_\mu {C}_\nu \sigma_\nu |_{\hat{n}_1 = \hat{n}_2 = 1} \\
= J \hat{S}_1 \cdot \hat{S}_2 + \text{const}
\]

exchange coupling

**Exercise**: Demonstrate the "particle-hole symmetry" of the model at half-filling by showing that

\[
\hat{H}_U = \frac{U}{Z} \sum_j \hat{n}_j \hat{n}_j = \frac{U}{Z} \sum_j (\hat{n}_j - 1)^2
\]
Now consider the Hubbard model for an arbitrary N-site system

→ Start with the $U/t = \infty$ result and expand perturbatively in powers of $\frac{t}{U}$

→ Schrödinger equation $H\Psi = E\Psi$

   can be written as

   $$H(P + Q)\overline{\Psi} = E(P + Q)\overline{\Psi}$$

   where $P$ is a projector onto the subspace with no double occupancies and $Q = 1 - P$

→ Note that $P^2 = P$ and $Q^2 = Q$ (always true for projectors)

   and $PQ = QP = P - P^2 = P - P = 0$

→ We're interested in the low-energy states $P\Psi$; we want to discard the high-energy states $Q\Psi$
→ multiply from the left with \( Q \)

\[
Q H (P + Q) Y = E Q (P + Q) Y
\]

\[
\downarrow
\]

\[
(Q H P + Q H Q) Y = E (Q P + Q Q^2) Y
\]

\[
= E Q Y
\]

→ rearrange to get

\[
(Q H Q - E) Y Y = - Q H P Y
\]

\[
\lor
\]

\[
Y Y = -(Q H Q - E)^{-1} Q H P Y
\]

→ insert into

\[
H (P + Q) Y = E (P + Q) Y
\]

\[
(Q H P - H (Q H Q - E)^{-1} Q H P) Y
\]

\[
= \partial Y [H - H (Q H Q - E)^{-1} Q H] Y Y = E P Y + E Q Y
\]

→ act from the left with \( P \)

\[
P [H - H (Q H Q - E)^{-1} Q H] P Y Y = E P Y + E P Q Y
\]
We now have a Schrödinger equation for $P_2$

$$P[\mathcal{H} - \mathcal{H}(QH Q - E)^{\dagger}Q H] (P_2) = E(P_2)$$

effective Hamiltonian for the low-energy space with no double occupancies.

→ Specialize to our case, with

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_t + \hat{\mathcal{H}}_U$$

$\hat{T}$ diagonal in the occupation number representation.

Hopping can move the system between the $P$ and $Q$ sectors.

and $P = \prod_j (1 - \hat{n}^{\dagger}_j \hat{n}_j)$.

NB $PH \not{P} = PH_0 P = 0$

$PHQ = PH_\tau Q_j, QHP = QH_\tau P$
→ return to effective Hamiltonian expression

\[ P \left[ H - H(QHQ - E)^{-1} QHQ \right] P \]

\[ \text{to leading order } QHQ \approx U \]

\[ \text{and } E \approx 0 \]

\[ P \rightarrow P HP - \frac{1}{U} (PHQHP) \]

\[ \rightarrow P \rightarrow P^0 HP - \frac{1}{U} (PHQHP) = - \frac{1}{U} PH^{\frac{1}{2}} P \]

→ Let \[ \hat{H}_t = -\sum_{ij} \tilde{t}_{ij} \, c_{i\alpha}^+ c_{j\alpha} \]

with \[ \tilde{t}_{ij} = t_{ij}^* \] and \[ \tilde{t}_{jj} = 0 \]

Then \[ PH^{\frac{1}{2}} P = \sum_{\alpha\beta} \sum_{ij} \tilde{t}_{ij} \tilde{t}_{ij}^* \, P c_{i\alpha}^+ c_{j\beta} \, c_{i\beta}^+ c_{j\alpha} P \]

→ electron created at \( i' \) must be removed

\[ \Rightarrow i' = j \]
So \( \hat{H}_{L}^{2} P = \sum_{\alpha \beta} \sum_{ij} t_{ij} t_{ji} P c_{i \alpha}^{+} c_{j \beta} P c_{j \beta}^{+} c_{i \alpha} P \). 

= \sum_{\alpha \beta} \sum_{ij} l t_{ij} l^{2} P c_{i \alpha}^{+} c_{i \beta} P . P c_{j \alpha}^{+} c_{j \beta} P 

\text{EXERCISE: Prove these identities} 

\[ c_{j \alpha}^{+} c_{j \beta} = \frac{1}{2} \delta_{\alpha \beta} (\hat{n}_{j \alpha}^{\dagger} + \hat{n}_{j \alpha}) + \frac{1}{2} \hat{s}_{j} \cdot \hat{\sigma}_{\alpha \beta} \]

\[ c_{j \alpha}^{+} c_{j \beta} = \delta_{\alpha \beta} (1 - \frac{\hat{n}_{j \beta} + \hat{n}_{j \alpha}}{2}) - \hat{s}_{j} \cdot \hat{\sigma}_{\alpha \beta} \]

where \( \frac{1}{2} \sum_{j} \sum_{\alpha \beta} c_{j \alpha}^{+} \hat{\sigma}_{\alpha \beta} c_{j \beta} \)

→ at half-filling \( (\hat{n}_{j \alpha}^{\dagger} + \hat{n}_{j \alpha} = \hat{n}_{j} = 1) \), these expressions simplify, so that

\[ \hat{H}_{L}^{2} P = \sum_{\alpha \beta} \sum_{ij} l t_{ij} l^{2} \left( \frac{1}{2} \delta_{\alpha \beta} + \frac{1}{2} \hat{s}_{j} \cdot \hat{\sigma}_{\alpha \beta} \right) \left( \frac{1}{2} \delta_{\alpha \beta} - \frac{1}{2} \hat{s}_{j} \cdot \hat{\sigma}_{\alpha \beta} \right) \]

\[ = \sum_{ij} l t_{ij} l^{2} \text{Tr} \left[ \left( \frac{1}{2} 1 + \sum_{a} \hat{s}_{a} \cdot \hat{\sigma}^{a} \right) \left( \frac{1}{2} 1 - \sum_{b} \hat{s}_{b} \cdot \hat{\sigma}^{b} \right) \right] \]

\[ \text{trace over true matrix products in real space} \]

\[ \text{2x2 unit matrix} \]

\[ \text{vectors in spin space} \]

\[ \text{indices in real space} \]
To get

\[ P A_{t}^{\uparrow \downarrow} \mathcal{P} = \sum_{i<j} |t_{ij}|^2 \left( \frac{1}{2} - Z \hat{s}_i \cdot \hat{s}_j \right) \]

\[ = \frac{1}{2} \sum_{i<j} |t_{ij}|^2 \left( 1 - 4 \hat{s}_i \cdot \hat{s}_j \right) \]

Hence \( \hat{H}_{\text{eff}} = -\frac{1}{U} P A_{t}^{\uparrow \downarrow} \mathcal{P} \)

\[ = \sum_{i<j} J_{ij} \hat{s}_i \cdot \hat{s}_j + \text{const} \]

where \( \sum_{ij} \frac{1}{U} |t_{ij}|^2 > 0 \)

is the antiferromagnetic exchange coupling.