Strong disorder in strongly correlated matter

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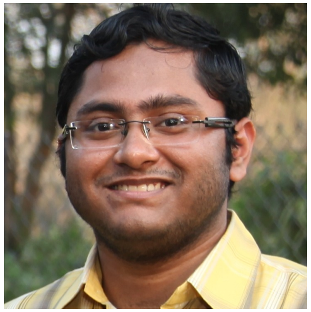


Student: Debmalya Chakraborty

Collaborator: Rajdeep Sensarma (TIFR)

Reference: NJP, 16, 103018 (2014) + preprint

Interplay of correlations and disorder in condensed phases
→ an outstanding challenge in solid-state physics

- We consider 2D system of spin-1/2 electrons, described by Hubbard model:

$$\mathcal{H}_{\text{Hubb}} = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) + U \sum_{j} n_{j\uparrow} n_{j\downarrow}$$

- Strong repulsion between electrons, **system in proximity of a Mott-insulator**

$$U \gg t$$

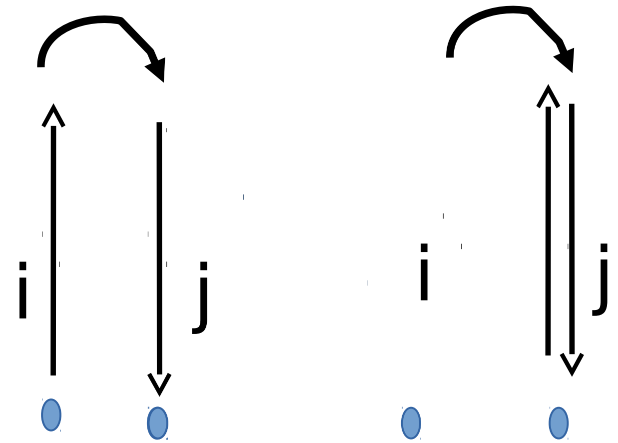
- T=0, the broken symmetry state (@ ρ=0.8) is a d-wave superconductor.

- Finally, we will add **disorder** in the system, **disorder strength being V**

Focus on parameter-space:

$$U \gg t, V \begin{cases} V \leq t & \text{"weak" disorder} \\ V > t & \text{"strong" disorder} \end{cases}$$

Key Role of Strong Repulsive Correlations:



With Strong Correlation

Without Strong Correlation

- hop(i $\longrightarrow$ j) : prohibited by strong repulsion, 'corrln-less' physics doesn't care!
  - with strong correlation, hopping allowed only if j was empty!

Incorporating strong electronic repulsion:

- effective hopping reduces, as local $\rho \leq 1$
- effective J (exchange coupling) enhanced, as large number of sites singly occupied

Gutzwiller Projection (removes **all** double occupancy: repulsion!)

Gutzwiller approximation:

$$t \rightarrow g_t t \quad \text{with} \quad g_t = \frac{(1-\rho)}{(1-\rho/2)} \qquad J \rightarrow g_J J \quad \text{with} \quad g_J = (1-\rho/2)^{-2}$$

Gutzwiller Approximation:

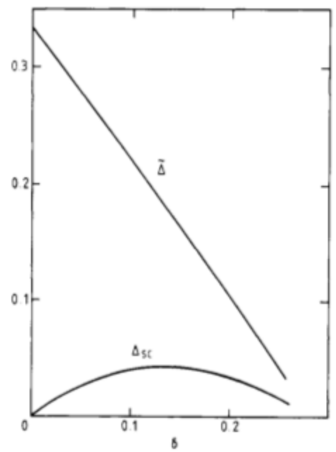
- **An *approximate* implementation of of Gutzwiller projection**

– full blown calculations via QMC. Paramekanti et. Al ('02), Andersonet.al ('04)

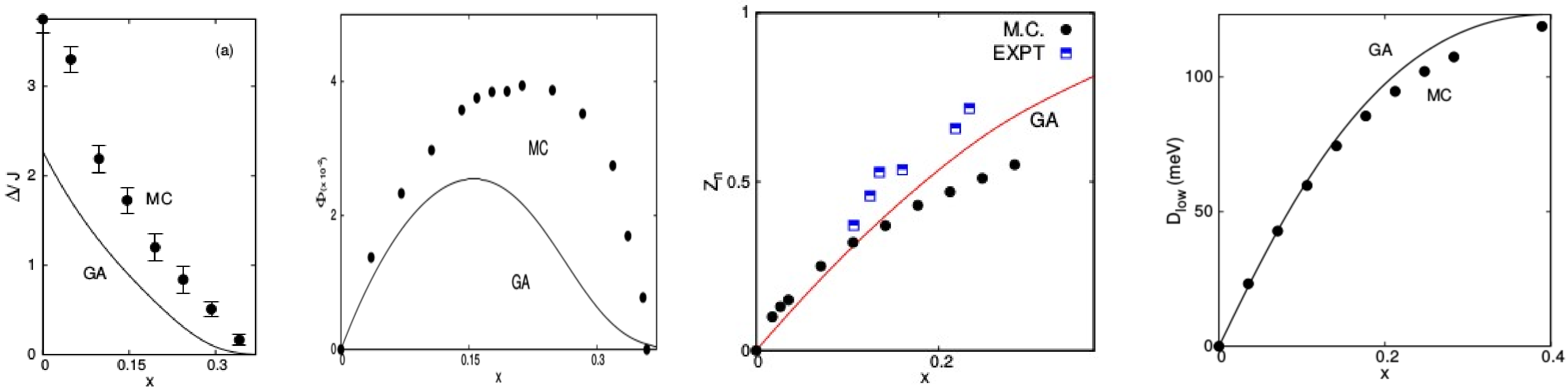
A renormalised Hamiltonian approach to a resonant valence bond wavefunction

F C Zhang, C Gros, T M Rice and H Shiba†
Theoretische Physik, ETH-Hönggerberg, CH 8093 Zurich, Switzerland

Received 1 March 1988, in final form 22 April 1988



- Strong non-BCS features (e.g. Mott limit @ half-filling), from strong correlations achieved within renormalized mean-field theory!!

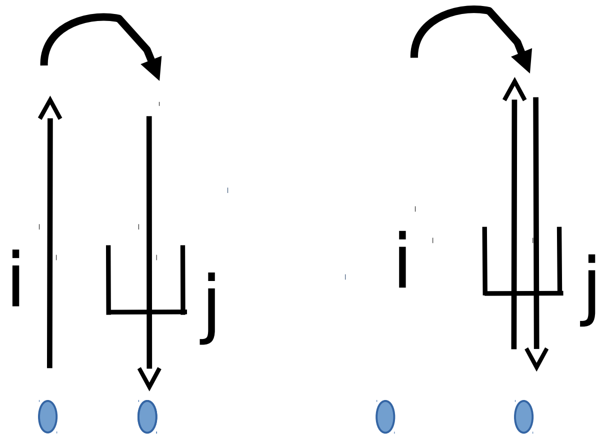


Ph.D. Thesis – Rajdeep Sensarma (2007)

Now deal with disorder...

- Amplitude fluctuations, Hartree-Fock-Bogoliubov BdG calculations (IMT):
  AG, Randeria & Trivedi; Atkinson, MacDonald & Hirschfeld (2000) and many others.

→ Δ fluctuates spatially @ length scale ξ_{coh} creating "islands"



With attractive potential @ j:

With Strong Correlation

Without Strong Correlation

happy hopping in simple BdG,
still forbidden with strong correlations!

- Gutzwiller **g-factors** (still removes **all** double occupancy!) now **depend** on **local densities!**

Ko et al, PRB, **76** (2007); Fukushima, PRB, 78 (2008)

$$t' \rightarrow g_t t$$
$$J' \rightarrow g_J J$$

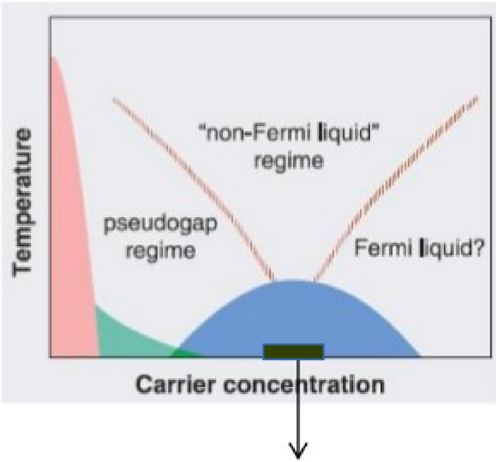
$$\left\langle c_{i\sigma}^{\dagger} c_{j\sigma} \right\rangle \approx g_{ij}^{t} \left\langle c_{i\sigma}^{\dagger} c_{j\sigma} \right\rangle_0 \text{ where } g_{ij}^{t} = \sqrt{\frac{4(1-n_i)(1-n_j)}{(2-n_i)(2-n_j)}}$$

...and corresponding modification of g_J in the same spirit.

Within this framework:

- Robustness of SC-DOS first found by Garg, Randeria & Trivedi, Nat Phys (08)

Model and Parameters:



Focus on this region

$$\mathcal{H}_{\rm Hubb} = -t\sum_{\langle ij\rangle\sigma}(c^\dagger_{i\sigma}c_{j\sigma}+h.c.)+U\sum_j n_{j\uparrow}n_{j\downarrow}$$

Schrieffer-Wolf transformation:

$$\mathcal{H}_{\rm t-J} = -t\sum_{\langle ij\rangle\sigma}\left(\ \tilde{c}^\dagger_{i\sigma}\tilde{c}_{j\sigma}+{\rm h.c.}\ \right)+\sum_{\langle ij\rangle}J\Big(\tilde{\mathbf{S}}_i.\tilde{\mathbf{S}}_j-\frac{\tilde{n}_i\tilde{n}_j}{4}\Big)$$

$$+\ \text{“Other terms”}$$

$$+\sum_{i,\sigma}(V_i-\mu)\,n_{i\sigma}$$

Cuprates:
Norman et al. PRB 52, 615 (1995)

$$t' = t/4,\ U = 12t$$

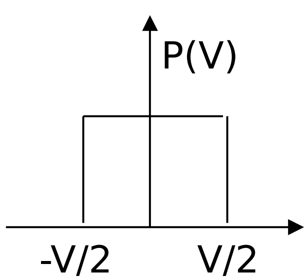
$$\langle n\rangle = 0.8\,(\text{optimal doping})$$

$$t_{ij} = -t, \text{for } \langle ij\rangle \qquad J_{ij} = \frac{4t_{ij}^2}{U} = J, \text{for } \langle ij\rangle$$

$$= t', \text{for } \langle\langle ij\rangle\rangle \qquad = J', \text{for } \langle\langle ij\rangle\rangle$$

Disorder:

$$\sum_{i,\sigma}(V_i-\mu)\,n_{i\sigma}$$



30X30 system
Disorder averaged over 10-15 realizations

Other models of disorder also considered!

Important Findings:

Strongly correlated matter responds differently at weak & strong disorder!

- Nature & degree of inhomogeneity differs upon including strong correlations; Nature changes substantially when approaching strong disorder.

- Superconducting-`islands' **absent** at disorder strengths where simple BdG finds them. Stronger disorder brings them back!

- Defining signatures of superconductivity ***robust to impurities*** up to disorder strength ~ "*few times t*". However, They decay sharply at larger disorder – **providing intriguing mechanism for the destruction of d-wave superconductivity.**

- "**Mottness**" relevant @ strong disorder even @ optimal doping!

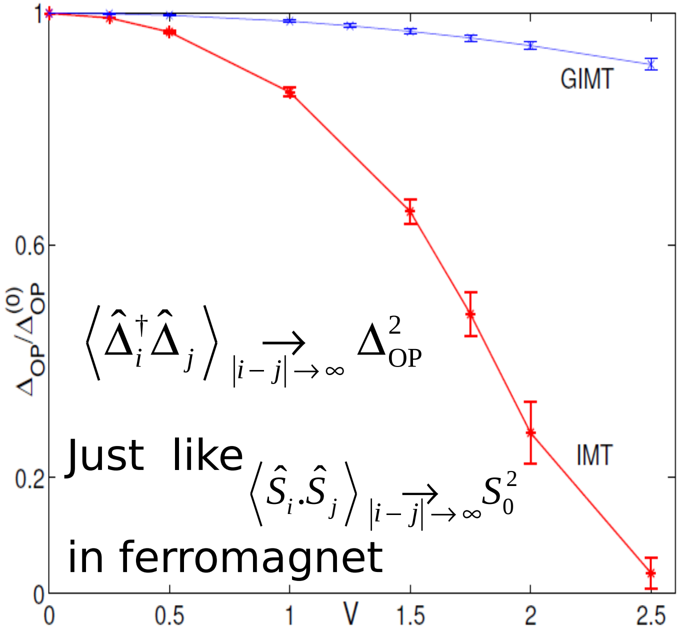
Results: Part - I

Up to moderate disorder, $V \leq 3t$

Nature and degree of inhomogeneity substantially different between results that includes or excludes strong correlations!

Debmalya Chakraborty & AG, NJP, 16, 103018 (2014)

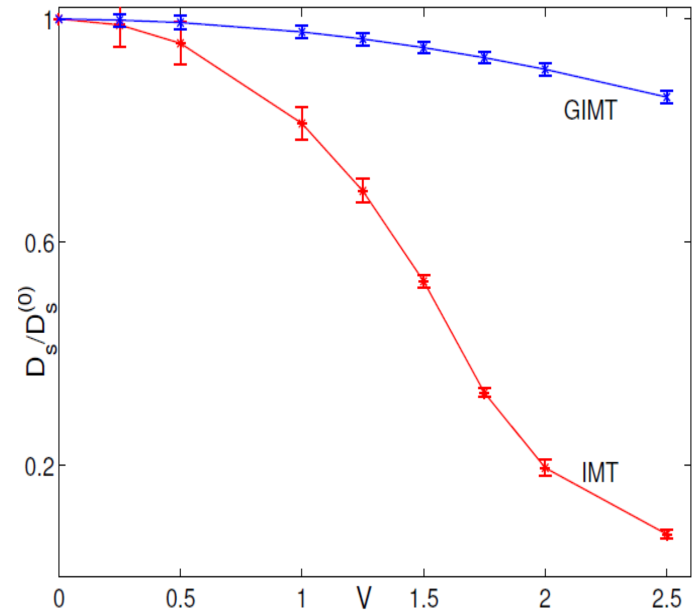
Off-diagonal Long Range Order and Superfluid Density



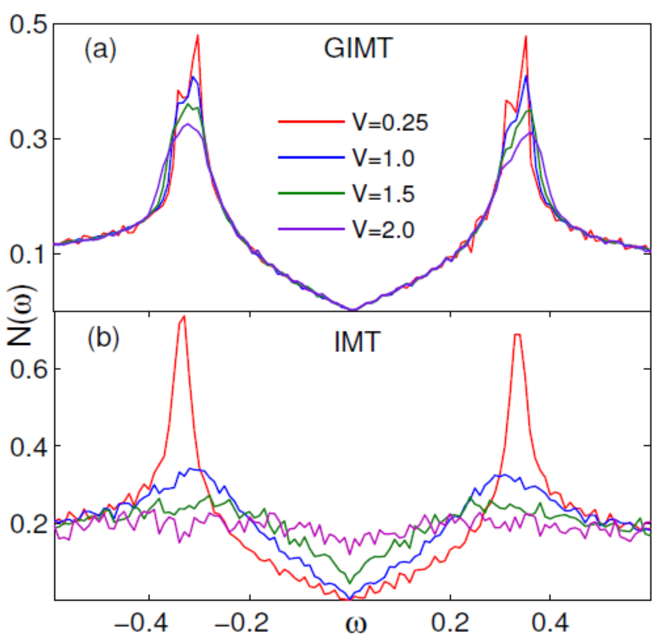
$$\left\langle \hat{\Delta}_i^{\dagger}\hat{\Delta}_j \right\rangle \xrightarrow[|i-j|\to\infty]{} \Delta_{OP}^2$$

Just like $\left\langle \hat{S}_i.\hat{S}_j \right\rangle \xrightarrow[|i-j|\to\infty]{} S_0^2$

in ferromagnet

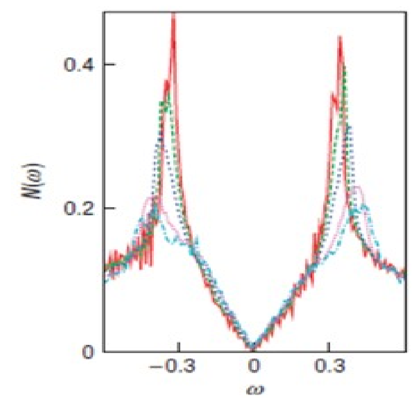


Calculated from "Kubo Formula"



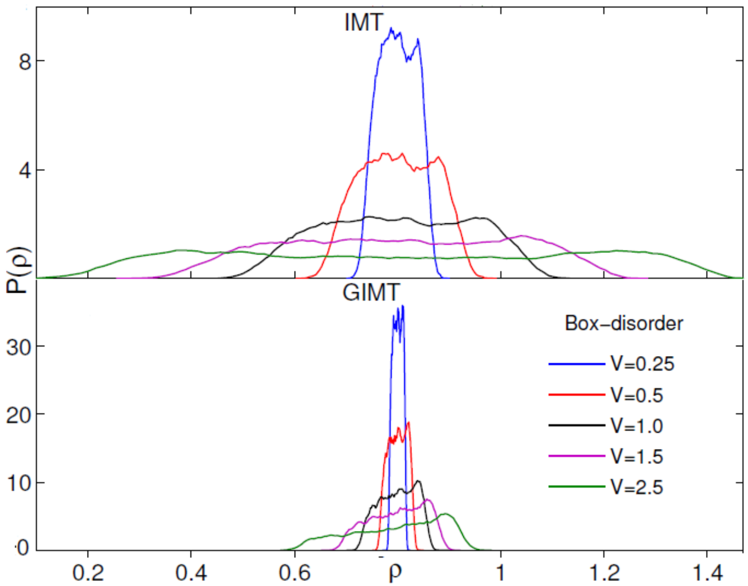
Density of States

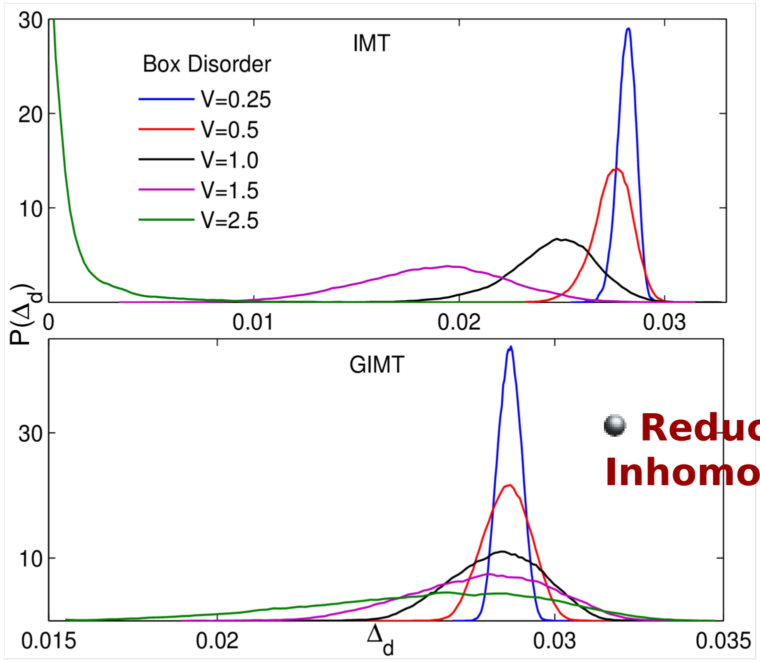
$$N(\omega) = \frac{1}{N}\sum_{i,n} g_{ii}^t \{ |u_{i,n}|^2 \, \delta(\omega - E_n) + |v_{i,n}|^2 \, \delta(\omega + E_n) \}$$



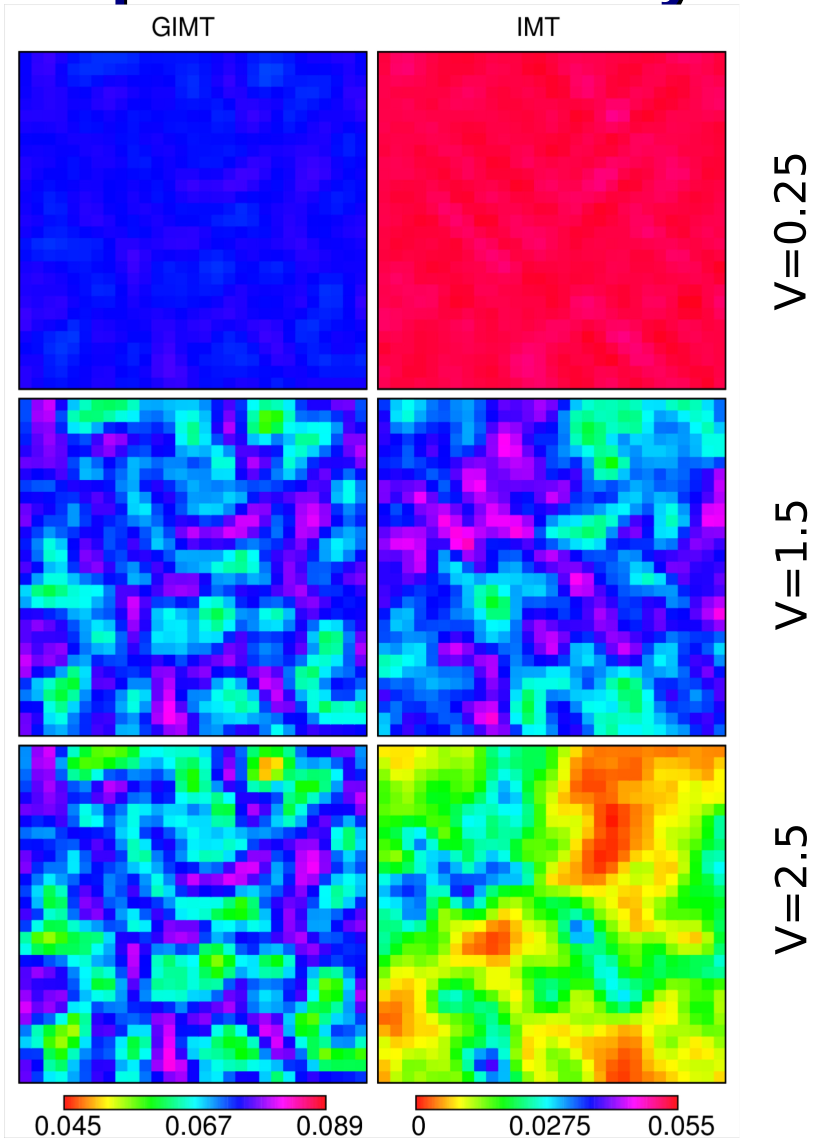
Similar to Garg et. al, Nat Phys., 4, (2008)

Distribution of d-wave pairing amplitude and density





- **Reduction of Inhomogeneity!!**



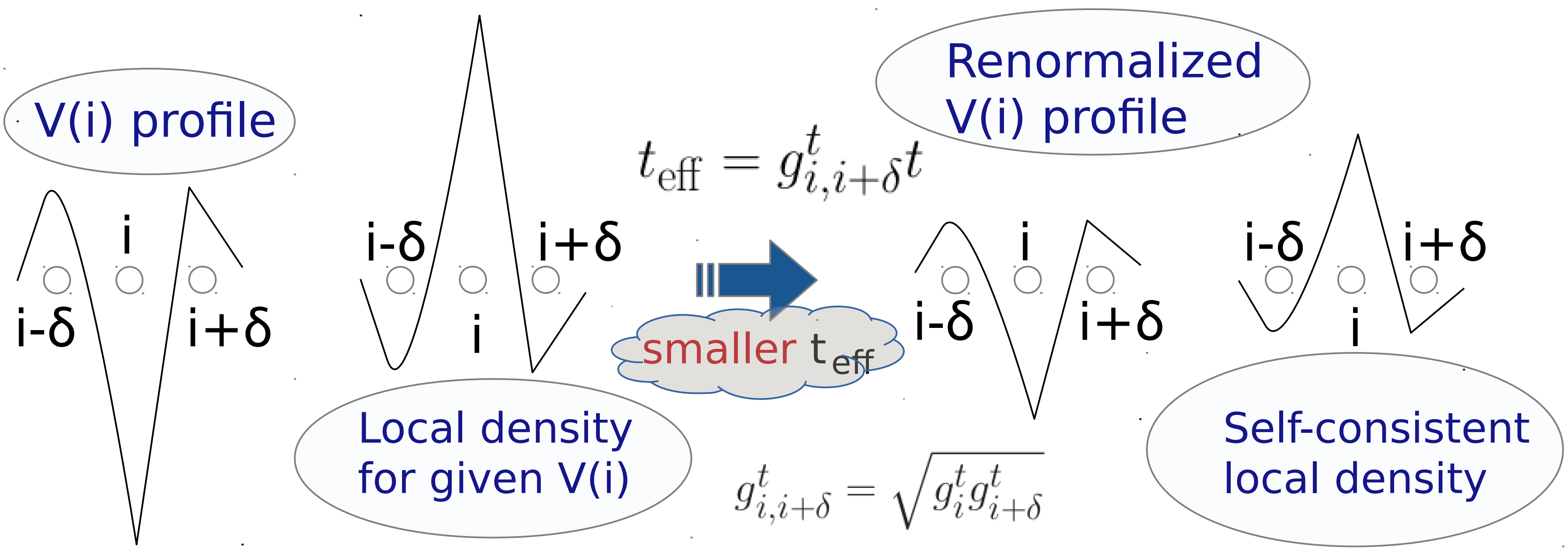
- GIMT: No SC-"island"
- GIMT: Δ-profile unaltered with V

What does homogenize ρ? : effective hopping-disorder

Effective Hamiltonian

$$H_{MF} = -\sum_{i,\delta,\sigma} t_{eff}(i,\delta) c^{\dagger}_{i\sigma} c_{i+\delta\sigma} + \sum_{i,\sigma} V_{eff}(i) n_{i\sigma}$$
$$+ \{\text{pairing terms involving } \Delta_i^{\delta}\}$$

$t_{eff}(i,\delta)$ → Probability of hopping of an electron onto the site i from neighbor @ i+δ



$$g_t = \frac{2\delta}{1+\delta}$$

Similar arguments work for hills of disorder

Strong correlations homogenize density!

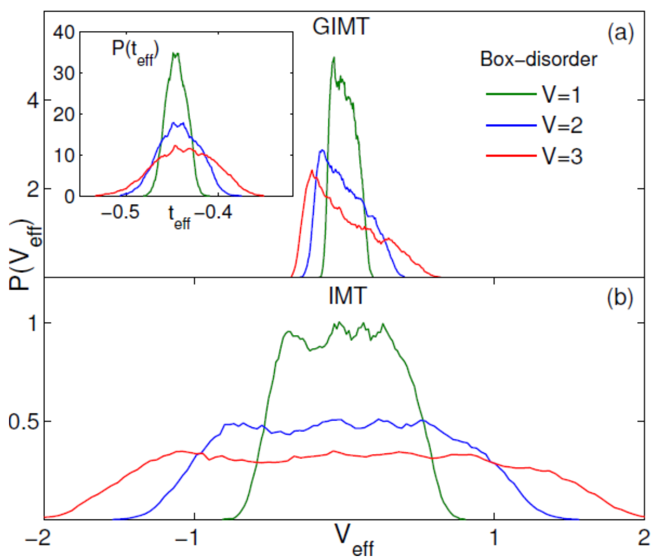
See also: Fukushima, PRB ('09); Tang et.al. PRB ('15), PRB ('16)

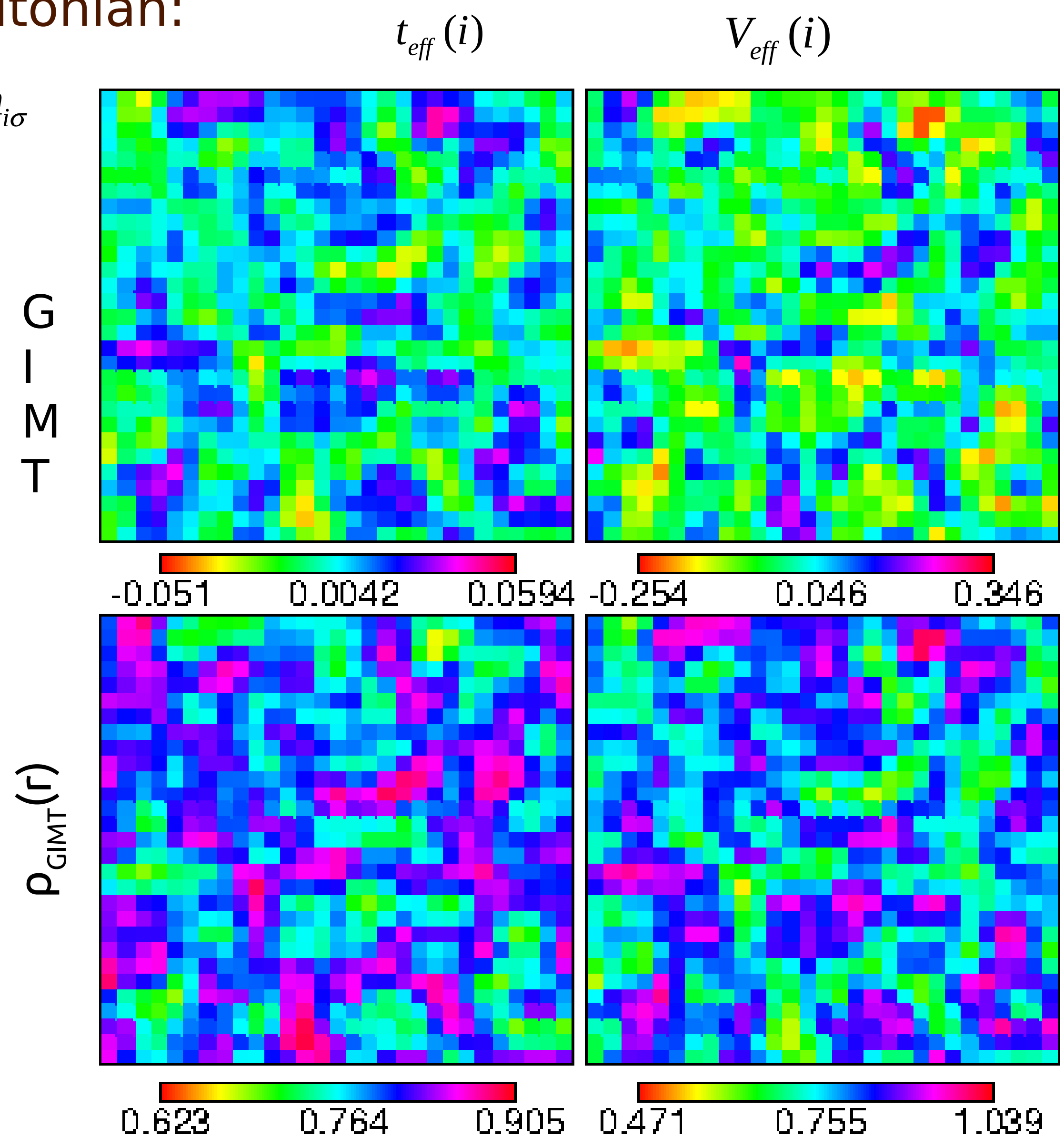
Effective Disorder

Effective one-particle Hamiltonian:

$$H_{MF} = -\sum_{i,\delta,\sigma} t_{eff}(i,\delta) c^{\dagger}_{i\sigma} c_{i+\delta\sigma} + \sum_{i,\sigma} V_{eff}(i) n_{i\sigma}$$

$$+ \{\text{pairing terms involving } \Delta_i^{\delta}\}$$





- Renormalization of $V_{eff}(i)$

- $V_{eff}(i)$ and $t_{eff}(i)$ work against each other

➡ ***homogenize!!***

Results: Part - II

Marching towards strong disorder, $V \geq 3t$

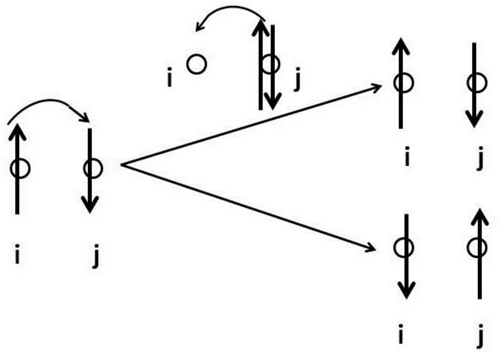
Quenched hopping on certain bonds provide mechanism for destruction of dSC!

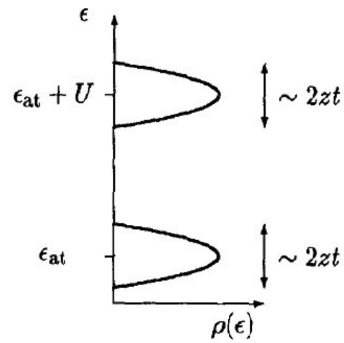
Emergent “Mottness” drives the inhomogeneity, creating puddles!

(preprint)

How to extend GIMT at Strong disorder?

- **Recap:** conventional SW (For $V \leq t$)





- Effective low energy Hamiltonian
- Unmixing of high and low energy sectors.

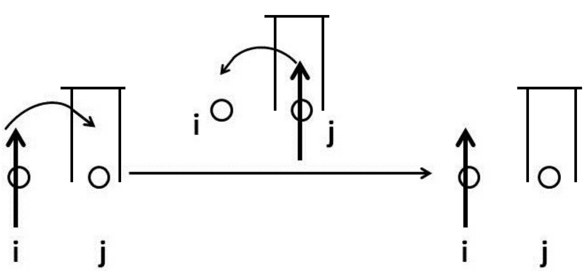
- **With disorder??**

- **SW-transformation for U >> V >> t:**

$$\mathcal{H}_{\text{Hubb}} = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) + U \sum_{j} n_{j\uparrow} n_{j\downarrow} + \sum_{i,\sigma} (V_i - \mu) n_{i\sigma}$$

SW ⇒ **"t-J"??**

New: direct hopping (1st order) prohibited, virtual hopping (2nd order) takes place!



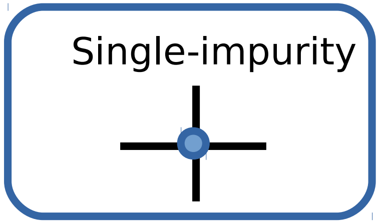
- No direct hopping, ***but*** virtual hopping
- Unmixing of high and low energy sectors depending on ***local*** disorder
- Leading to "t-J model" with independent parameters on ***each bond***

Inhomogenous "J":

$$J_{ij} = \frac{4t^2 U}{U^2 - (V_i - V_j)^2}$$

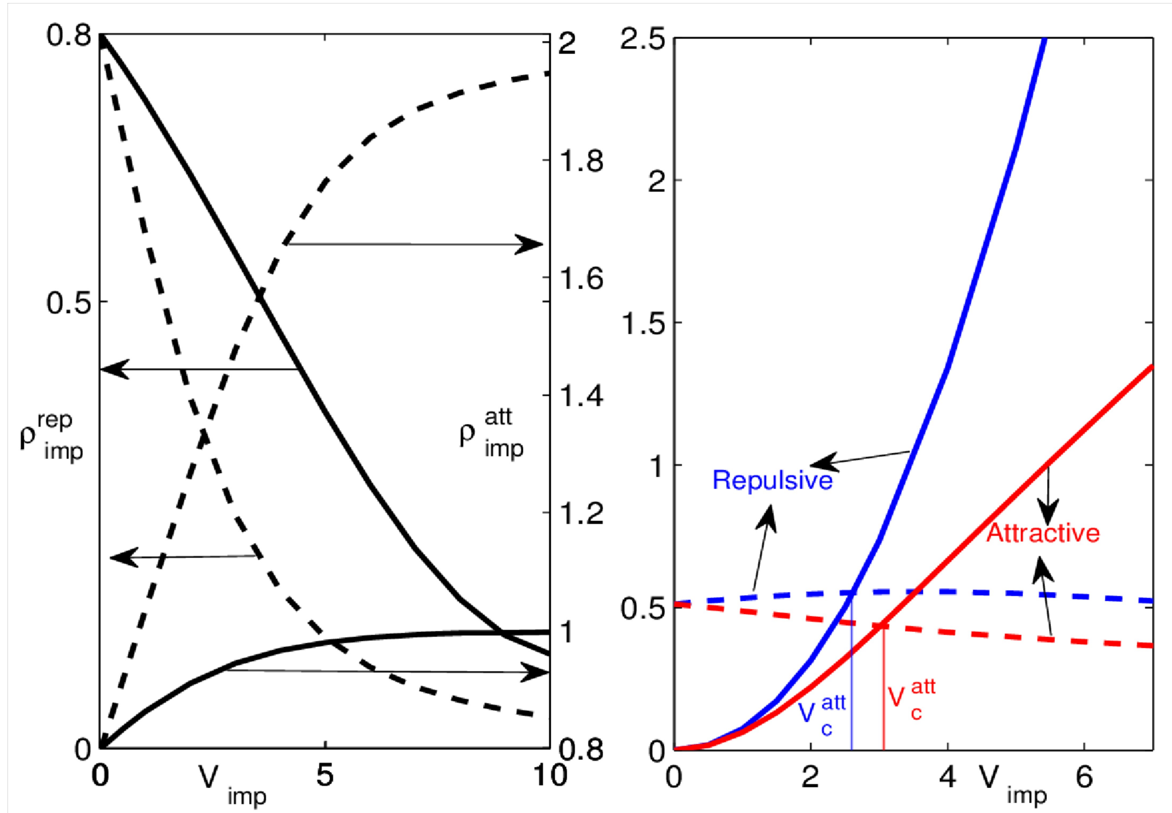
Nunner et.al. Physica C ('07)

How to extend GIMT at Strong disorder?



- Repulsive, as well as attractive impurities, with large strengths, localize electrons on them.

- Making locally Anderson or Mott insulator!



$$\langle H_{eff} \rangle = \langle H_{gain} \rangle + \langle H_{loss} \rangle$$

Loss $\sim V_i \Delta\rho_i$

Gain $\sim g_t(i,j) \langle c^{\dagger}_{i\sigma} c_{j\sigma} \rangle_0$

$$\langle H_{gain} \rangle \rightarrow \textit{Primarily Kinetic Energy}$$

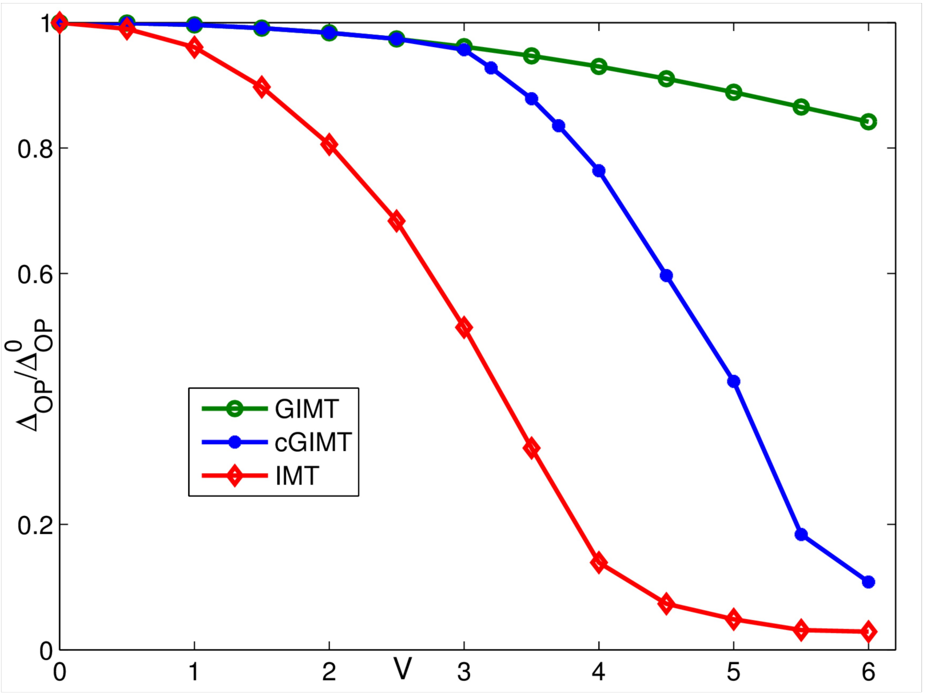
$$\langle H_{loss} \rangle \rightarrow \textit{Disorder Energy} \equiv V_i \Delta\rho_i$$

$$\Delta\rho_i = \rho - \rho_i$$

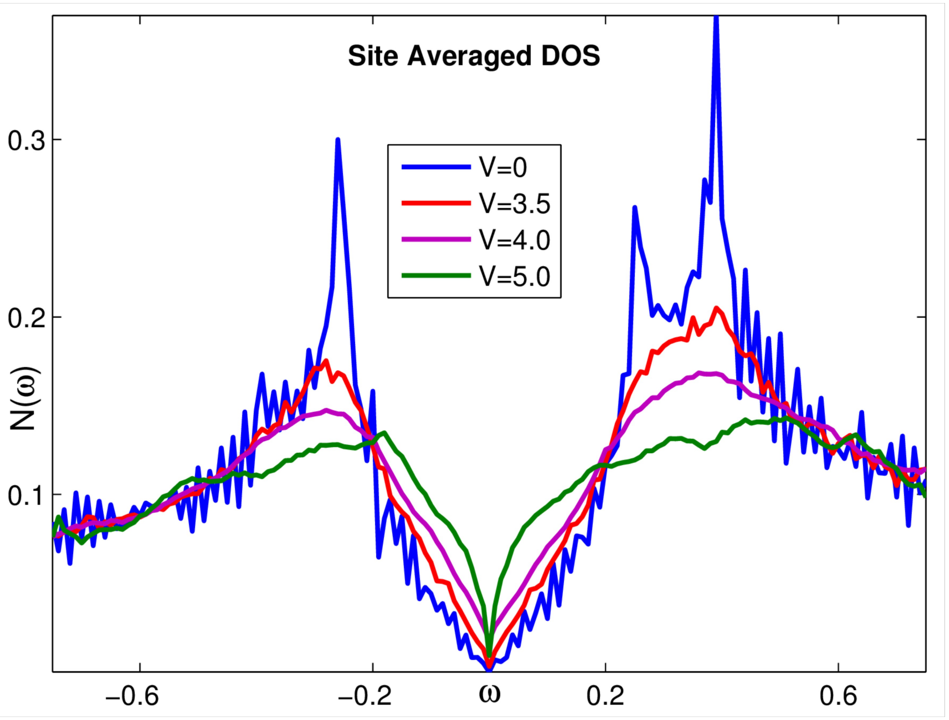
V_c: Critical impurity strength beyond which *gain* & *loss* terms crosses each other

Results: Physical observables

ODLRO

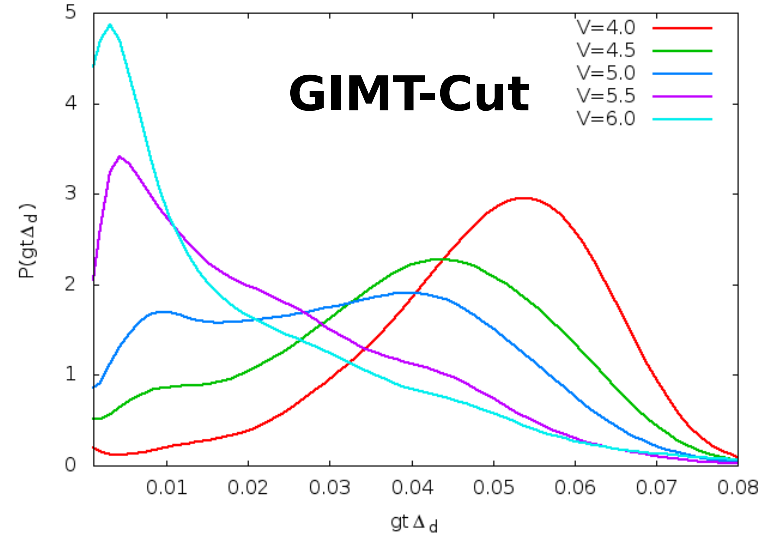


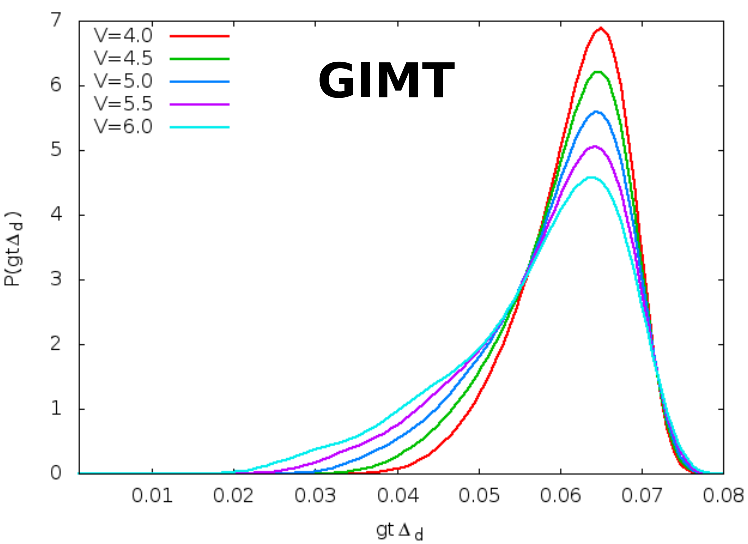
DOS

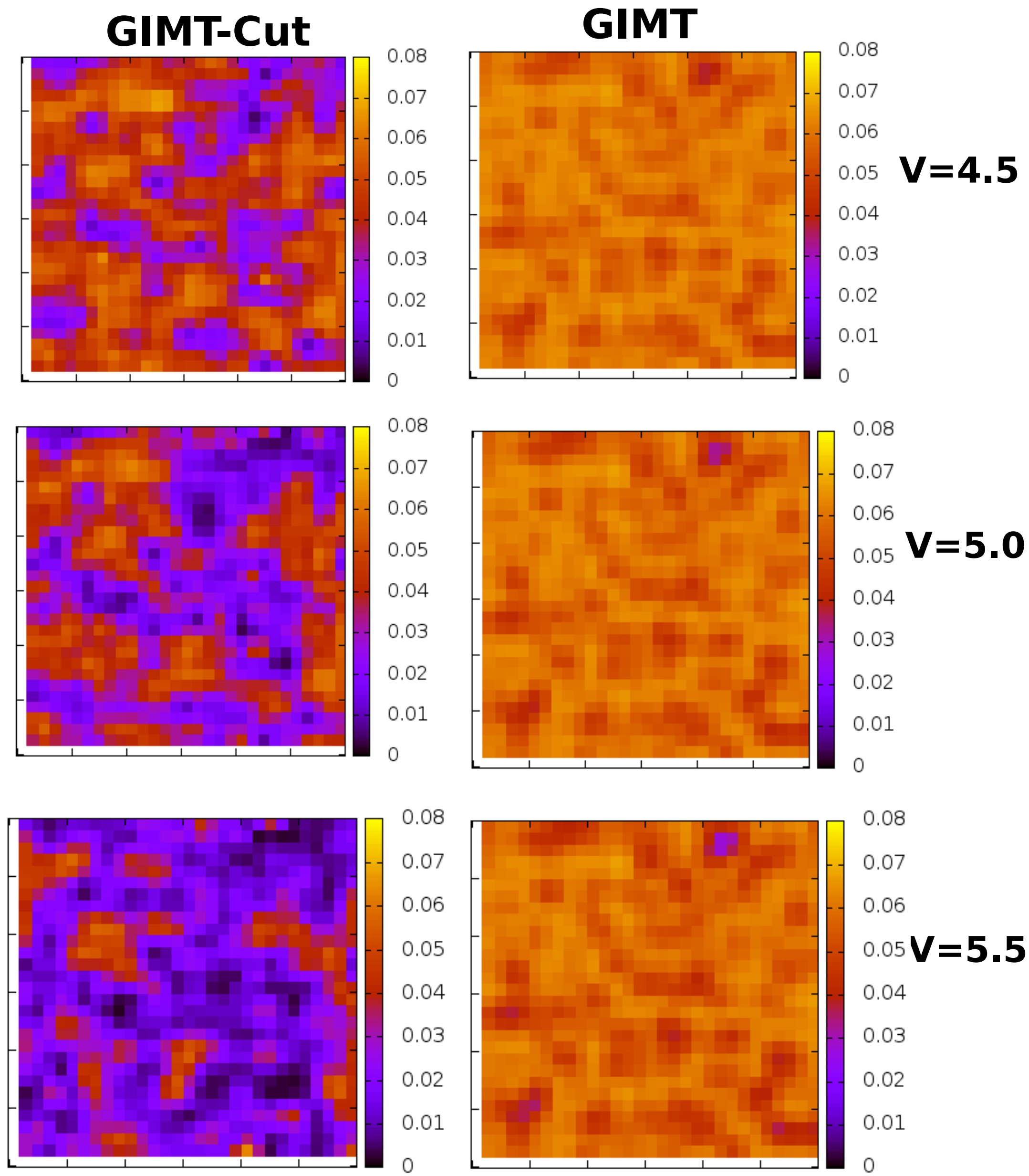


- **GIMT calculation with "cut"-bonds provides mechanism for destruction of superconductivity**
- **Partial filling up of Low energy DOS**
- **Qualitative physics <u>insensitive</u> to specific value of V_c**

Superconducting Order Parameter ~ $g_t |\Delta|$

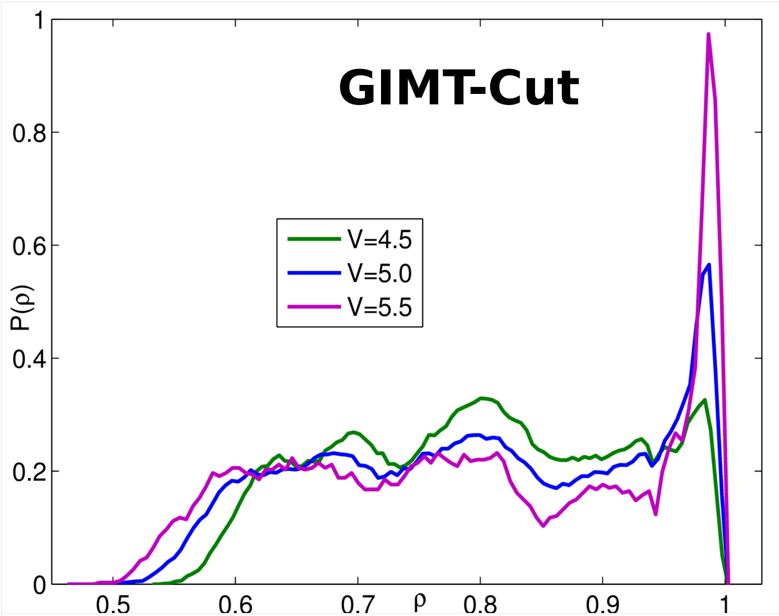


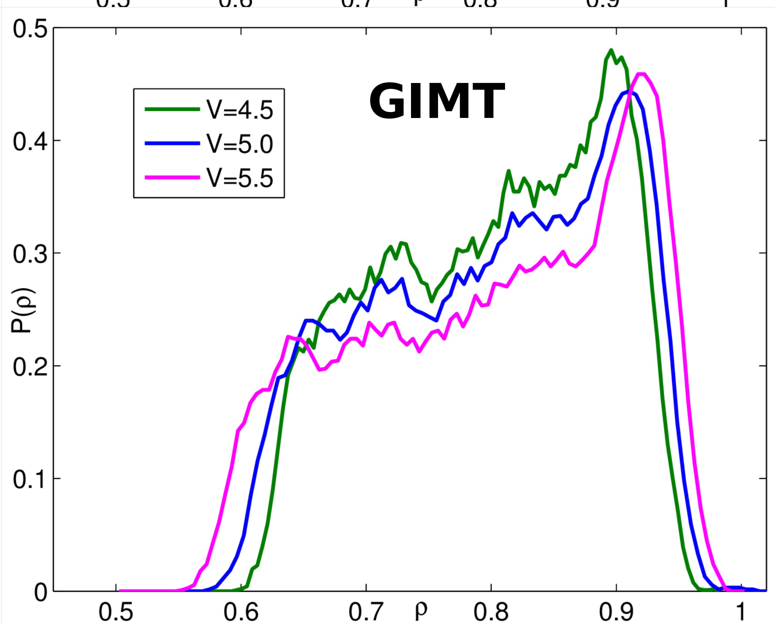


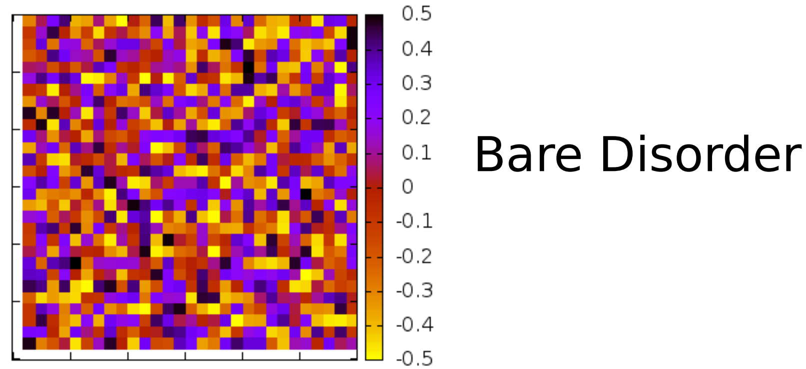


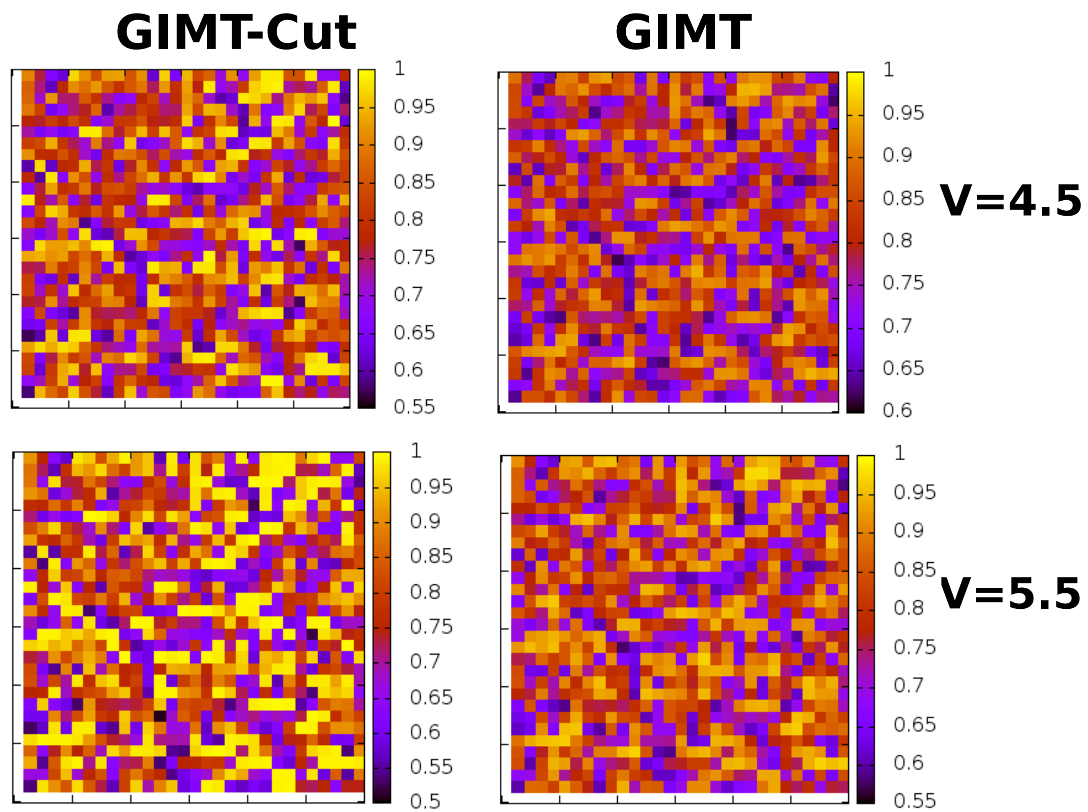
- Formation of ``islands”

Density



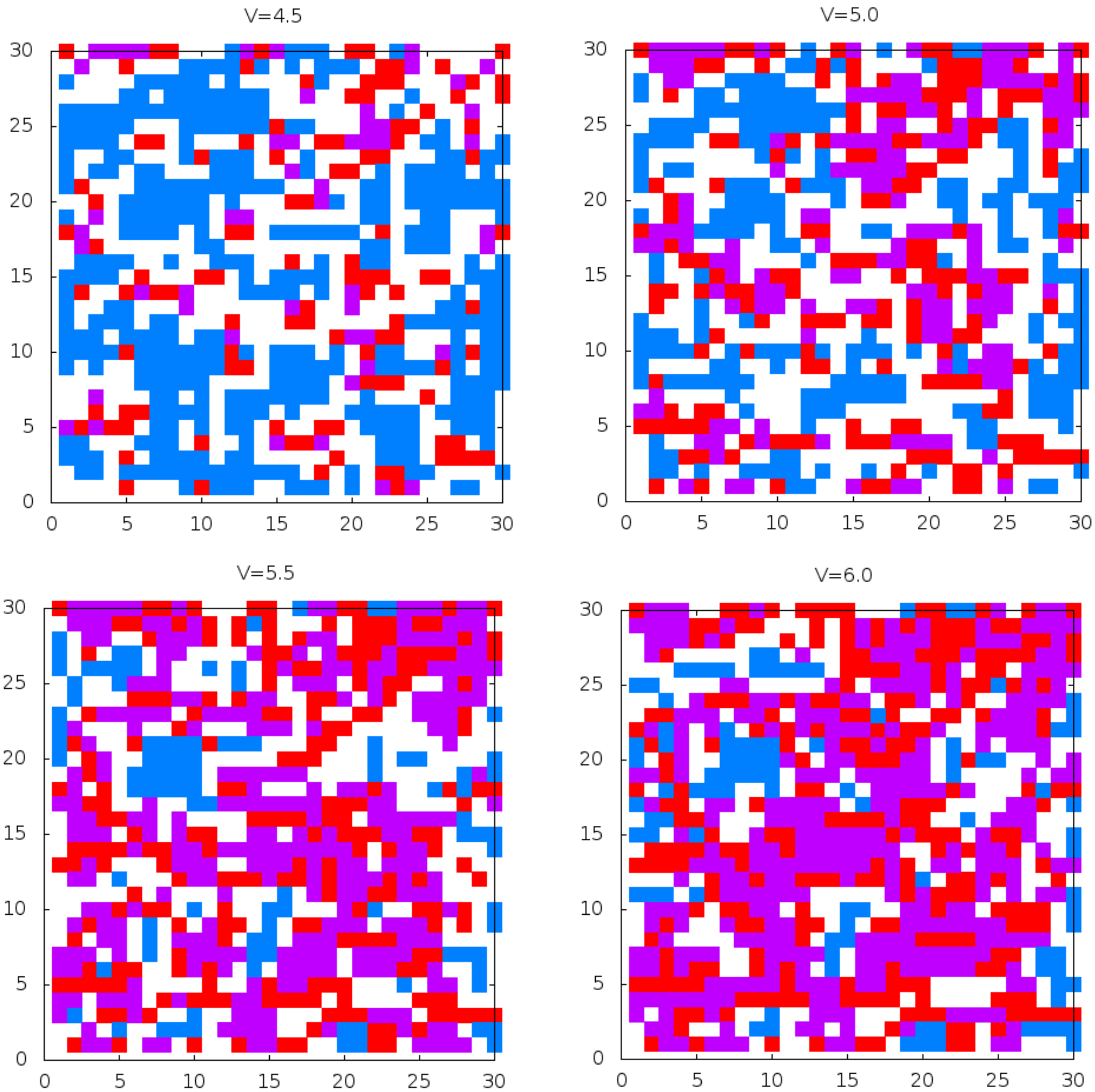






- Sites with ρ=1 keeps increasing sharply

Coarse-grained spatial regions



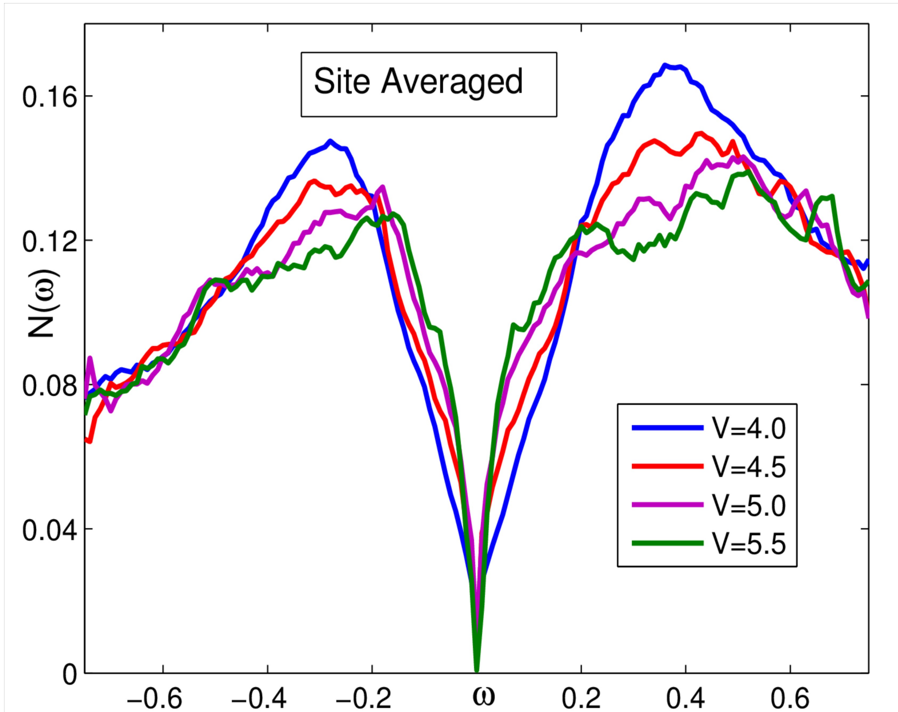
Blue: $g_t*|\Delta| > 0.045$, wide range of ρ (locally SC)

Red: $g_t*|\Delta| \leq 0.02$, and $\rho \geq 0.98$ (locally "Mott")

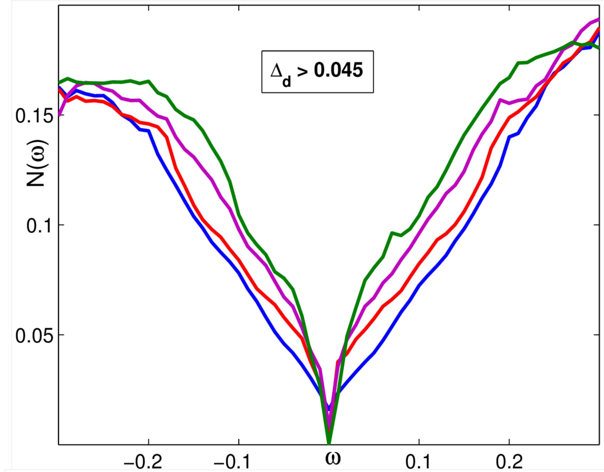
Violet: $g_t*|\Delta| \leq 0.02$, and $\rho \leq 0.95$ (surrounds Mott sites/regions)

"Mott"-sites nucleates non-SC regions!

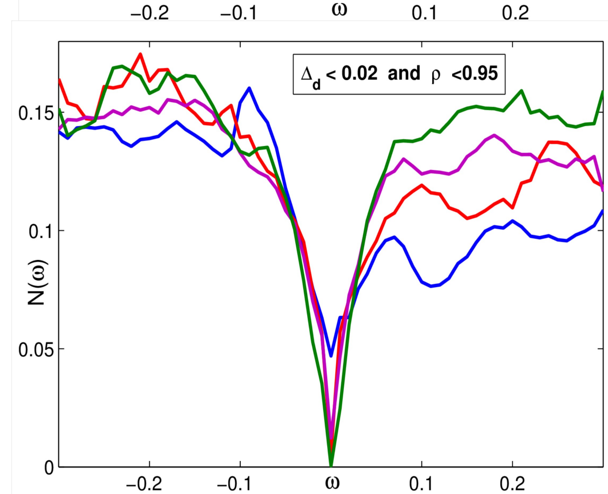
LDOS in coarse-grained spatial regions:



Average DOS

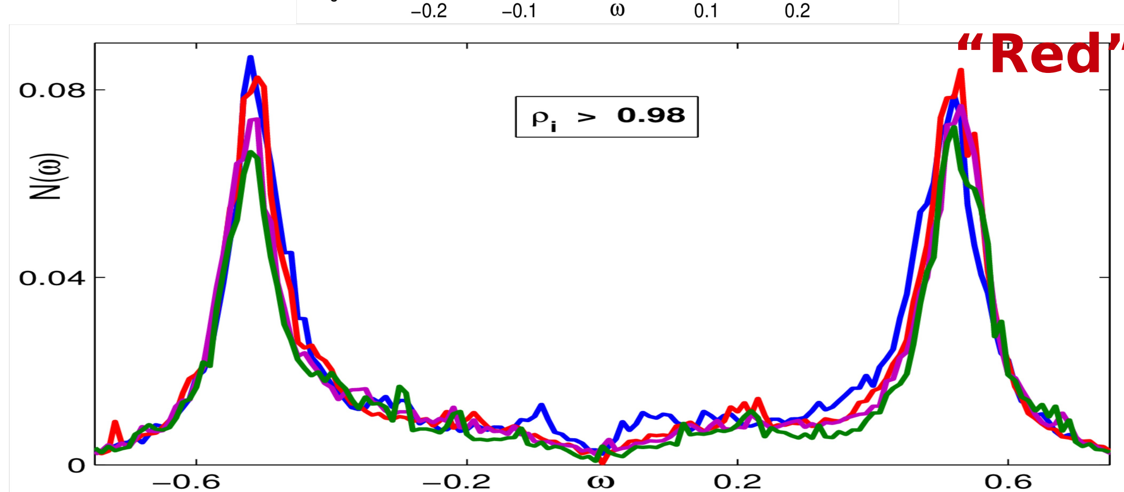


"Blue"



"Violet"

"Red"

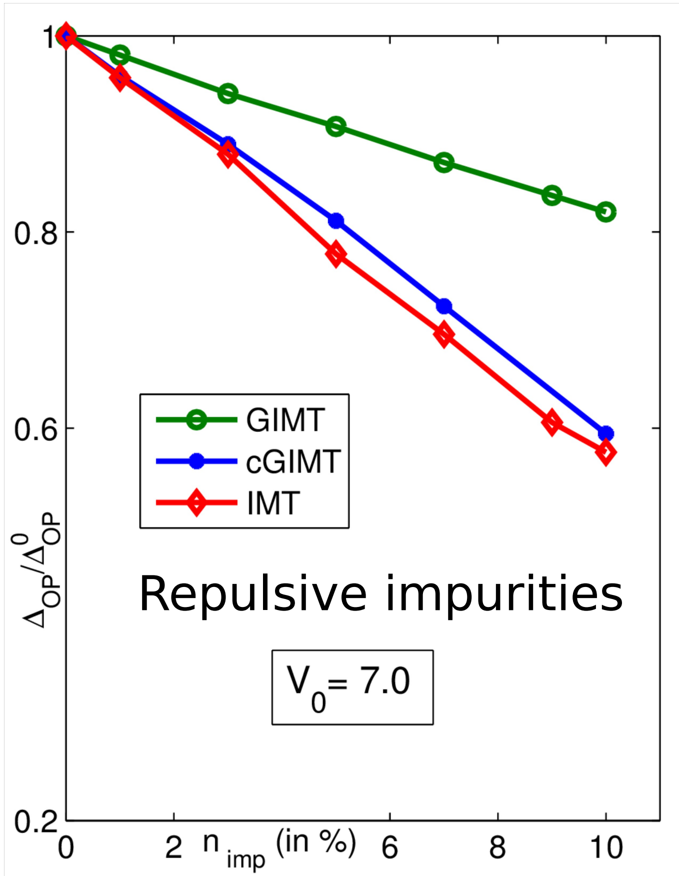


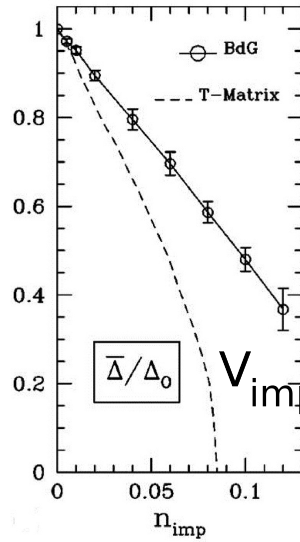
Thin gap:

- Nersesyan et.al. PRL (1994)
- Senthil, Fisher PRB (1999)
- Atkinson et.al PRL (2000)
- AG et.al. PRB (2000)

"Concentration" disorder:

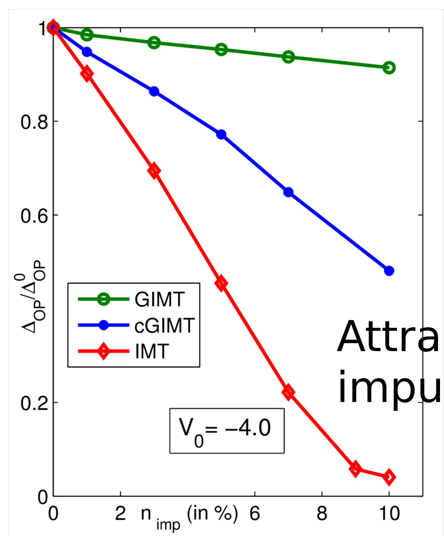
- Impurities (***same*** strength V_{imp}) on n_{imp} fraction of ***random*** sites.



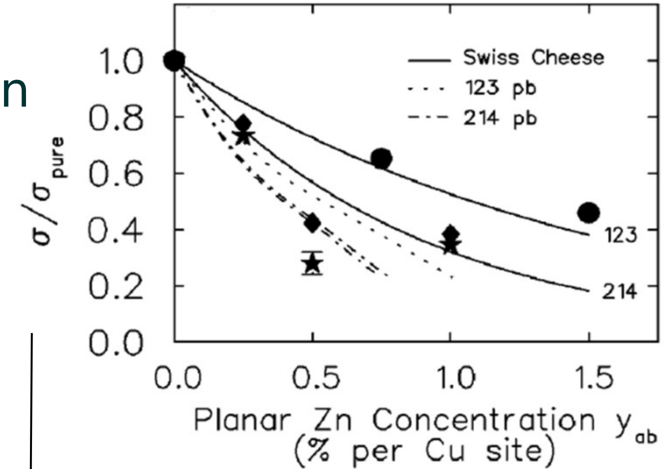


V_{imp} = 100

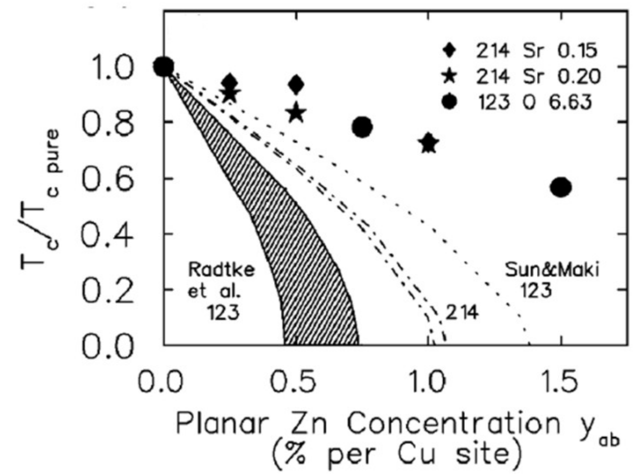
AG, Randeria, Trivedi (2000)



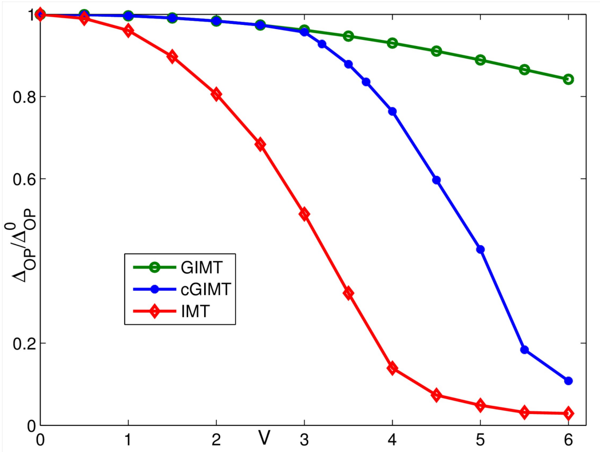
Attractive impurities

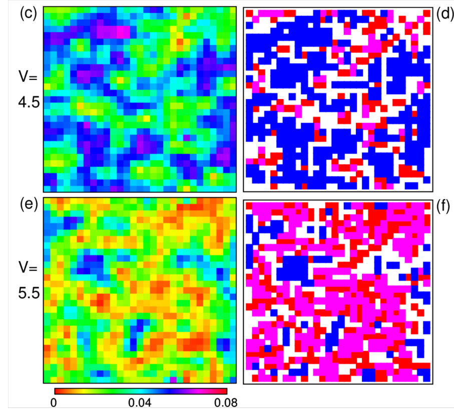


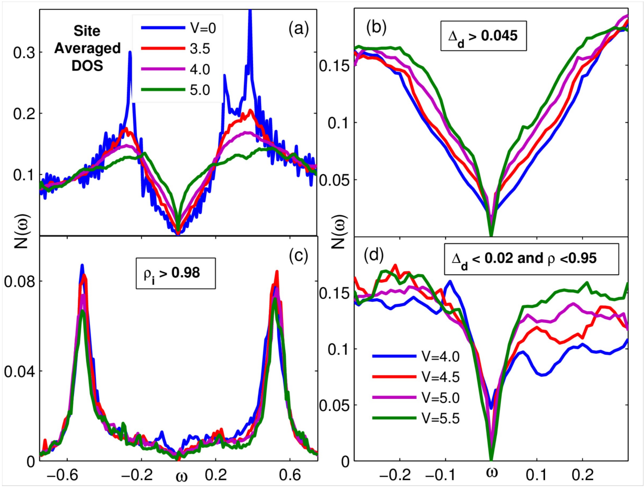
Nachumi, PRL, ('96)



- Zn substituting Cu in cuprates.







Conclusions:

- dSC amazingly **robust to impurities** up to moderate disorder.
  ➡ Due to (spatially correlated) renormalization of one-particle potential due to strong correlations.

For large disorder, $|V_i - V_j| \geq 3t$, direct hopping is prohibited on some bonds and homognizing ceases.
  ➡ superconductivity decays rapidly!

- At large V, "Mottness" of cut-bond & attractive site-energy nucleates non-SC regions, that rapidly engulfs whole system!
  ➡ "Mottness" relevant @ large disorder at optimal doping!
  ➡ heterogeneous system susceptible to phase fluctuations.
-

Why thin gap in DOS?

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Disorder-Induced Stabilization of the Pseudogap in Strongly Correlated Systems

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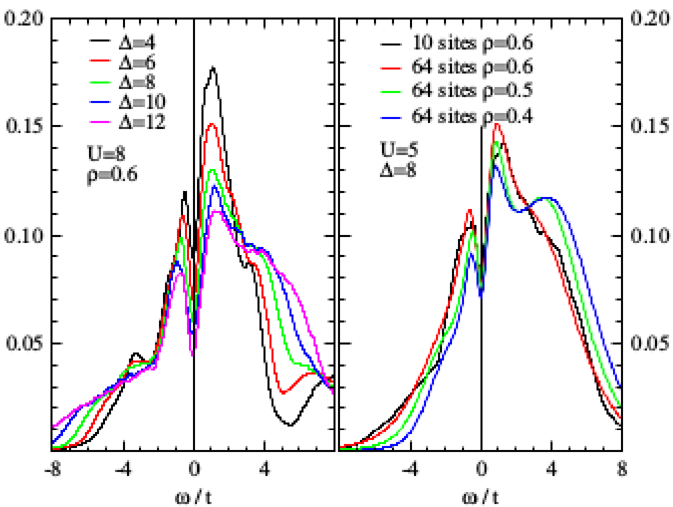
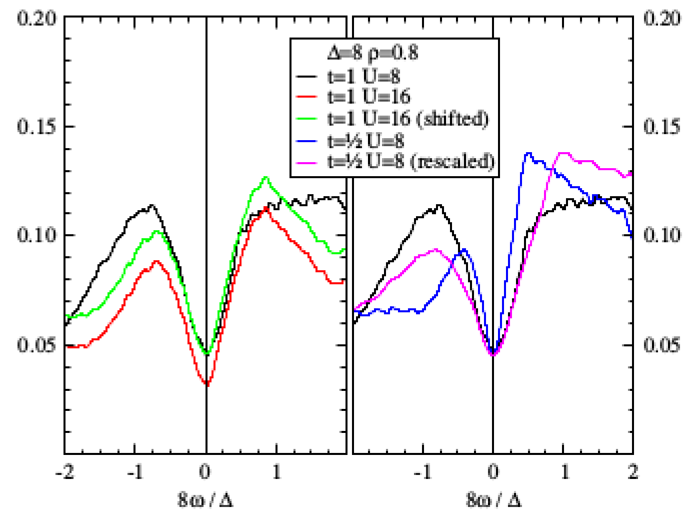
Department of Physics, University of California, Davis, California 95616, USA
(Received 29 April 2008; published 20 August 2008)

$$\mathcal{H}_{\mathrm{AH}} = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + h.c.) + \sum_{i} V_i n_i + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



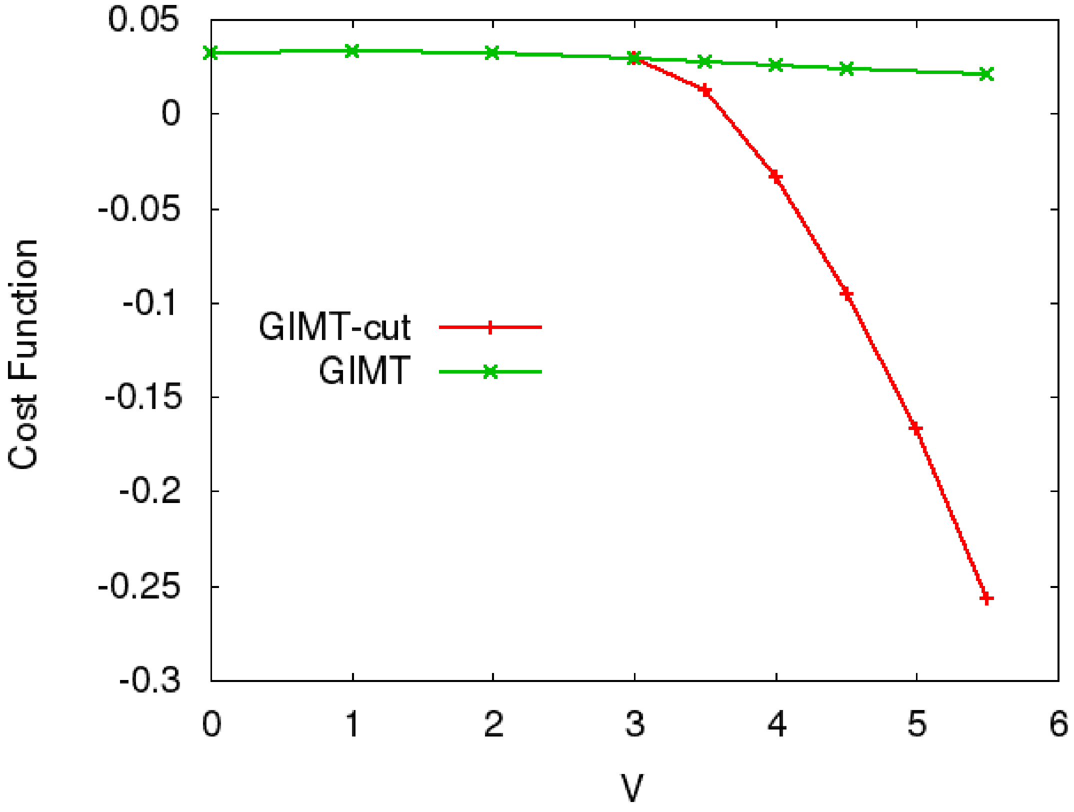


<u>Also:</u>
Shinaoka & Imada, PRL (2009)

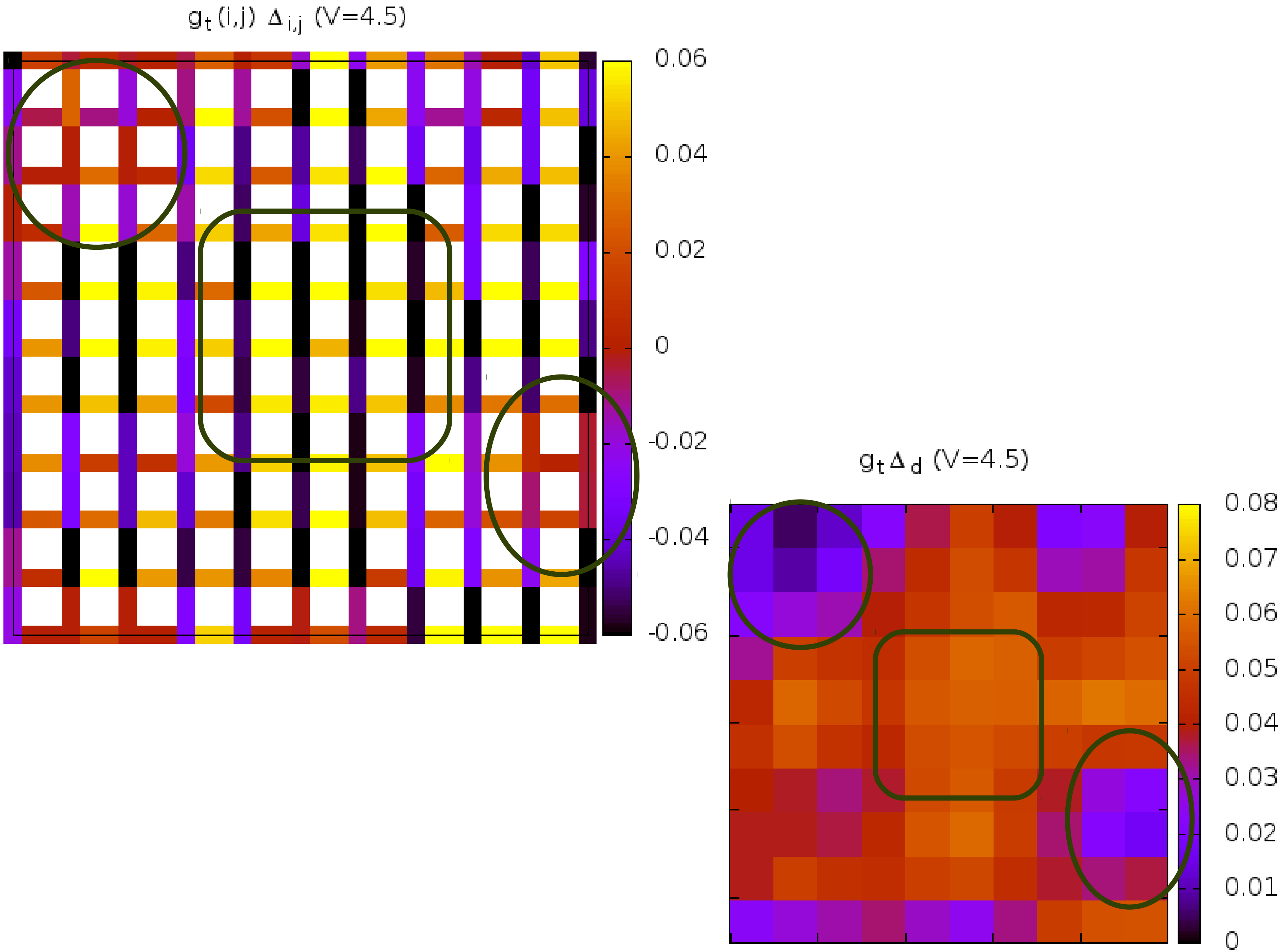
Wortis & Atkinson, PRB (2010)

Anderson-Hubbard model opens up pseudogap @ μ, for <u>strong U and V for a wide range of <ρ></u>.
Gap scale <u>independent of U and V</u>, but d<u>epends on t.</u>

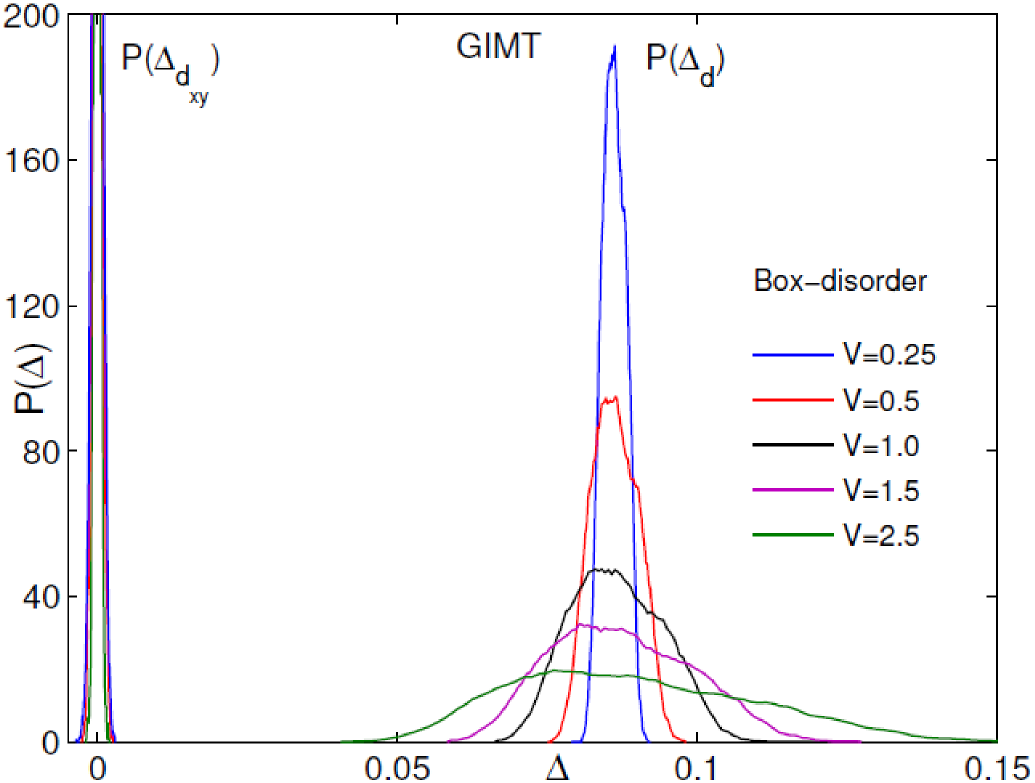
Sanity check: Is there any variational gain by cut-GIMT?



... Yes indeed!


$g_t(i,j)\,\Delta_{i,j}$ (V=4.5)
0.06
0.04
0.02
0
-0.02
-0.04
-0.06
$g_t\,\Delta_d$ (V=4.5)
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0

Other Cooper-channel Orders?



- Small width, tiny values & V-independence of the sub-dominant orders

$$\Delta_{xs}(\boldsymbol{k}) = \Delta_{xs}(\cos k_x + \cos k_y)/2$$

$$\Delta_{s_{xy}}(\boldsymbol{k}) = \Delta_{s_{xy}} \cos k_x \cos k_y$$

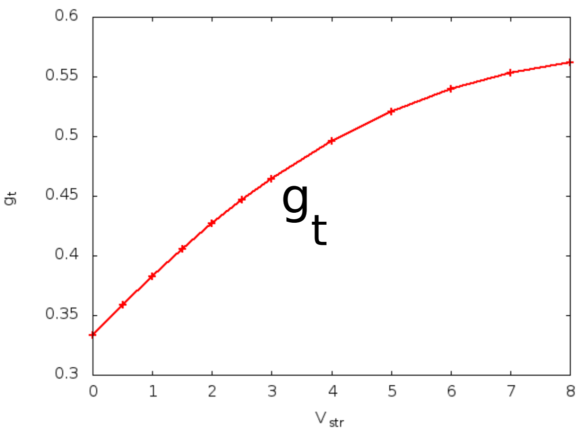
$$\Delta_{d_{xy}}(\boldsymbol{k}) = \Delta_{d_{xy}} \sin k_x \sin k_y$$

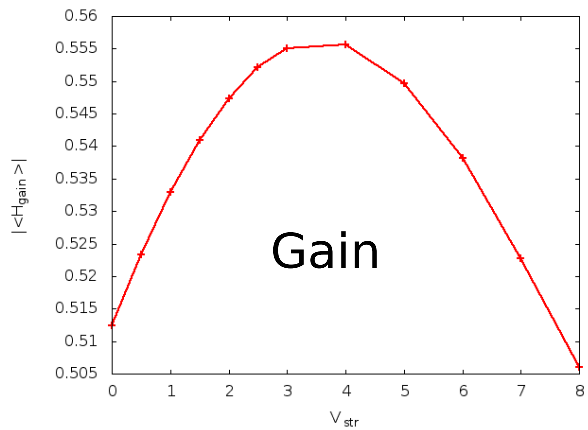
Hence suppress $\Delta_{d_{xy}}, \Delta_{s_{xy}}, \Delta_{xs}$ and work with simpler $t-J$ model:

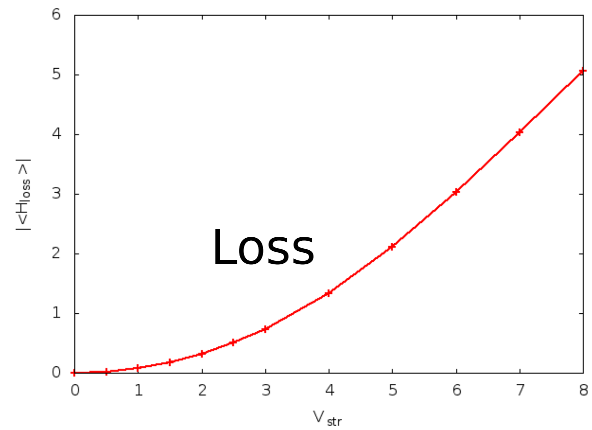
$$H_{"t-J"} = -\sum_{ij\sigma} t_{ij}(\tilde{c}^{\dagger}_{i\sigma}\tilde{c}_{j\sigma} + h.c.) + \sum_{\langle ij \rangle} J\left(\tilde{\boldsymbol{S}}_i.\tilde{\boldsymbol{S}}_j - \frac{\tilde{n}_i\tilde{n}_j}{4}\right)$$

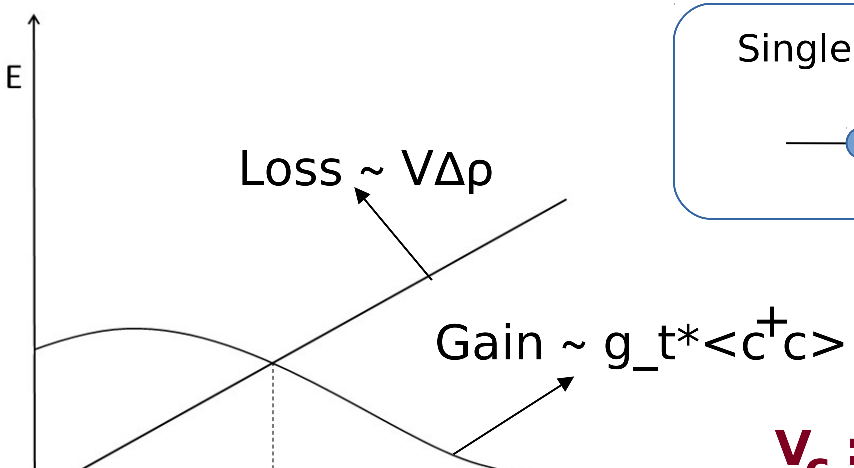
How to extend GIMT at Strong disorder?

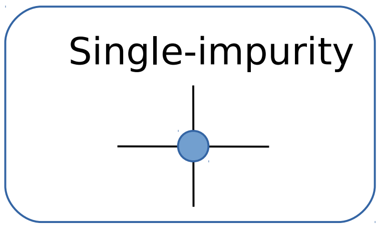
- Strong correlations homogenize the system by increasing g_t on links connecting to a repulsive impurity-site, and enhanced charge transport across such bonds weakens the effective repulsive site-energy.











$$\langle H_{eff} \rangle = \langle H_{gain} \rangle + \langle H_{loss} \rangle$$

$$\langle H_{gain} \rangle \rightarrow \text{ primarily Kinetic Energy}$$

$$\langle H_{loss} \rangle \rightarrow \text{Disorder Energy} \equiv V_i \Delta\rho_i$$

$$\Delta\rho_i = \rho - \rho_i$$

V_c : Critical impurity strength, beyond which hopping on bonds prohibited