What is the form of the interaction term?

$$\hat{V}_{ee} = \sum_{\substack{i,i' \\ j,j'}} \mathcal{U}_{ii'jj'}\, a^{\dagger}_{i\sigma}\, a^{\dagger}_{i'\sigma'}\, a_{j'\sigma'}\, a_{j\sigma}$$

$$V_{ee} \rightsquigarrow \mathcal{U}_{ii'jj'} = \frac{1}{2}\int d^d r\, d^d r'\, \psi^*_{R_i}(\vec{r})\, \psi^*_{R_{i'}}(\vec{r}')\, \psi_{R_{j'}}(\vec{r}')\, \psi_{R_j}(\vec{r}) \times \times V(\vec{r}-\vec{r}')$$

What are the important terms?

* Direct: $\mathcal{U}_{ii'ii'} = V_{ii'} \quad i \neq i'$

$$\rightsquigarrow \sum_{i \neq i'} V_{ii'}\, \hat{n}_i\, \hat{n}_{i'} \qquad \hat{n}_i = \sum_{\sigma} a^{\dagger}_{i\sigma} a_{i\sigma} = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$$

Coulomb interaction between electrons.

* Exchange: gives magnetic coupling!

$\mathcal{U}_{ijji} = J^F_{ij}$

$$\hat{V}_{ee} \rightsquigarrow \sum_{i \neq j} \mathcal{U}_{ijji}\, a^{\dagger}_{i\sigma}\, a^{\dagger}_{j\sigma'}\, a_{i\sigma'}\, a_{j\sigma}$$

Using a spin operator: $\vec{S}_i = \frac{1}{2} a^{\dagger}_{i\sigma}\, \underbrace{\vec{\sigma}_{\sigma\sigma'}}_{\text{Pauli matrices}}\, a_{i\sigma'}$, one gets:

$$V_{ee} \rightsquigarrow -2 \sum_{i \neq j} J^F_{ij} \left(\vec{S}_i \cdot \vec{S}_j + \frac{1}{4} \hat{n}_i \hat{n}_j \right)$$

Coulomb is repulsive, so $J^F_{ij} > 0$, gives a

* ferromagnetic spin interaction!

$$\left(\vec{\sigma}_{\alpha\beta} \cdot \vec{\sigma}_{\gamma\delta} = 2\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{\alpha\beta}\delta_{\gamma\delta} \right)$$

Local (Hubbard) Term:

$$V_{ee} \rightsquigarrow \sum_{i,\sigma\sigma'} \underbrace{U_{iiii}}_{U_i/2} a^\dagger_{i\sigma} a^\dagger_{i\sigma'} a_{i\sigma'} a_{i\sigma}$$

$$= \sum_{i,\sigma,\sigma'} \frac{U_i}{2} \left(\hat{n}_{i\sigma} \hat{n}_{i\sigma'} - \hat{n}_{i\sigma} \delta_{\sigma\sigma'} \right)$$

$$= \cancel{U} \sum_i U_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

On-site term, dominates if atoms are far ~~ap~~ apart.

(t_{ij}, J^F_{ij} small)

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* Physics: two overlapping orbitals:

If spins align, WF is <u>anti</u>-symmetric, so zero where Coulomb interaction is largest, Coulomb energy minimised.

If we only keep kinetic & local term, we get Hubbard model:

$$H = -t \sum_{\langle i j \rangle} a^{\dagger}_{i\sigma} a_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \mu \sum_i n_i$$

μ: chemical potential, $n_i = (n_{i\uparrow} + n_{i\downarrow})$

Important model!

① $t \gg U$: tight binding approx. of single band Hamiltonian.

μ ~~sets~~ sets the physics: metal if μ in band (half filling) band insulator; μ outside of band.

② At $U \gg t$ and half filling:

GS is

$$\begin{matrix} \uparrow & \downarrow & \uparrow & \downarrow \\ \downarrow & \uparrow & \downarrow & \uparrow \\ \uparrow & \downarrow & \uparrow & \downarrow \end{matrix}$$

Antiferromagnetic insulator: Mott insulator

No charge transport due to large onsite U

Away from half filling very hard to solve, ~~transitio~~ transition between ① (metal) & ② poorly understood.

Origin of AF behaviour:

Assume: large U; small overlap between wf's at different sites; $t \ll U$; half filling (one e^- per site).

Two site problem: 4 8 states:

$|\uparrow\downarrow\ 0\rangle$; $|0\ \uparrow\downarrow\rangle$: $E = U$ ← $t=0$.

$|\uparrow\ \downarrow\rangle$; $|\downarrow\ \uparrow\rangle$ $E = 0$

Perturbation theory in t. 1st order vanishes.

$$|\uparrow\ \downarrow\rangle \begin{array}{c} \xrightarrow{t} |\uparrow\downarrow\ 0\rangle \xrightarrow{t} \\ \xrightarrow{t} |0\ \downarrow\uparrow\rangle \xrightarrow{t} \end{array} |\uparrow\ \downarrow\rangle$$

$$\Delta E = (-t)^2 \sum_\alpha \frac{|\langle\alpha| \sum_{i,j,\sigma} a^\dagger_{i\sigma} a_{j\sigma} |\uparrow\downarrow\rangle|^2}{\underset{\underset{0}{\parallel}}{E_0} - E_\alpha}$$

$$= 2t^2/(-U) \quad \text{singlet}$$

$$\Delta E = 0 \quad \text{triplet}$$

In terms of $\vec{S}_i$:
$$2\vec{S}_1 \cdot \vec{S}_2 = (\vec{S}_1 + \vec{S}_2)^2 - 2\vec{S}_1^2$$
$$= \vec{S}_{tot}^2 - 2 \cdot 3/4$$

$$\Rightarrow \vec{S}_1 \cdot \vec{S}_2 = -3/4 \quad \text{singlet}$$
$$\vec{S}_1 \cdot \vec{S}_2 = +\tfrac{1}{4} \quad \text{triplet}$$

The effective hamiltonian becomes:

$$H = \frac{2t^2}{U} \sum_{\langle i,j \rangle} \left(\vec{S}_i \vec{S}_j - \frac{1}{4} \right)$$

Dropping the shift, we get the Heisenberg anti-ferromagnet model.

Hard to solve in general, but can be done in 1-d systems (NN-coupling).

Ferro case: $H = -J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \quad (J > 0)$

g.s.: all spins aligned, f.i. $|\uparrow\uparrow\cdots\uparrow\rangle$, but works in any direction ϑ.

$d > 1$: rot. sym. spontaneously broken in groundstate.

Low energy excitations: spin waves w/ large wavelength.

We demonstrate this for large S, in 1-d.
(see exercise).

SU(2) algebra: α, etc: x, y, z

$$[S_i^\alpha, S_j^\beta] = i\delta_{i,j}\varepsilon^{\alpha\beta\gamma}S_i^\gamma$$

tot. antisym. symbol.

In terms of $S_i^\pm = S_i^x \pm i S_i^y$:

$$[S_i^z, S_j^\pm] = \pm\delta_{i,j}S_i^\pm \;;\; [S_i^+, S_j^-] = 2\delta_{i,j}S_i^z$$

Rep. in terms of bosons: Holstein Primakov

For spin-S:

$$S_i^- = a_i^\dagger(2S-\hat{n}_i)^{\frac{1}{2}} \quad S_i^+ = (2S-\hat{n}_i)^{\frac{1}{2}}a_i$$

$$S_i^z = S-\hat{n}_i \;;\; \hat{n}_i = a_i^\dagger a_i \;;\; [a_i, a_j^\dagger] = \delta_{ij}$$

Ex: show that $S_i^\pm, S_i^z$ satisfy SU(2) alg!

A groundstate: $|\uparrow\uparrow\ldots\uparrow\rangle = |0,0,\ldots,0\rangle = |0\rangle$

has $S_i^z|0\rangle = S|0\rangle$, or $\hat{n}_i|0\rangle = 0$

Acting w/ $a_i^\dagger$, one finds $\Delta S_i^z \sim 1$, or $\frac{\Delta S_i^z}{S} \ll 1$

for large S: small fluctuations around $|0\rangle$

are found by expanding in $1/S$.

Use HP on Heisenberg model (ex!).

$$H = -J\sum_i \underbrace{\tfrac{1}{2}(S_i^{+}S_{i+1}^{-} + S_i^{-}S_{i+1}^{+})}_{= S_i^x S_{i+1}^x + S_i^y S_{i+1}^y} + S_i^z S_{i+1}^z$$

$$= -JS\sum_i \left(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i - 2a_i^\dagger a_i\right)$$

$$-NJS^2 + O(S^0)$$

Use FT: $a_j = \frac{1}{\sqrt{N}}\sum_k e^{-ikj} a_k$

$H = -JNS^2 + \sum_k \hbar\omega_k a_k^\dagger a_k + O(S^0)$, where

$\hbar\omega_k = 4JS\sin^2(k/2) \sim JSk^2$ for $k \to 0$.

So: low energy excitations have quadratic dispersion

$\rightsquigarrow$ magnons

Anti-ferromag. case: $H = +J\sum_i \vec{S}_i \vec{S}_{i+1}$ $J > 0$.

g.s. for bi-partite system: $\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$

A B A B ...

To find bosonic rep, we first rotate spins on

B sublattice: $S_B^x \to \tilde{S}_B^x$; $S_B^y \to -\tilde{S}_B^y$, $S_B^z \to -\tilde{S}_B^z$,

So GS is like a ferromagnet again

The hamiltonian can be written as

$$H = -J\sum_j \tilde{S}^z_{2j-1}\tilde{S}^z_{2j} + \tilde{S}^z_{2j} S^z_{2j+1}$$
$$-\tfrac{1}{2}\left[S^+_{2j-1}\tilde{S}^+_{2j} + \tilde{S}^+_{2j} S^+_{2j+1} + S^-_{2j-1}\tilde{S}^-_{2j} + \tilde{S}^-_{2j} S^-_{2j+1}\right]$$

The $\tilde{S}^z_i$ are just spin operators, so we can drop the $\sim$, and perform a HP Transformation as in the ferromagnetic case, which gives (in limit of large S)

$$H = -NJS^2 + JS\sum_i \left[a^+_i a_i + a^+_{i+1} a_{i+1} + a_i a_{i+1} + a^+_i a^+_{i+1}\right] + O(S^0)$$

We need to take care of the anomalous $a_i a_{i+1}$ terms.
First, one does a FT:

$$H = -NJS(S+1) + JS\sum_k (a^+_k, a_{-k})\begin{pmatrix} 1 & \cos k \\ \cos k & 1\end{pmatrix}\begin{pmatrix} a_k \\ a^+_{-k}\end{pmatrix} + O(S^0).$$

This can be diagonalised ~~with~~ with a Bogoliubov Transformation, which gives $H = JS\sum_k \sqrt{1-\cos^2 k}\,\left[\alpha^+_k \alpha_k + \tfrac{1}{2}\right]$,

so the spectrum is linear for small k: $\sqrt{1-\cos^2 k} = |\sin k| \to k$ for k small.

This result is true even ~~to~~ for small half integer spins!
Integer ~~a~~ case: system has a gap! No low energy ~~excitation~~ excitations.
Difference between integer & half integer case: Topological origin! Haldane