§8. Exact solution of (HM) in $d=\infty$ limit – dynamical mean-field theory

History of mean-field theory

Van der Waals (1873) – 1st order
Pierre Weiss (1907) – 2nd order, SSB
L.D. Landau (1937) – effective theory of continuous phtr. } phenomenology

~~Landau~~

L. Onsager (1944) – microscopic theory → role of critical fluctuations around mean field theory

Widom (1965)
Kadanoff (1966) } scaling

K. Wilson (1971) – RG

Domb and Green (1973) – linked cluster expansion, high temp

Baym (1962) – formulated criteria a self consistent theory must fulfill to be thermodynamically consistent and conserving, obeying Ward identities

> Any approximation of mean-field character has to offer a global and thermodynamically consistent theory simulating behaviour of an exact solution.

How to find the best mean-field theory for the Hubbard model?

Look for a non-trivial exactly solvable limit.

$$[\hat{H}_{kin}, \hat{H}_{int}] \neq 0$$

From statistical physics we learned that $d \to \infty$ ($z \to \infty$) limit offers such possibility

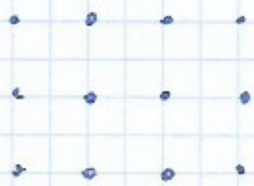
$z = 4$ $\quad$ $z = 8$ $\quad$ $z = \infty$

However, $$\langle H \rangle = J \sum_{\langle ij \rangle} \langle S_i S_j \rangle = J \sum_{i=1}^{N} \underbrace{\sum_{j(i)}}_{\sim z \to \infty} \langle S_i S_j \rangle$$

remedy $J = \frac{J^*}{z}$ then $\langle H \rangle$ finite.

<u>High dimension limit for HM</u>

$d = 1$  $z = 2$ chain

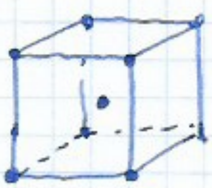
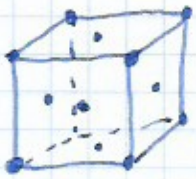
$d = 2$  $z = 4$ square

$d = 3$  $z = 6$ sc cubic

⋮

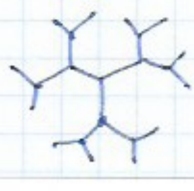
d $\quad$ $z = 2d$ hypercubic

other lattices in $d = 3$

bcc   fcc

$z = 8$ $\quad$ $z = 12$

$\boxed{z \to \infty}$



Bethe tree
Cayley graph

Consider hopping energy $\qquad T=0,\ U=0$

$$E^0_{kin} = -t \sum_{\langle ij\rangle \sigma} \rho^0_{ij\sigma} \qquad \rho^0_{ij\sigma} = \langle a^\dagger_{i\sigma} a_{j\sigma} \rangle$$

one particle density matrix

$\rho^0_{ij\sigma}$ – transition amplitude from j to i.

$P_{ij} = |\rho^0_{ij\sigma}|^2$ – probability of transition

$$\sum_{j(i)}^{Z} P_{ij} = \underbrace{\sum_{j(i)}^{Z}}_{\sim Z} \underbrace{|\rho^0_{ij\sigma}|^2}_{\sim \frac{1}{Z}} = 1$$

$$\Rightarrow \quad \rho^0_{ij\sigma} \sim O\left(\frac{1}{\sqrt{Z}}\right)$$

$$E^0_{kin} = -t \underbrace{\sum_{i=1}^{N}}_{N} \underbrace{\sum_{j(i)}^{Z}}_{\sim Z} \underbrace{\rho^0_{ij\sigma}}_{\frac{1}{\sqrt{Z}}} \sim \sqrt{Z} \xrightarrow[Z\to\infty]{} \infty \quad !$$

Metzner and Vollhardt (1989)

$$t \to \frac{t^*}{\sqrt{Z}}$$

$$E^0_{kin} = -\frac{t^*}{\sqrt{Z}} \underbrace{\sum_{i=1}^{N}}_{N} \underbrace{\sum_{j(i)}^{Z}}_{\sim Z} \underbrace{\rho^0_{ij\sigma}}_{\frac{1}{\sqrt{Z}}} \sim \frac{Z}{\sqrt{Z}\sqrt{Z}} \underset{Z\to\infty}{\sim} 1 \cdot N$$

$$\frac{E^0_{kin}}{N} \sim 1 \quad \text{in } Z\to\infty \ (d\to\infty) \text{ limit}$$

Note $\qquad U \underbrace{\sum_i}_{\sim N} \langle n_{i\uparrow} n_{i\downarrow} \rangle \sim U \cdot N \quad$ for all Z (d)

Note
$$\rho^0_{ij\sigma} = \lim_{t\to 0} G^0_{ij\sigma}(t) = \lim_{t\to 0^+} i\langle T\, a_{i\sigma}(t)\, a^\dagger_{j\sigma}(0)\rangle$$

$$G^0_{ij\sigma}(\omega) = \int dt\, e^{i\omega t}\, G^0_{ij\sigma}(t)$$

$$E^0_{kin} = -\frac{t}{2\pi i} \sum_{\langle ij\rangle\sigma} \int_{-\infty}^{\infty} d\omega\, e^{-i\omega\eta}\, G^0_{ij\sigma}(\omega)$$

$$\Rightarrow \quad G^0_{ij\sigma}(\omega) \sim \frac{1}{\sqrt{z}} \quad \text{as well.}$$

For general (i,j)

$$\boxed{G^0_{ij\sigma} \sim \mathcal{O}\left(\frac{1}{z^{\frac{\|\vec R_i - \vec R_j\|}{2}}}\right) \qquad t_{ij} \to \frac{t^*_{ij}}{z^{\frac{\|\vec R_i - \vec R_j\|}{2}}}} \qquad \|\vec R\| = \sum_{n=1}^{d} |R_n|$$

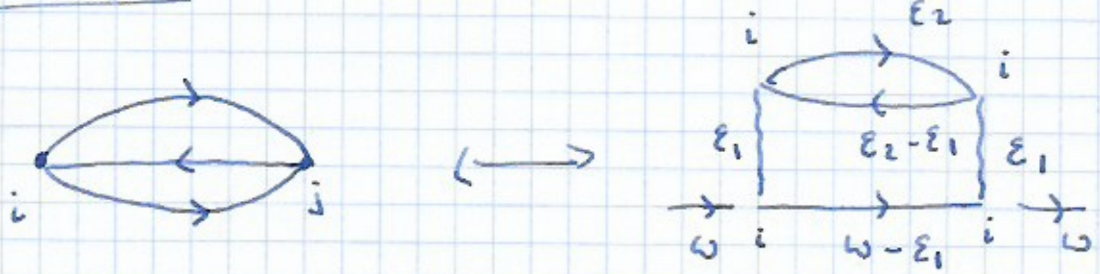
New-York metric
(taxi cab metric)

$\|\vec R\| = 7$

Diagrammatic simplification

All self-energy diagrams are local in lattice space and $\vec k$-independent in momentum space.

Example

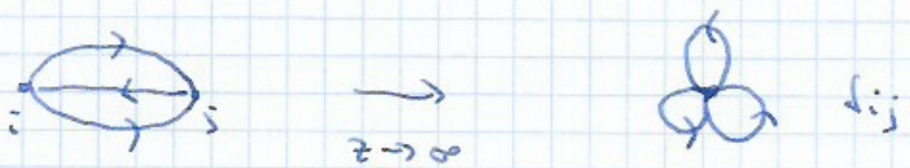


$$\sim \; U^2 \, i^2 (-1) \int d\varepsilon_1 \int d\varepsilon_2 \; \underbrace{G^{(0)}_{ij\sigma}(\omega-\varepsilon_1)}_{\frac{1}{\sqrt{z}}} \; \underbrace{G^{(0)}_{ji\bar\sigma}(\varepsilon_2-\varepsilon_1)}_{1/\sqrt{z}} \; \underbrace{G^{(0)}_{ij\bar\sigma}(\varepsilon_2)}_{1/\sqrt{z}}$$

due to a local interaction on internal lattice sum

$$\Sigma_{ij\sigma}(\omega) = U \langle n_{i\bar\sigma}\rangle \delta_{ij} + \Sigma^{(2)}_{ij\sigma}(\omega)$$

$$\Sigma^{(2)}_{ij\sigma}(\omega) \xrightarrow[z\to\infty]{} \Sigma^{(2)}_{ii}(\omega)$$



"petal shaped diagrams" only
(płatek)

$$\boxed{\begin{aligned} &\Sigma_{ij\sigma}(\omega) \xrightarrow[z\to\infty]{} \Sigma_{ii\sigma}(\omega)\,\delta_{ij} \\ &\Sigma_{\vec{k}}(\omega) \xrightarrow[z\to\infty]{} \Sigma(\omega) \end{aligned}}$$

Dynamical mean-field theory - cavity method

$$\hat{H} = \sum_{ij\sigma}{}' t_{ij}\, a^\dagger_{i\sigma} a_{j\sigma} + \sum_{i\sigma} (\varepsilon_i - \mu)\, a^\dagger_{i\sigma} a_{i\sigma} + \frac{u}{2} \sum_{i\sigma\sigma'}{}' n_{i\sigma} n_{i\sigma'}$$

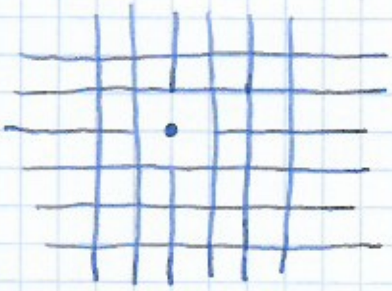
$$Z = \int \prod_i D[a^*_{i\sigma} a_{i\sigma}]\, e^{-S'}$$

$$\langle \hat{A} \rangle_S = \frac{\int \prod_i D[a^*_{i\sigma} a_{i\sigma}]\, e^{-S'}\, A[a^*_{i\sigma}, a_{i\sigma}]}{\int \prod_i D[a^*_{i\sigma} a_{i\sigma}]\, e^{-S'}}$$

$$S' = \int_0^\beta d\tau \sum_{i\sigma} a^*_{i\sigma}(\tau) (\partial_\tau - \mu) a_{i\sigma}(\tau) +$$

$$\int_0^\beta d\tau \sum_{ij\sigma} t_{ij}\, a^*_{i\sigma}(\tau) a_{j\sigma}(\tau) + \sum_{i\sigma} \varepsilon_i\, a^*_{i\sigma} a_{i\sigma} +$$

$$+ \frac{u}{2} \sum_{i\sigma\sigma'}{}' a^*_{i\sigma}(\tau) a_{i\sigma}(\tau)\, a^*_{i\sigma'}(\tau) a_{i\sigma'}(\tau)$$



select $i=0$ site - cavity

$$H_0 = \sum_\sigma \varepsilon_0\, a^\dagger_{0\sigma} a_{0\sigma} + \frac{u}{2} \sum_{\sigma\sigma'}{}' n_{0\sigma} n_{0\sigma'}$$

$$H_c = \sum_{i\sigma} (t_{i0}\, a^\dagger_{i\sigma} a_{0\sigma} + t_{0i}\, a^\dagger_{0\sigma} a_{i\sigma})$$

$$H^{(0)} = \sum_{j,i\neq 0\sigma} t_{ij}\, a^\dagger_{i\sigma} a_{j\sigma} + \frac{u}{2} \sum_{i\sigma\sigma'}{}' n_{i\sigma} n_{i\sigma'}$$

Integrate out all degrees of freedom with $i \neq 0$ to obtain an effective theory on a single site.

$$S_0 = \int_0^\beta d\tau \sum_\sigma a_{0\sigma}^* (\partial_\tau - \mu + \varepsilon_0) a_{0\sigma} + \frac{U}{2} \int_0^\beta d\tau \sum_{\sigma\sigma'} n_{0\sigma} n_{0\sigma'}$$

$$\Delta S = \int_0^\beta d\tau \Big[\sum_{i\sigma} t_{i0}\, a_{i\sigma}^* a_{0\sigma} + t_{0i}\, a_{0\sigma}^* a_{i\sigma} \Big] = \int_0^\beta d\tau \, \Delta S(\tau)$$

$$S^{(0)} = \int_0^\beta d\tau \Big[\sum_{i\neq 0,\sigma} a_{i\sigma}^* (\partial_\tau - \mu + \varepsilon_i) a_{i\sigma} +$$

$$+ \sum_{\substack{ij\sigma \\ \neq 0}}{}' t_{ij}\, a_{i\sigma}^* a_{j\sigma} + \frac{U}{2} \sum_{i\neq 0\, \sigma\sigma'} n_{i\sigma} n_{i\sigma'} \Big]$$

$$Z = \int D[a_{0\sigma}^* a_{0\sigma}]\, e^{-S_0} \int \prod_{i\neq 0} D[a_{i\sigma}^* a_{i\sigma}]\, e^{-S^{(0)}} \, e^{-\int_0^\beta d\tau\, \Delta S(\tau)}$$

Expand (like $O(t^2/\sqrt{z})$ expansion)

$$e^{-\int_0^\beta d\tau\, \Delta S(\tau)} = 1 - \int_0^\beta d\tau\, \Delta S(\tau) + \frac{1}{2!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2\, \Delta S(\tau_1) \Delta S(\tau_2) + \dots$$

Then

$$Z = \int D[a_\sigma^* a_\sigma]\, e^{-S_0}\, Z^{(0)} \Big[1 - \int_0^\beta d\tau \, \langle \Delta S(\tau) \rangle_{S^{(0)}} +$$

$$+ \frac{1}{2!} \int_0^\beta d\tau_1 \int_0^\beta d\tau_2 \, \langle \Delta S(\tau_1) \Delta S(\tau_2) \rangle_{S^{(0)}} + \dots \Big]$$

where $Z^{(0)} = \int \prod_{i\neq 0} D[a_{i\sigma}^* a_{i\sigma}]\, e^{-S^{(0)}}$

$$\frac{Z}{Z^{(0)}} = \int D[a_{0\sigma}^{+} a_0]\, e^{-S_0} \cdot \frac{1}{Z^{(0)}} \int_{\neq 0} D[a_{i\sigma}^{+} a_i]\, e^{-S^{(0)}} \cdot \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \cdot$$

$$\cdot \sum_{\substack{i_1 \dots i_n \\ j_1 \dots j_n}} \int d\tau_{i_1} \dots d\tau_{i_n}\, d\tau_{j_1} \dots d\tau_{j_n}\; t_{0 i_1} a_{0\sigma}^{+}(\tau_{i_1})\, t_{0 i_2} a_{0\sigma}^{+}(\tau_{i_2}) \dots t_{0 i_n} a_{0\sigma}^{+}(\tau_{i_n})$$

$$\cdot\, t_{j_1 0}\, a_{0\sigma}(\tau_{j_1})\, t_{j_2 0}\, a_{0\sigma}(\tau_{j_2}) \dots t_{j_n 0} (\tau_{j_n}) \,\cdot$$

$$\cdot\, c_{i_1}(\tau_{i_1}) \dots c_{i_n}(\tau_{i_n})\, c_{j_1}^{+}(\tau_{j_1}) \dots c_{j_n}^{+}(\tau_{j_n})$$

$$=$$

$$= \int D[a_{0\sigma}^{+} a_{0\sigma}]\, e^{-S_0}\, e^{-\sum_{n=1}^{\infty} \sum_{\substack{i_1 \dots i_n \\ j_1 \dots j_n}} \int \dots \int t_{0 i_1} a_{0\sigma}^{+}(\tau_{i_1}) \dots t_{0 i_n} a_{0\sigma}(\tau_{i_n})} \cdot$$

$$t_{j_1 0} \cdot a_{0\sigma}(\tau_{j_1}) \dots t_{j_n 0}\, a_{0\sigma}(\tau_{j_n}) \cdot G^{[0]}_{i_1 \dots i_n j_1 \dots j_n}(\tau_{i_1} - \tau_{i_n} \tau_{j_1} \dots \tau_{j_n})$$

$\uparrow$

Connected Green's functions on the cavity lattice with the HM.

<u>Linked cluster theorem</u>

$$\sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \langle \dots \rangle_{2n} = e^{-\sum_{k=0}^{\infty} \langle \dots \rangle_{2k}^{c}}$$

Now, only correlation functions with the same a^{+} and a operators survive $\rightarrow$ particle number conservation.

$\underline{n=1 \text{ term}}$ $\qquad G^{(0)}_{ij} \sim \left(\frac{1}{\sqrt{z}}\right)^{|i-j|}$

$$\underbrace{\sum_{ij}}_{\sim z^2} \int d\tau_i\, d\tau_j\, a^\dagger_{0i}(\tau_i)\, a_{0i}(\tau_j)\, \underbrace{t_{0i}\, t_{j0}\, G^{0}_{ij}}_{\sim \frac{1}{z^2}} \sim O(1)$$

$$\underbrace{\left(\frac{1}{\sqrt{z}}\right)^{|0-i|} \cdot \left(\frac{1}{\sqrt{z}}\right)^{|0-j|} \left(\frac{1}{\sqrt{z}}\right)^{|i-j|}}_{\sim \frac{1}{z^2}}$$

$|i-j| \geq 2$

$|0-i| \geq 1$

$|0-j| \geq 1$

$\underline{n=2 \text{ term}}$ $\qquad G^{(0)}_{ijkl} \sim \left(\frac{1}{\sqrt{z}}\right)^{|i-j|} \left(\frac{1}{\sqrt{z}}\right)^{|i-k|} \left(\frac{1}{\sqrt{z}}\right)^{|i-l|}$

a) $i \neq j \neq k \neq l$

$|i-j| \geq 2$

$|i-k| \geq 2$

$|i-l| \geq 2$

$$\underbrace{\sum_{ijkl}}_{\sim z^4} \int d\tau \dots a^\dagger_{0i} \dots a_{0c}\, \underbrace{t_{0i}\, t_{0j}\, t_{k0}\, t_{l0}}_{\left(\frac{1}{\sqrt{z}}\right)^4 = \frac{1}{z^2}}\, \underbrace{G^{(0)}_{ijkl}}_{\left(\frac{1}{\sqrt{z}}\right)^{3\cdot 2} \text{ or more}} \sim$$

$$\sim z^4 \cdot \frac{1}{z^2} \cdot \frac{1}{z^3} \sim O\left(1/z\right)$$

b) $i = j \neq k \neq l$

$|i-k| \geq 2$

$|i-l| \geq 2$

$$\underbrace{\sum_{ikl}}_{\sim z^3} \int d\tau \dots a^\dagger \dots a\, \underbrace{t_{0i}\, t_{0i}\, t_{k0}\, t_{l0}}_{\left(\frac{1}{\sqrt{z}}\right)^4 = \frac{1}{z^2}}\, \underbrace{G^{(0)}_{iikl}}_{\frac{1}{z^2}} \sim$$

$$\sim O\left(\frac{1}{z}\right)$$

c) $i = j = k \neq l$

$$\underbrace{\sum_{il}}_{\sim z^2} \int d\tau \dots a^\dagger \dots a\, \underbrace{t_{0i}\, t_{0i}\, t_{i0}\, t_{l0}}_{\frac{1}{z^2}}\, \underbrace{G^{(0)}_{iiil}}_{\frac{1}{z}} \qquad |i-l| \geq 2$$

$$\sim O\left(1/z\right)$$

d) $i = j = k = l$

$$\underbrace{\sum_{i}}_{\sim z} \int d\tau \dots a^\dagger \dots a\, \underbrace{t_{0i}\, t_{0i}\, t_{i0}\, t_{i0}}_{1/z^2}\, \underbrace{G^{(0)}_{iiii}}_{\sim O(1)} \sim O\left(1/z\right)$$

→ All higher order contributions vanish in $z \to \infty$ limit.

The effective theory is simple

$$\frac{\Xi}{\Xi_0} = \int D[a_{0\sigma}^+ a_{0\sigma}]\, e^{\left(-\int_0^\beta d\tau \int_0^\beta d\tau' \left(a_{0\sigma}^+(\tau)(\partial_\tau - \mu + \varepsilon_0) a_{0\sigma}(\tau)\, \delta(\tau-\tau') - \sum_{ij} t_{0i} t_{j0}\, G_{ij\sigma}^{(0)}(\tau-\tau')\, a_{0\sigma}^+(\tau)\, a_{0\sigma}(\tau') \right) - \int_0^\beta d\tau\, U\, n_{0\uparrow}(\tau)\, n_{0\downarrow}(\tau) \right)} =$$

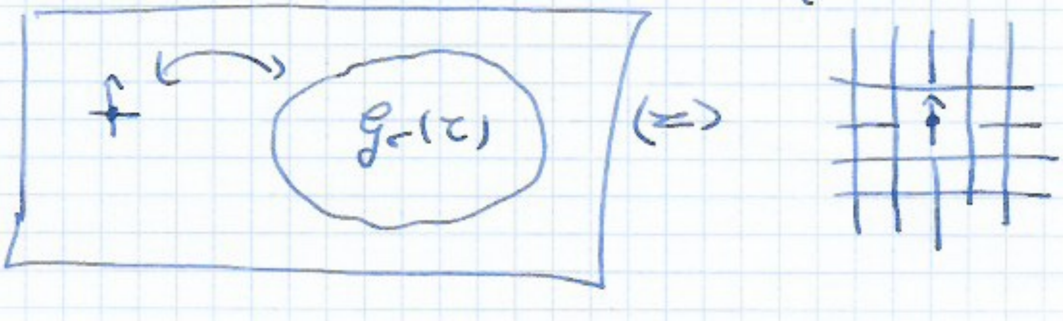
$$= \int D[a_{0\sigma}^+ a_{0\sigma}]\, e^{-\int_0^\beta d\tau \int_0^\beta d\tau'\, a_{0\sigma}^+(\tau)\, \mathcal{G}_\sigma^{-1}(\tau-\tau')\, a_{0\sigma}(\tau') - \int_0^\beta d\tau\, U n_{0\uparrow} n_{0\downarrow}}$$

$$\mathcal{G}_\sigma^{-1}(\tau-\tau') = \underbrace{(\partial_\tau - \mu + \varepsilon_0)\,\delta(\tau-\tau')}_{\text{free propagator}} - \overbrace{\underbrace{\sum_{ij} t_{0i} t_{j0}\, G_{ij}^{0}(\tau-\tau')}_{\text{hybridization of } i=0 \text{ site with the rest of the lattice}}}^{\Delta_\sigma(\tau-\tau')}$$

Weiss mean-field

exact single site dynamics in time!

DMFT



We need to find $G^{[0]}_{ij}(\tau-\tau')$ in terms of $G_{ij}(\tau-\tau')$

Fact

$$G^{[0]}_{ij}(\omega) = G_{ij}(\omega) - G_{i0}(\omega)\,G_{00}^{-1}(\omega)\,G_{0j}(\omega)$$

or $\int_0^\beta d\tau'\, G_{i0}(\tau-\tau')\,G_{0j}(\tau') = \int_0^\beta d\tau' \left[G_{ij}(\tau-\tau') - G^{[0]}_{ij}(\tau-\tau')\right] G_{00}(\tau')$

proof EOM $\sum_j \big(\overbrace{-t_{ij} + (i\omega_n + \mu)\delta_{ij} - \Sigma_i(\omega_n)\delta_{ij}}^{G_{ij}(\omega_n)^{-1}} \big) G_{jk}(\omega_n) = \delta_{ik}$

Let at site $i=0$ there is a potential $V_{ij} = \varepsilon_0\,\delta_{i0}\,\delta_{ij}$.

The EOM $\quad \sum_j \left(G^{-1}_{ij}(\omega_n) - V_{ij} \right) G^{(\varepsilon_0)}_{jk}(\omega_n) = \delta_{ik} \quad / \sum_i G_{\ell i}(\omega)$

$$\sum_i G_{\ell i} \sum_j \left(G^{-1}_{ij} - V_{ij} \right) G^{(\varepsilon_0)}_{jk} = \sum_i G_{\ell i}\,\delta_{ik}$$

rearranging $\quad G^{(\varepsilon_0)}_{\ell k} = G_{\ell k} + \sum_{i_1 j_1} G_{\ell i_1} V_{i_1 j_1} G^{(\varepsilon_0)}_{j_1 k}$

iterating

$$\boxed{G^{(\varepsilon_0)}_{\ell k} = G_{\ell k} + \sum_{i_1 j_1} G_{\ell i_1} T_{i_1 j_1} G_{j_1 k}} \qquad (*)$$

with $\quad T_{i_1 j_1} = V_{i_1 j_1} + \sum_{i_2 j_2} V_{i_1 i_2} G_{i_2 j_2} V_{j_2 j_1} + \dots$

for $V_{ij} = \varepsilon_0\,\delta_{i0}\,\delta_{ij}$

$$T_{i_1 j_1} = \delta_{i_1 0}\,\delta_{i_1 j_1}\,\varepsilon_0 \left(1 + \varepsilon_0 G_{00} + (\varepsilon_0 G_{00})^2 + \dots\right) =$$

$$= \delta_{i_1 0}\,\delta_{i_1 j_1}\,\varepsilon_0 \frac{1}{1-\varepsilon_0 G_{00}} = \delta_{i_1 0}\,\delta_{i_1 j_1} \left[\frac{1}{\frac{1}{\varepsilon_0} - G_{00}} \right]$$

$G^{[0]}_{ij} = \lim_{\varepsilon_0 \to \infty} G^{[\varepsilon_0]}_{ij} \quad \Rightarrow \quad T_{i_1 j_1} = -\delta_{i_1 0}\,\delta_{i_1 j_1} \dfrac{1}{G_{00}}$

and from $(*)$

$$\boxed{G^{[0]}_{ij} = G_{ij} - G_{i0}\,\frac{1}{G_{00}}\,G_{0j}} \qquad \square$$

Hence,

$$\mathcal{G}^{-1}(i\omega_n) = i\omega_n + \mu - \sum_{ij} t_{i0} t_{0j} G^{(0)}_{ij}(\omega_n) =$$

$$= i\omega_n + \mu - \sum_{ij} t_{i0} t_{0j} \left[G_{ij}(\omega_n) - G_{i0}(\omega_n) \frac{1}{G_{00}(\omega_n)} G_{0j}(\omega_n) \right]$$

For translationally invariant system we use Fourier transform

$$G_{ij}(\omega_n) = \sum_{\vec{k}} e^{i\vec{k}\vec{R}_{ij}} G_{\vec{k}}(\omega_n)$$

$$\cancel{\sum_i t_{i0} G_{i0} = \sum_{\vec{k}} e^{i\vec{k}\vec{R}_{i0}} G_{\vec{k}} = \sum_{\vec{k}}}$$

$$\sum_i t_{i0} G_{i0} = \sum_i t_{i0} \sum_{\vec{k}} e^{i\vec{k}\vec{R}_{i0}} G_{\vec{k}} = \sum_{\vec{k}} \varepsilon_{\vec{k}} G_{\vec{k}}(\omega_n)$$

$$\sum_{ij} t_{i0} t_{0j} G_{ij} = \sum_{ij} t_{i0} t_{0j} \sum_{\vec{k}} e^{i\vec{k}\vec{R}_{ij}} G_{\vec{k}} =$$

$$= \sum_{\vec{k}} \sum_i t_{i0} e^{i\vec{k}\vec{R}_{i0}} \sum_j t_{0j} e^{i\vec{k}\vec{R}_{0j}} G_{\vec{k}} = \sum_{\vec{k}} \varepsilon_{\vec{k}}^2 G_{\vec{k}}$$

Dyson equation $\quad G_{\vec{k}}^{-1} = i\omega_n + \mu - \varepsilon_{\vec{k}} - \underbrace{\Sigma(i\omega_n)}_{\text{self-energy}}$

Let $\zeta = i\omega_n + \mu - \Sigma(\omega_n)$

$$G_{\vec{k}}^{-1} = \zeta - \varepsilon_{\vec{k}}$$

$$\sum_{\vec{k}} \varepsilon_{\vec{k}} G_{\vec{k}} = \sum_{\vec{k}} \frac{\varepsilon_{\vec{k}}}{\zeta - \varepsilon_{\vec{k}}} = \sum_{\vec{k}} \frac{\varepsilon_{\vec{k}} - \zeta + \zeta}{\zeta - \varepsilon_{\vec{k}}} = -1 + \sum_{\vec{k}} \frac{\zeta}{\zeta - \varepsilon_{\vec{k}}} =$$

$$= -1 + \zeta \sum_{\vec{k}} G_{\vec{k}} = -1 + \zeta G_{00}(\omega_n)$$

$$\sum_{\vec{k}} \varepsilon_{\vec{k}}^2 G_{\vec{k}} = \sum_{\vec{k}} \frac{\varepsilon_{\vec{k}}^2}{\zeta - \varepsilon_{\vec{k}}} = \sum_{\vec{k}} \frac{\varepsilon_{\vec{k}}(\varepsilon_{\vec{k}} - \zeta) + \varepsilon_{\vec{k}}\zeta}{\zeta - \varepsilon_{\vec{k}}} = -\overbrace{\sum_{\vec{k}} \varepsilon_{\vec{k}}}^{=0} + \zeta \sum_{\vec{k}} \frac{\varepsilon_{\vec{k}}}{\zeta - \varepsilon_{\vec{k}}} =$$

$$= \zeta(-1 + \zeta G_{00}) = -\zeta + \zeta^2 G_{00}$$

$$\mathcal{G}^{-1}(i\omega_n) = i\omega_n + \mu - \sum_{k} \varepsilon_k^2 G_{\bar{k}} + \Big(\sum_k \varepsilon_{\bar{k}} G_k\Big)^2 G_{00}^{-1} =$$

$$= i\omega_n + \mu + \zeta - \zeta^2 G_{00} + (-1 + \zeta G_{00})(-G_{00}^{-1} + \zeta) =$$

$$= i\omega_n + \mu + \cancel{\zeta} - \zeta^2 \cancel{G_{00}} + G_{00}^{-1} - \cancel{\zeta} - \zeta \underbrace{G_{00} \cdot G_{00}^{-1}}_{1} + \zeta^2 \cancel{G_{00}} =$$

$$= i\omega_n + \mu - \zeta + G_{00}^{-1} =$$

$$= \Sigma(i\omega_n) + G_{00}^{-1}$$

$$\Rightarrow \qquad \boxed{G_{00}^{-1} = \mathcal{G}^{-1}(i\omega_n) - \Sigma(i\omega_n)}$$

local Dyson equation

DMFT scheme

$$\begin{tikzcd}
 & \boxed{G_{00} = \langle c_0 c_0^+ \rangle_{S[\mathcal{G}]}} \arrow[dr] & \\
\boxed{\mathcal{G}^{-1} = G_{00}^{-1} + \Sigma} \arrow[ur] & & \boxed{\Sigma = \mathcal{G}^{-1} - G_{00}^{-1}} \arrow[dl] \\
 & \boxed{G_{00} = \sum_k G_k = \sum_k \frac{1}{i\omega_n + \mu - \varepsilon_{\bar{k}} - \Sigma}} \arrow[ul] &
\end{tikzcd}$$

For inhomogeneous systems 08.01.08 52

Dyson equation

$$\mathbb{G} = \mathbb{G}_0^{-1} - \mathbb{\Sigma} \quad \leftarrow N_L \times N_L \text{ matrices}$$

$$\mathbb{\Sigma} = \begin{pmatrix} \Sigma_{11} & & 0 \\ & \Sigma_{22} & \\ 0 & & \ddots \; \Sigma_{N_L N_L} \end{pmatrix}$$

Local Dyson equation

$$G_i \equiv G_{ii} \quad \forall i$$

$$\Sigma_i = \mathcal{G}_i^{-1} - G_i^{-1} \qquad \Sigma_i \equiv \Sigma_{ii}$$

$$\forall j \quad S_\ell = \int_0^\beta\!\!\int_0^\beta d\tau\, d\tau'\, a_i^{+}(\tau)\, \mathcal{G}_\ell^{-1}(\tau-\tau') \sum_{ij} t_{i\ell}\, t_{\ell j}\, G_{ij}^{[\ell]} + $$

$$+ U \int_0^\beta d\tau\, n_{\ell\uparrow}\, n_{\ell\downarrow}$$

Now

$$G_{ij}^{[\ell]} = G_{ij} - \frac{G_{i\ell}\, G_{\ell j}}{G_{\ell\ell}}$$

$$\Delta_\ell = \sum_{ij} t_{i\ell}\, t_{\ell j}\, G_{ij}^{[\ell]} = [\mathbb{t}\; \mathbb{G}\; \mathbb{t}]_{\ell\ell} - \frac{[\mathbb{t}\,\mathbb{G}]_{\ell\ell}\,[\mathbb{G}\,\mathbb{t}]_{\ell\ell}}{G_{\ell\ell}}$$

$$\mathbb{G} = [\zeta - \mathbb{t} - \mathbb{\Sigma}]^{-1} \qquad \zeta_{ij} = (i\omega_n + \mu - \varepsilon_i)\,\delta_{ij}$$

$$\mathbb{t}\,\mathbb{G}\,\mathbb{t} = \mathbb{t}\cdot\mathbb{G}\cdot[\zeta - \mathbb{\Sigma} - \mathbb{G}^{-1}] =$$

$$= \mathbb{t}\cdot\mathbb{G}\,(\zeta - \mathbb{\Sigma}) - \mathbb{t} \qquad \mathbb{t} = \zeta - \mathbb{\Sigma} - \mathbb{G}^{-1}$$

$$\mathbb{t}\,\mathbb{G} = [\zeta - \mathbb{\Sigma} - \mathbb{G}^{-1}]\cdot\mathbb{G} =$$

$$= (\zeta - \mathbb{\Sigma})\cdot\mathbb{G} - \mathbb{1}$$

$$\Delta_i = \left([\zeta - \Sigma - G^{-1}] \cdot G \cdot (\zeta - \Sigma) \right)_{ii} - t_{ii} -$$

$$- [(\zeta - \Sigma) G - 1]_{ii} \, [G (\zeta - \Sigma) - 1]_{ii} / G_{ii} =$$

$$= -(\zeta - \Sigma)_{ii} + \left([(\zeta - \Sigma)] G [\zeta - \Sigma] \right)_{ii} -$$

$$- [(\zeta - \Sigma) G - 1]_{ii} \, [G (\zeta - \Sigma) - 1]_{ii} / G_{ii}$$

$t_{ii} = 0$, ζ and Σ are diagonal

hence

$$\mathcal{G}_i^{-1} = \underbrace{i\omega_n + \mu - \Sigma_i}_{\zeta - \Sigma} - \Delta_i =$$

$$= (\zeta - \Sigma)_{ii} - (\zeta - \Sigma)_{ii}$$

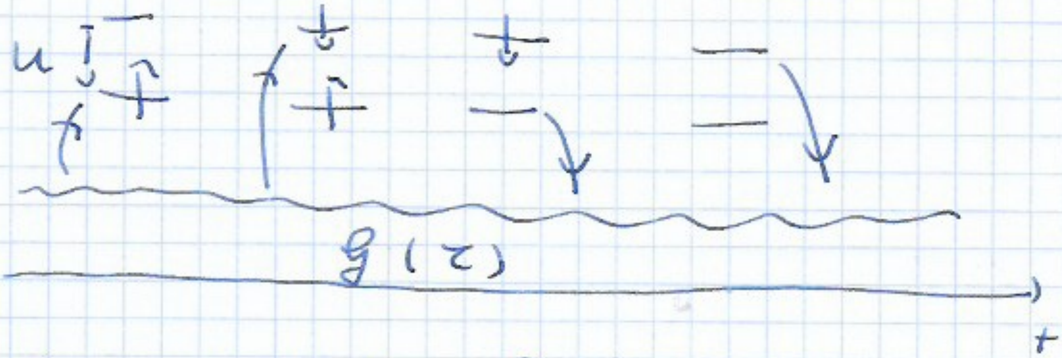
$$\Rightarrow \boxed{\mathcal{G}_i^{-1} = \Sigma_i + G_{ii}^{-1}}$$

<u>R-DMFT</u> real-space DMFT

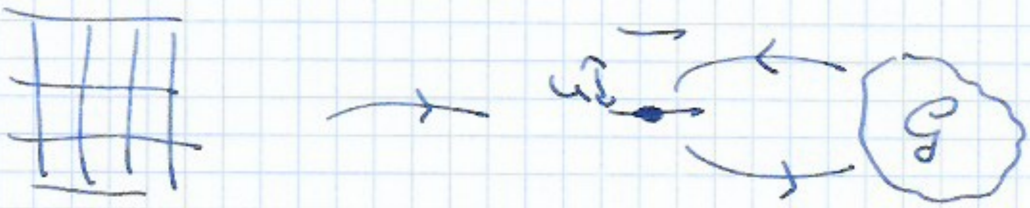
DMFT exact

$$\left.\begin{array}{l} t_{ij} = 0 \\ U = 0 \end{array}\right\} \text{ any } d$$

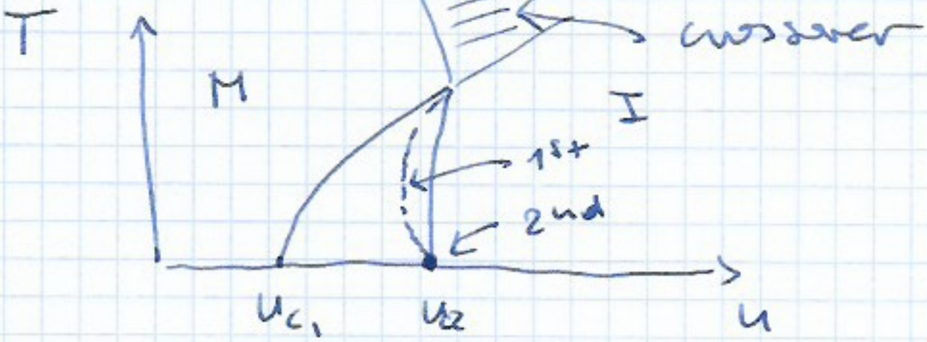
$d \to \infty$, any t_{ij} , U

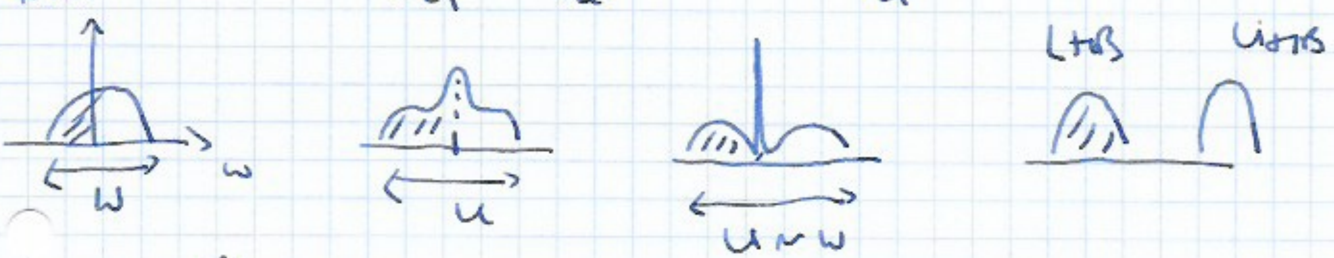


- Local dynamics exact in time
- spatial fluctuations neglected



Most important result Mott-Hubbard MIT





$n = \frac{N_e}{N_L} = 1$ half filling