§ 6. Two site Hubbard model

Two site Hubbard model

Hamiltonian

$$\boxed{\hat{H} = \hat{H}^{(1)}_{loc} + \hat{H}^{(2)}_{loc} + \hat{H}_t}$$

$$\boxed{\hat{H}^{(1)}_{loc} = \varepsilon \sum_\sigma (\hat{n}_{1\sigma} + \hat{n}_{2\sigma}) + E \sum_\sigma (\hat{n}_{1\sigma} - \hat{n}_{2\sigma}) + B \sum_\sigma \sigma (\hat{n}_{1\sigma} + \hat{n}_{2\sigma})}$$

ε - local on-site (atomic) energy

E - electric field

B - magnetic (Zeeman) field

$$\boxed{\hat{H}^{(2)}_{loc} = U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} + n_{2\downarrow})}$$

U - local (Hubbard) interaction

$$\boxed{\hat{H}_t = t \sum_\sigma (a^+_{1\sigma} a_{2\sigma} + a^+_{2\sigma} a_{1\sigma})}$$

t - hopping amplitude

$\# = \binom{2N_L}{N}$

$\sum_{N=0}^{2N_L} \binom{2N_L}{N} = 2^{2N_L}$

particle number sectors $N = 0, 1, 2, 3, 4$

$N=0$, $S_z = 0$ — 1

$N=1$, $S_z = 1/2$, $S_z = -1/2$ — 4

$N=2$, $S_z = -1$, $S_z = 0$ - 4x, $S_z = +1$ — 6

$N=3$, $S_z = 1/2$, $S_z = -1/2$ — 4

$N=4$, $S_z = 0$ — 1

total # of states $= 16 = 2^4$

∘) $\underline{N=0}$, $\underline{S = S_z = 0}$

$$|1\rangle = |v\rangle$$

$$\langle 1|\hat{H}|1\rangle = 0 = H_{N=0,\, S=0,\, S_z=0}$$

∘) $\underline{N=1}$, $\underline{S = 1/2 ,\ S_z = \pm 1/2}$

$$\left.\begin{aligned} |2\rangle &= a^{+}_{1\uparrow}|v\rangle \\ |3\rangle &= a^{+}_{2\uparrow}|v\rangle \end{aligned}\right\} S_z = 1/2$$

$$\left.\begin{aligned} |4\rangle &= a^{+}_{1\downarrow}|v\rangle \\ |5\rangle &= a^{+}_{2\downarrow}|v\rangle \end{aligned}\right\} S_z = -1/2$$

$$\hat{H}^{(1)}_{loc}|2\rangle = (\varepsilon + E + B)|2\rangle$$

$$\hat{H}^{(1)}_{loc}|3\rangle = (\varepsilon - E + B)|3\rangle$$

$$\hat{H}^{(1)}_{loc}|4\rangle = (\varepsilon + E - B)|4\rangle$$

$$\hat{H}^{(1)}|5\rangle = (\varepsilon - E - B)|5\rangle$$

$$\hat{H}_t^{(1)}|2\rangle = t|3\rangle , \quad \hat{H}_t^{(1)}|3\rangle = t|2\rangle$$

$$\hat{H}^{(1)}_t|4\rangle = t|5\rangle , \quad \hat{H}_t^{(1)}|5\rangle = t|4\rangle$$

$$H_{N=1} = \begin{array}{c} \left(\begin{array}{cc|cc} \varepsilon+E+B & t & 0 & 0 \\ t & \varepsilon-E+B & 0 & 0 \\ \hline 0 & 0 & \varepsilon+E-B & t \\ 0 & 0 & t & \varepsilon-E-B \end{array}\right) \begin{array}{c} |2\rangle \\ |3\rangle \\ |4\rangle \\ |5\rangle \end{array} \\ \begin{array}{cccc} |2\rangle & |3\rangle & |4\rangle & |5\rangle \end{array} \end{array}$$

$$H\bar{v} = \lambda\bar{v}$$

$$\begin{pmatrix} \varepsilon + E + B - \lambda & t \\ t & \varepsilon - E + B - \lambda \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0$$

$$(\varepsilon + E + B - \lambda)(\varepsilon - E + B - \lambda) - t^2 = 0$$

$$(\varepsilon + B - \lambda + E)(\varepsilon + B - \lambda - E) - t^2 = 0$$

$$(\varepsilon + B - \lambda)^2 - E^2 - t^2 = 0$$

$$(\varepsilon + B - \lambda)^2 = t^2 + E^2$$

$$\varepsilon + B - \lambda = \pm\sqrt{t^2 + E^2}$$

$$\lambda_\pm = \varepsilon + B \pm \sqrt{t^2 + E^2}$$

λ_+

$$\begin{pmatrix} \cancel{\varepsilon} + E + \cancel{B} - \cancel{\varepsilon} - \cancel{B} - \sqrt{t^2+E^2} & t \\ t & \cancel{\varepsilon} - E + \cancel{B} - \cancel{\varepsilon} - \cancel{B} - \sqrt{t^2+E^2} \end{pmatrix}\begin{pmatrix} \alpha_+ \\ \beta_+ \end{pmatrix} = 0$$

$$\begin{pmatrix} E - \sqrt{t^2+E^2} & t \\ t & -E - \sqrt{t^2+E^2} \end{pmatrix}\begin{pmatrix} \alpha_+ \\ \beta_+ \end{pmatrix} = 0$$

$$\alpha_+ (E - \sqrt{\ }) + t\beta_+ = 0 \qquad \alpha_+ = -\frac{t}{E - \sqrt{\ }}\beta_+$$

$$\left(-\frac{t^2}{E - \sqrt{\ }} - (E + \sqrt{\ })\right)\beta_+ = \frac{t^2 - (E - \sqrt{\ })(E + \sqrt{\ })}{E - \sqrt{\ }}\beta_+ =$$

$$= \frac{-t^2 - (\cancel{E^2} - t^2 - \cancel{E^2})}{E - \sqrt{\ }}\beta_+ = 0$$

$$\begin{cases} (E - \sqrt{\ })\alpha_+ + t\beta_+ = 0 \\ t\alpha_+ - (E + \sqrt{\ })\beta_+ = 0 \end{cases} \Rightarrow \alpha_+ = \frac{E + \sqrt{\ }}{t}\beta_+$$

$$\det(\,) = -E^2 + t^2 + E^2 - t^2 = 0$$

$$\left(\frac{(E - \sqrt{\ })(E + \sqrt{\ })}{t} + t\right)\beta_+ = \frac{E^2 - t^2 - E^2 + t^2}{t}\beta_+ = 0$$

$$\begin{pmatrix}\alpha_+\\ \beta_+\end{pmatrix} = N_+ \begin{pmatrix}\frac{E+\surd}{t}\\ 1\end{pmatrix}$$

$$1 = \alpha_+^2 + \beta_+^2 = N_+^2\left(\frac{(E+\surd)^2}{t^2} + 1\right) = N_+^2\,\frac{E^2 + 2E\surd + E^2 + t^2 + t^2}{t^2} =$$

$$= N_+^2\,\frac{2(E^2 + t^2 + E\surd)}{t^2}$$

$$N_+ = \frac{t}{\sqrt{E^2 + t^2 + E\sqrt{t^2+E^2}}}\,\frac{1}{\sqrt{2}}$$

$$\lambda_- \quad \begin{pmatrix}\cancel{\varepsilon} + E + \cancel{B} - \cancel{\varepsilon} - \cancel{B} + \surd & t\\ t & \cancel{\varepsilon} - E + \cancel{B} - \cancel{\varepsilon} - \cancel{B} + \surd\end{pmatrix}\begin{pmatrix}\alpha_-\\ \beta_-\end{pmatrix} = 0$$

$$\begin{pmatrix}E+\surd & t\\ t & -E+\surd\end{pmatrix}\begin{pmatrix}\alpha_-\\ \beta_-\end{pmatrix} = 0$$

$$\begin{cases}(E+\surd)\alpha_- + t\beta_- = 0\\ t\alpha_- - (E-\surd)\beta_- = 0\end{cases} \Rightarrow \alpha_- = \frac{E-\surd}{t}\beta_-$$

$$\begin{pmatrix}\alpha_-\\ \beta_-\end{pmatrix} = N_- \begin{pmatrix}\frac{E-\surd}{t}\\ 1\end{pmatrix}$$

$$1 = \alpha_-^2 + \beta_-^2 = N_-^2\left(\frac{(E-\surd)^2 + t^2}{t^2}\right) = N_-^2\,\frac{1}{t^2}\left(E^2 - 2E\surd + E^2 + t^2 + t^2\right) =$$

$$= N_-^2\,\frac{2}{t^2}\left(E^2 + t^2 - E\surd\right)$$

$$\boxed{N_- = \frac{t}{\sqrt{2}}\,\frac{1}{\sqrt{E^2 + t^2 - E\sqrt{E^2+t^2}}}}$$

N = 1 – summary

$$\lambda_+^{\uparrow} = \varepsilon + B + \sqrt{t^2+E^2}$$

$$|\lambda_+^{\uparrow}\rangle = \frac{t}{\sqrt{2}} \frac{1}{\sqrt{t^2+E^2+E\sqrt{t^2+E^2}}}\left(\frac{E+\sqrt{t^2+E^2}}{t}\, a_{1\uparrow}^{\dagger} + a_{2\uparrow}^{\dagger}\right)|v\rangle$$

$$\lambda_-^{\uparrow} = \varepsilon + B - \sqrt{t^2+E^2}$$ bonding

$$|\lambda_-^{\uparrow}\rangle = \frac{t}{\sqrt{2}} \frac{1}{\sqrt{t^2+E^2-E\sqrt{t^2+E^2}}}\left(\frac{E-\sqrt{t^2+E^2}}{t}\, a_{1\uparrow}^{\dagger} + a_{2\uparrow}^{\dagger}\right)|v\rangle$$

$$\lambda_+^{\downarrow} = \varepsilon - B + \sqrt{t^2+E^2}$$

$$|\lambda_+^{\downarrow}\rangle = \cancel{|\lambda_+^{\uparrow}\rangle}\, \frac{t}{\sqrt{2}} \frac{1}{\sqrt{\ +\ }}\left(\frac{E+\sqrt{t^2+E^2}}{t}\, a_{1\downarrow}^{\dagger} + a_{2\downarrow}^{\dagger}\right)|v\rangle$$

$$\lambda_-^{\downarrow} = \varepsilon - B - \sqrt{t^2+E^2}$$ bonding

$$|\lambda_-^{\downarrow}\rangle = \cancel{|\lambda_-^{\uparrow}\rangle} = \frac{t}{\sqrt{2}} \frac{1}{\sqrt{\ -\ }}\left(\frac{E-\sqrt{t^2+E^2}}{t}\, a_{1\downarrow}^{\dagger} + a_{2\downarrow}^{\dagger}\right)|v\rangle$$

o) $E = 0$ case

$\lambda_+^{\uparrow} = \varepsilon + B + t$ $\quad |\lambda_+^{\uparrow}\rangle = \frac{1}{\sqrt{2}}(a_{1\uparrow}^{\dagger} + a_{2\uparrow}^{\dagger})|v\rangle$

$\lambda_-^{\uparrow} = \varepsilon + B - t$ $\quad |\lambda_-^{\uparrow}\rangle = \frac{1}{\sqrt{2}}(-a_{1\uparrow}^{\dagger} + a_{2\uparrow}^{\dagger})|v\rangle$ bonding

$\lambda_+^{\downarrow} = \varepsilon - B + t$ $\quad |\lambda_+^{\downarrow}\rangle = \frac{1}{\sqrt{2}}(a_{1\downarrow}^{\dagger} + a_{2\downarrow}^{\dagger})|v\rangle$

$\lambda_-^{\downarrow} = \varepsilon - B - t$ $\quad |\lambda_-^{\downarrow}\rangle = \frac{1}{\sqrt{2}}(-a_{1\downarrow}^{\dagger} + a_{2\downarrow}^{\dagger})|v\rangle$ bonding

o) $t = 0$ case

$\lambda_+^{\uparrow} = \varepsilon + B + E$ $\quad |\lambda_+^{\uparrow}\rangle = a_{1\uparrow}^{\dagger}|v\rangle$

$\lambda_-^{\uparrow} = \varepsilon + B - E$ $\quad |\lambda_-^{\uparrow}\rangle = a_{2\uparrow}^{\dagger}|v\rangle$

$\lambda_+^{\downarrow} = \varepsilon - B + E$ $\quad |\lambda_+^{\downarrow}\rangle = a_{1\downarrow}^{\dagger}|v\rangle$

$\lambda_-^{\downarrow} = \varepsilon - B - E$ $\quad |\lambda_-^{\downarrow}\rangle = a_{2\downarrow}^{\dagger}|v\rangle$

$$H = t\sum_\sigma \left(a_{1\sigma}^+ a_{2\sigma} + a_{2\sigma}^+ a_{1\sigma}\right) + U n_{1\uparrow} n_{1\downarrow} + U n_{2\uparrow} n_{2\downarrow} +$$

$$\Delta \sum_\sigma \left(\underbrace{a_{1\sigma}^+ a_{1\sigma}}_{n_{1\sigma}} - \underbrace{a_{2\sigma}^+ a_{2\sigma}}_{n_{2\sigma}}\right) + B \sum_\sigma \left(\sigma n_{1\sigma} + \sigma n_{2\sigma}\right)$$

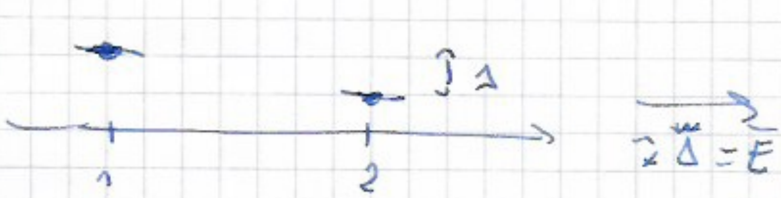
$N_e = 2, \quad N_L = 2$

$\sqrt{1 \pm x} = 1 \pm \frac{1}{2} x - \frac{1}{8} x^2 + \dots$

$\frac{1}{\sqrt{1 \pm x}} = 1 \mp \frac{1}{2} x + \frac{3}{8} x^2 + \dots$

$S=1$:
$|1\rangle = a_{1\uparrow}^+ a_{2\uparrow}^+ |v\rangle$ $\quad S_z = 1$
$|2\rangle = \frac{1}{\sqrt{2}}\left[a_{1\uparrow}^+ a_{2\downarrow}^+ + a_{1\downarrow}^+ a_{2\uparrow}^+\right]|v\rangle$ $\quad S_z = 0$
$|3\rangle = a_{1\downarrow}^+ a_{2\downarrow}^+ |v\rangle$ $\quad S_z = -1$
triplet states

$S=0$, $S_z=0$:
$|4\rangle = \frac{1}{\sqrt{2}}\left[a_{1\uparrow}^+ a_{2\downarrow}^+ - a_{1\downarrow}^+ a_{2\uparrow}^+\right]|v\rangle$ singlet state
$|5\rangle = \frac{1}{\sqrt{2}}\left[a_{1\uparrow}^+ a_{1\downarrow}^+ + a_{2\uparrow}^+ a_{2\downarrow}^+\right]|v\rangle$
$|6\rangle = \frac{1}{\sqrt{2}}\left[a_{1\uparrow}^+ a_{1\downarrow}^+ - a_{2\uparrow}^+ a_{2\downarrow}^+\right]|v\rangle$
doublet states



$H = H_t + H_U + H_\Delta + H_B$

$H_t|1\rangle = 0$

$H_t|2\rangle = \frac{t}{\sqrt{2}}\sum_\sigma \left(a_{1\sigma}^+ a_{2\sigma} + a_{2\sigma}^+ a_{1\sigma}\right)\left(a_{1\uparrow}^+ a_{2\downarrow}^+ + a_{1\downarrow}^+ a_{2\uparrow}^+\right)|v\rangle =$

$\delta_{\sigma\downarrow}$ $\quad \delta_{\sigma\uparrow}$ $\quad \delta_{\sigma\uparrow}$ $\quad \delta_{\sigma\uparrow}$

$= \frac{t}{\sqrt{2}}\sum_\sigma \left[a_{1\sigma}^+ \underbrace{a_{2\sigma} a_{1\uparrow}^+ a_{2\downarrow}^+}_{-\delta_{\sigma\downarrow}} + a_{1\sigma}^+ \underbrace{a_{2\sigma} a_{1\downarrow}^+ a_{2\uparrow}^+}_{-\delta_{\sigma\uparrow}} + a_{2\sigma}^+ \underbrace{a_{1\sigma} a_{1\uparrow}^+}_{\delta_{\sigma\uparrow}} a_{2\downarrow}^+ + a_{2\sigma}^+ \underbrace{a_{1\sigma} a_{1\downarrow}^+}_{\delta_{\sigma\downarrow}} a_{2\uparrow}^+\right]$

$= \frac{t}{\sqrt{2}}\left[-a_{1\downarrow}^+ a_{1\uparrow}^+ - a_{1\uparrow}^+ a_{1\downarrow}^+ + a_{2\uparrow}^+ a_{2\downarrow}^+ + a_{2\downarrow}^+ a_{2\uparrow}^+\right]|v\rangle = 0$

$H_t|3\rangle = 0$

(1)

$H_t|4\rangle = \frac{t}{\sqrt{2}}\sum_\sigma \left(a_{1\sigma}^+ a_{2\sigma} + a_{2\sigma}^+ a_{1\sigma}\right)\left(a_{1\uparrow}^+ a_{2\downarrow}^+ - a_{1\downarrow}^+ a_{2\uparrow}^+\right)|v\rangle =$

$= t/\sqrt{2} \sum_\sigma \left(a_{1\sigma}^+ \underbrace{a_{2\sigma} a_{1\uparrow}^+ a_{2\downarrow}^+}_{-\delta_{\sigma\downarrow}} - a_{1\sigma}^+ \underbrace{a_{2\sigma} a_{1\downarrow}^+ a_{2\uparrow}^+}_{-\delta_{\sigma\uparrow}} + a_{2\sigma}^+ \underbrace{a_{1\sigma} a_{1\uparrow}^+}_{\delta_{\sigma\uparrow}} a_{2\downarrow}^+ - a_{2\sigma}^+ \underbrace{a_{1\sigma} a_{1\downarrow}^+}_{\delta_{\sigma\downarrow}} a_{2\uparrow}^+\right)|v\rangle$

$\parallel$
$2H_t|5\rangle$

$= t/\sqrt{2}\left\{-a_{1\downarrow}^+ a_{1\uparrow}^+ + a_{1\uparrow}^+ a_{1\downarrow}^+ + a_{2\uparrow}^+ a_{2\downarrow}^+ - a_{2\downarrow}^+ a_{2\uparrow}^+\right\} = \frac{2}{\sqrt{2}} t \left[a_{1\uparrow}^+ a_{1\downarrow}^+ + a_{2\uparrow}^+ a_{2\downarrow}^+\right]$

$$H_t|5\rangle = \frac{t}{\sqrt{2}}\sum_\sigma (a_{1\sigma}^+ a_{2\sigma} + a_{2\sigma}^+ a_{1\sigma})(a_{1\uparrow}^+ a_{1\downarrow}^+ + a_{2\uparrow}^+ a_{2\downarrow}^+)|v\rangle =$$

$$= \frac{t}{\sqrt{2}}\sum_\sigma \Big[\underbrace{a_{1\sigma}^+ a_{2\sigma} a_{1\uparrow}^+ a_{1\downarrow}^+}_{=0} + a_{1\sigma}^+ a_{2\sigma} a_{2\uparrow}^+ a_{2\downarrow}^+ + a_{2\sigma}^+ a_{1\sigma} a_{1\uparrow}^+ a_{1\downarrow}^+ + \underbrace{a_{2\sigma}^+ a_{1\sigma} a_{2\uparrow}^+ a_{2\downarrow}^+}_{=0}\Big]|v\rangle$$

$$= \frac{t}{\sqrt{2}}\Big[a_{1\uparrow}^+ a_{2\downarrow}^+ - a_{1\downarrow}^+ a_{2\uparrow}^+ + a_{2\uparrow}^+ a_{1\downarrow}^+ - a_{2\downarrow}^+ a_{1\uparrow}^+\Big]|v\rangle =$$

$$= \frac{2t}{\sqrt{2}}(a_{1\uparrow}^+ a_{2\downarrow}^+ - a_{2\downarrow}^+ a_{1\uparrow}^+) = 2H_t|4\rangle$$

$$H_t|6\rangle = \frac{t}{\sqrt{2}}\sum_\sigma (a_{1\sigma}^+ a_{2\sigma} + a_{2\sigma}^+ a_{1\sigma})(a_{1\uparrow}^+ a_{1\downarrow}^+ - a_{2\uparrow}^+ a_{2\downarrow}^+)|v\rangle =$$

$$= \frac{t}{\sqrt{2}}\sum_\sigma \Big(\underbrace{a_{1\sigma}^+ a_{2\sigma} a_{1\uparrow}^+ a_{1\downarrow}^+}_{=0} - a_{1\sigma}^+ a_{2\sigma} a_{2\uparrow}^+ a_{2\downarrow}^+ + a_{2\sigma}^+ a_{1\sigma} a_{1\uparrow}^+ a_{1\downarrow}^+ - \underbrace{a_{2\sigma}^+ a_{1\sigma} a_{2\uparrow}^+ a_{2\downarrow}^+}_{=0}\Big)|v\rangle$$

$$= \frac{t}{\sqrt{2}}\Big(-a_{1\uparrow}^+ a_{2\downarrow}^+ + a_{1\downarrow}^+ a_{2\uparrow}^+ - a_{2\uparrow}^+ a_{1\downarrow}^+ - a_{2\downarrow}^+ a_{1\uparrow}^+\Big)|v\rangle = 0$$

$$H_u|1\rangle = H_u|2\rangle = H_u|3\rangle = H_u|4\rangle = 0$$

$$H_u|{5 \atop 6}\rangle = \frac{U}{\sqrt{2}}(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow})(a_{1\uparrow}^+ a_{1\downarrow}^+ \pm a_{2\uparrow}^+ a_{2\downarrow}^+)|v\rangle =$$

$$= \frac{U}{\sqrt{2}}\Big[a_{1\uparrow}^+ a_{1\downarrow}^+ \pm a_{2\uparrow}^+ a_{2\downarrow}^+\Big] = U|{5 \atop 6}\rangle$$

$$H_B|1\rangle = B\sum_\sigma (\sigma n_{1\sigma} + \sigma n_{2\sigma})\, a_{1\uparrow}^+ a_{2\uparrow}^+|v\rangle = 2B\, a_{1\uparrow}^+ a_{2\uparrow}^+|v\rangle = 2B|1\rangle$$

$$H_B|2\rangle = \frac{B}{\sqrt{2}}\sum_\sigma \sigma(n_{1\sigma} + n_{2\sigma})(a_{1\uparrow}^+ a_{2\downarrow}^+ + a_{1\downarrow}^+ a_{2\uparrow}^+)|v\rangle =$$

$$= \frac{B}{\sqrt{2}}\sum_\sigma[\sigma n_{1\sigma} a_{1\uparrow}^+ a_{2\downarrow}^+ + \sigma n_{1\sigma} a_{1\downarrow}^+ a_{2\uparrow}^+ + \sigma n_{2\sigma} a_{1\uparrow}^+ a_{2\downarrow}^+ + \sigma n_{2\sigma} a_{1\downarrow}^+ a_{2\uparrow}^+] = \frac{B}{\sqrt{2}}[a_{1\uparrow}^+ a_{2\downarrow}^+ - a_{1\downarrow}^+ a_{2\uparrow}^+ - a_{1\uparrow}^+ a_{2\downarrow}^+ + a_{1\downarrow}^+ a_{2\uparrow}^+] = 0$$

$$H_B|3\rangle = B\sum_\sigma \sigma(n_{1\sigma} + n_{2\sigma})\, a_{1\downarrow}^+ a_{2\downarrow}^+|v\rangle = -2B|3\rangle$$

$$H_B|4\rangle = \frac{B}{\sqrt{2}}\sum_\sigma \sigma(n_{1\sigma} + n_{2\sigma})(a_{1\uparrow}^+ a_{2\downarrow}^+ - a_{1\downarrow}^+ a_{2\uparrow}^+)|v\rangle =$$

$$= \frac{B}{\sqrt{2}}\Big[\sigma n_{1\sigma} a_{1\uparrow}^+ a_{2\downarrow}^+ - \sigma n_{1\sigma} a_{1\downarrow}^+ a_{2\uparrow}^+ + \sigma n_{2\sigma} a_{1\uparrow}^+ a_{2\downarrow}^+ - \sigma n_{2\sigma} a_{1\downarrow}^+ a_{2\uparrow}^+\Big]|v\rangle =$$

$$= \frac{B}{\sqrt{2}}\Big(a_{1\uparrow}^+ a_{2\downarrow}^+ + a_{1\downarrow}^+ a_{2\uparrow}^+ - a_{1\uparrow}^+ a_{2\downarrow}^+ - a_{1\downarrow}^+ a_{2\uparrow}^+\Big)|v\rangle = 0$$

$$H_B|{5 \atop 6}\rangle = \frac{B}{\sqrt{2}}(\sigma n_{1\sigma} a_{1\uparrow}^+ a_{1\downarrow}^+ \pm \sigma n_{2\sigma} a_{2\uparrow}^+ a_{2\downarrow}^+)|v\rangle = 0$$

$$H_\Delta|1\rangle = \Delta\sum_\sigma (n_{1\sigma}-n_{2\sigma})\, a^+_{1\uparrow}a^+_{2\uparrow}|V\rangle = (1-1) = 0$$

$$= \Delta\sum_\sigma \left(n_{1\sigma}a^+_{1\uparrow}a^+_{2\uparrow} - n_{2\sigma}a^+_{1\uparrow}a^+_{2\uparrow}\right)|V\rangle = \Delta\left(a^+_{1\uparrow}a^+_{2\uparrow} - a^+_{1\uparrow}a^+_{2\uparrow}\right)|V\rangle = 0$$

$$H_\Delta|2\rangle = \frac{\Delta}{\sqrt{2}}\sum_\sigma (n_{1\sigma}-n_{2\sigma})\left(a^+_{1\uparrow}a^+_{2\downarrow} + a^+_{1\downarrow}a^+_{2\uparrow}\right)|V\rangle =$$

$$= \frac{\Delta}{\sqrt{2}}\sum_\sigma \left[n_{1\sigma}a^+_{1\uparrow}a^+_{2\downarrow} + n_{1\sigma}a^+_{1\downarrow}a^+_{2\uparrow} - n_{2\sigma}a^+_{1\uparrow}a^+_{2\downarrow} - n_{2\sigma}a^+_{1\downarrow}a^+_{2\uparrow}\right]|V\rangle =$$

$$= \frac{\Delta}{\sqrt{2}}\left(a^+_{1\uparrow}a^+_{2\downarrow} + a^+_{1\downarrow}a^+_{2\uparrow} - a^+_{1\uparrow}a^+_{2\downarrow} - a^+_{1\downarrow}a^+_{2\uparrow}\right)|V\rangle = 0$$

$$H_\Delta|3\rangle = \Delta\left(a^+_{1\downarrow}a^+_{2\downarrow} - a^+_{1\downarrow}a^+_{2\downarrow}\right)|V\rangle = 0$$

$$H_\Delta|4\rangle = \frac{\Delta}{\sqrt{2}}\sum_\sigma\left[n_{1\sigma}a^+_{1\uparrow}a^+_{2\downarrow} - n_{1\sigma}a^+_{1\downarrow}a^+_{2\uparrow} - n_{2\sigma}a^+_{1\uparrow}a^+_{2\downarrow} + n_{2\sigma}a^+_{1\downarrow}a^+_{2\uparrow}\right]|V\rangle =$$

$$= \frac{\Delta}{\sqrt{2}}\left(a^+_{1\uparrow}a^+_{2\downarrow} - a^+_{1\downarrow}a^+_{2\uparrow} - a^+_{1\uparrow}a^+_{1\downarrow} + a^+_{1\downarrow}a^+_{2\uparrow}\right)|V\rangle = 0$$

$$H_\Delta|{}^5_6\rangle = \frac{\Delta}{\sqrt{2}}\sum_\sigma (n_{1\sigma}-n_{2\sigma})\left(a^+_{1\uparrow}a^+_{1\downarrow} \pm a^+_{2\uparrow}a^+_{2\downarrow}\right)|V\rangle =$$

$$= \frac{\Delta}{\sqrt{2}}\sum_\sigma\left(n_{1\sigma}a^+_{1\uparrow}a^+_{1\downarrow} - (\pm)\, n_{2\sigma}a^+_{2\uparrow}a^+_{2\downarrow}\right)|V\rangle =$$

$$= \frac{2\Delta}{\sqrt{2}}\left(a^+_{1\uparrow}a^+_{1\downarrow} \mp a^+_{2\uparrow}a^+_{2\downarrow}\right)|V\rangle = 2\Delta\,|{}^6_5\rangle$$

$$
\langle i|H|j\rangle = \begin{array}{cc}
 & \begin{array}{cccccc} |1\rangle & |2\rangle & |3\rangle & |4\rangle & |5\rangle & |6\rangle \end{array} \\
\begin{array}{c} S=1 \\ \\ \\ S=0 \\ \\ \end{array} & \left(\begin{array}{ccc|ccc}
2B & & & & & \\
 & 0 & & & & \\
 & & -2B & & & \\
\hline
 & & & 0 & 2t & 0 \\
 & & & 2t & U & \Delta \\
 & & & 0 & \Delta & U
\end{array}\right)\begin{array}{c} |1\rangle \\ |2\rangle \\ |3\rangle \\ |4\rangle \\ |5\rangle \\ |6\rangle \end{array} \\
 & \begin{array}{cc} S=1 & \qquad S=0 \end{array}
\end{array}
$$

$$
\left.\begin{array}{l} \lambda_1 = 2B \\ \lambda_2 = 0 \\ \lambda_3 = -2B \end{array}\right\} \quad \begin{array}{l} |\lambda_1\rangle = |1\rangle \\ |\lambda_2\rangle = |2\rangle \\ \text{triplet states,} \\ |\lambda_3\rangle = |3\rangle \end{array}
$$

$\frac{3\times}{B=0}$ $\uparrow\uparrow$ $S_z=1$, $\uparrow\downarrow$ $S_z=0$, $\downarrow\downarrow$ $S_z=-1$

Diagonalization in $S=0$ channel

•) $\Delta = 0$ case – simpler

$\lambda_6 = U$, $|\lambda_6\rangle = |6\rangle$

$$
\begin{vmatrix} -\lambda & 2t \\ 2t & U-\lambda \end{vmatrix} = -\lambda(U-\lambda) - 4t^2 = 0 \Leftrightarrow \lambda^2 - \lambda U - 4t^2 = 0
$$

$$
\lambda_{4,5} = \frac{U \pm \sqrt{U^2+16t^2}}{2} = \frac{U}{2} \pm \sqrt{\left(\frac{U}{2}\right)^2 + (2t)^2} =
$$

$$
= \frac{U}{2} \pm D
$$

eigenvectors

$$
\begin{pmatrix} -\frac{U}{2} \pm D & 2t \\ 2t & U - \frac{U}{2} \mp D \end{pmatrix} \begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} = 0
\qquad D \equiv \sqrt{\left(\frac{U}{2}\right)^2 + (2t)^2}
$$

$$|\lambda_{4,5}\rangle = |\lambda_\pm\rangle = a_\pm |4\rangle + b_\pm |5\rangle$$

$$\begin{pmatrix} -\lambda_\pm & 2t \\ 2t & U-\lambda_\pm \end{pmatrix} \begin{pmatrix} a_\pm \\ b_\pm \end{pmatrix} = 0 \quad , \quad a_\pm^2 + b_\pm^2 = 1$$

$$\begin{cases} -\lambda_\pm a_\pm + 2t\, b_\pm = 0 \\ -2t\, a_\pm + (U-\lambda_\pm)\, b_\pm = 0 \end{cases} \Rightarrow \left(\frac{a_\pm}{b_\pm}\right) = \frac{2t}{\lambda_\pm}$$

$$\left(\frac{a_\pm}{b_\pm}\right)^2 = \frac{4t^2}{\lambda_\pm^2}$$

$$a_\pm^2 = \frac{4t^2}{\lambda_\pm^2} b_\pm^2$$

$$\left(\frac{4t^2}{\lambda_\pm^2} + 1\right) b_\pm^2 = 1 \Rightarrow b_\pm^2 = \frac{1}{\frac{4t^2}{\lambda_\pm^2} + 1} = \frac{\lambda_\pm^2}{4t^2 + \lambda_\pm^2}$$

$$a_\pm^2 = \frac{4t^2}{4t^2 + \lambda_\pm^2}$$

$$\begin{cases} |\lambda_4\rangle = \dfrac{2t}{\sqrt{4t^2+\lambda_+^2}} |4\rangle + \dfrac{\lambda_+}{\sqrt{4t^2+\lambda_+^2}} |5\rangle \ , \quad \lambda_+ = \frac{U}{2} + \sqrt{\left(\frac{U}{2}\right)^2 + (2t)^2} \\ |\lambda_5\rangle = \dfrac{2t}{\sqrt{4t^2+\lambda_-^2}} |4\rangle + \dfrac{\lambda_-}{\sqrt{4t^2+\lambda_-^2}} |5\rangle \ , \quad \lambda_- = \frac{U}{2} - \sqrt{\left(\frac{U}{2}\right)^2 + (2t)^2} \end{cases}$$

singlet

$$\frac{a_{1\uparrow}^\dagger a_{2\downarrow}^\dagger - a_{1\downarrow}^\dagger a_{2\uparrow}^\dagger}{\sqrt{2}}$$

ionic combination

$$\frac{a_{1\uparrow}^\dagger a_{1\downarrow}^\dagger + a_{2\uparrow}^\dagger a_{2\downarrow}^\dagger}{\sqrt{2}}$$

$u \ll t$

$$\lambda_{4,5} = \frac{u}{2} \pm 2t\sqrt{1+\left(\frac{u}{4t}\right)^2} \simeq \frac{u}{2} \pm 2t\left[1+\frac{1}{2}\left(\frac{u}{4t}\right)^2+\dots\right] =$$

$$= \frac{u}{2} \pm 2t \pm \frac{u^2}{\cancel{32}\,16\,t} \xrightarrow[u\to 0]{} \pm 2t$$

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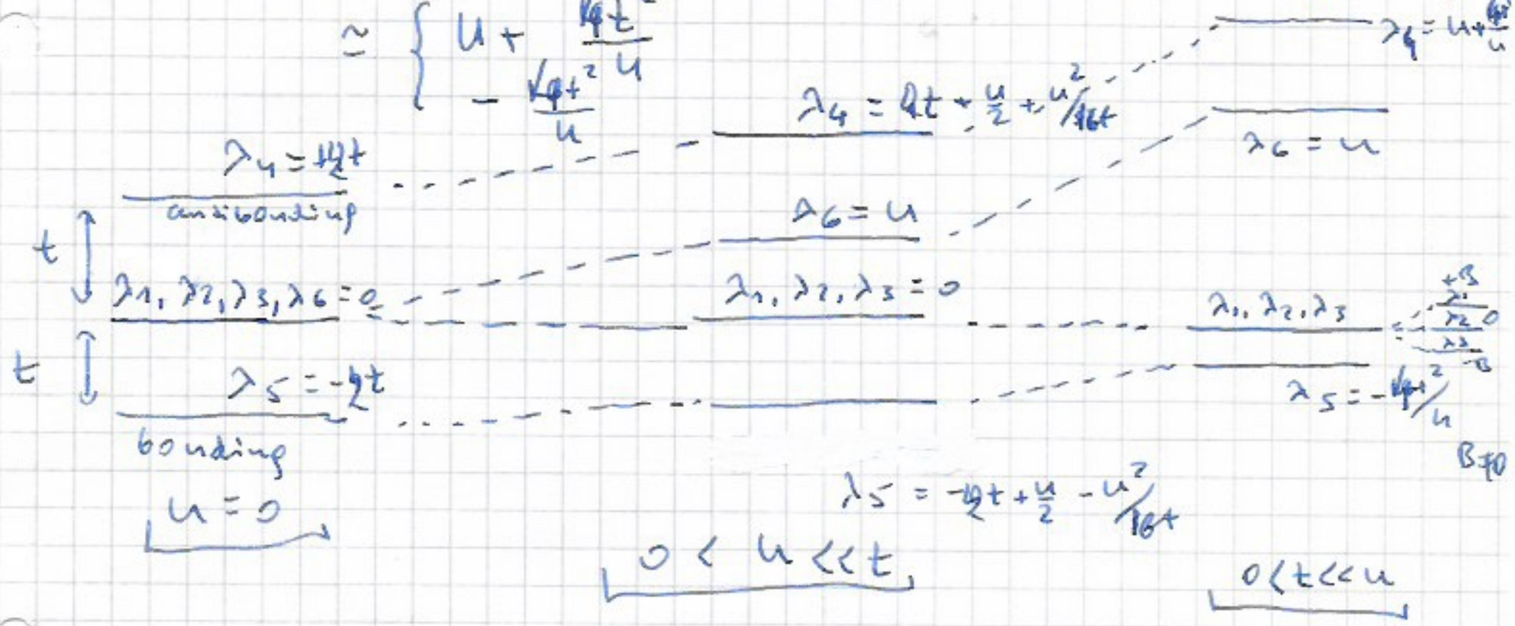
$u \gg t$

$$\lambda_{4,5} = \frac{u}{2} \pm \frac{u}{2}\sqrt{1+\left(\frac{4t}{u}\right)^2} \simeq \frac{u}{2} \pm \frac{u}{2}\left[1+\frac{1}{2}\left(\frac{4t}{u}\right)^2+\dots\right]$$

$$\simeq \begin{cases} u + \dfrac{4t^2}{u} \\ -\dfrac{4t^2}{u} \end{cases}$$



$|\lambda_1\rangle = a^\dagger_{1\uparrow} a^\dagger_{2\uparrow}|0\rangle$

$|\lambda_2\rangle = \frac{1}{\sqrt{2}}\left(a^\dagger_{1\uparrow} a^\dagger_{2\downarrow} + a^\dagger_{1\downarrow} a^\dagger_{2\uparrow}\right)|0\rangle$ — triplet states

$|\lambda_3\rangle = a^\dagger_{1\downarrow} a^\dagger_{2\downarrow}|0\rangle$

$|\lambda_6\rangle = \frac{1}{\sqrt{2}}\left[a^\dagger_{1\uparrow} a^\dagger_{1\downarrow} - a^\dagger_{2\uparrow} a^\dagger_{2\downarrow}\right]|0\rangle$ antibonding ionic combination