Simulations for correlated and disordered systems in two dimensions

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Outline

I. Motivation and model

II. Methods and results

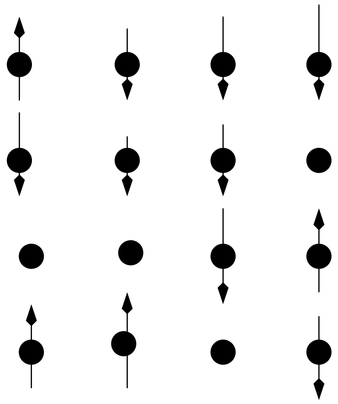
  A. 2nd-order perturbation theory
  B. Dynamical mean-field theory
  C. Dynamical cluster approximation

III. Summary, future directions

I. Motivation and model

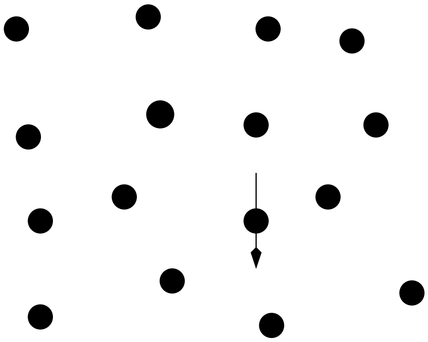
The curious case of two dimensions

- Interaction physics



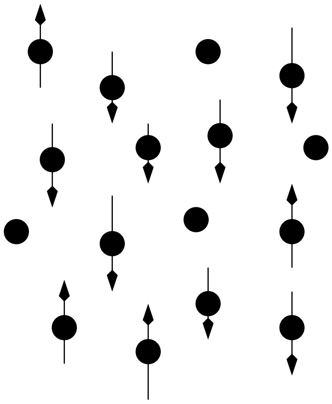
  - Lack of ordering (Mermin-Wagner-Hohenberg)
    - Only Ising-like order at finite T
    - Fluctuation effects over range of T
    - KTB transition for superconductors
  - Fermi-liquid (3D) and non-Fermi-liquid (1D) states
  - Mott transitions

- Disorder



  - Insulating state in 2D for any disorder strength

- Interactions and disorder

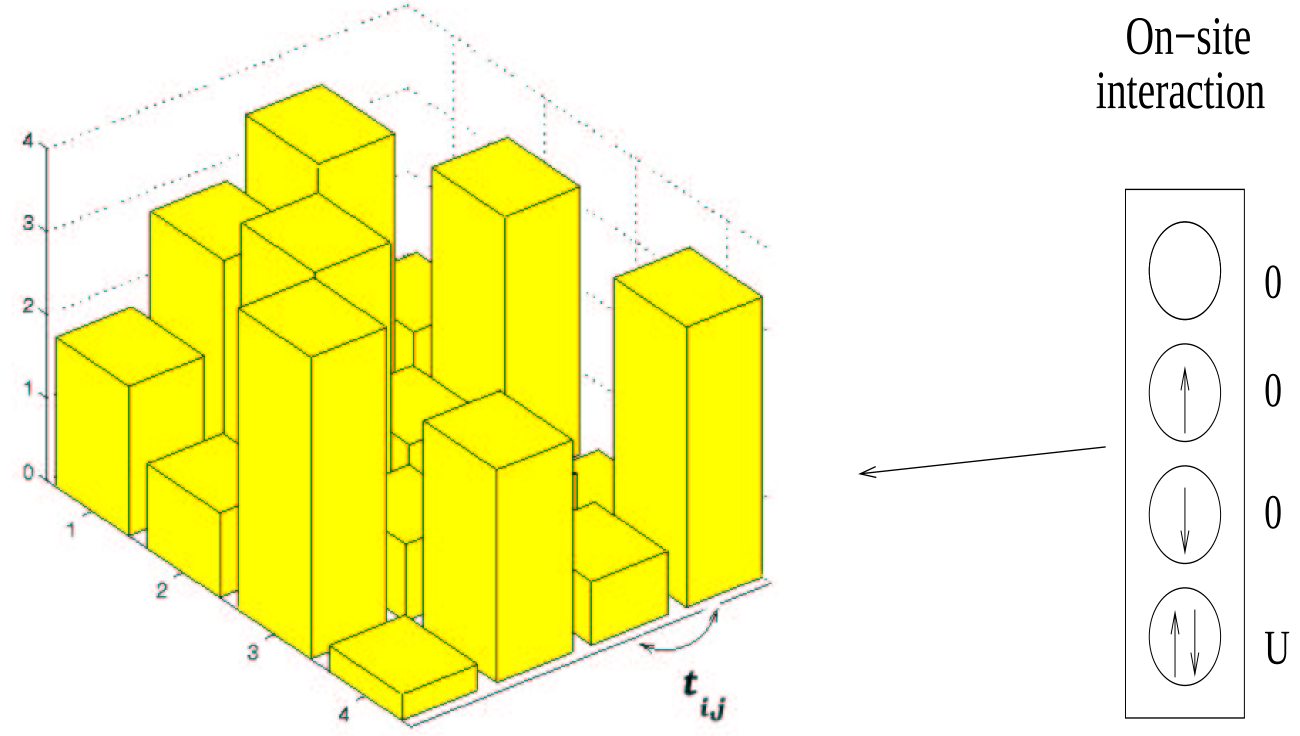


  - Mott-Hubbard-Anderson transitions
  - Density driven metal-insulator transition
  - Superconductor-insulator transition
  - Competing length scales: localization length, $v_F\tau$, correlation length, coherence length

Model

Lattice model with a local interactions, i.e. the disordered Hubbard model

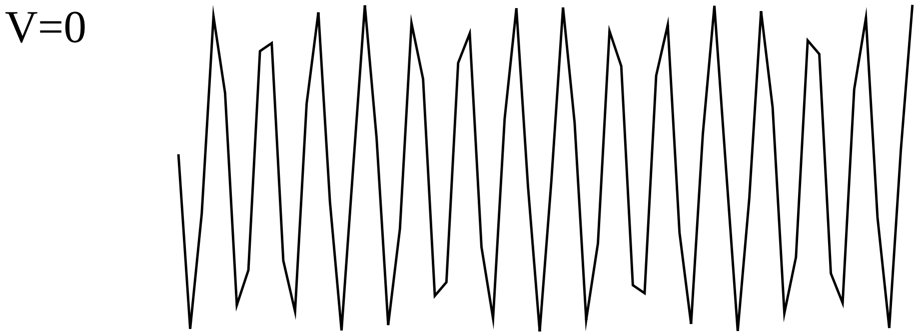
$$H = - \sum_{<i,j>,\sigma} (t_{i,j}\, c^{\dagger}_{i,\sigma} c_{j,\sigma} + H.c) + \sum_{i} U_i\, n_{i,\uparrow} n_{i,\downarrow} + \sum_{i,\sigma} (V_i - h_{i,z}\, \sigma) n_{i,\sigma}$$

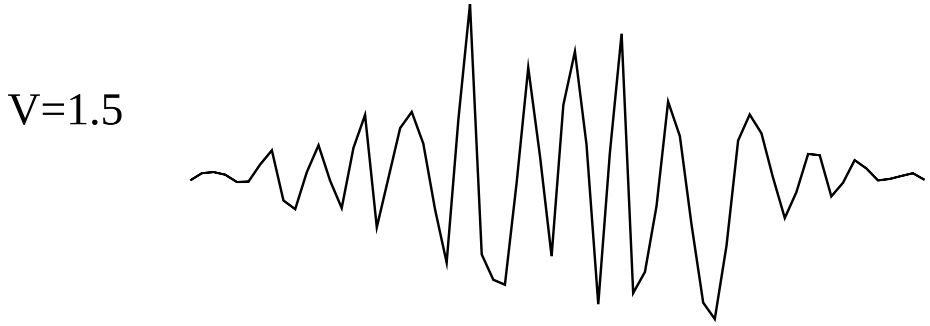


$0 \leq V_i < 2V, V = 2$

Bloch (1928): Wave functions are extended in
periodic structures

Anderson (1958): - Disorder localizes wave functions





Inverse participation ratio:

$$P_{H,l} = \sum_{\mathbf{r}} |\psi_l(\mathbf{r})|^4 \quad \sim \quad 1 \text{ (site localized)}$$

$$\sim \quad 1/N \text{ (extended)}$$

Strong correlation effects are evaluated with Hubbard model

- $|U|$ is an appreciable fraction of the bandwidth
- In the clean limit ($V = 0$) system evolves toward a low-temperature ordered state.
- Several ordered states with this model: s-wave SC, CDW, AFM, FM?, d-wave SC?, p-wave SC?
- Non Fermi liquid behavior (?)
- Model contains $U > W$ Mott-Hubbard transition

Competition in low dimensions

- Ordering
- Order parameter fluctuations
- Quasiparticle localization
- Quasiparticle scattering (NFL)
- Mott insulating behavior

Numerical challenges

- No translational invariance to simplify calculations
- For $N = L_x \times L_y$, there are 4^N states
  - 4.3×10^9 states for $N = 16$ w/o symmetries
  - Kotlyar and Das Sarma (2001) - 313,600 states with 6 electrons
- Quantum Monte Carlo (Scalletar, Huscroft, *et al.*)
  - 10×10 lattices at moderate T
  - Algorithm does not use translational invariance
  - $(1/T)^3$ scaling
  - Sign problem for positive U
  - Difficult to extend the interaction range

Goals

- Develop, analyze, and implement numerical methods for this problem.
  - Non-perturbative treatment of single-particle disorder terms.
  - Demonstrate the broad applicability of these methods, *i.e.* $-U$, $+U$, $|U| < W$, $|U| > W$, wide range for V
  - Parallel

- Apply to interacting and disordered systems in 2D
  - Search for unique characteristics of 2D
  - Fill in gaps, *i.e.* $U \sim W$, $l \sim \xi$

- Extend the method to studies of other non-periodic systems.
  - Vortex configurations
  - Grain boundaries
  - Interfaces (S/N, S/I, etc.)

Perturbation theory versus quantum Monte Carlo, physical considerations

- PT is valid at best for $U < W$
  - No Mott-Hubbard, preformed pairs
  - Non-convergent (order-by-order) for low temperatures
  - QMC can access $U < W$ and $U > W$
- PT enables analysis of different interaction effects
  - First order: tendency to order
  - Second order: quasiparticle scattering, strong coupling effects
  - Flex: quasiparticle-collective mode coupling
  - Perhaps enhances interpretation of QMC results

Perturbation theory vs. quantum Monte Carlo, numerical considerations

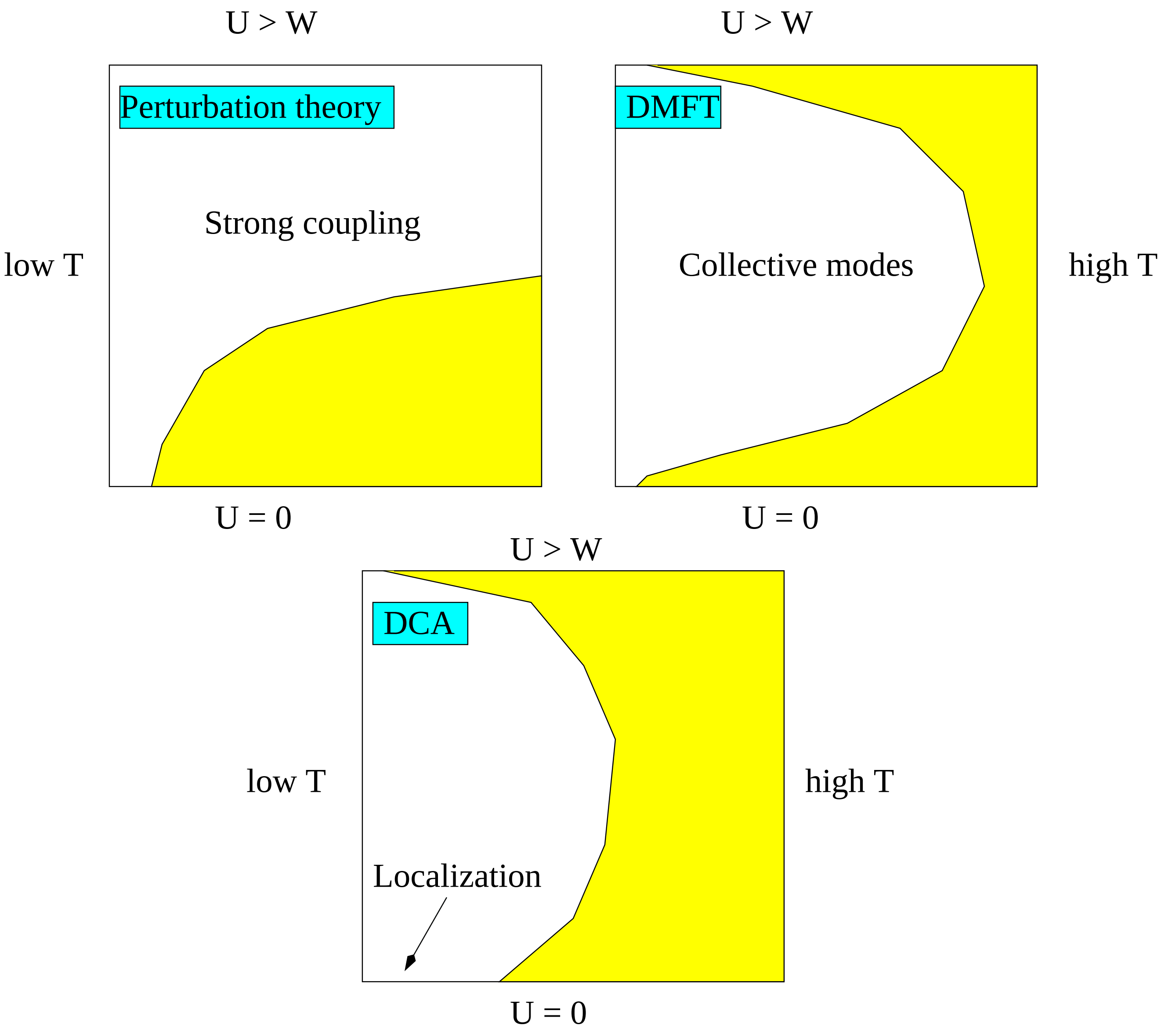
- QMC size scaling: $(N/T)^3 \rightarrow 10 \times 10$ at T = 0.1

- PT size scaling: $(N^3/T)\,\ln(1/T) \rightarrow 20 \times 20$ at T = 0.1

- Localization and fluctuations are cut-off

- Relevant boundary conditions:
  - Open, periodic, embedded

Perturbation theory and quantum Monte Carlo, application limits



II.A. Self-consistent 2nd-order perturbation theory (with Buhrow)

Algorithm

Based on Dyson's equation,

$$G(\varepsilon_n) = [G^{(0)}(\varepsilon_n)^{-1} - \Sigma(\varepsilon_n)]^{-1}$$

$$G(\varepsilon_n) \equiv G_{i\sigma,i'\sigma'}(\varepsilon_n),$$

where G_o includes the disorder potential.

- Operation scales as (N^3/T) ln$(1/T)$ versus (N/T) ln(N/T) for periodic systems.
- Parallelize by dividing data according to ε_n values. Data redistribution occurs during Fourier transforms $\varepsilon_n \to \tau$.
- High frequencies are treated analytically.

Approximations for the self energy

$$\Sigma \approx \Sigma^{(1)} + \Sigma^{(2)} + \Sigma^{(3)} + \Sigma^{(fluct)}$$

$\Sigma^{(1)}$ (Ghosal, Randeria, and Trivedi - 1998)

$\Sigma^{(2)}$:

$\Sigma^{(fluct)}$

Analysis

The grand thermodynamic potential is calculated via:

$$\Omega(T,\mu) = -\mathrm{Tr}[\Sigma G + \ln(-[G^{(0)}]^{-1} + \Sigma)] + \Phi[G]$$

Electronic excitations are examined by using Padé approximates to continue the self-energy to the real frequency axis.

$$\Sigma_{i\sigma,i'\sigma'}(z) = \frac{\sum_n P_{i\sigma,i'\sigma'}(n)\, z^n}{\sum_n Q_{i\sigma,i'\sigma'}(n)\, z^n}$$

Density of states is evaluated by taking

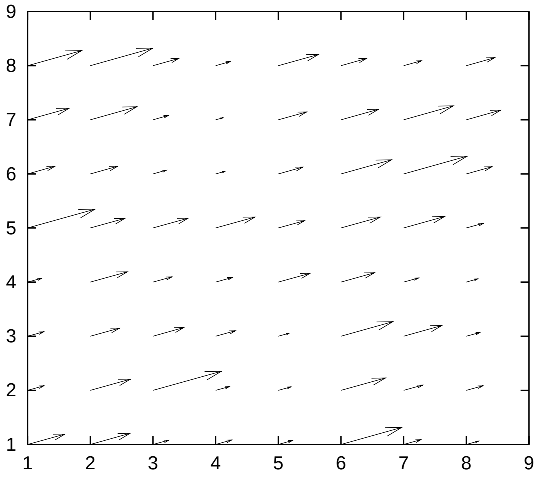
$$A(\varepsilon) = \frac{-1}{\pi N}\ \mathrm{Tr}\ \mathrm{Im}\, G_{\uparrow,\uparrow}(\varepsilon + i\delta)$$

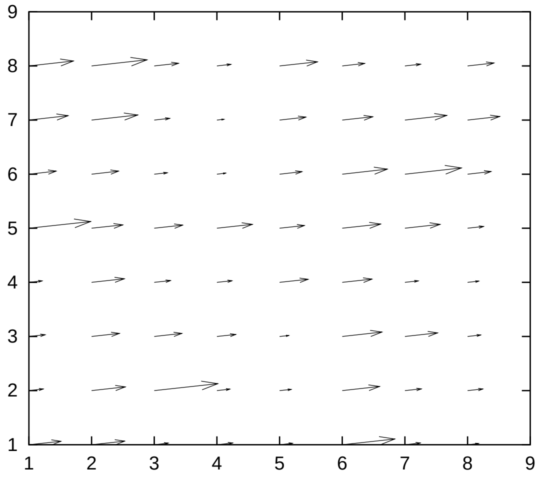
and quasiparticle wave functions and eigenvalues are obtained using

$$[H_{eff} + \Sigma(z)]\, \psi_{qp} = z\, \psi_{qp}.$$

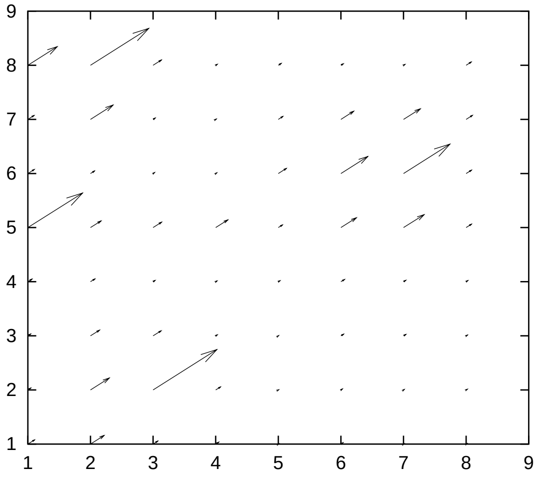
Superconducting order for $U = -4t$

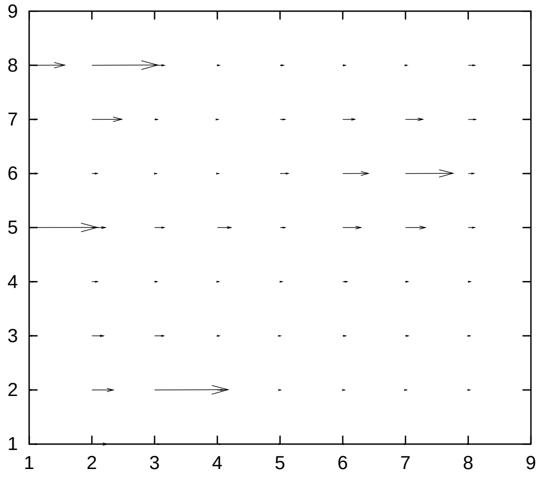
$V = t$


1st order

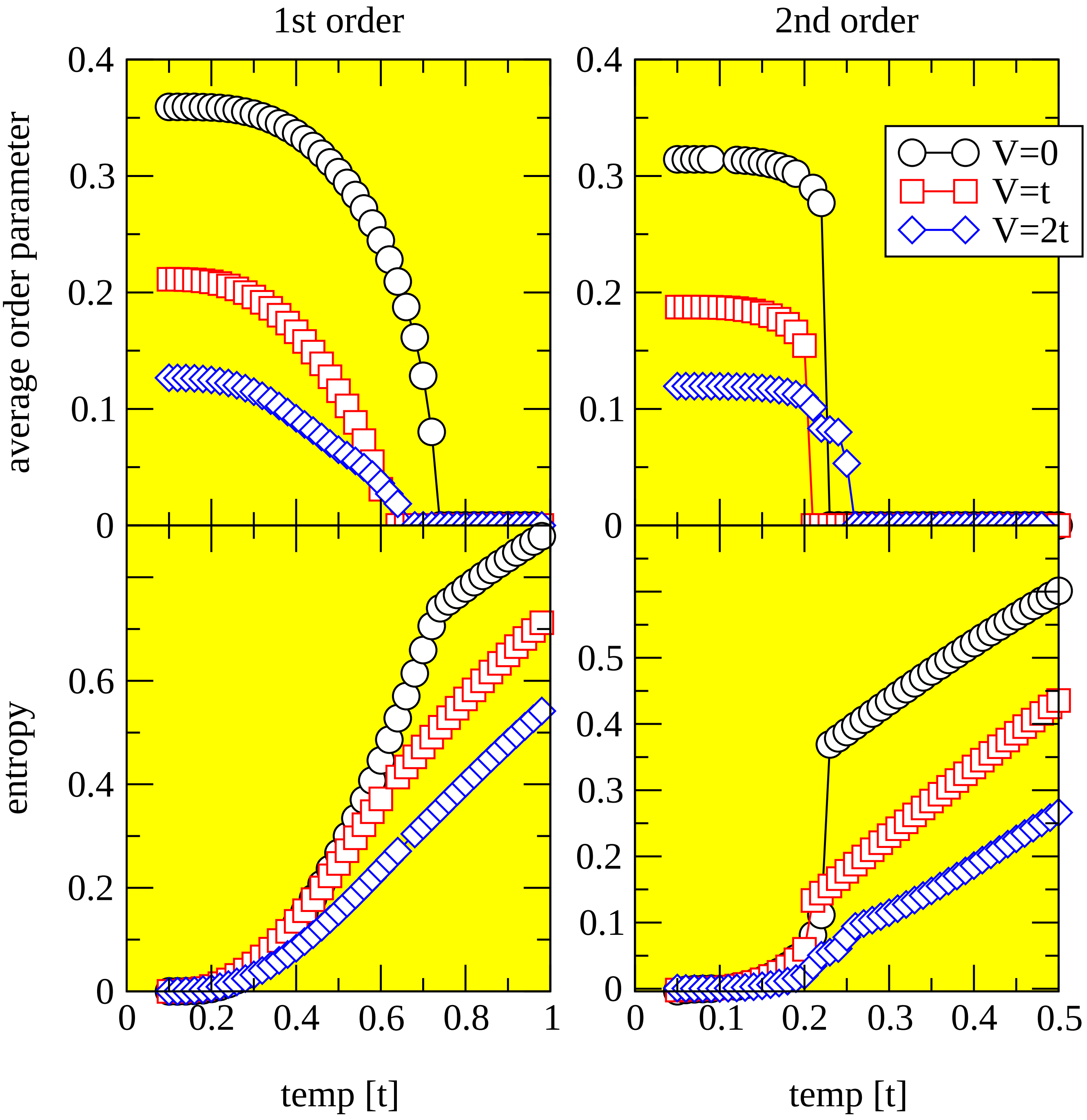

2nd order

$V = 2t$


1st order

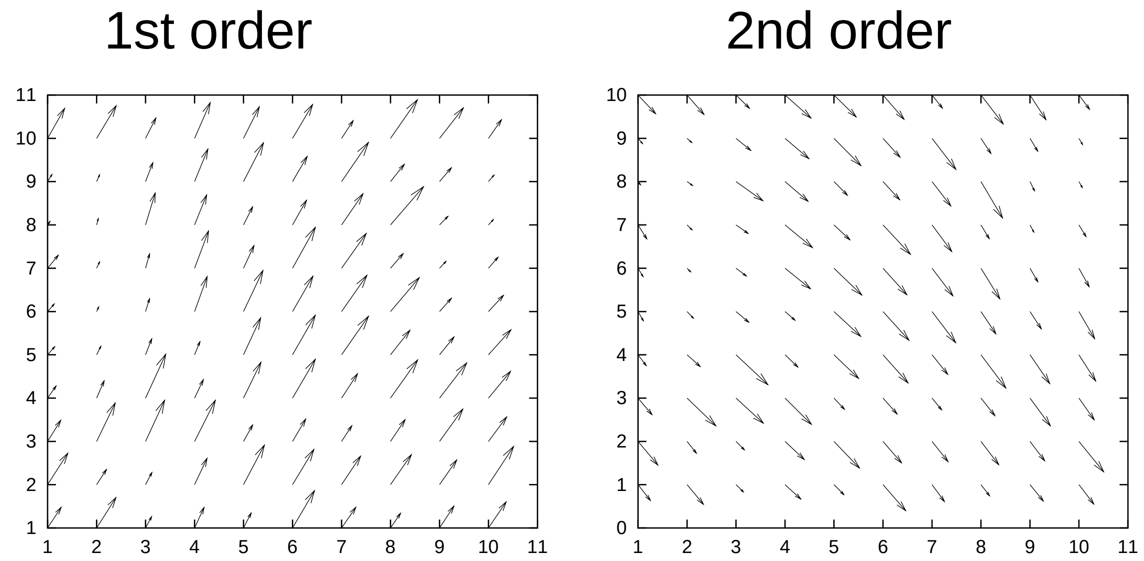

2nd order

Thermodynamics



Stiffness for V=t

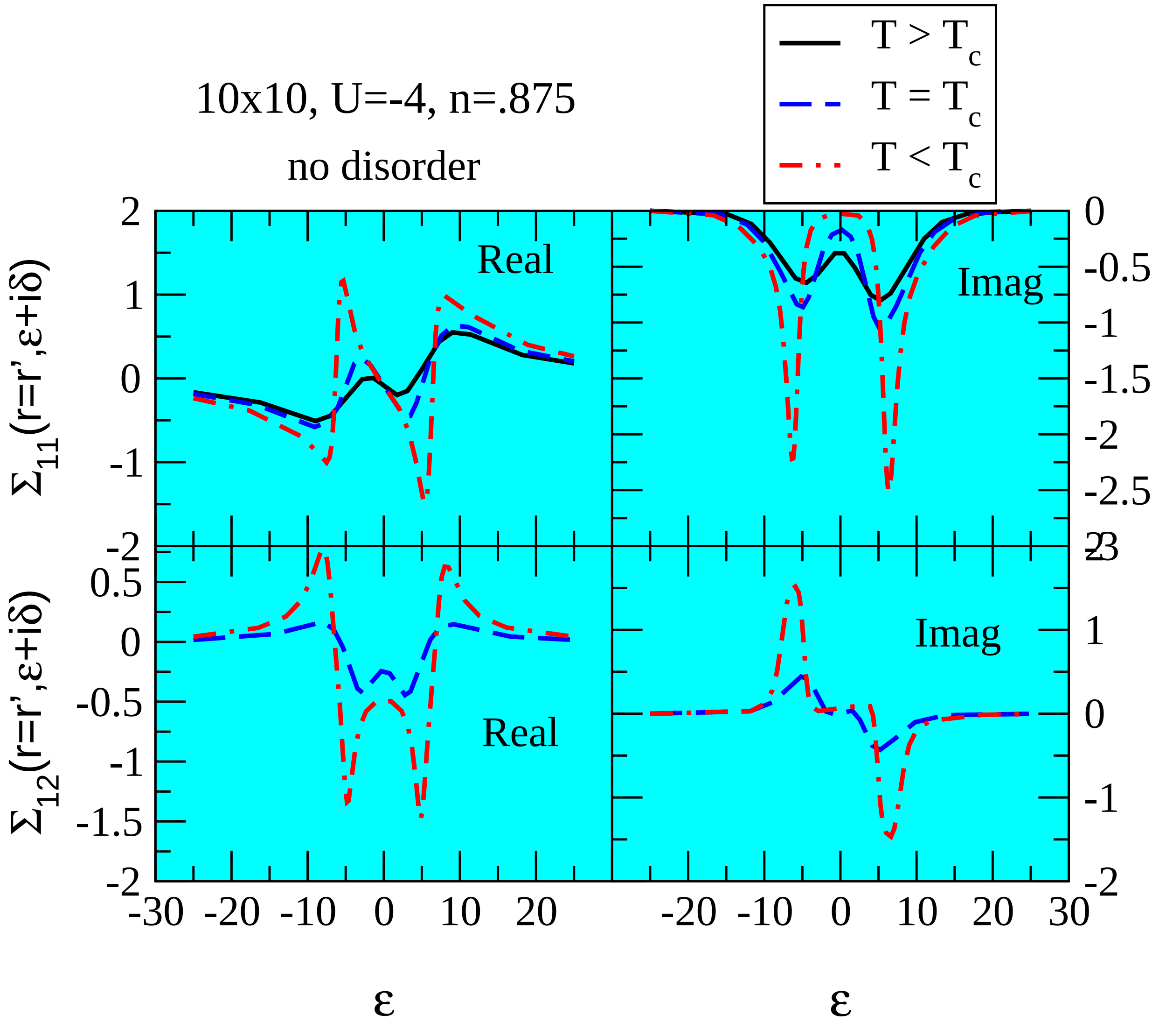
Threaded field induces gradients in in the pairing phase.



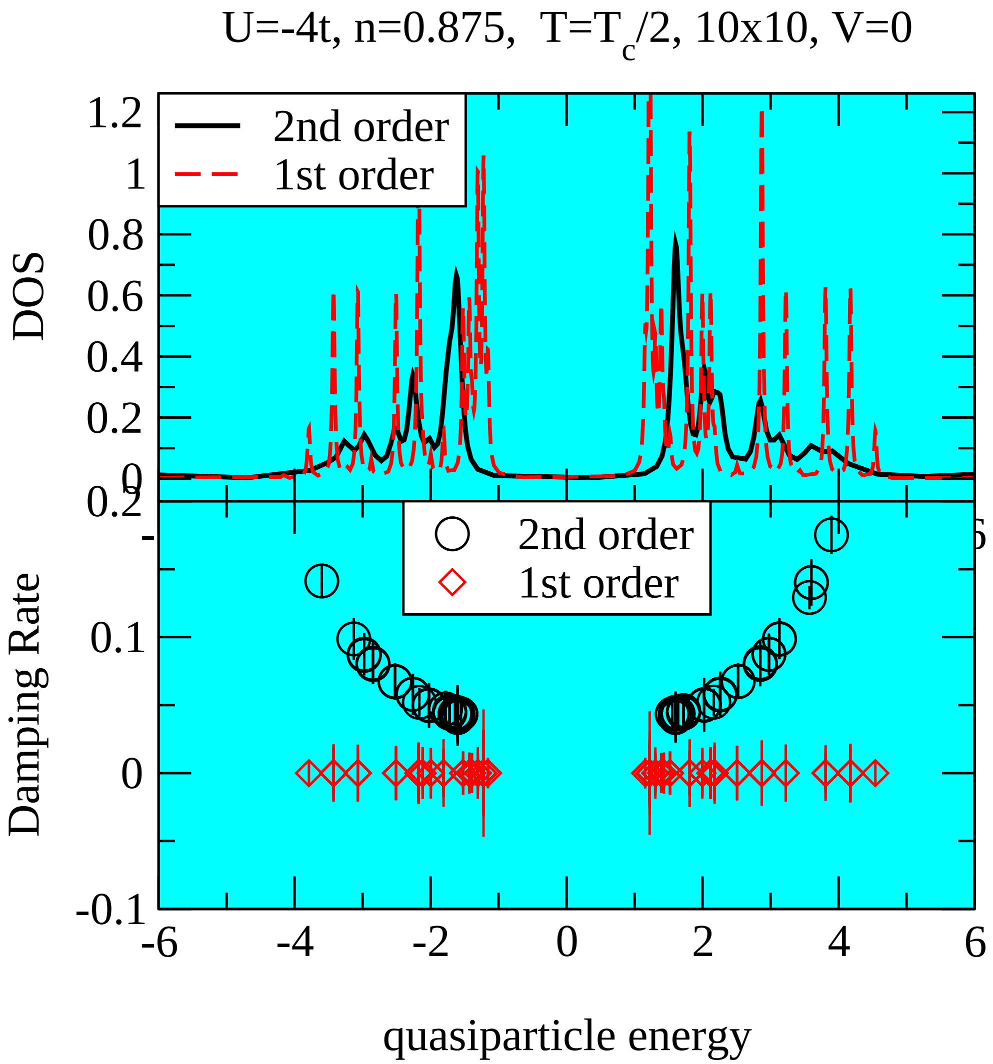
- Strong reduction in stiffness with V.
- Greater stiffness in 2nd order.
- Likely unstable to fluctuations for $V > t$.

Electronic excitations

Properties of electronic excitations are obtained through an analytic continuation of the self-energy from the imaginary-frequency axis to the real-frequency axis.

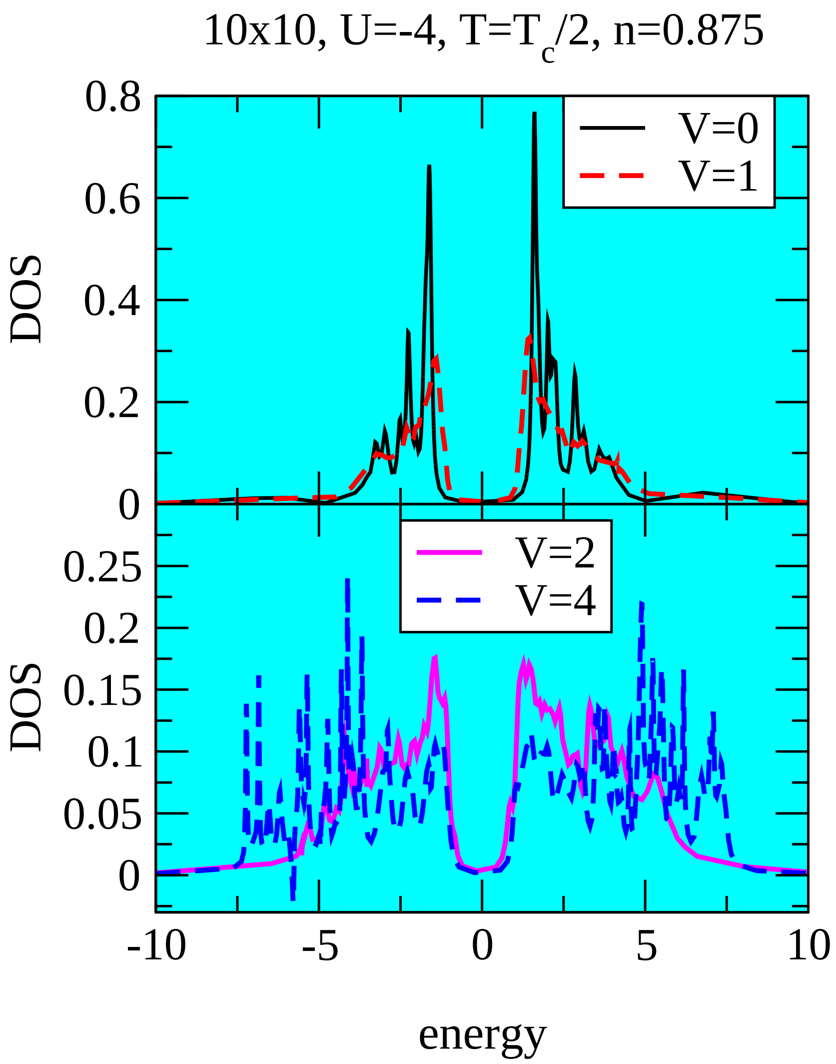


1st and 2nd order P.T. for $V = 0$



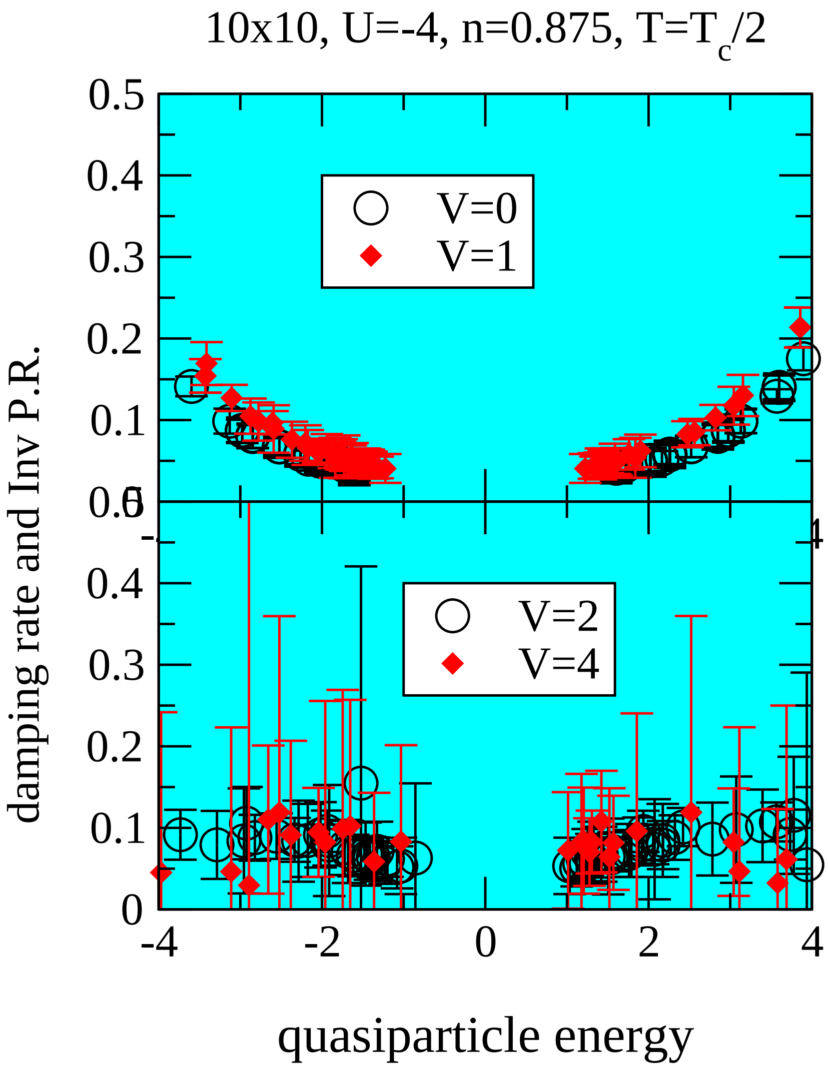
- Vertical lines in bottom graph indicate size of the inverse participation ratio for that excitation.

DOS vs. disorder strength (2nd order)



- Gap persists to large disorder values.
- Analytic continuation problems for large V.

Quasiparticle excitations



- Increased localization (larger IPR) as disorder increases.

Perturbation theory summary

1. Dominant ordering pattern is insensitive to strong coupling corrections, but the calculated phase stability strongly depends on the approximation.

2. Superconducting gap persists to large disorder (as observed earlier with QMC and 1st order p.t.). Excitations are localized even near the gap edges.

3. Demonstrated that such calculations are computationally practical. System sizes of order 25×25 are feasible.

II.B. Dynamical mean-field approximation (w/ Jarrell and Hess)

Algorithm

1. Each unit cell is embedded in a correlated two-dimensional host.
2. The interactions in the unit cell are treated exactly (to within statistical precision) using an impurity quantum Monte Carlo algorithm.
3. Newly recalculated cell properties determine new effective host for each site.
4. Iterated to self-consistency (5 to 10 iterations).

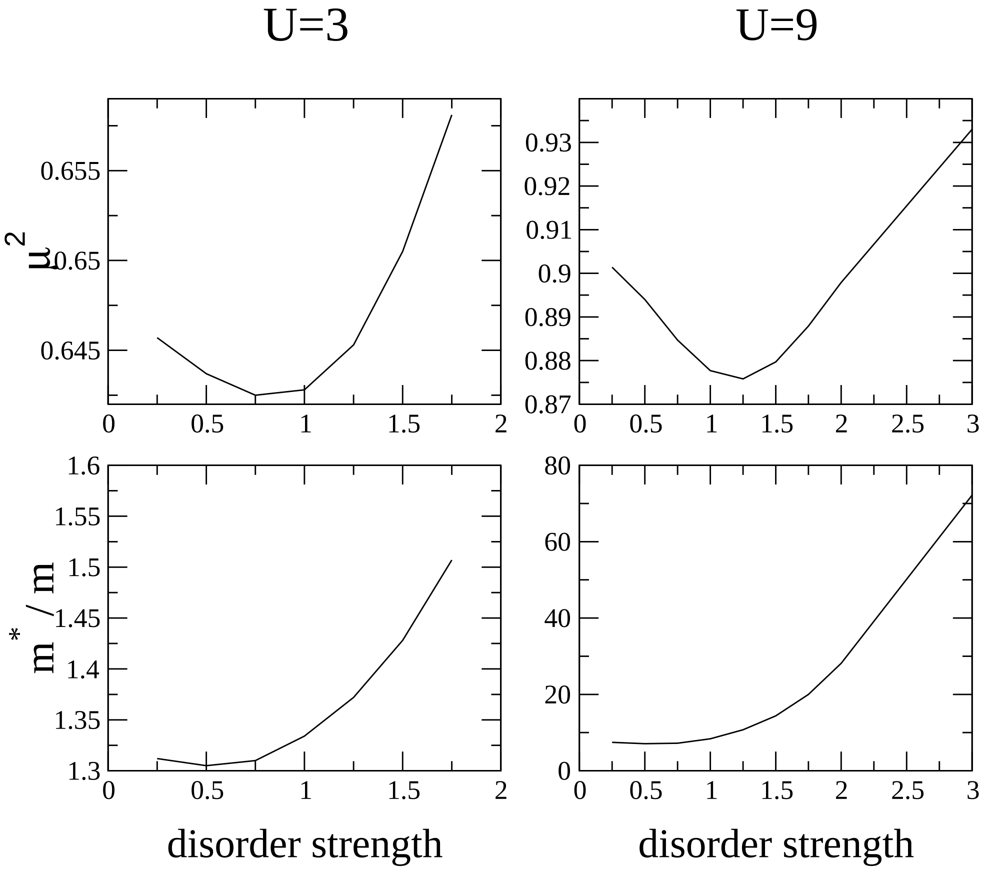
Advantages

- Anderson and Mott transition mechanisms are included
- Linear scaling
- Large lattices, up to 64×64 sites

Disadvantages

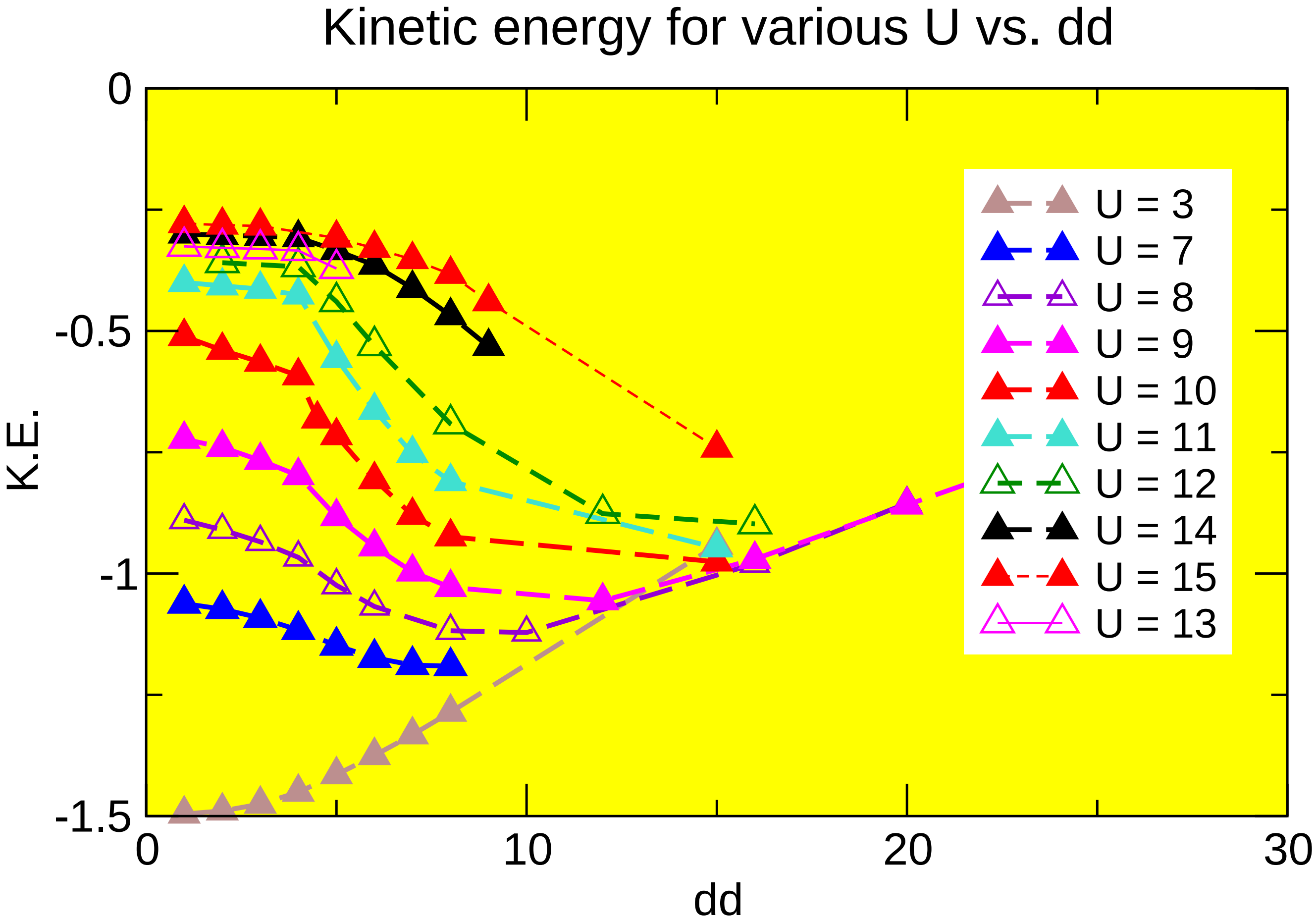
- No fluctuation effects
- 1-particle calculations are straightforward, 2-particle calculations (conductivity) are difficult

Some results



- Disorder tends to increase the effective mass (m^*) of the electrons (localization?).

- Disorder tends to initially fight the effect of interactions and then it enhances interaction effects (more Mott-like).


Kinetic energy for various U vs. dd
0
-0.5
-1
-1.5
K.E.
0
10
20
30
dd
U = 3
U = 7
U = 8
U = 9
U = 10
U = 11
U = 12
U = 14
U = 15
U = 13

II.C. Dynamical cluster approximation (w/ Jarrell, *et al.*)

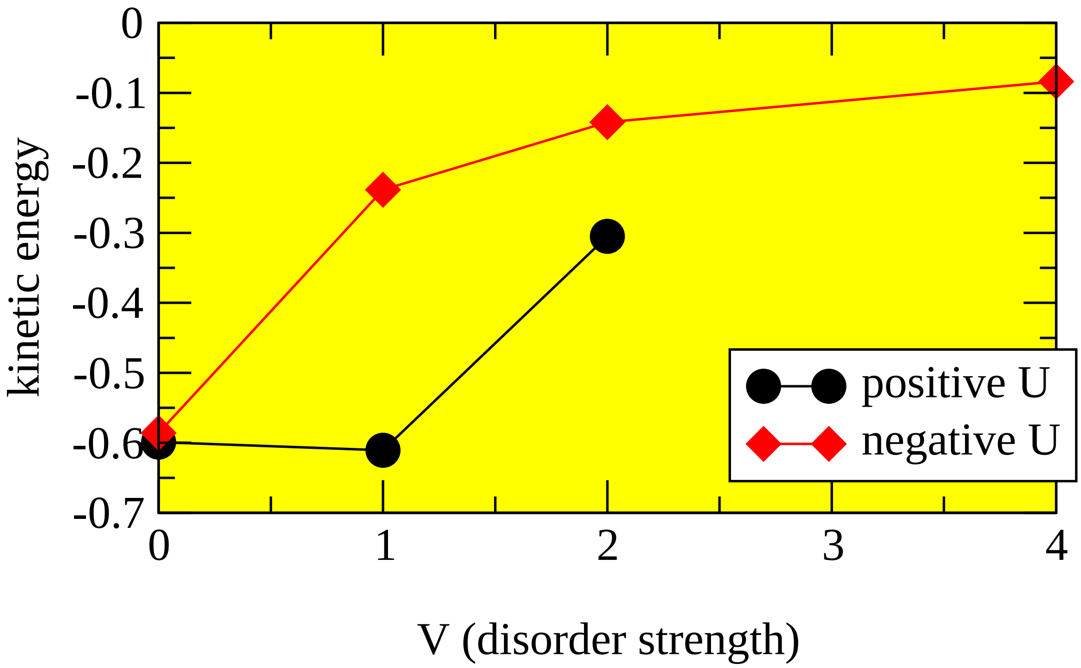
Algorithm (Jarrell and Krishnamurty, 2001)

Clusters of size N_c are embedded in a disorder-averaged host

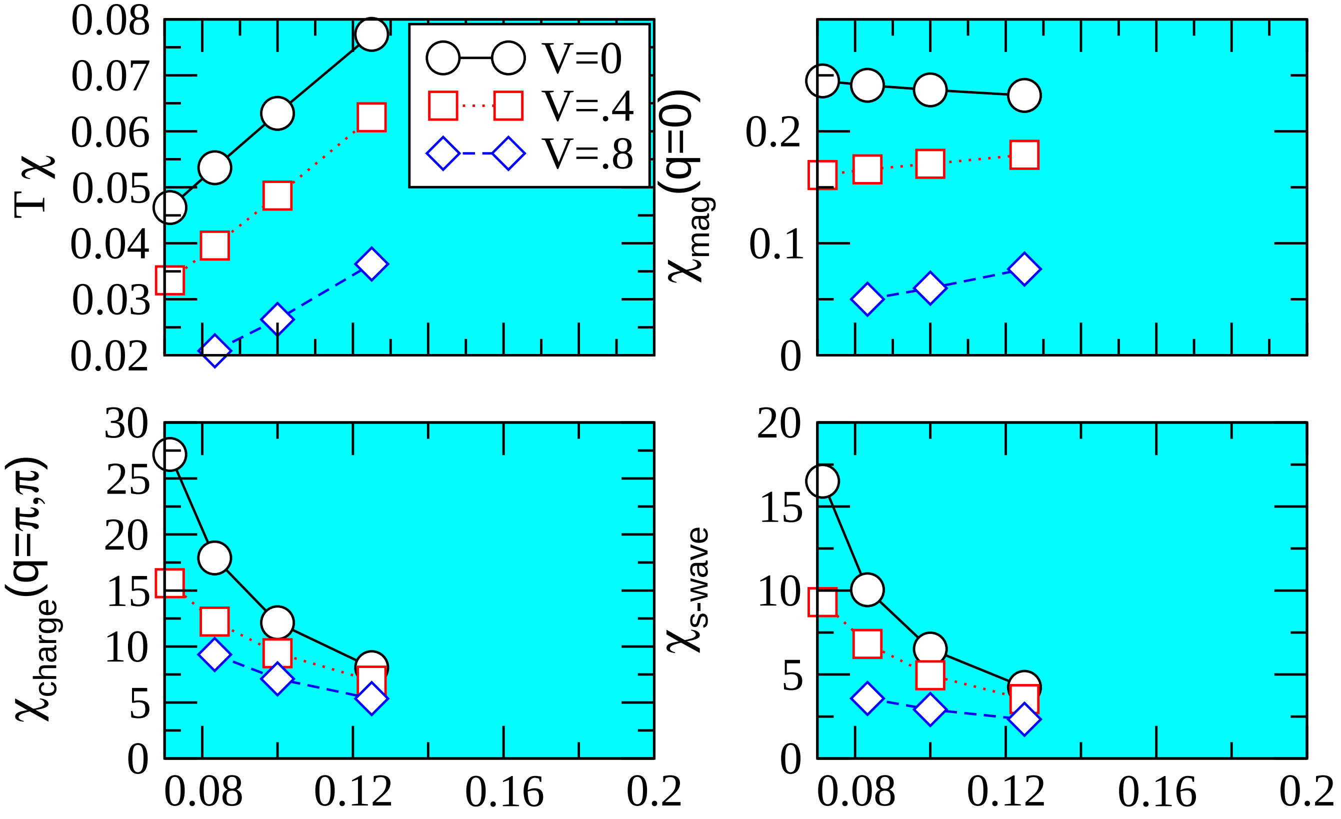
- Generalization of CPA
- Intersite correlations are cut-off on a length scale determined by N_c. For larger length scales, averaging restores periodicity.
- Always in the thermodynamic limit.
- Cluster problem is solved with QMC.

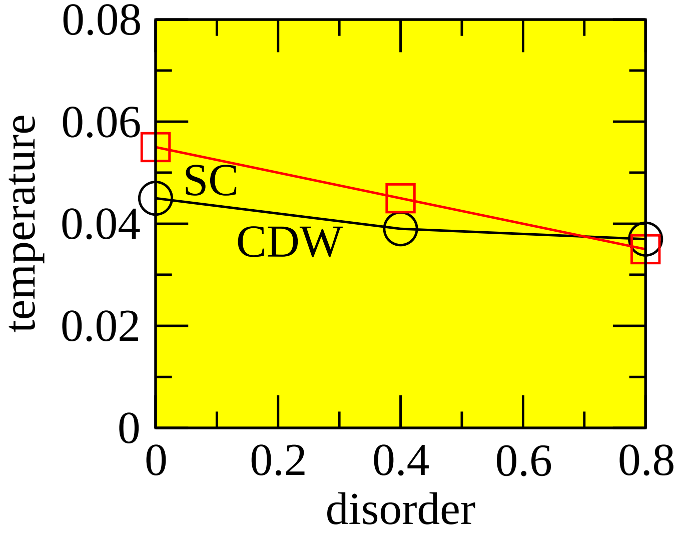
Results: negative U vs. positive U

$|U|=8, \beta=0.5, n=.9$



- Repulsion fights potential variation, attraction enhances it.


T χ
$\chi_{mag}(q=0)$
$\chi_{charge}(q=\pi,\pi)$
$\chi_{s\text{-wave}}$
V=0
V=.4
V=.8
0.02
0.03
0.04
0.05
0.06
0.07
0.08
0
0.1
0.2
0
5
10
15
20
25
30
0
5
10
15
20
0.08
0.12
0.16
0.2
0.08
0.12
0.16
0.2


temperature
disorder
SC
CDW
0
0.02
0.04
0.06
0.08
0
0.2
0.4
0.6
0.8