LECTURE: Kinetic antiferromagnetic exchange from Hubbard dimer

abstract Hilbert space

- Single-particle QM: $\hat{A}$, $|\psi\rangle \in \mathcal{H}$ or $\langle \vec{r}|\psi\rangle \in L^2(\mathbb{R})$

Hilbert space of square integrable functions

- Many-particle QM: $\hat{A} = f(\hat{c}_{i\sigma}, \hat{c}^{+}_{i\sigma})$, $|\psi\rangle \in \overline{\mathcal{F}}$

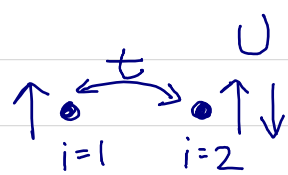
completion

$$\mathcal{F} = \mathbb{C} \oplus \mathcal{H} \oplus \hat{\mathcal{A}}(\mathcal{H}\otimes\mathcal{H}) \oplus \underbrace{\hat{\mathcal{A}}(\mathcal{H}\otimes\mathcal{H}\otimes\mathcal{H})}_{\text{antisymmetrized 3-fold tensor product}} \oplus \ldots$$

direct sum

Fock space for fermions

- Hubbard dimer:



$$\hat{H} = -t \sum_{\sigma} \left(\hat{c}^{+}_{1\sigma} \hat{c}_{2\sigma} + \hat{c}^{+}_{2\sigma} \hat{c}_{1\sigma} \right) + U \sum_{i=1,2} c^{+}_{i\uparrow} c_{i\uparrow} c^{+}_{i\downarrow} c_{i\downarrow}$$

$\dim \mathcal{F} = 4^2 = 16$ as each site can host four states $|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$

$$\hat{c}^{+}_{1\uparrow} \mapsto \begin{array}{c|cccc} & 0 & \uparrow & \downarrow & \uparrow\downarrow \\ \hline 0 & 0 & 0 & 0 & 0 \\ \uparrow & 1 & 0 & 0 & 0 \\ \downarrow & 0 & 0 & 0 & 0 \\ \uparrow\downarrow & 0 & 0 & 1 & 0 \end{array} \qquad \hat{c}_{1\uparrow} \mapsto \begin{array}{c|cccc} & 0 & \uparrow & \downarrow & \uparrow\downarrow \\ \hline 0 & 0 & 1 & 0 & 0 \\ \uparrow & 0 & 0 & 0 & 0 \\ \downarrow & 0 & 0 & 0 & 1 \\ \uparrow\downarrow & 0 & 0 & 0 & 0 \end{array}$$

"half-filled" lattice

- In the sector of $\mathcal{F}$ with 2 electrons, vector subspace is spanned by six vectors:

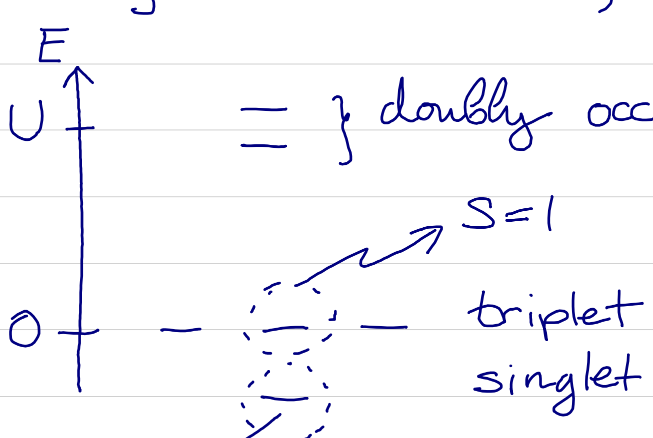
$$|\uparrow\downarrow, 0\rangle,\ |0, \uparrow\downarrow\rangle,\ |\uparrow, \downarrow\rangle,\ |\downarrow, \uparrow\rangle,\ |\uparrow, \uparrow\rangle,\ |\downarrow, \downarrow\rangle$$

$$\hat{H} \mapsto \left(\begin{array}{cccc|cc} U & 0 & t & -t & 0 & 0 \\ 0 & U & t & -t & 0 & 0 \\ t & t & 0 & 0 & 0 & 0 \\ -t & -t & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{array}\right)_{6\times 6}$$

$\Rightarrow$ eigenenergies: U, $\dfrac{U \pm \sqrt{U^2 + 16t^2}}{2}$

0, 0, 0 with spin triplet eigenstates $\begin{cases} \frac{1}{\sqrt{2}}\left(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle\right) \\ |\uparrow,\uparrow\rangle \\ |\downarrow,\downarrow\rangle \end{cases}$

$\Rightarrow$ for $t \ll U$: U, $U + \dfrac{4t^2}{U}$, $-\dfrac{4t^2}{U} < 0$



$\hookrightarrow U/t \to 0$ eigenstate becomes singlet $\frac{1}{\sqrt{2}}\left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right)$

$\rightarrow$ $S=0$ is the lowest energy, so antiferromagnetic interaction is favored as kinetic energy is lowered for antiparallel spins

→ for $S=1$, hopping between two sites is blocked by the Pauli principle, so hopping parameter t does not even show up in the corresponding eigenenergies

→ the eigenenergies of $S=0$ and $S=1$ "low-energy" states can be mimicked by using effective spin-$1/2$ Hamiltonian

$$\hat{H}_{eff} = -J\,\hat{\vec{S}}_1\cdot\hat{\vec{S}}_2 = -\frac{J}{2}\left(\hat{\vec{S}}\cdot\hat{\vec{S}} - \hat{\vec{S}}_1\cdot\hat{\vec{S}}_1 - \hat{\vec{S}}_2\cdot\hat{\vec{S}}_2\right)$$

$$\hat{\vec{S}}_1 = \frac{1}{2}\hat{\vec{\sigma}}\otimes\hat{I} \qquad\qquad = -\frac{J}{2}\Big[S(S+1)\underbrace{-\frac{3}{4}-\frac{3}{4}}_{\text{const.}}\Big]$$

$$\hat{\vec{S}}_2 = \hat{I}\otimes\frac{1}{2}\hat{\vec{\sigma}} \qquad\qquad = \text{const.} - J\,S(S+1)$$

$$\hat{\vec{S}} = \hat{\vec{S}}_1 + \hat{\vec{S}}_2 \qquad\qquad = \text{Const.}\begin{cases} +\,0 & \text{for } S=0 \\ -\,J & \text{for } S=1 \end{cases}$$

so, $\hat{H}_{eff} = \dfrac{4t^2}{U}\,\hat{\vec{S}}_1\cdot\hat{\vec{S}}_2$ with $J = -\dfrac{4t^2}{U}$

mimics low-energy levels of Hubbard dimer in the limit $U \gg t$

■ Generalization of this to cubic lattice leads to biquadratic exchange $\propto (\hat{\vec{S}}_i\cdot\hat{\vec{S}}_j)^2$, as well as ring exchange $\propto (\hat{\vec{S}}_i\cdot\hat{\vec{S}}_j)(\hat{\vec{S}}_k\cdot\hat{\vec{S}}_l) + (\hat{\vec{S}}_i\cdot\hat{\vec{S}}_l)(\hat{\vec{S}}_k\cdot\hat{\vec{S}}_j) - (\hat{\vec{S}}_i\cdot\hat{\vec{S}}_k)(\hat{\vec{S}}_j\cdot\hat{\vec{S}}_l)$ at order t^4/U^3