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- $S(q)$, check difference b/w $S(\pi)$ & m : $\langle \vec{S}(i)\cdot\vec{S}(j)\rangle$ Analytical
- Print $\langle S^2\rangle$ and $\langle S_i^2\rangle$
- Print $S(q)$
- Print Δ_{DOS}
- Print $|\psi_i|^2 \leftarrow$ fermi-state
- Analytical $\rightarrow \sigma(\omega) \rightarrow$? & print $\sigma(\omega)$
- $\langle n_{i\uparrow} n_{i\downarrow}\rangle \leftarrow$ double occupancy

$\leftarrow$ To add

- $\langle S^+(i)\, S^-(j)\rangle = \langle c_{i\uparrow}^\dagger c_{i\downarrow} c_{j\downarrow}^\dagger c_{j\uparrow}\rangle$

$$= \sum_{\substack{n,m\\k,l}} (\psi_{i\uparrow}^n)^* (\psi_{i\downarrow}^m) (\psi_{j\downarrow}^k)^* (\psi_{j\uparrow}^l) \langle c_n^\dagger c_m c_k^\dagger c_l\rangle$$

$$= \sum_{n\neq m} (\psi_{i\uparrow}^n)^* (\psi_{i\downarrow}^m)\, \psi_{j\downarrow}^{m*} \psi_{j\uparrow}^{n} \langle c_n^\dagger c_m c_m^\dagger c_n\rangle$$

$$\sum_{n,m} \psi_{i\uparrow}^{n*} \psi_{i\downarrow}^{n}\, \psi_{j\downarrow}^{m*} \psi_{j\uparrow}^{m} \langle c_n^\dagger c_n c_m^\dagger c_m\rangle$$

$$= \sum_{n\neq m} \Big[\psi_{i\uparrow}^{n*} \psi_{i\downarrow}^{m} \psi_{j\downarrow}^{m*} \psi_{j\uparrow}^{n} \langle c_n^\dagger c_n c_m c_m^\dagger\rangle + \psi_{i\uparrow}^{n*} \psi_{i\downarrow}^{n} \psi_{j\downarrow}^{m*} \psi_{j\uparrow}^{m} \langle \underbrace{c_n^\dagger c_n}\, \underbrace{c_m^\dagger c_m}\rangle \Big]$$

$$+ \sum_{n} \psi_{i\uparrow}^{n*} \psi_{i\downarrow}^{n}\, \psi_{j\downarrow}^{m*} \psi_{j\uparrow}^{m} \langle c_n^\dagger c_n c_n^\dagger c_n\rangle$$

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$$\Rightarrow \boxed{\sum_{n\neq m}\Big[\psi^{n*}_{i\uparrow}\psi^{m}_{i\downarrow}\psi^{m*}_{j\downarrow}\psi^{n}_{j\uparrow}f(\varepsilon_n)(1-f(\varepsilon_m)) + \psi^{n*}_{i\uparrow}\psi^{n}_{i\downarrow}\psi^{m*}_{j\downarrow}\psi^{m}_{j\uparrow}f(\varepsilon_n)f(\varepsilon_m)\Big] + \sum_{n}\psi^{n*}_{i\uparrow}\psi^{n}_{i\downarrow}\psi^{n*}_{j\downarrow}\psi^{n}_{j\uparrow}f(\varepsilon_n)}$$

$$= \langle S^{+}(i)\, S^{-}(j)\rangle$$

$$\langle S^{+}(i)\, S^{-}(j)\rangle^{*} = \langle S^{+}(j)\, S^{-}(i)\rangle$$

$$= \underline{\langle S^{-}(i)\, S^{+}(j)\rangle}$$

$$\cancel{\langle S^{+} S^{+}}$$

$$\boxed{\begin{aligned}\langle S^{-}(i)\, S^{+}(j)\rangle = &\sum_{n\neq m}\psi^{n*}_{i\downarrow}\psi^{m}_{i\uparrow}\psi^{m*}_{j\uparrow}\psi^{n}_{j\downarrow}f(\varepsilon_n)(1-f(\varepsilon_m)) \\ &+ \psi^{n*}_{i\downarrow}\psi^{n}_{i\uparrow}\psi^{m*}_{j\uparrow}\psi^{m}_{j\downarrow}f(\varepsilon_n)f(\varepsilon_m) \\ &+ \sum_{n}\psi^{n*}_{i\downarrow}\psi^{n}_{i\uparrow}\psi^{n*}_{j\uparrow}\psi^{n}_{j\downarrow}f(\varepsilon_n)\end{aligned}}$$

• $\langle S^z(i)\, S^z(j) \rangle$

$$= \frac{1}{4} \langle (n^i_\uparrow - n^i_\downarrow)\,(n_\uparrow(j) - n_\downarrow(j)) \rangle$$

$$\cancel{E} = \langle (c^\dagger_{i\uparrow} c_{i\uparrow} - c^\dagger_{i\downarrow} c_{i\downarrow})(c^\dagger_{j\uparrow} c_{j\uparrow} - c^\dagger_{j\downarrow} c_{j\downarrow}) \rangle$$

$$= \langle c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{j\uparrow} c_{j\uparrow} \rangle^{①} - \langle c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{j\downarrow} c_{j\downarrow} \rangle^{②}$$

$$- \langle c^\dagger_{i\downarrow} c_{i\downarrow} c_{j\uparrow} c_{j\uparrow} \rangle^{③} + \langle c^\dagger_{i\downarrow} c_{i\downarrow} c^\dagger_{j\downarrow} c_{j\downarrow} \rangle^{④}$$

①

$$\langle c^\dagger_{i\uparrow} c_{i\uparrow} c^\dagger_{j\uparrow} c_{j\uparrow} \rangle = \sum_{n,m,k,l} \psi^{n*}_{i\uparrow} \psi^{m}_{i\uparrow} \psi^{k*}_{j\uparrow} \psi^{l}_{j\uparrow} \underline{\langle c^\dagger_n c_m c^\dagger_k c_l \rangle}$$

$$= \sum_{n \neq m} \psi^{n*}_{i\uparrow} \psi^{m}_{i\uparrow} \psi^{m*}_{j\uparrow} \psi^{n}_{j\uparrow} \langle c^\dagger_n c_m c^\dagger_m c_n \rangle$$

$$+ \sum_{n,m} \psi^{n*}_{i\uparrow} \psi^{n}_{i\uparrow} \psi^{m*}_{j\uparrow} \psi^{m}_{j\uparrow} \langle c^\dagger_n c_n c^\dagger_m c_m \rangle$$

$$= \sum_{n \neq m} \Big[\psi^{n*}_{i\uparrow} \psi^{m}_{i\uparrow} \psi^{m*}_{j\uparrow} \psi^{n}_{j\uparrow} f(\varepsilon_n)(1 - f(\varepsilon_m))$$

$$+ \psi^{n*}_{i\uparrow} \psi^{n}_{i\uparrow} \psi^{m*}_{j\uparrow} \psi^{m}_{j\uparrow} f(\varepsilon_n) f(\varepsilon_m) \Big]$$

$$+ \sum_{n} \psi^{n*}_{i\uparrow} \psi^{n}_{i\uparrow} \psi^{n*}_{j\uparrow} \psi^{n}_{j\uparrow} f(\varepsilon_n)$$

(2) $\langle c^{+}_{i\uparrow} c_{i\uparrow} c^{+}_{j\downarrow} c_{j\downarrow} \rangle$

$$= \sum_{n \neq m} \left[\psi^{n*}_{i\uparrow} \psi^{m}_{i\uparrow} \psi^{m*}_{j\downarrow} \psi^{n}_{j\downarrow} f(\varepsilon_n)(1-f(\varepsilon_m)) + \psi^{n*}_{i\uparrow} \psi^{n}_{i\uparrow} \psi^{m*}_{j\downarrow} \psi^{m}_{j\downarrow} f(\varepsilon_n) f(\varepsilon_m) \right]$$

$$+ \sum_{n} \psi^{n*}_{i\uparrow} \psi^{n}_{i\uparrow} \psi^{n*}_{j\downarrow} \psi^{n}_{j\downarrow} f(\varepsilon_n)$$

$$\Rightarrow \frac{1}{4} \Big[\sum_{n \neq m} f(\varepsilon_n)(1-f(\varepsilon_m)) \big\{ \psi^{n*}_{i\uparrow} \psi^{m}_{i\uparrow} \psi^{m*}_{j\uparrow} \psi^{n}_{j\uparrow} - \psi^{n*}_{i\uparrow} \psi^{m}_{i\uparrow} \psi^{m*}_{j\downarrow} \psi^{n}_{j\downarrow} + \psi^{n*}_{i\downarrow} \psi^{m}_{i\downarrow} \psi^{m*}_{j\downarrow} \psi^{n}_{j\downarrow} - \psi^{n*}_{i\downarrow} \psi^{m}_{i\downarrow} \psi^{m*}_{j\uparrow} \psi^{n}_{j\uparrow} \big\}$$

$$+ \sum_{n \neq m} f(\varepsilon_n) f(\varepsilon_m) \big\{ \psi^{n*}_{i\uparrow} \psi^{n}_{i\uparrow} \psi^{m*}_{j\uparrow} \psi^{m}_{j\uparrow} - \psi^{n*}_{i\uparrow} \psi^{n}_{i\uparrow} \psi^{m*}_{j\downarrow} \psi^{m}_{j\downarrow} + \psi^{n*}_{i\downarrow} \psi^{n}_{i\downarrow} \psi^{m*}_{j\downarrow} \psi^{m}_{j\downarrow} - \psi^{n*}_{i\downarrow} \psi^{n}_{i\downarrow} \psi^{m*}_{j\uparrow} \psi^{m}_{j\uparrow} \big\}$$

$$+ \sum_{n} f(\varepsilon_n) \big\{ \psi^{n*}_{i\uparrow} \psi^{n}_{i\uparrow} \psi^{n*}_{j\uparrow} \psi^{n}_{j\uparrow} - \psi^{n*}_{i\uparrow} \psi^{n}_{i\uparrow} \psi^{n*}_{j\downarrow} \psi^{n}_{j\downarrow} + \psi^{n*}_{i\downarrow} \psi^{n}_{i\downarrow} \psi^{n*}_{j\downarrow} \psi^{n}_{j\downarrow} - \psi^{n*}_{i\downarrow} \psi^{n}_{i\downarrow} \psi^{n*}_{j\uparrow} \psi^{n}_{j\uparrow} \big\} \Big]$$

$\langle \vec{S}(i) \vec{S}(j) \rangle$

$$\sigma^{xx}(\omega) = \frac{\pi t^2 e^2 (1 - e^{-\beta\omega})}{\omega L} \times$$

$$\sum_{n \neq m} \frac{\left| \sum_{i\sigma} \left(\psi^{n^*}_{i+\hat{x}\sigma} \psi^{m}_{i\sigma} - \psi^{n^*}_{i\sigma} \psi^{m}_{i+\hat{x}\sigma} \right) \right|^2}{\left(1 + e^{\beta(\varepsilon_n - \mu)}\right)\left(1 + e^{-\beta(\varepsilon_m - \mu)}\right)}$$

$$\times \delta(\omega + \varepsilon_n - \varepsilon_m)$$

For $\langle S^+(i)\, S^-(j) \rangle$

$$\sum_{n,m} \psi_{i\uparrow}^{n*} \psi_{i\downarrow}^{m} \psi_{j\downarrow}^{m*} \psi_{j\uparrow}^{n} f(\varepsilon_n)\,(1 - f(\varepsilon_m))$$

$$+ \psi_{i\uparrow}^{n*} \psi_{i\downarrow}^{n} \psi_{j\downarrow}^{m*} \psi_{j\uparrow}^{m} f(\varepsilon_n)\, f(\varepsilon_m)$$

$$+ \sum_{n} \cancel{\psi_{i\uparrow}^{n*} \psi_{i\downarrow}^{n} \psi_{j\downarrow}^{n*} \psi_{j\uparrow}^{n} f(\varepsilon_n)}$$

$$- \cancel{\psi_{i\uparrow}^{n*} \psi_{i\downarrow}^{n} \psi_{j\downarrow}^{n*} \psi_{j\uparrow}^{n} f(\varepsilon_n)}\,(\cancel{1} - f(\varepsilon_n))$$

$$- \cancel{\psi_{i\uparrow}^{n*} \psi_{i\downarrow}^{n} \psi_{j\downarrow}^{n*} \psi_{j\uparrow}^{n} f(\varepsilon_n)}\, f(\varepsilon_n)$$

$$\boxed{\begin{aligned} \langle S^+(i)\, S^-(j) \rangle = & \left[\sum_{n} \psi_{i\uparrow}^{n*} \psi_{j\uparrow}^{n} f(\varepsilon_n)\right] \times \left[\sum_{m} \psi_{i\downarrow}^{m} \psi_{j\downarrow}^{m*} (1 - f(\varepsilon_m))\right] \\ & + \left[\sum_{n} \psi_{i\uparrow}^{n*} \psi_{i\downarrow}^{n} f(\varepsilon_n)\right] \times \left[\sum_{m} \psi_{j\downarrow}^{m*} \psi_{j\uparrow}^{m} f(\varepsilon_m)\right] \end{aligned}}$$

$\langle S^-(i) S^+(j) \rangle$

$$= \sum_{n,m} \psi^{n*}_{i\downarrow} \psi^{m}_{i\uparrow} \psi^{m*}_{j\uparrow} \psi^{n}_{j\downarrow} f(\varepsilon_n)(1-f(\varepsilon_m))$$

$$+ \psi^{n*}_{i\downarrow} \psi^{n}_{i\uparrow} \psi^{m*}_{j\uparrow} \psi^{m}_{j\downarrow} f(\varepsilon_n) f(\varepsilon_m)$$

$$\boxed{\begin{aligned}\langle S^-(i) S^+(j) \rangle = \Big\{ & \Big[\sum_n \psi^{n*}_{i\downarrow} \psi^{n}_{j\downarrow} f(\varepsilon_n)\Big]\Big[\sum_m \psi^{m}_{i\uparrow} \psi^{m*}_{j\uparrow} (1-f(\varepsilon_m))\Big] \\ & + \Big[\sum_n \psi^{n*}_{i\downarrow} \psi^{n}_{i\uparrow} f(\varepsilon_n)\Big]\Big[\sum_m \psi^{m*}_{j\uparrow} \psi^{m}_{j\downarrow} (f(\varepsilon_m))\Big]\Big\}\end{aligned}}$$

$\langle S^z(i) S^z(j) \rangle$

$$= \frac{1}{4}\Big\{ \Big[\sum_n \psi^{n*}_{i\uparrow} \psi^{n}_{j\uparrow} f(\varepsilon_n)\Big] \times \Big[\sum_m (1-f(\varepsilon_m)) \psi^{m}_{i\uparrow} \psi^{m*}_{j\uparrow}\Big]$$

$$- \Big[\sum_n \psi^{n*}_{i\uparrow} \psi^{n}_{j\downarrow} f(\varepsilon_n)\Big]\Big[\sum_m \psi^{m}_{i\uparrow} \psi^{m*}_{j\downarrow} (1-f(\varepsilon_m))\Big]$$

$$+ \Big[\sum_n \psi^{n*}_{i\downarrow} \psi^{n}_{j\downarrow} f(\varepsilon_n)\Big]\Big[\sum_m \psi^{m}_{i\downarrow} \psi^{m*}_{j\downarrow} (1-f(\varepsilon_m))\Big]$$

$$- \Big[\sum_n \psi^{n*}_{i\downarrow} \psi^{n}_{j\uparrow} f(\varepsilon_n)\Big]\Big[\sum_m \psi^{m}_{i\downarrow} \psi^{m*}_{j\uparrow} (1-f(\varepsilon_m))\Big]$$

p.t.o.

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$$+\left[\sum_n \psi_{i\uparrow}^{n*}\psi_{i\uparrow}^{n} f(\varepsilon_n)\right]\left[\sum_m \psi_{j\uparrow}^{m*}\psi_{j\uparrow}^{m} f(\varepsilon_m)\right]$$

$$-\left[\sum_n \psi_{i\uparrow}^{n*}\psi_{i\uparrow}^{n} f(\varepsilon_n)\right]\left[\sum_m \psi_{j\downarrow}^{m*}\psi_{j\downarrow}^{m} f(\varepsilon_m)\right]$$

$$+\left[\sum_n \psi_{j\downarrow}^{n*}\psi_{i\downarrow}^{n} f(\varepsilon_n)\right]\left[\sum_m \psi_{j\downarrow}^{m*}\psi_{j\downarrow}^{m} f(\varepsilon_m)\right]$$

$$-\left[\sum_n \psi_{i\downarrow}^{n*}\psi_{i\downarrow}^{n} f(\varepsilon_n)\right]\left[\sum_m \psi_{j\uparrow}^{m*}\psi_{j\uparrow}^{m} f(\varepsilon_m)\right]\Bigg\}$$