Phys 726 - Lecture 13

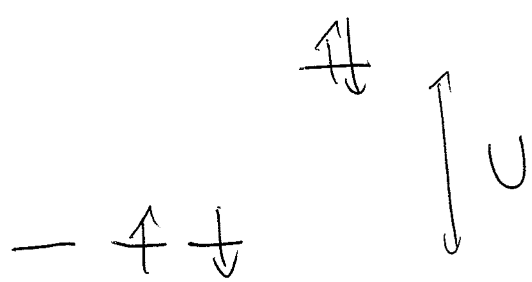
Heisenberg model

* 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

$$\hat{H} = \underbrace{-t \sum_{\alpha=\uparrow\downarrow} \left(c_{1\alpha}^{\dagger} c_{2\alpha} + c_{2\alpha}^{\dagger} c_{1\alpha}\right)}_{\text{hopping between the two sites}} + \underbrace{U \sum_{j=1,2} \hat{n}_{j\uparrow} \hat{n}_{j\downarrow}}_{\text{repulsion term that discourages double occupancy}}$$



separation of energy scales

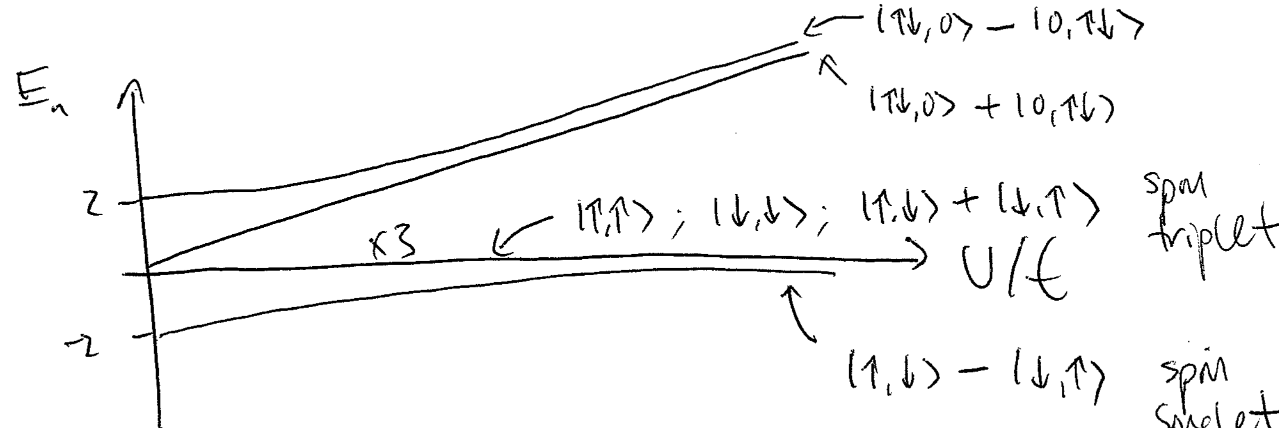
→ at half-filling (exactly 2 electrons on the two sites) the number of vacancies ("holes") is exactly equal to the number of double occupancies

i.e. $\underline{\uparrow}\ \underline{\downarrow}$ and $\underline{\downarrow}\ \underline{\uparrow}$

are connected by the hopping term

to $\underline{\ \ }\ \underline{\uparrow\downarrow}$ and $\underline{\uparrow\downarrow}\ \underline{\ \ }$

→ At large U, the vacancies and double occupancies are "gapped away", and the model becomes ever closer to satisfying $\hat{n}_j = \hat{n}_{j\uparrow} + \hat{n}_{j\downarrow} = 1$ in the low-lying states



→ the four lowest energy states seem to be described by an effective spin model

$$\hat{H}_{eff} = \frac{4t^2}{U} \cdot \frac{1}{2}\sum_{\alpha\beta} c^\dagger_{1\alpha}\vec{\sigma}_{\alpha\beta}c_{1\beta} \cdot \frac{1}{2}\sum_{\mu\nu} c^\dagger_{2\mu}\vec{\sigma}_{\mu\nu}c_{2\nu} \Big|_{\hat{n}_1 = \hat{n}_2 = 1}$$

$$\equiv \underbrace{J}_{\text{exchange coupling}} \hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2 + \text{const}$$

<u>EXERCISE</u>: Demonstrate the "particle-hole symmetry" of the model at half-filling by showing that

$$H_U = U \sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow} = \frac{U}{2}\sum_j (\hat{n}_j - 1)^2$$

* Now consider the Hubbard model for an arbitrary N-site system

→ Start with the $U/t = \infty$ result and expand perturbatively in ~~???~~ powers of $\frac{t}{U} \ll 1$

→ Schrödinger equation $H\Psi = E\Psi$ can be written as

$$H(P+Q)\Psi = E(P+Q)\Psi$$

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

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

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

<u>disjoint</u> subspaces

→ 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

$$QH(P+Q)\psi = EQ(P+Q)\psi$$

$$(QHP + QHQ)\psi \qquad\qquad E(\cancelto{0}{QP} + Q^2)\psi$$

$$= EQ\psi$$

→ rearrange to get

$$(QHQ - E)Q\psi = -QHP\psi$$

or $$Q\psi = -(QHQ-E)^{-1}QHP\psi$$

→ insert into

$$H(P+\overbrace{Q)\psi} = E(P+Q)\psi$$

$$(HP - H(QHQ-E)^{-1}QHP)\psi$$

$$= [H - H(QHQ-E)^{-1}QH]P\psi = EP\psi + EQ\psi$$

→ act from the left with P

$$P[H - H(QHQ-E)^{-1}QH]P\psi = E\cancelto{P}{P^2}\psi + E\cancelto{0}{PQ}\psi$$

→ We now have a Schrödinger equation for $P\psi$

$$\underbrace{P[H - H(QHQ-E)^{-1}QH]}_{\text{effective Hamiltonian for the low-energy space with no double occupancies}}(P\psi) = E(P\psi)$$

→ Specialize to our case, with

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

$\hat{H}_U$: diagonal in the occupation number representation

$\hat{H}_t$: hopping can move the system between the P and Q sectors

and $P = \prod_j (1 - \hat{n}_{j\uparrow}\hat{n}_{j\downarrow})$

<u>NB</u> $PHP = PH_UP = 0$

$PHQ = PH_tQ$; $QHP = QH_tP$

→ return to effective Hamiltonian expression

$$P[H - H(QHQ-E)^{-1}QH]P$$

to leading order $QHQ \simeq U$

and $E \simeq 0$

$$= PHP - \frac{1}{U}(PHQHP)$$

$$= \cancel{PHP}^{\,0} - \frac{1}{U}(PHQ)(QHP) = -\frac{1}{U} P H_t^2 P$$

→ Let $\hat{H}_t = -\sum_{\alpha}\sum_{ij} t_{ij} c^\dagger_{i\alpha} c_{j\alpha}$ with $t_{ij} = t^*_{ji}$ and $t_{jj} = 0$

Then $$P\hat{H}_t^2 P = \sum_{\alpha\beta} \sum_{\substack{ij\\ i'j'}} t_{ij} t_{i'j'} P c^\dagger_{i\alpha} c_{j\alpha} c^\dagger_{i'\beta} c_{j'\beta} P$$

electron created at i' must be removed

$\Rightarrow i' = j$

electron annihilated at j' must reappear in the same place

$\Rightarrow j' = i$

$$\text{So } P\hat{H}_t^2 P = \sum_{\alpha\beta}\sum_{\substack{ij\\(i\neq j)}} t_{ij}t_{ji}\, P c^\dagger_{i\alpha} \underbrace{c_{j\alpha} c^\dagger_{j\beta} c_{i\beta}}_{(-1)^2} P$$

$$= \sum_{\alpha\beta}\sum_{\substack{ij\\(i\neq j)}} |t_{ij}|^2 P c^\dagger_{i\alpha} c_{i\beta} P \cdot P c_{j\alpha} c^\dagger_{j\beta} P$$

EXERCISE: Prove these identities

$$c^\dagger_{j\alpha} c_{j\beta} = \frac{1}{2}\delta_{\alpha\beta}(\hat{n}_{j\uparrow} + \hat{n}_{j\downarrow}) + \hat{\vec{S}}_j \cdot \vec{\sigma}_{\beta\alpha}$$

$$c_{j\alpha} c^\dagger_{j\beta} = \delta_{\alpha\beta}\left(1 - \frac{\hat{n}_{j\uparrow} + \hat{n}_{j\downarrow}}{2}\right) - \hat{\vec{S}}_j \cdot \vec{\sigma}_{\alpha\beta}$$

where $\hat{\vec{S}}_j = \frac{1}{2}\sum_{\alpha\beta} c^\dagger_{j\alpha}\vec{\sigma}_{\alpha\beta} c_{j\beta}$

→ at half-filling ($\hat{n}_{j\uparrow} + \hat{n}_{j\downarrow} = \hat{n}_j = 1$), these expressions simplify, so that

$$P\hat{H}_t^2 P = \sum_{\alpha\beta}\sum_{ij} |t_{ij}|^2 \left(\frac{1}{2}\delta_{\alpha\beta} + \hat{\vec{S}}_i \cdot \vec{\sigma}_{\beta\alpha}\right)\left(\frac{1}{2}\delta_{\alpha\beta} - \hat{\vec{S}}_j \cdot \vec{\sigma}_{\alpha\beta}\right)$$

vectors in real space; indices in spin space

2×2 unit matrix

$$= \sum_{ij} |t_{ij}|^2 \,\mathrm{Tr}\left[\left(\frac{1}{2}\mathbb{1} + \sum_{a=x,y,z} \hat{S}^a_i \sigma^a\right)\left(\frac{1}{2}\mathbb{1} - \sum_{b=x,y,z} S^b_j \sigma^b\right)\right]$$

trace over the matrix products; indices in real space

→ make use of the 2x2 matrix identities

$$\mathrm{Tr}\,\mathbb{1} = 2$$

$$\mathrm{Tr}\,\sigma^a = 0 \quad \text{for each of } a = x, y, z$$

$$\mathrm{Tr}\,\sigma^a \sigma^b = 2\delta^{ab}$$

to get

$$P \hat{H}_t^2 P = \sum_{ij} |t_{ij}|^2 \left(\tfrac{1}{2} - 2 \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j \right)$$

$$= \frac{1}{2} \sum_{ij} |t_{ij}|^2 \left(1 - 4 \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j \right)$$

unrestricted sum that double counts

$$= \sum_{i<j} |t_{ij}|^2 \left(1 - 4 \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j \right)$$

Hence $\hat{H}_{eff} = -\frac{1}{U} P \hat{H}_t^2 P$

$$= \sum_{i<j} J_{ij} \, \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j + \text{const}$$

where $J_{ij} = 4 \frac{|t_{ij}|^2}{U} > 0$

is the antiferromagnetic exchange coupling