Study of multiband disordered systems using the typical medium dynamical cluster approximation

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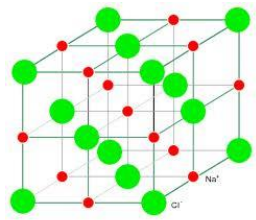
Outline

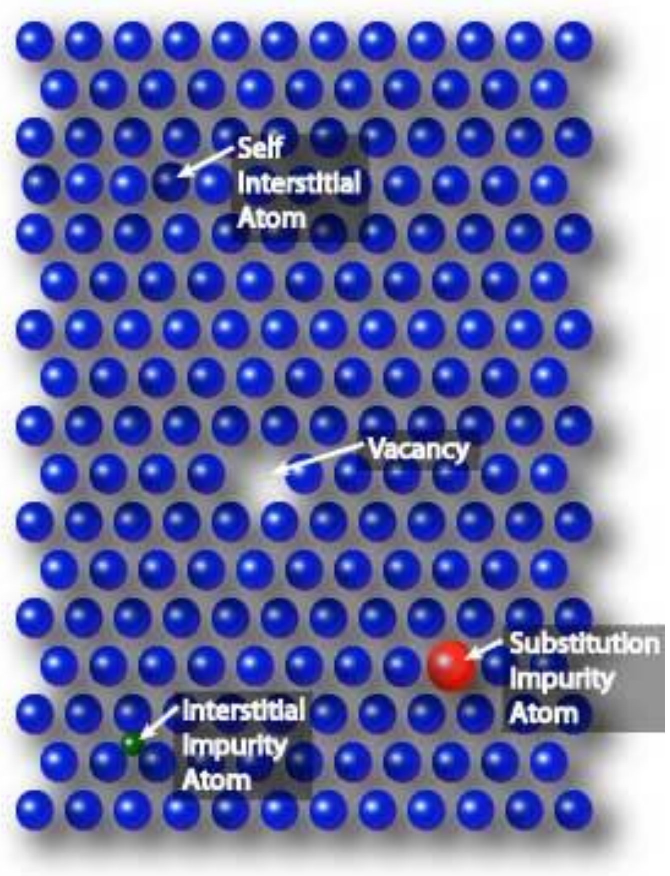
1. Introduction
- Disorder and Anderson localization
2. Theoretical approaches of disorder systems:
- Coherent potential approximation
- Dynamical cluster approximation
- Typical medium theory
3. Extension to multiband systems
4. Current Results
5. Summary and Future work

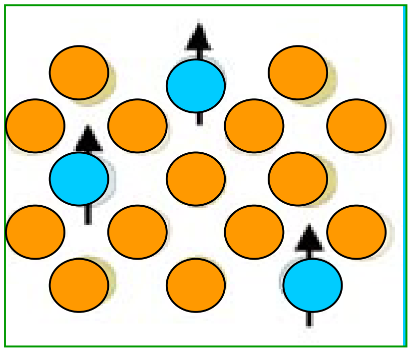
Disorder - a common feature of many materials



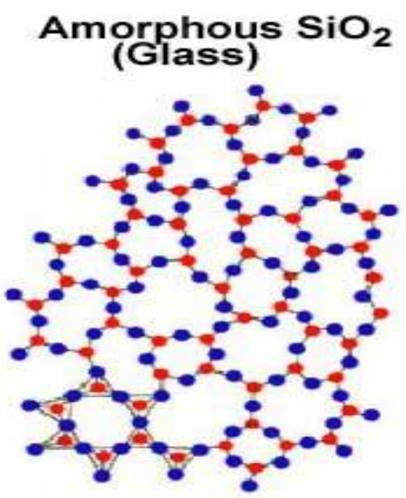
In real life, the crystalline state is exception rather than a rule!

impurities or defects

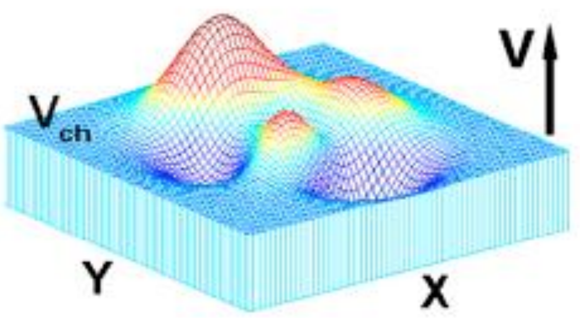




Random (magnetic) impurities

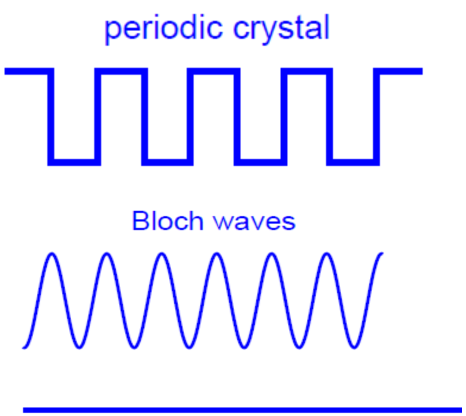


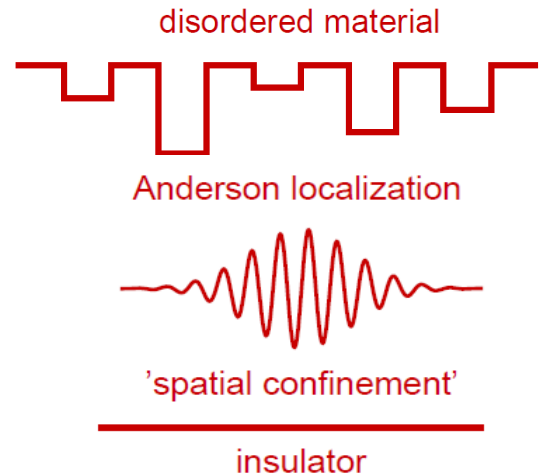
Amorphous network



External spatially random potential

Physical Problem: Anderson localization in disordered systems





Localized states can NOT carry electric current :

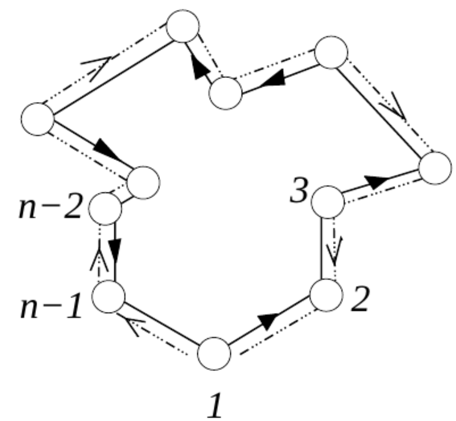
$\sigma(T=0) \neq 0$

Metal-Insulator Transition

$\sigma(T=0) = 0$

Wc=0, d=1,2, Wc>0, d=3

Anderson, 1958

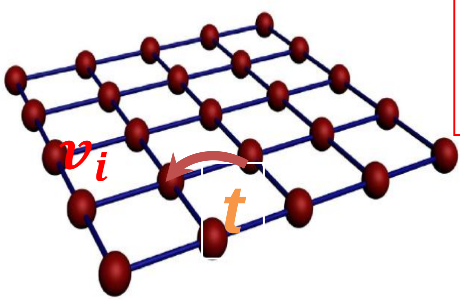


Localization due to backscattering processes.

We need to understand and control such behavior in real materials

Theoretical approaches (mean field) of disorder systems

Model



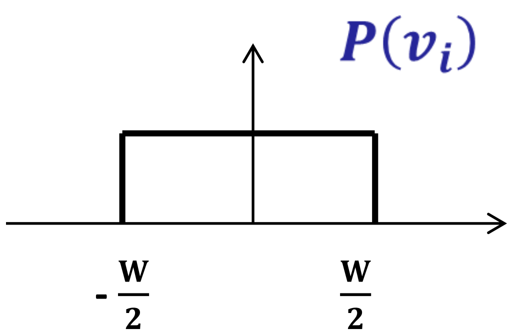
$$\boxed{H = \sum_{<ij>} t_{ij}(c_i^\dagger c_j + h.c.) + \sum_i v_i n_i}$$

$\boldsymbol{v}_i$ - random potential with PDF $\boldsymbol{P}(\boldsymbol{v}_i)$

$$<O_i>=\int P(v_i)O(v_i)dv_i$$

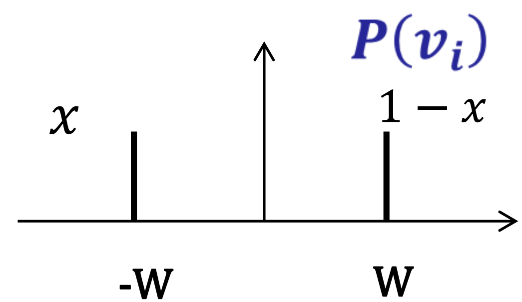
Disorder distribution, e.g.:

Box disorder:



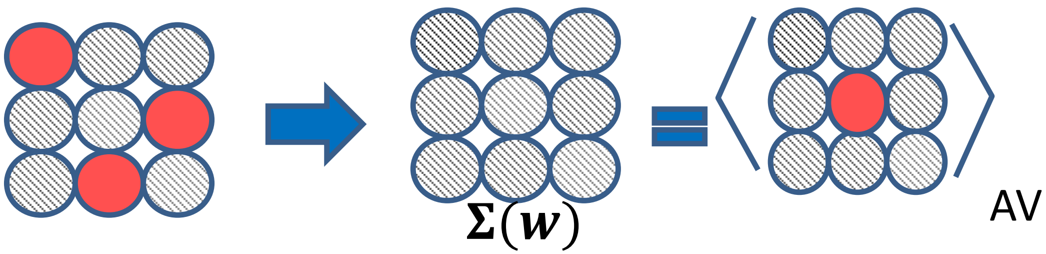
$$P(v_i)=\frac{1}{W}\theta(\frac{W}{2} - |v_i|)$$

Binary alloy disorder: $Fe_{1-x}Co_x$



$$P(v_i)=x\delta(v_i + W) + (1-x)\delta(v_i - W)$$

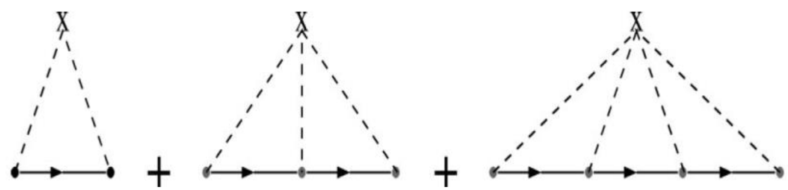
Coherent Potential Approximation - (P. Soven, Phy. Rev. 1967)



$$< g_{imp} >_{av} = G_{00}^{eff.med.}(\Sigma)$$

disordered system → effective medium, Σ(w)

Local Σ(w)=

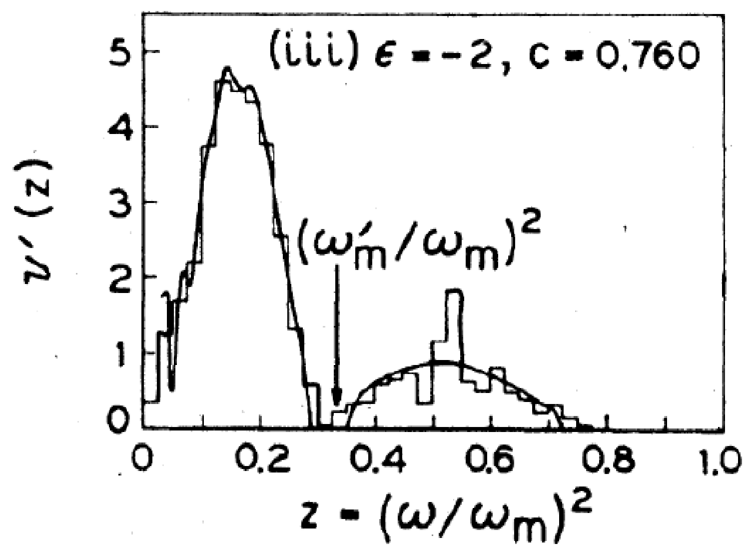


CPA: best single-site approximation with <u>robust</u> results for aver. DOS (Soven, 1967)

- eff. med. Σ(w) is local with no k dependence

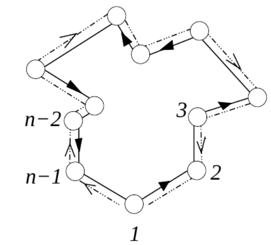
- good for description of DOS in model and materials (alloys)

- fails to describe Anderson localization



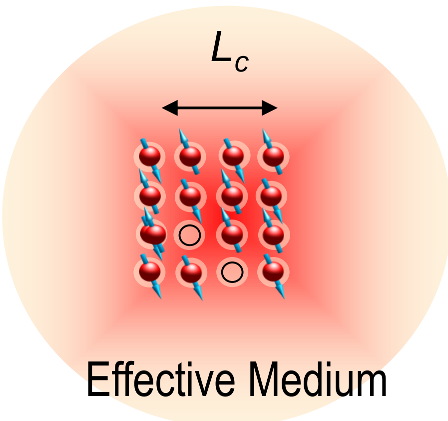
Phonon DOS for cubic lattice, solid line –CPA and the machine calculations, 1974

Beyond single-site CPA: DCA

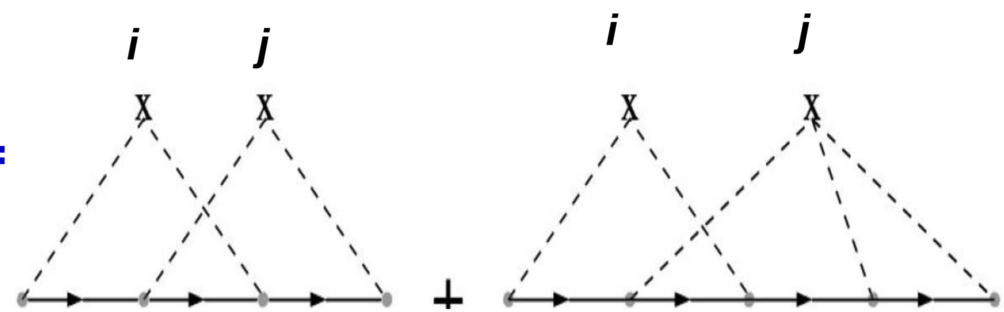


- **Cluster extensions of CPA : DCA+disorder**

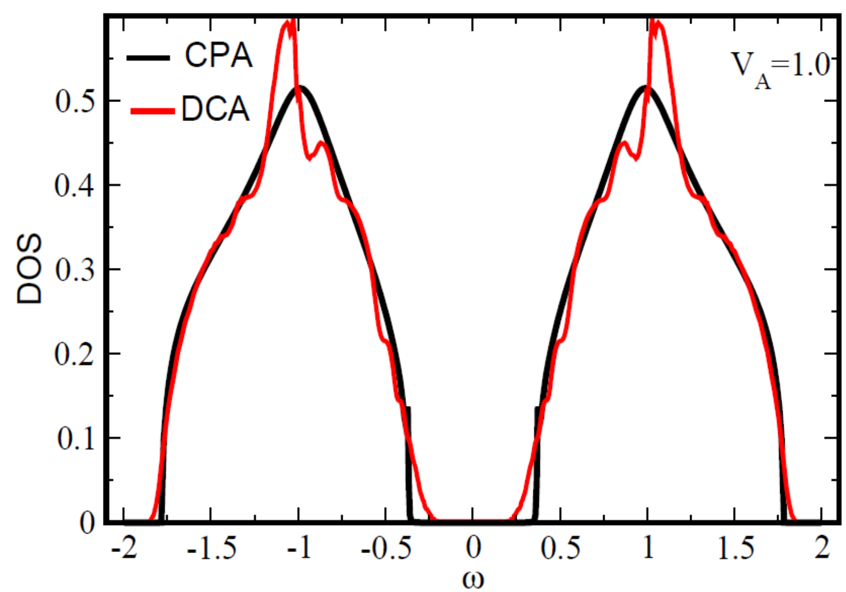
(**M. Jarrell and H.Krishnamurthy, PRB, 2001**), D. D. Johnson, KKR-DCA, etc)



Σ(w,K)=



- CPA, DCA: multi-scale approaches
- DCA provides **non-local corrections** **but NOT localization;**

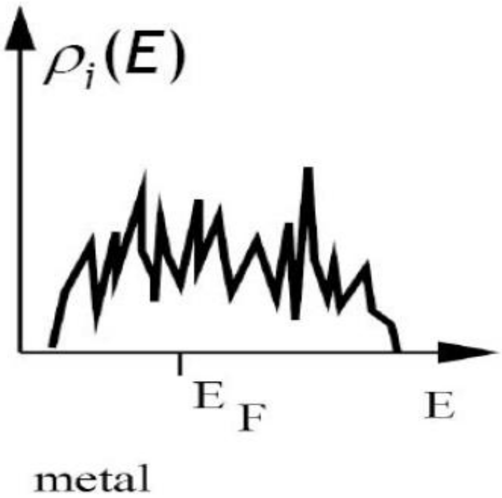


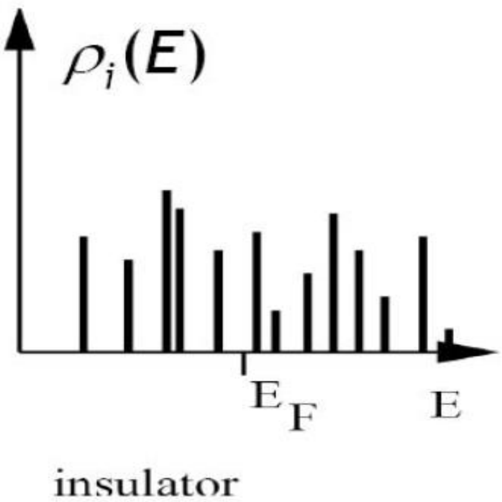
Localization in Typical Medium Theory

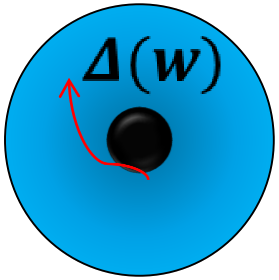
TMT: V. Dobrosavljevic, 2003

- **Provides a *proper order parameter* for localization: typical LDOS , not the average DOS**
- **Consider typical not average effective medium**

local density of states (LDOS) $$\rho_i(E) = \sum_n \delta(E - E_n)|\psi_n(i)|^2$$

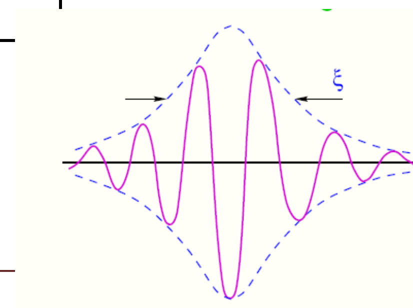


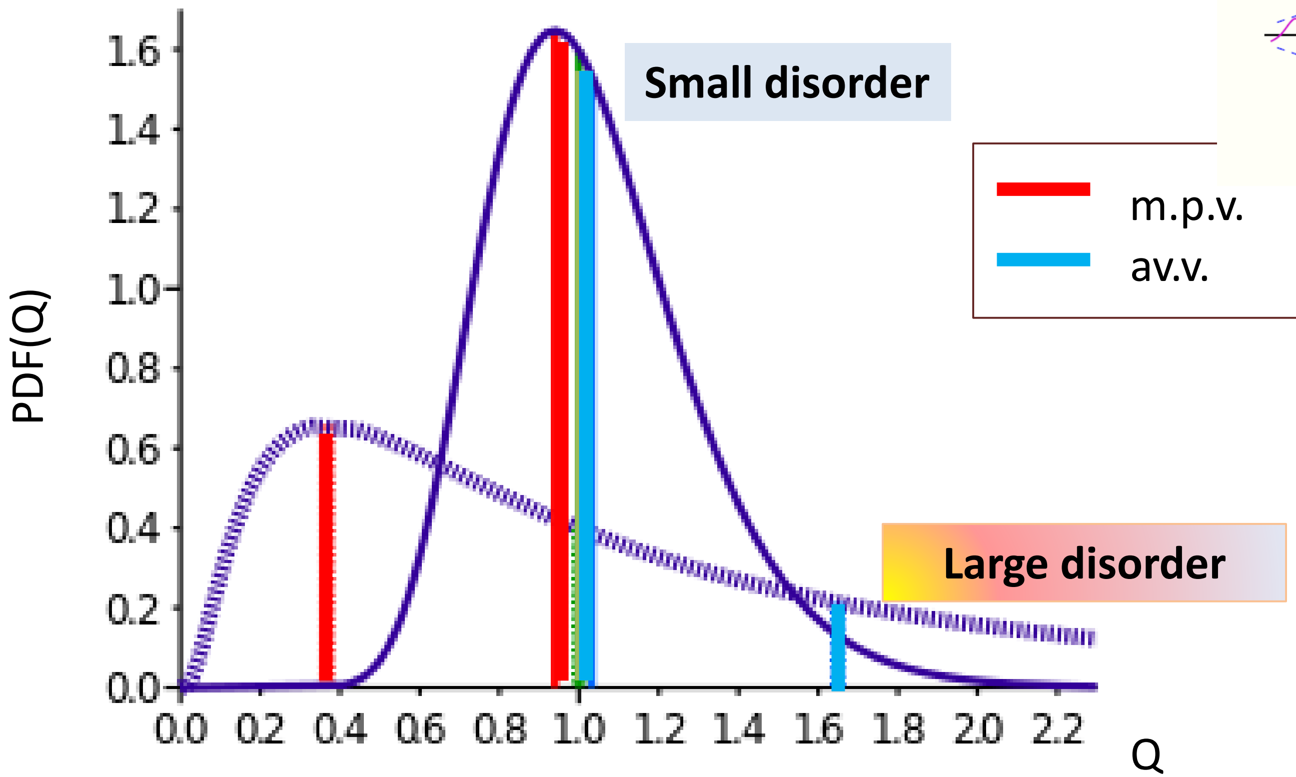




Average (global) DOS is NOT critical at the transition, while LDOS qualitatively changes upon localization: from continuous to discrete->typical LDOS will vanishes

PDF of disordered systems: very broad with long tails
→ system not self-averaging **m.p.v. ≠ av.v.**





m.p.v. **av. v.**

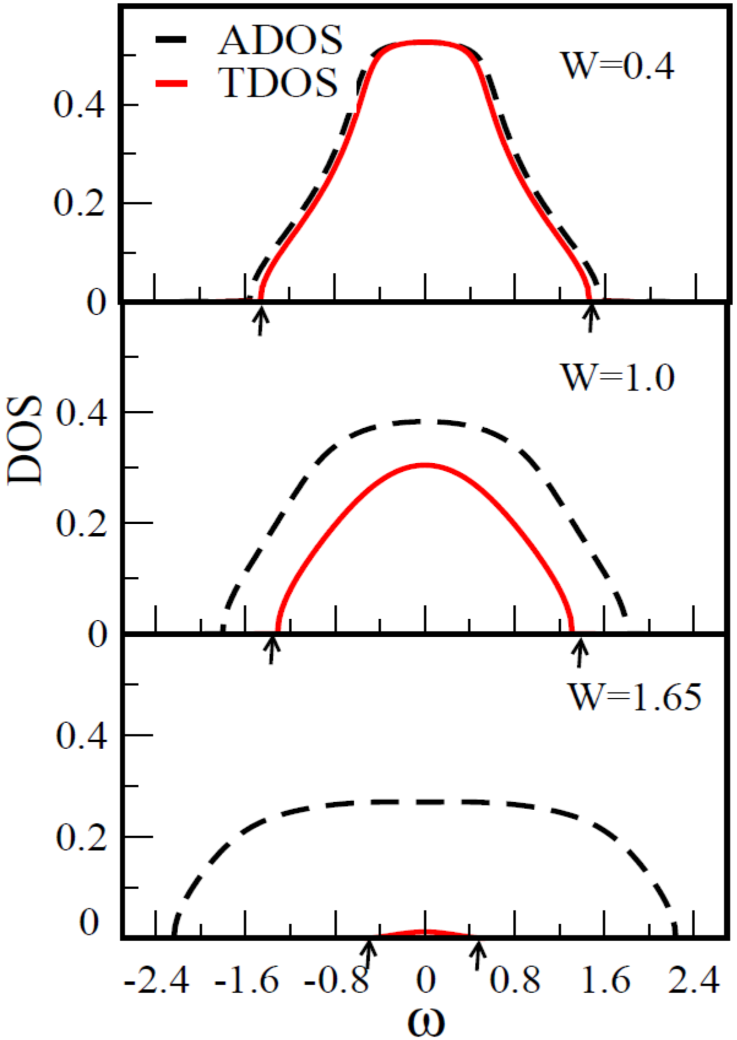
M.p.v. (typical) decreases with disorder, and vanishes at ALT

$\langle \rho_i(E) \rangle_{\text{arith}} > 0$ does not detect localization

$$\rho_i(E)\big|_{\text{typical}} = \langle \rho_i(E) \rangle_{\text{geometric}} = e^{\langle \ln \rho_i(E) \rangle}$$ **=0 at ALT**

Results for Typical Medium Theory (Nc=1): $< g_{imp} >_{typ} = G_{00}^{eff.med.}(\Sigma)$

Evolution of ADOS and TDOS with disorder

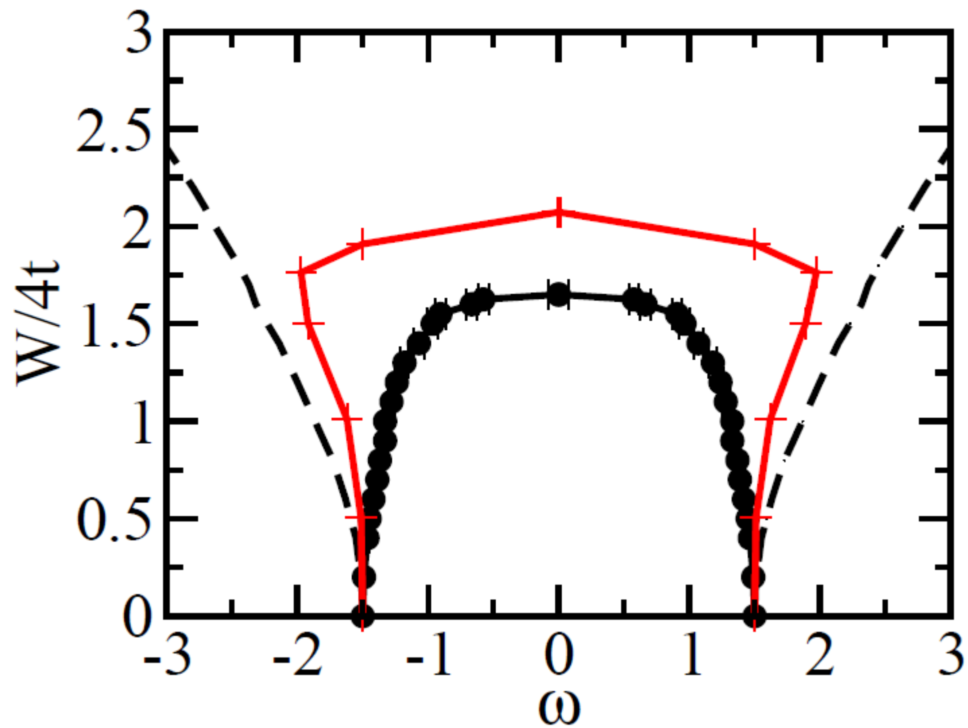


TDOS≠0 – extended states

TDOS=0 – localized states

TDOS is an ***order parameter for AL***

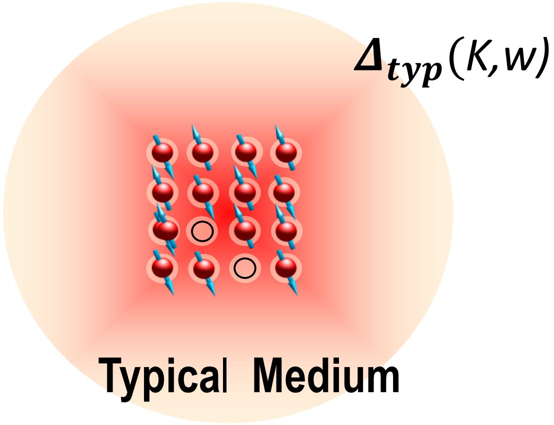
TMT (Nc=1) phase diagram



TMT underestimates Wc=1.65;
no re-entrance of mobility edge

Beyond Typical Medium Theory-TMDCA

by Hanna Terletska, C. Ekuma, C. Moore, K.M. Tam, J. Moreno, M. Jarrell (2014)



Anderson localization: $\rho_i(E)\big|_{\text{typical}} = \big\langle \rho_i(E) \big\rangle_{\text{geometric}} = e^{\langle \ln \rho_i(E) \rangle}$

$$G(\omega, \epsilon_i) \rightarrow \rho_i(\omega) = -\frac{1}{\pi}\mathrm{Im}\mathrm{G}(\omega, \epsilon_\mathrm{i})$$

$\rho_g(\omega) = e^{\langle \ln \rho_i(\omega) \rangle}; \quad G(\omega) = \int d\omega' \frac{\rho_g(\omega)}{\omega - \omega'}$: lattice Green function

Self consistent loop of TMDCA

$$\rho^c_{typ}(K,\omega) = \overbrace{\exp\left(\frac{1}{N_c}\sum_{i=1}^{N_c}\langle \ln \rho^c_i(\omega,V)\rangle\right)}^{\text{local TDOS}} \underbrace{\left\langle \frac{\rho^c(K,\omega,V)}{\frac{1}{N_c}\sum_i \rho^c_i(\omega,V)} \right\rangle}_{\text{non-local}}$$

$$\boxed{G_c^{typ}(K,w) = \int \frac{\rho^c_{typ}(K,w')dw'}{w-w'}}$$

$$\boxed{\bar{G}_c(K,w) = \frac{1}{N}\sum_k \frac{1}{G_c^{typ}(K)^{-1} + \Delta(\mathrm{K}) - \varepsilon_k + \overline{\epsilon(K)}}}$$

$$\boxed{\Delta_{\mathrm{new}}(\mathrm{K}) = \Delta_{\mathrm{old}}(\mathrm{K}) + \xi(G_c^{typ}(K)^{-1} - \bar{G}_c^{-1}(K))}$$

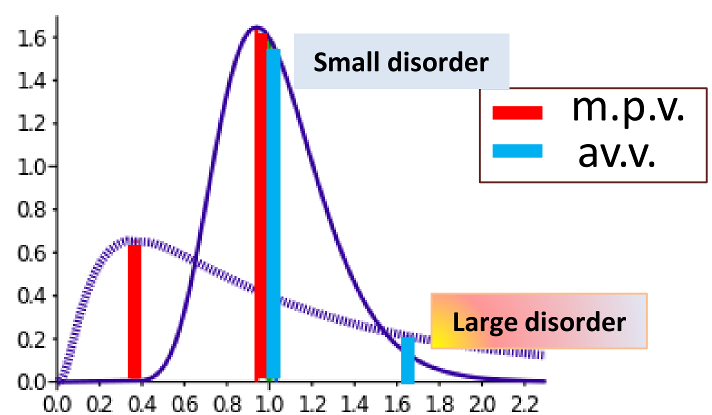
$$\boxed{G^{-1}_{script}(K,w) = \mathrm{w} - \Delta_{\mathrm{new}}(\mathrm{K,w}) - \bar{\epsilon}(\mathrm{K})}$$

Limits:

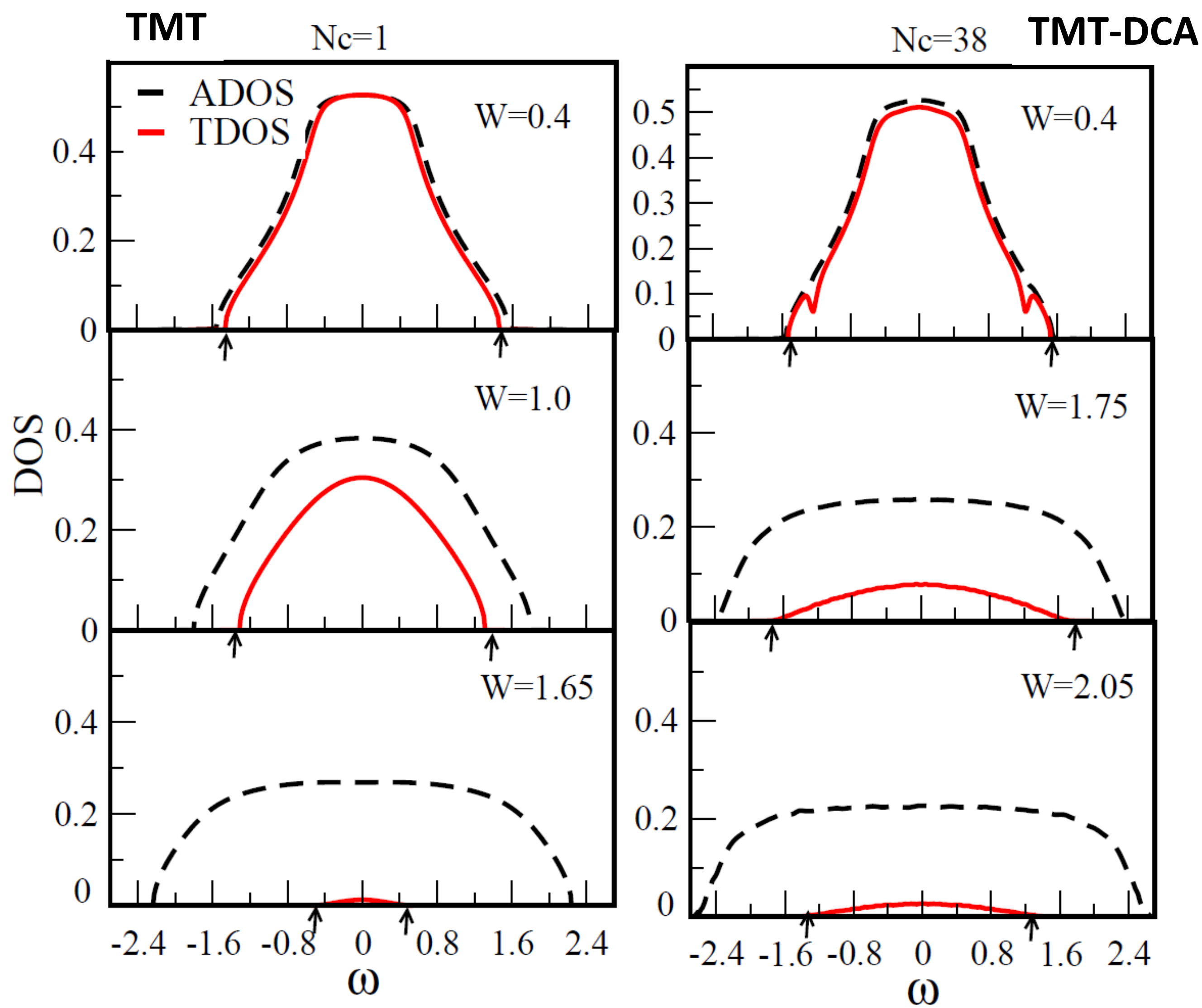
1) $N_c = 1$: $\rho^c_{typ} \to \exp < ln\rho^c(w,V) >$

- single site TMT

2) $at\, W \ll W_c,\ \rho^c_{typ} \to < \rho^c(K,w,V) >$

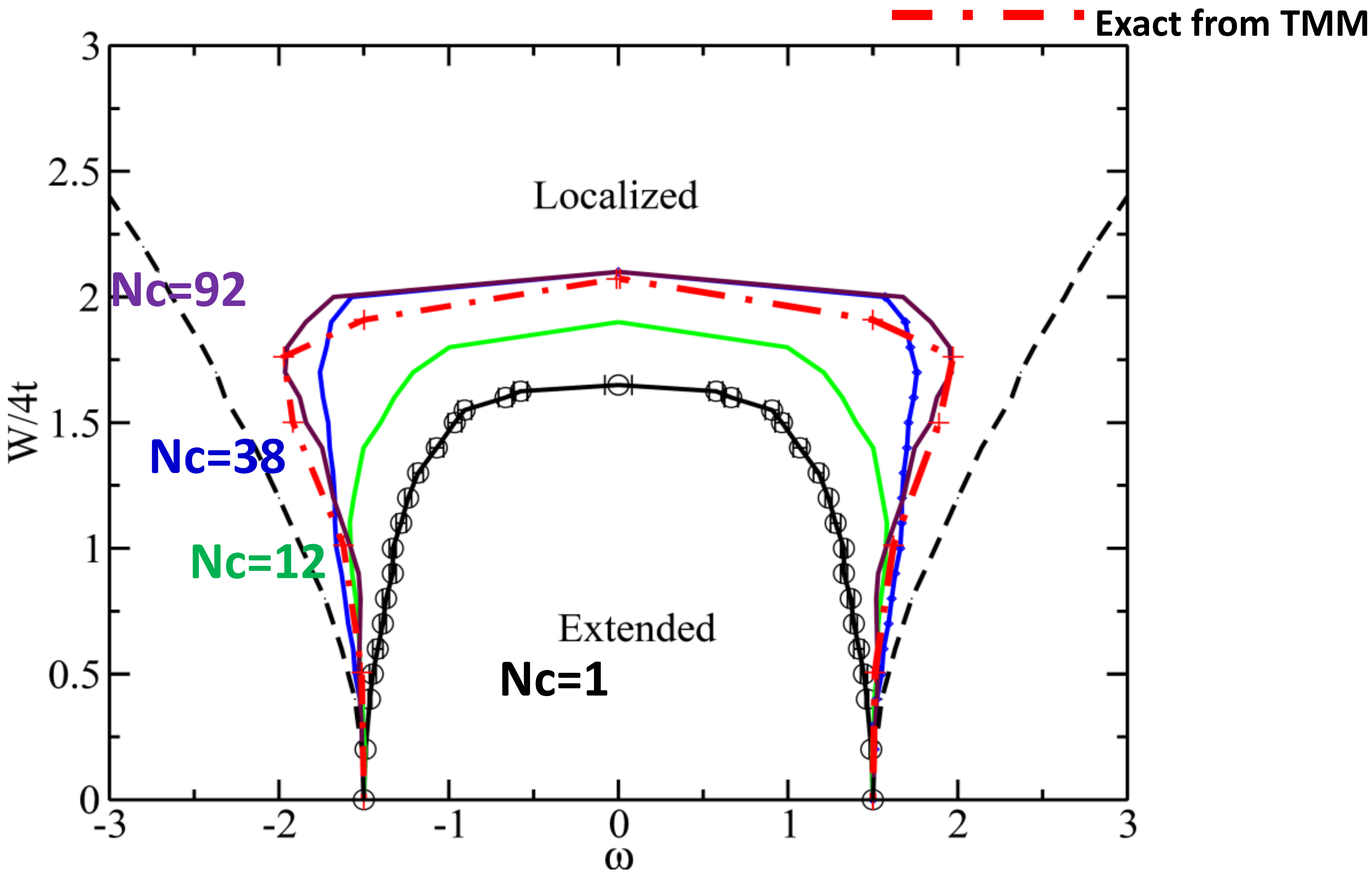


TMDCA results



TDOS-serves as an O.P. ->vanishes at the transition.
Extended states: TDOS-finite, localized-TDOS-zero.

TMT-DCA results: phase diagram



Systematic convergence of mobility edge with increase of the cluster size

Extension to the multiband systems

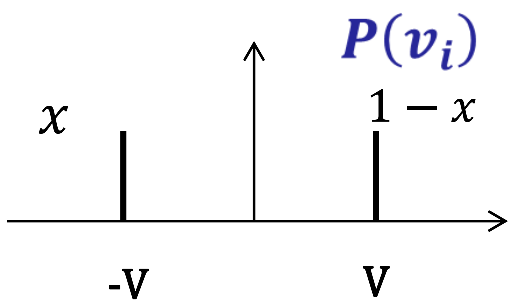
Model for multiband systems

$$H = \sum_{<ij>\alpha\beta} t_{\alpha\beta}(c_{i\alpha}^{+} c_{j\beta} + h.c.) + \sum_i V_{i\alpha\beta} c_{i\alpha}^{+} c_{i\beta}$$

For system with two bands a,b

$$t = \begin{pmatrix} t_{aa} & t_{ab} \\ t_{ab} & t_{bb} \end{pmatrix} \qquad V_i = \begin{pmatrix} V_{iaa} & V_{iab} \\ V_{iab} & V_{ibb} \end{pmatrix}$$

$V_{i\alpha\beta}$ - random potential with PDF $\boldsymbol{P}(V_{i\alpha\beta})$

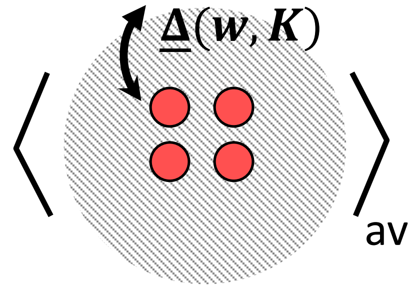


P$(V_{i\alpha\beta})$=$x\delta\left(V_{i\alpha\beta} + V_{\alpha\beta}\right) + (1-x)\delta\left(V_{i\alpha\beta} - V_{\alpha\beta}\right)$ with x=0.5

Multiband extension for DCA

$$\underline{\boldsymbol{\Delta}}(K,w) = \begin{pmatrix} \Delta_{aa}(K,w) & \Delta_{ab}(K,w) \\ \Delta_{ab}(K,w) & \Delta_{bb}(K,w) \end{pmatrix}$$

$$\underline{\boldsymbol{G}}(K,w) = \begin{pmatrix} G_{aa}(K,w) & G_{ab}(K,w) \\ G_{ab}(K,w) & G_{bb}(K,w) \end{pmatrix}$$



$$< \underline{\boldsymbol{G}}^{c}(K,w) >_{av}$$

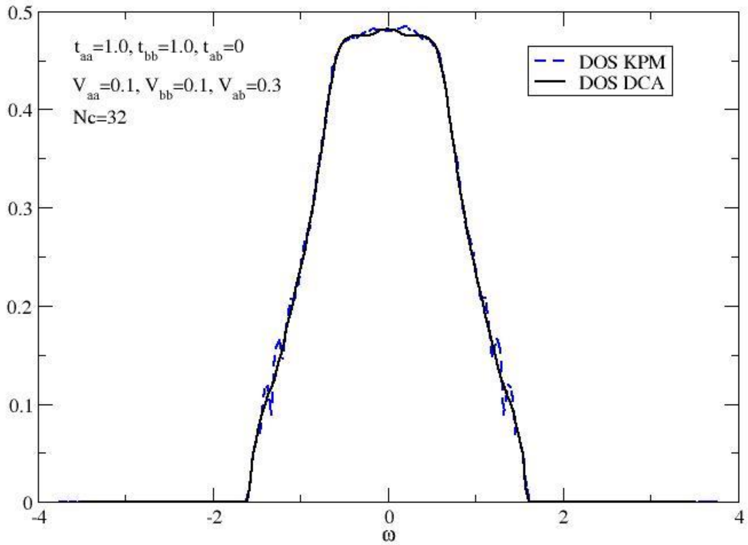
$$\boxed{\underline{\boldsymbol{G}}_{c}^{av}(K,w) =< \underline{\boldsymbol{G}}_{c}(K,w,V) >}$$

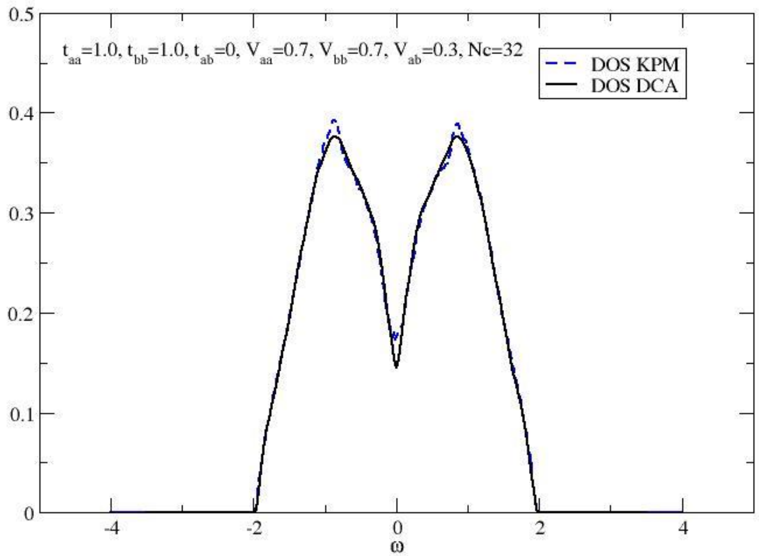
$$\boxed{\overline{\underline{\boldsymbol{G}}}_{c}(K,w) = \frac{1}{N}\sum_{k}\frac{1}{\underline{\boldsymbol{G}}_{c}^{av}(K)^{-1} + \underline{\boldsymbol{\Delta}}(\mathrm{K}) - \underline{\boldsymbol{\varepsilon}_{k}} + \underline{\overline{\epsilon(K)}}}}$$

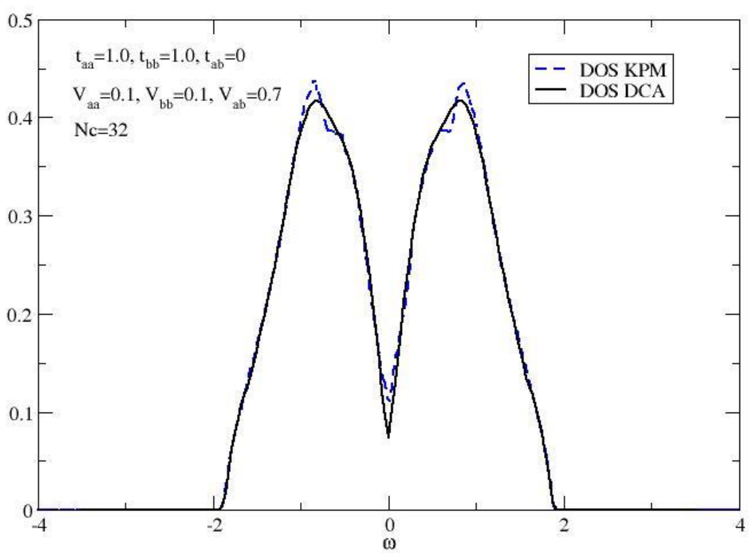
$$\boxed{\underline{\boldsymbol{\Delta}}_{\mathrm{new}}(\mathrm{K}) = \underline{\boldsymbol{\Delta}}_{\mathrm{old}}(\mathrm{K}) + \xi(\underline{\boldsymbol{G}}_{c}^{av}(K)^{-1} - \overline{\underline{\boldsymbol{G}}}_{c}(K)^{-1})}$$

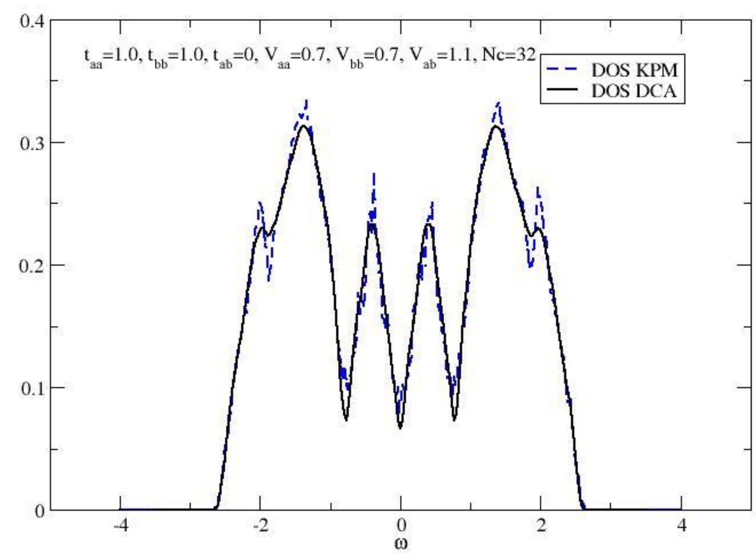
$$\boxed{\underline{\boldsymbol{G}}_{script}^{-1}(K,w) = \underline{\boldsymbol{w}} - \underline{\boldsymbol{\Delta}}_{\mathrm{new}}(\mathrm{K,w}) - \underline{\overline{\epsilon(K)}}}$$

Results: Multiband DCA









Multiband extension for TMDCA

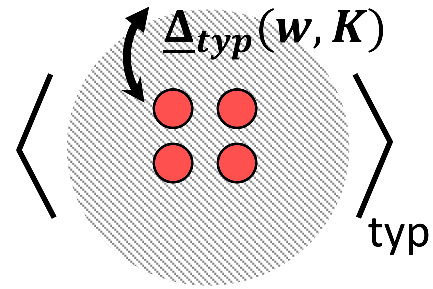
$$\rho^c_{typ}(K,\omega) = \overbrace{\exp\left(\frac{1}{N_c}\sum_{i=1}^{N_c}\langle \ln \rho_i^c(\omega,V)\rangle\right)}^{\text{local TDOS}} \underbrace{\left\langle \frac{\rho^c(K,\omega,V)}{\frac{1}{N_c}\sum_i \rho_i^c(\omega,V)}\right\rangle}_{\text{non-local}}$$

Difficulties:

1. $\underline{\boldsymbol{\rho}}_{\boldsymbol{i}}$ is not positive definite
2. $\boldsymbol{\rho}_{\boldsymbol{i}}^{\boldsymbol{ab}}$ is not positive definite

$$\underline{\rho}_{typ}(K,\omega) = \begin{pmatrix} e^{\frac{1}{Nc}\sum_i <ln\rho_{ii}^{aa}>} < \frac{\rho^{aa}(K,\omega)}{\frac{1}{Nc}\sum_i \rho_{ii}^{aa}} > & e^{\frac{1}{Nc}\sum_i <ln|\rho_{ii}^{ab}|>} < \frac{\rho^{ab}(K,\omega)}{\frac{1}{Nc}\sum_i |\rho_{ii}^{ab}|} > \\ e^{\frac{1}{Nc}\sum_i <ln|\rho_{ii}^{ba}|>} < \frac{\rho^{ba}(K,\omega)}{\frac{1}{Nc}\sum_i |\rho_{ii}^{ba}|} > & e^{\frac{1}{Nc}\sum_i <ln\rho_{ii}^{bb}>} < \frac{\rho^{bb}(K,\omega)}{\frac{1}{Nc}\sum_i \rho_{ii}^{bb}} > \end{pmatrix}$$

Self consistent loop for MBTMDCA



$< \underline{G}^c(K,w) >_{typ}$

$$\underline{\rho}_{typ}(K,\omega) = \begin{pmatrix} e^{\frac{1}{Nc}\sum_i <ln\rho_{ii}^{aa}>} < \frac{\rho^{aa}(K,\omega)}{\frac{1}{Nc}\sum_i \rho_{ii}^{aa}} > & e^{\frac{1}{Nc}\sum_i <ln|\rho_{ii}^{ab}|>} < \frac{\rho^{ab}(K,\omega)}{\frac{1}{Nc}\sum_i |\rho_{ii}^{ab}|} > \\ e^{\frac{1}{Nc}\sum_i <ln|\rho_{ii}^{ba}|>} < \frac{\rho^{ba}(K,\omega)}{\frac{1}{Nc}\sum_i |\rho_{ii}^{ba}|} > & e^{\frac{1}{Nc}\sum_i <ln\rho_{ii}^{bb}>} < \frac{\rho^{bb}(K,\omega)}{\frac{1}{Nc}\sum_i \rho_{ii}^{bb}} > \end{pmatrix}$$

$$\boxed{\underline{G}_c^{typ}(K,w) = \int \frac{\underline{\rho}_{typ}^{c}(K,w')dw'}{w-w'}}$$

$$\boxed{\underline{\overline{G}}_c(K,w) = \frac{1}{N}\sum_k \frac{1}{\underline{G}_c^{typ}(K)^{-1} + \underline{\Delta}(\mathrm{K}) - \underline{\varepsilon_k} + \underline{\overline{\epsilon(K)}}}}$$

$$\boxed{\underline{\Delta}_{\mathrm{new}}(\mathrm{K}) = \underline{\Delta}_{\mathrm{old}}(\mathrm{K}) + \xi(\underline{G}_c^{typ}(K)^{-1} - \underline{\overline{G}}_c(K)^{-1})}$$

$$\boxed{\underline{G}_{script}^{-1}(K,w) = \underline{w} - \underline{\Delta}_{\mathrm{new}}(\mathrm{K,w}) - \underline{\overline{\epsilon(K)}}}$$

Limits:

$$\underline{\rho}_{typ}(K,\omega) = \begin{pmatrix} e^{\frac{1}{Nc}\sum_i <ln\rho_{ii}^{aa}>} < \frac{\rho^{aa}(K,\omega)}{\frac{1}{Nc}\sum_i \rho_{ii}^{aa}} > & e^{\frac{1}{Nc}\sum_i <ln|\rho_{ii}^{ab}|>} < \frac{\rho^{ab}(K,\omega)}{\frac{1}{Nc}\sum_i |\rho_{ii}^{ab}|} > \\ e^{\frac{1}{Nc}\sum_i <ln|\rho_{ii}^{ba}|>} < \frac{\rho^{ba}(K,\omega)}{\frac{1}{Nc}\sum_i |\rho_{ii}^{ba}|} > & e^{\frac{1}{Nc}\sum_i <ln\rho_{ii}^{bb}>} < \frac{\rho^{bb}(K,\omega)}{\frac{1}{Nc}\sum_i \rho_{ii}^{bb}} > \end{pmatrix}$$

1. If t_{ab}=0 and V_{ab}=0

$$\underline{\rho}_{typ}(K,\omega) = \begin{pmatrix} e^{\frac{1}{Nc}\sum_i <ln\rho_{ii}^{aa}>} < \frac{\rho^{aa}(K,\omega)}{\frac{1}{Nc}\sum_i \rho_{ii}^{aa}} > & 0 \\ 0 & e^{\frac{1}{Nc}\sum_i <ln\rho_{ii}^{bb}>} < \frac{\rho^{bb}(K,\omega)}{\frac{1}{Nc}\sum_i \rho_{ii}^{bb}} > \end{pmatrix}$$

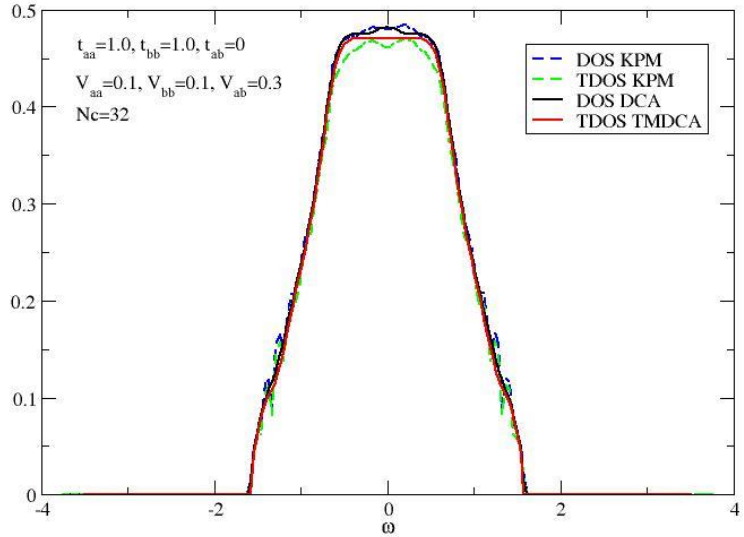
$\Longrightarrow$ two decoupled single band TMDCA

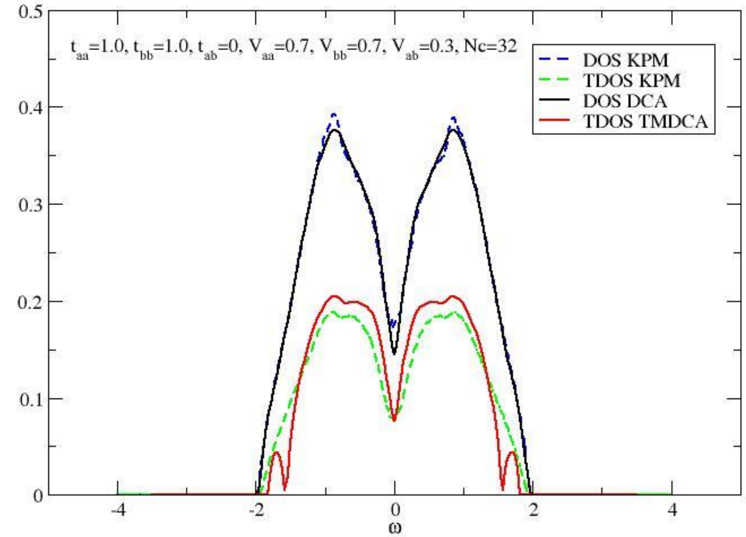
2. If $V_{\alpha\beta}$<<$V_{\alpha\beta}^{c}$

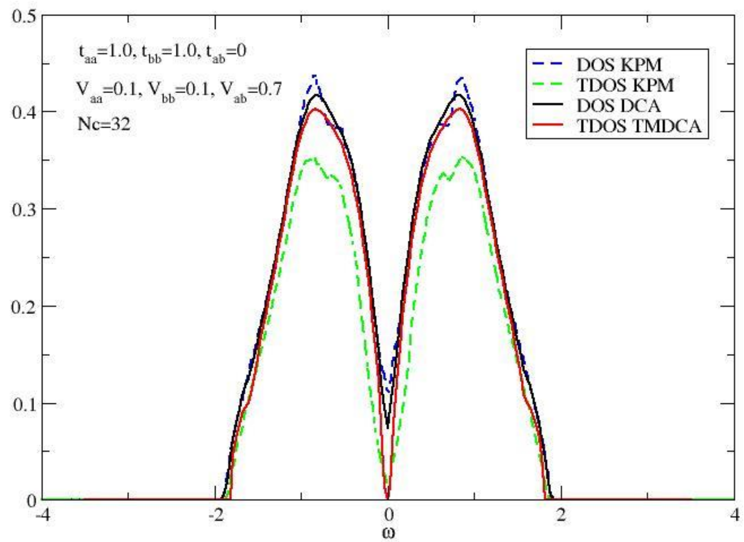
$$\underline{\rho}_{typ}(K,\omega) = \begin{pmatrix} <\rho^{aa}(K,\omega)> & <\rho^{ab}(K,\omega)> \\ <\rho^{ba}(K,\omega)> & <\rho^{bb}(K,\omega)> \end{pmatrix} = <\underline{\rho}(K,\omega,V)>$$

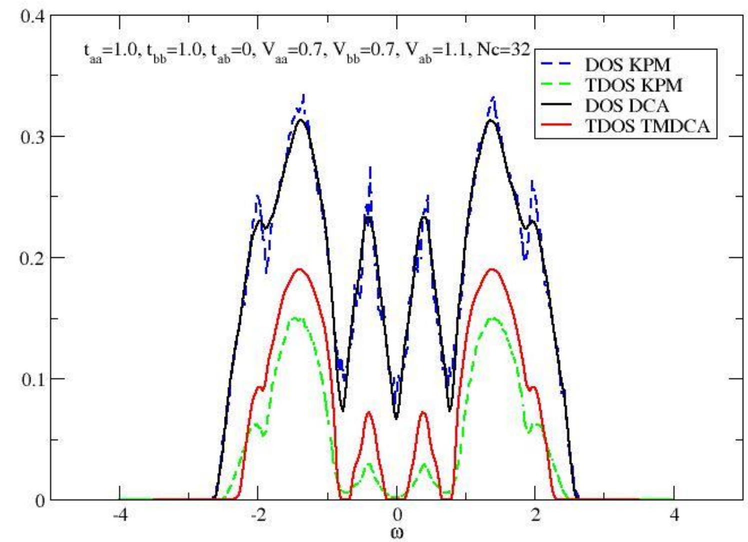
$\Longrightarrow$ Multiband DCA

Results: Multiband TMDCA

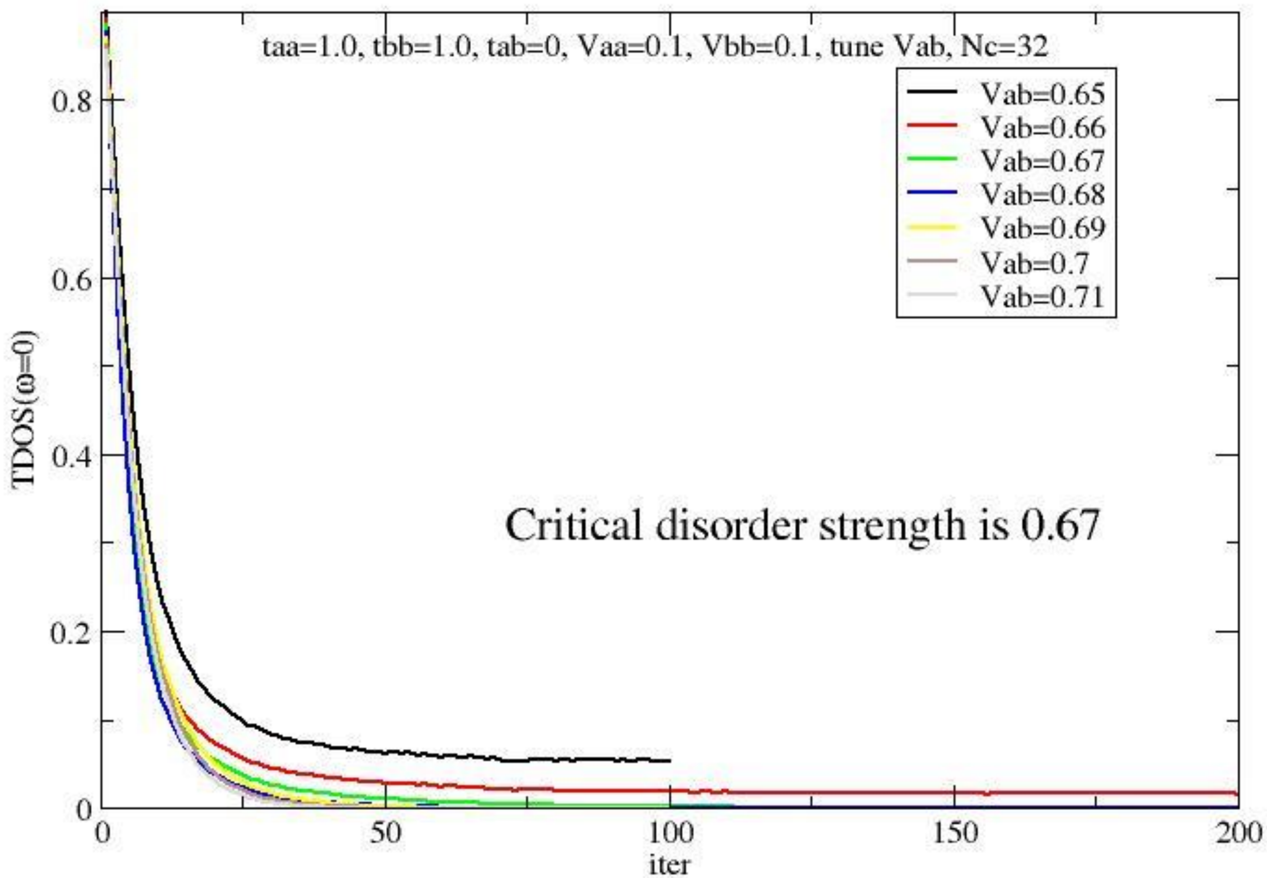




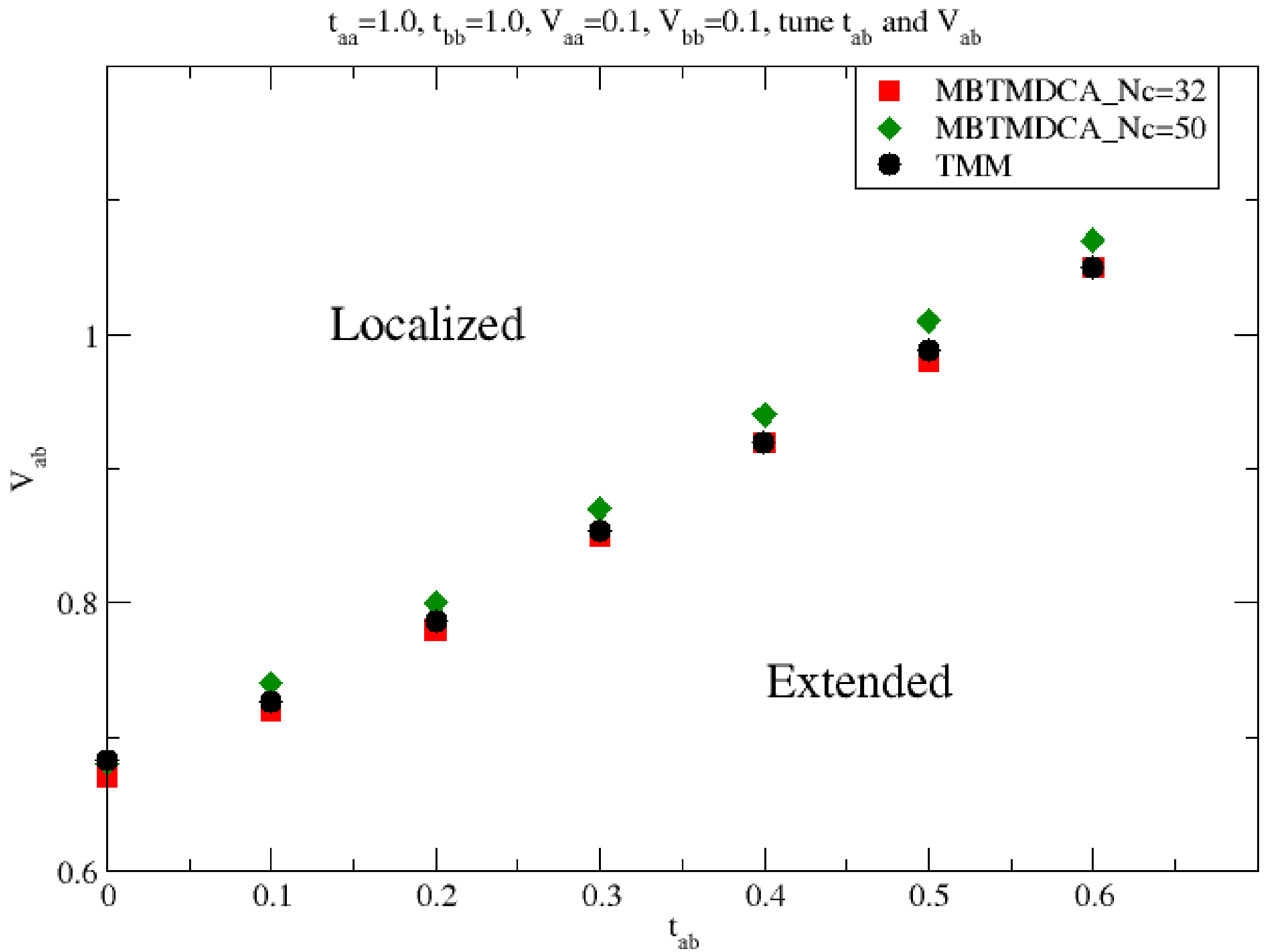




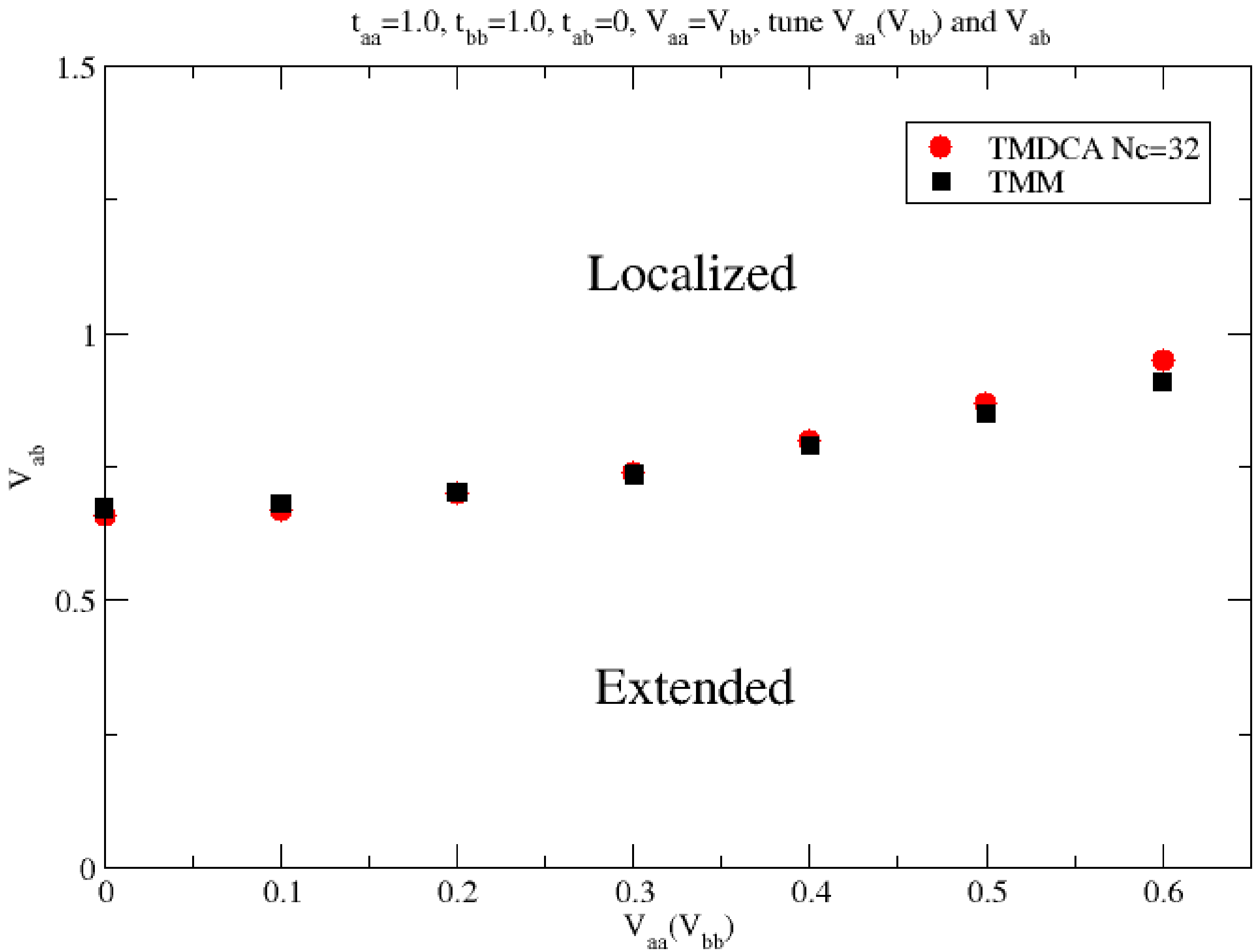
Determine the critical disorder strength



Effect of inter-band hopping t_{ab}
Comparison with transfer matrix method



Effect of intra-band disorder to inter-band critical disorder V_{ab}
Comparison with transfer matrix method



Summary and future work

- We generalize typical medium DCA to multiband systems and study the effects of inter-band disorder and inter-band hopping to Anderson localization.
- The predicted critical disorder strength is consistent with transfer matrix method, but the calculated typical density of states are not quite consistent with KPM. More work need to be done to resolve this discrepancy.
- This method sets up a starting point to study Anderson localization in real systems.
- It can be extended to system with interaction.

Thank you!