

II. Hubbard model and HTSC

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- Tight-binding model Hamiltonian
- Coulomb interaction and Hubbard model
- Hubbard model in terms of Hubbard operators $X^{\alpha\beta}$
- strongly correlated system $\Rightarrow U \gg W$

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Tight-binding Hamiltonian

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- Hamiltonian for solid with N electrons
- $$H_e = T + H_{el} + H_c$$

↓

$$\begin{aligned} H_e &= \int d^3r \hat{\psi}^\dagger(\mathbf{r}) \epsilon_0(\hat{p}) \hat{\psi}(\mathbf{r}) + \\ &+ \frac{1}{2} \int d^3r d^3r' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) V_c(\mathbf{r} - \mathbf{r}') \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}') \end{aligned} \quad (1)$$

↓

$$\{\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\} = \delta(\mathbf{r} - \mathbf{r}') \quad (2)$$

↓

$\epsilon_0(\hat{p}) = \hat{p}^2/2m$ - kinetic energy of electron

$V_c(\mathbf{r} - \mathbf{r}') = \frac{e^2}{|\mathbf{r}-\mathbf{r}'|}$ - Coulomb **e-e** interaction

↓

$$\hat{\psi}(\mathbf{r}) = \sum_i \phi_i(\mathbf{r}) \hat{f}_i \quad (3)$$

↓

- complete basis $\{\phi_j(\mathbf{r})\}$

$$\int d^3r \phi_j^*(\mathbf{r}) \phi_i(\mathbf{r}) = \delta_{ji} \quad (4)$$

↓

$$\{\hat{f}_i \hat{f}_j^\dagger\} = \delta_{ij}$$

↓

- in solids two set of basis are usually used:
plane waves and tight-binding

Plane waves basis

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$$\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}\sigma} \hat{f}_{\mathbf{k}\sigma} e^{i\mathbf{kr}} \chi_\sigma \quad (5)$$

↓

$$\hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{k}\sigma} \hat{\rho}_{\mathbf{k}} e^{-i\mathbf{kr}} \quad (6)$$

$$\hat{\rho}_{\mathbf{k}} = \sum_{\mathbf{q}\sigma} \hat{f}_{\mathbf{k}+\mathbf{q}\sigma}^\dagger \hat{f}_{\mathbf{q}\sigma}$$

↓

- kinetic energy T

$$T = \sum_{\mathbf{k}\sigma} \epsilon_{\mathbf{k}} \hat{f}_{\mathbf{k}\sigma}^\dagger \hat{f}_{\mathbf{k}\sigma} \quad (7)$$

↓

- Electron-lattice interaction (**G**-reciprocal lattice vectors)

↓

$$H_{el} = \sum_{\mathbf{G}} V_{el,\mathbf{G}} \hat{\rho}_{\mathbf{G}} \quad (8)$$

↓

- e-e Coulomb interaction

↓

$$H_c = \sum_{\mathbf{k}} V_{c,\mathbf{k}} \hat{\rho}_{\mathbf{k}}^\dagger \hat{\rho}_{\mathbf{k}} \quad (9a)$$

↓

- Coulomb interaction $V_{c,\mathbf{k}}$,

$$V_{c,\mathbf{k}} = \frac{4\pi e^2}{k^2 \epsilon_\infty \Omega} \quad (9b)$$

↓

ϵ_∞ - dielectric function (high energy screening)

↓

$$\Omega = V/N$$

Tight-binding basis

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- Wannier orbitals $\phi(\mathbf{r} - \mathbf{R}_m)$

↓

$$T = \sum_{m\sigma} T_{0,m} \hat{f}_{m\sigma}^\dagger \hat{f}_{m\sigma} + \sum_{m \neq n\sigma} T_{mn} \hat{f}_{m\sigma}^\dagger \hat{f}_{n\sigma}$$

(10)

↓

$$T_{mn} = \frac{\hbar^2}{2m} \int d^3 r \nabla \phi^*(\mathbf{r} - \mathbf{R}_m) \nabla \phi(\mathbf{r} - \mathbf{R}_n)$$

(11)

↓

- electron-lattice interaction

↓

$$H_{el} = \sum_{m\sigma} V_{el,0,m} \hat{f}_{m\sigma}^\dagger \hat{f}_{m\sigma} + \sum_{m \neq n\sigma} V_{el,mn} \hat{f}_{m\sigma}^\dagger \hat{f}_{n\sigma}$$

(12)

↓

$$V_{el,mn} = \int d^3r \phi^*(\mathbf{r} - \mathbf{R}_m) V_{el}(\mathbf{r}) \phi(\mathbf{r} - \mathbf{R}_n)$$

(13)

↓

- e-e Coulomb interaction (only two-center terms included)

$$H_{el} = \frac{U}{2} \sum_{m\sigma_1\sigma_2} \hat{n}_{m\sigma_1} \hat{n}_{m\sigma_2} + \frac{1}{2} \sum_{m \neq n \sigma \sigma'} V_{c,mn} \hat{n}_{m\sigma} \hat{n}_{n\sigma'}$$

(14)

↓

$$\hat{n}_{m\sigma} = \hat{f}_{m\sigma}^\dagger \hat{f}_{m\sigma}$$

↓

$$V_{c,mn} = e^2 \int \int \frac{d^3r d^3r'}{| \mathbf{r} - \mathbf{r}' |}$$

(15)

$$\times | \phi^*(\mathbf{r} - \mathbf{R}_m) |^2 | \phi(\mathbf{r} - \mathbf{R}_n) |^2$$

↓

- for well localized $\phi(\mathbf{r} - \mathbf{R}_n) \Rightarrow V_{c,mn} \approx \frac{e^2}{R_{mn}}$
- note $\hat{n}_{m\sigma}^2 = \hat{n}_{m\sigma}$
- "atomic level" $\epsilon_{a,m} = T_{0,m} + V_{el,0,m} < 0$



EXTENDED HUBBARD MODEL



$$\begin{aligned}
 H_H^e = & \sum_{m\sigma} \epsilon_{a,m} \hat{n}_{m\sigma} - \sum_{m \neq n\sigma} t_{mn} \hat{f}_{m\sigma}^\dagger \hat{f}_{n\sigma} \\
 & + U \sum_m \hat{n}_{m\uparrow} \hat{n}_{m\downarrow} + \frac{1}{2} \sum_{m \neq n\sigma\sigma'} V_{c,mn} \hat{n}_{m\sigma} \hat{n}_{n\sigma'}
 \end{aligned} \tag{16}$$



- Note, $t_{mn} = -(T_{mn} + V_{el,mn})$



- Brillouin zone wave vector basis



$$\hat{f}_{n\sigma} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \hat{f}_{\mathbf{k}\sigma} e^{i\mathbf{kR}_n} \tag{17}$$



$$\sum_n \hat{f}_{n\sigma}^\dagger \hat{f}_{n\sigma} = \sum_{\mathbf{k}} \hat{f}_{\mathbf{k}\sigma}^\dagger \hat{f}_{\mathbf{k}\sigma} \tag{18}$$



$$\begin{aligned}
H_H^e = & \epsilon_a \sum_{\mathbf{k}\sigma} \hat{n}_{\mathbf{k}\sigma} - \sum_{\mathbf{k}} t_{\mathbf{k}} \hat{f}_{\mathbf{k}\sigma}^\dagger \hat{f}_{\mathbf{k}\sigma} \\
& + \frac{U}{N} \sum_{\mathbf{k}} \rho_{k\uparrow}^\dagger \rho_{k\downarrow} + \frac{1}{2N} \sum_{\mathbf{k}\sigma\sigma'} V_{c,\mathbf{k}} \rho_{k\sigma}^\dagger \rho_{k\sigma'} \\
& \quad (19a)
\end{aligned}$$

↓

$$t_{\mathbf{k}} = \sum_{\mathbf{R}_n \neq 0} t_n e^{-i\mathbf{k}\mathbf{R}_n}$$

$$V_{c,\mathbf{k}} = \sum_{\mathbf{R}_n \neq 0} (e^2/R_n) e^{i\mathbf{k}\mathbf{R}_n} \quad (19b)$$

- note and
- usually is V_c neglected and assumed $t_n \neq 0$ for n.n.

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Small U Hubbard Model -metals

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- small $U \Rightarrow U \ll W$ (band width)

↓

- charge susceptibility (in imaginary frequency $i\omega_n$)

↓

$$\begin{aligned}\chi_c(\mathbf{k}, i\omega_n) &= -\frac{1}{N} \int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau \rho_{\mathbf{k}}(\tau) \rho_{\mathbf{k}}^\dagger(0) \rangle \\ &= 2(\chi_{\uparrow\uparrow} + \chi_{\uparrow\downarrow})\end{aligned}\quad (20)$$

↓

$$\rho_{\mathbf{k}} = \rho_{\mathbf{k}\uparrow} + \rho_{\mathbf{k}\downarrow} \quad (21)$$

↓

$$\chi_c(\mathbf{k}, i\omega_n) = \frac{2P(\mathbf{k}, i\omega_n)}{1 - (U + 2V_{c,\mathbf{k}})P(\mathbf{k}, i\omega_n)} \quad (22)$$

↓

- spin susceptibility $\chi_s(\mathbf{k}, i\omega_n)$

↓

$$\begin{aligned}\chi_s(\mathbf{k}, i\omega_n) &= -\frac{1}{N} \int_0^\beta d\tau e^{i\omega_n \tau} \langle T_\tau s_{\mathbf{k}}^z(\tau) s_{\mathbf{k}}^{z\dagger}(0) \rangle \\ &= 2(\chi_{\uparrow\uparrow} - \chi_{\uparrow\downarrow})\end{aligned}\quad (23)$$

↓

$$s_{\mathbf{k}}^z(\tau) = \rho_{\mathbf{k}\uparrow} - \rho_{\mathbf{k}\downarrow} \quad (24)$$

↓

$$\chi_s(\mathbf{k}, i\omega_n) = \frac{2P(\mathbf{k}, i\omega_n)}{1 + UP(\mathbf{k}, i\omega_n)} \quad (25)$$

↓

$$\begin{aligned} P_{\sigma}^{RPA}(\mathbf{k}, i\omega_n) &= -\frac{1}{N} \sum_q G(q)G(k+q) \\ &= \frac{1}{N} \sum_{\mathbf{q}} \frac{n_F(\xi_{\mathbf{q}}) - n_F(\xi_{\mathbf{k+q}})}{i\omega_n + \xi_{\mathbf{q}} - \xi_{\mathbf{k+q}}} \end{aligned} \quad (26)$$

↓

$$\chi_c(\mathbf{k}) = -\frac{N(0)}{1 + N(0)U + \frac{k_{sc}^2}{k^2}} \quad (27)$$

↓

- in metals $\chi_c(\mathbf{k} \rightarrow \mathbf{0}) \rightarrow 0$

Charge collective modes for $U \ll W$

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- define $x = \frac{\omega}{kv_F}$

- for $x \rightarrow 0$

$$P_{\sigma}^{RPA}(0) = -N(0) \quad (28)$$

- for $x \rightarrow \infty$ (in d-dimensions)

↓

$$P_{\sigma}^{RPA}(k) = \frac{k^2 a^2 E}{\omega^2 d} \quad (29)$$

↓

- average "kinetic" energy E

↓

$$E = \frac{1}{N} \sum_{\mathbf{k}} t_{\mathbf{k}} n_F(\xi_{\mathbf{k}})$$

↓

$$\xi_{\mathbf{k}} = -t_{\mathbf{k}} - \mu$$

↓

- in metals

$$\chi_c(\mathbf{k} \rightarrow \mathbf{0}, \omega) = -\frac{2n_0 a^2 k^2 E}{\omega^2 - \omega_{pl}^2} \quad (30)$$

↓

$$\omega_{pl}^2 = \frac{4\pi^2 n_0 e^2}{\epsilon_\infty m} \quad (31)$$

↓

- in metals plasma collective mode with ω_{pl}

↓

- neutral systems $\Rightarrow V_c = 0 \Rightarrow$ pure Hubbard model

↓

$$\chi_c(\mathbf{k} \rightarrow \mathbf{0}, \omega) = -\frac{2n_0 a^2 k^2 E}{\omega^2 - \omega_k^2} \quad (32a)$$

- sound-like mode ($v_c^2 = a^2 U E / d$)

$$\omega_k^2 = v_c^2 k^2 \quad (32b)$$

↓

a - nearest neighbour distance

↓

n_0 - density of electrons

↓

Antiferromagnetism and spin collective modes

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- limit $x \rightarrow \infty$

↓

$$\chi_s(\mathbf{k} \rightarrow \mathbf{0}, \omega) = \frac{2v_c^2 k^2 / U}{\omega^2 + v_c^2 k^2} \quad (33)$$

↓

- there is relaxation mode $\omega_{rel} = iv_c k$

↓

AF instability - 2D system with

↓

- Case: half-filling $n_0 = 1$ and $\mu = 0$)
- for 2D n.n. $\epsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a)$

↓

- density of states

$$N(\omega) = \frac{1}{2\pi^2 t} \ln \frac{16t}{\omega} \quad (34)$$

- static $\chi_s(\mathbf{k})$

↓

$$\chi_s(\mathbf{k}) = \frac{2P(\mathbf{k})}{1 + UP(\mathbf{k})} \quad (35)$$

- at $T > 0$

\downarrow

- at $\mathbf{k} = 0$

$$P^{RPA}(\mathbf{0}) \sim -\frac{1}{t} \ln \frac{t}{T} \quad (36)$$

- at $\mathbf{Q} = (\pi, \pi)$

$$P(\mathbf{k} = \mathbf{Q}) \sim -\frac{1}{t} \ln^2 \frac{t}{T} \quad (37)$$

\downarrow

- AF (SDW) instability at T_{SDW}

\downarrow

$$1 + UP(\mathbf{Q}) = 0 \quad (38)$$

\downarrow

$$T_{SDW} \sim t e^{-2\pi(t/U)^2} \quad (39)$$

\downarrow

- for $n \lesssim 1$ AF fluctuations are inherent
(Fig.AF)

\downarrow

Hubbard model with large $U \gg W$

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$$H = -t \sum_{m \neq n\sigma} \hat{f}_{m\sigma}^\dagger \hat{f}_{n\sigma} + U \sum_m \hat{n}_{m\uparrow} \hat{n}_{m\downarrow} \quad (40)$$

↓

- doubly occupation ("doublons") is suppressed for $U \gg W$

↓

- novel types of screening is expected

↓

- Hilbert space $\{ | \alpha \rangle \Rightarrow | 0 \rangle, | 2 \rangle, | \uparrow \rangle, | \downarrow \rangle \}$
- Hubbard projection operators $X^{\alpha\beta}$;
 $\alpha, \beta = 0, 2, \sigma = \uparrow (+), \sigma = \downarrow (-)$

↓

$$X^{\alpha\beta} = | \alpha \rangle \langle \beta | \quad (41)$$

↓

$$X^{\alpha\beta} X^{\gamma\delta} = \delta_{\beta\gamma} X^{\alpha\delta} \quad (42)$$

↓

- "ugly" algebra

↓

$$X_i^{\alpha\beta} X_j^{\gamma\delta} \pm X_j^{\gamma\delta} X_i^{\alpha\beta} = \delta_{ij} (\delta_{\beta\gamma} X_i^{\alpha\delta} \pm \delta_{\delta\alpha} X_j^{\gamma\beta}) \quad (43)$$

↓

- completeness relation

↓

$$X_i^{00} + X_i^{22} + \sum_{\sigma} X_i^{\sigma\sigma} = 1 \quad (44)$$

↓

- $\hat{f}_{i\sigma}$ versus $X^{\alpha\beta}$

(if $\sigma = \uparrow \Rightarrow \bar{\sigma} = \downarrow$)

↓

$$\begin{aligned} \hat{f}_{i\sigma} &= X_i^{0\sigma} + \sigma X_i^{\bar{\sigma}2} \\ \hat{f}_{i\sigma}^\dagger &= X_i^{\sigma 0} + \sigma X_i^{2\bar{\sigma}} \end{aligned} \quad (45)$$

$$n_i = 1 - X_i^{00} + X_i^{22} \quad (46)$$

$$S_i^+ = \hat{f}_{i\uparrow}^\dagger \hat{f}_{i\downarrow} = X_i^{+-} = (S_i^-)^\dagger = (X_i^{-+})^\dagger$$

$$S_i^z = \frac{1}{2}(\hat{f}_{i\uparrow}^\dagger \hat{f}_{i\uparrow} - \hat{f}_{i\downarrow}^\dagger \hat{f}_{i\downarrow}) = \frac{1}{2}(X_i^{++} - X_i^{--}) \quad (47)$$

↓

$X^{\alpha\beta}$ **VERSUS** $\hat{f}_{i\sigma}$

↓

$$X^{\sigma 0} = \hat{f}_\sigma^\dagger (1 - \hat{n}_{\bar{\sigma}}); \quad X^{\sigma \bar{\sigma}} = \hat{f}_\sigma^\dagger \hat{f}_{\bar{\sigma}} \quad (48)$$

$$X^{\sigma\sigma} = \hat{n}_\sigma (1 - \hat{n}_{\bar{\sigma}}) \quad (49)$$

$$X^{00} = (1 - \hat{n}_\uparrow)(1 - \hat{n}_\downarrow) \quad (50)$$

$$X^{2\sigma} = \sigma \hat{f}_{\bar{\sigma}}^\dagger \hat{n}_\sigma; \quad X^{20} = \sigma \hat{f}_{\bar{\sigma}}^\dagger \hat{f}_\sigma \quad (51)$$

$$X^{22} = n_\uparrow n_\downarrow \quad (52)$$

↓

- Hamiltonian in terms of $X^{\alpha\beta} \Rightarrow$ correlated motion of holes (electrons)

↓

$$H = -t \sum_{ij\sigma} (X_i^{\sigma 0} X_j^{0\sigma} + X_i^{2\sigma} X_j^{\sigma 2})$$

$$\begin{aligned}
& -t \sum_{ij\sigma} \sigma (X_i^{\sigma 0} X_j^{\bar{\sigma} 2} + X_i^{2\bar{\sigma}} X_j^{0\sigma}) + U \sum_i X_i^{22} \\
& = H_1 + H_{12} + H_2 \tag{53}
\end{aligned}$$

$H_1 \Rightarrow$ single hole motion \Rightarrow lower Hubbard band

$H_2 \Rightarrow$ two holes \Rightarrow upper Hubbard band

$H_{12} \Rightarrow$ connect two bands

\downarrow

Effective Hamiltonian for $U \gg t$

\downarrow

VARIOUS METHODS

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- perturbation over U -term

\downarrow

- canonical transformation $S \Rightarrow$ mixes lower and upper band

\downarrow

$$\begin{aligned}
H_{eff} &= e^S H e^{-S} \\
&= H + [S, H] + \frac{1}{2} [S, [S, H]] + \dots \tag{54}
\end{aligned}$$

↓

$$S = \chi \sum_{ij\sigma} (X_i^{\sigma 0} X_j^{\bar{\sigma} 2} - X_i^{2\bar{\sigma}} X_j^{0\sigma}) \quad (55)$$

↓

$\chi \Rightarrow$ disappear all L-U processes $\sim t$

$$\chi = -\frac{t}{U}$$

$$H_{12} + [S, H_2] = 0 \quad (56)$$

↓

$$H_{eff} = -t \sum_{ij\sigma} X_i^{\sigma 0} X_j^{0\sigma} + H_{3s}$$

$$+ J \sum_{ij\sigma} (\mathbf{S}_i \mathbf{S}_j - \frac{1}{4} \hat{n}_i \hat{n}_j) + H_2 \quad (57)$$

↓

- exchange energy $J = 2t^2/U$

- $H_2 \Rightarrow$ motion of "doublons"

↓

$$H_2 = U \sum_i X_i^{22} - t \sum_{ij\sigma} X_i^{2\sigma} X_j^{\sigma 2} \quad (58)$$

↓

- three sites term H_{3s} (usually neglected in t-J model)

↓

$$H_{3s} = \frac{J}{2} \sum_{ijl\sigma} (X_i^{\bar{\sigma}0} X_l^{\sigma\bar{\sigma}} X_j^{0\sigma} - X_i^{\sigma0} X_l^{\bar{\sigma}\bar{\sigma}} X_j^{0\sigma}) \quad (59)$$

↓

- projection on the lower band

↓

$$PH_{eff}P = H_{tJ}$$

↓

$$H_{tJ} = -t \sum_{ij\sigma} X_i^{\sigma0} X_j^{0\sigma} + +J \sum_{ij\sigma} (\mathbf{S}_i \mathbf{S}_j - \frac{1}{4} \hat{n}_i \hat{n}_j)$$

$$= -t \sum_{ij\sigma} X_i^{\sigma0} X_j^{0\sigma} + \frac{J}{2} \sum_{ij\sigma} (X_i^{\sigma\bar{\sigma}} X_j^{\bar{\sigma}\sigma} - X_i^{\sigma\sigma} X_j^{\bar{\sigma}\bar{\sigma}})$$

(60)

↓

- Spin operators S^\pm, S^z do not describe correctly the electron spin!

$S = 0, 1/2$



$$[S_i^+, S_j^-] = 2\delta_{ij}S_i^z$$

$$[S_i^z, S_j^\pm] = \pm\delta_{ij}S_i^\pm \quad (61)$$

$$\mathbf{S}_i^2 = \frac{3}{4}\hat{n}_i \neq \frac{3}{4} \quad (62)$$



Ugly algebra of $X^{\alpha\beta} \Rightarrow$ How to treat H_{tJ} ?



Various representations of $X^{\alpha\beta}$



SLAVE BOSON METHOD



$F_{i\sigma}$ - fermion (spinon); B_i - boson (holon)



$$X^{0\sigma} = F_\sigma B^\dagger \quad (63)$$



- constraint on Hilbert space
(completeness)

↓

$$B^\dagger B + \sum_{\sigma} F_{i\sigma}^\dagger F_{i\sigma} = 1 \quad (64)$$

$$H_{tJ} = -t \sum_{ij\sigma} F_{i\sigma}^\dagger F_{j\sigma} B_i B_j^\dagger + \frac{J}{2} \sum_{ij\sigma\sigma'} F_{i\sigma}^\dagger F_{j\sigma} F_{j\sigma'}^\dagger F_{i\sigma'} \quad (65)$$

↓

- partition function ($F_{i\sigma}$ - Grassman variable)

↓

$$Z = \int D\lambda_i DB_i DB_i^* DF_{i\sigma} DF_{i\sigma}^* e^{-\int_0^\beta (L+H_{tJ}) d\tau} \quad (66)$$

↓

$$\begin{aligned} L = & \sum_{i\sigma} F_{i\sigma}^\dagger \left(\frac{\partial}{\partial \tau} - \mu \right) F_{j\sigma} + \sum_i B_i^\dagger \frac{\partial}{\partial \tau} B_i \\ & + \sum_i \lambda_i (B_i^\dagger B_i + \sum_{\sigma} F_{i\sigma}^\dagger F_{i\sigma} - 1) \end{aligned} \quad (67)$$

↓

- 1/N expansion as a controllable methods



SLAVE FERMION METHOD



$$X^{0\sigma} = B_\sigma^\dagger F \quad (68)$$



- constraint on Hilbert space



$$F^\dagger F + \sum_{\sigma} B_\sigma^\dagger B_\sigma = 1 \quad (69)$$



SPIN FERMION METHOD



$$\hat{f}_\uparrow^\dagger \hat{f}_\uparrow + \hat{f}_\downarrow^\dagger \hat{f}_\downarrow = 1 - F^\dagger F \quad (70)$$

$$\mathbf{S} = \mathbf{s}(1 - F^\dagger F) \quad (71)$$



$$H_{tJ} = 2t \sum_{ij} F_i^\dagger F_j (\mathbf{s}_i \mathbf{s}_j + \frac{1}{4})$$

$$+ J \sum_{ij} (1 - F_i^\dagger F_i) (\mathbf{s}_i \mathbf{s}_j - \frac{1}{4}) (1 - F_j^\dagger F_j)$$

(72)

↓

PROPERTIES OF REPRESENTATIONS

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- nonuniqueness (ambiguity)
- Fermi-Boson diagram technique possible
- constraint gives rise to singular kinematical interaction
- difficult to find controllable approximation