Advanced Computation for Complex Materials

- Computational Progress is brainpower limited, not machine limited
  - Algorithms
  - Physics
- Major progress in algorithms
  - Quantum Monte Carlo
  - Density Matrix Renormalization Group
- Building the right Hamiltonians
- Solving the dimensionality/sign problem

UCIrvine
University of California, Irvine

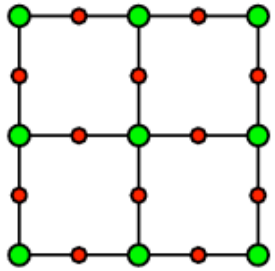
Getting started: density functional theory

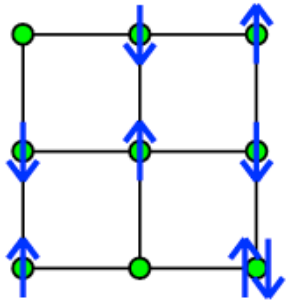
- "DFT is exact" is a silly statement.
- LDA and LDA++ are clever, useful calculation schemes
  - Always useful for getting started with a new material
  - Maybe all that's needed for weakly correlated systems
  - Maybe all you can do for complex structures
  - The Wrong Framework for strongly correlated systems
    - Strong interatomic correlations not treated
- Hybrids (LDA+DMFT) useful in some cases
- Many systems require reduction to a model: the correlations are too complicated.
- Getting the model:
  - The past: educated, insightful guesswork...
  - The future: systematic reduction from band structure?

Solving lattice models

- Direct attack (exact diagonalization): Exponential growth of effort with system size
  - Going from workstation to supercomputer only buys you a few more sites
- Clever algorithms: beating the exponential
  - Quantum Monte Carlo
    - Determinantal
    - World line, stochastic series expansions: loop algorithms!
  - Density matrix renormalization group
- History of previous advances:
  - An improved algorithm allows a new class of problems or new regime to be solved
  - Trying to go beyond the regime runs into exponential problems.

Example: QMC for the Hubbard Model





- First step: Blancenbecler, Sugar, Scalapino used the Trotter decomposition

$$e^{-\beta H} \approx e^{-\tau H} \ldots e^{-\tau H}$$

- and the Hubbard Stratonovich decomposition

$$e^{-\tau U n_{i\uparrow} n_{i\downarrow}} \sim \sum_{s_i} e^{-\gamma s_i (n_{i\uparrow} - n_{i\downarrow})}$$

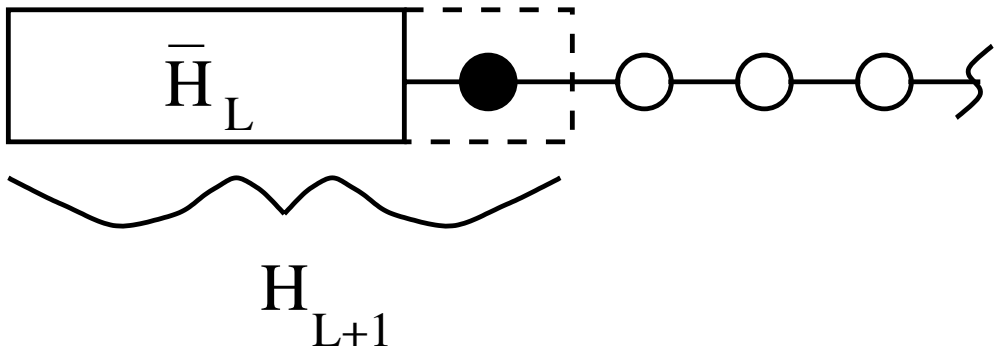
- to turn the quantum problem into a Ising-like noninteracting Monte Carlo calculation
- This was applied to get some of the first nonperturbative results for the Hubbard model in 1D and 2D

Example: QMC for the Hubbard Model (cont)

- First problem: for $\beta >\sim 4$, a numerical instability ruined the simulation, requiring quadruple precision
- Solution: we found a matrix factorization procedure that cured the instability at all β
- Second problem: once we could go to lower temperatures, we encountered the fermion sign problem ($\beta \sim 6$) away from half filling.
  - Universal problem related to Fermi statistics
  - Problem is in treating a nonpositive quantity as a probability
  - Simulations still possible (use $|P|$) but get exponentially hard as $\langle sign(P) \rangle$ vanishes
- All QMC methods still suffer the sign problem, but some approximate treatments have emerged (constrain sign with approximate wavefunction).

Example: Numerical RGs

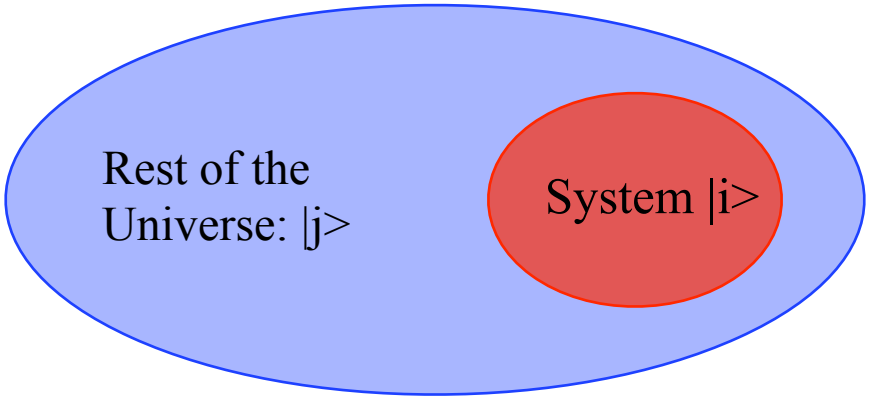
- The Kondo impurity problem was one of the big unsolved problems of the 60's and early 70's
- Wilson (1975) showed how to map it onto a special 1D half-chain and how to diagonalize the system one step at a time, adding sites:



- This showed how to solve a wide variety of impurity problems. For ordinary 1D lattice systems, the method failed.

Density Matrix Methods

- RG: throw away unimportant states, effective H in truncated basis
- Statistical Mechanics Viewpoint (Feynman SM lectures)



$$|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle |j\rangle$$

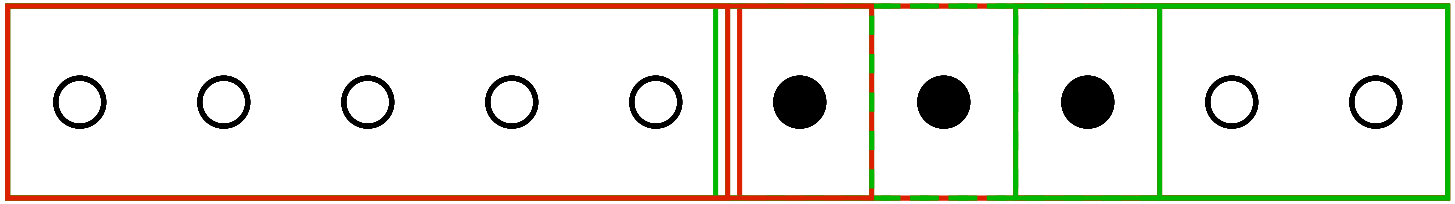
$$\rho_{ii'} = \sum_{j} \psi^*_{ij} \psi_{i'j}$$

$$\langle A \rangle = \sum_{\alpha} w_\alpha \langle \alpha | A | \alpha \rangle$$

- Quantum Information viewpoint
  - The entanglement between two systems is determined by its Schmidt decomposition.
  - The Schmidt decomposition is equivalent to changing basis to the density matrix eigenvectors!

DMRG Algorithm

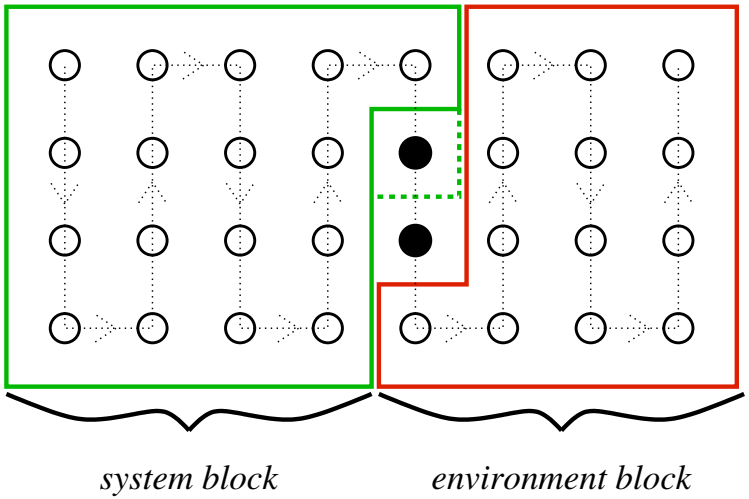
- Finite system method:



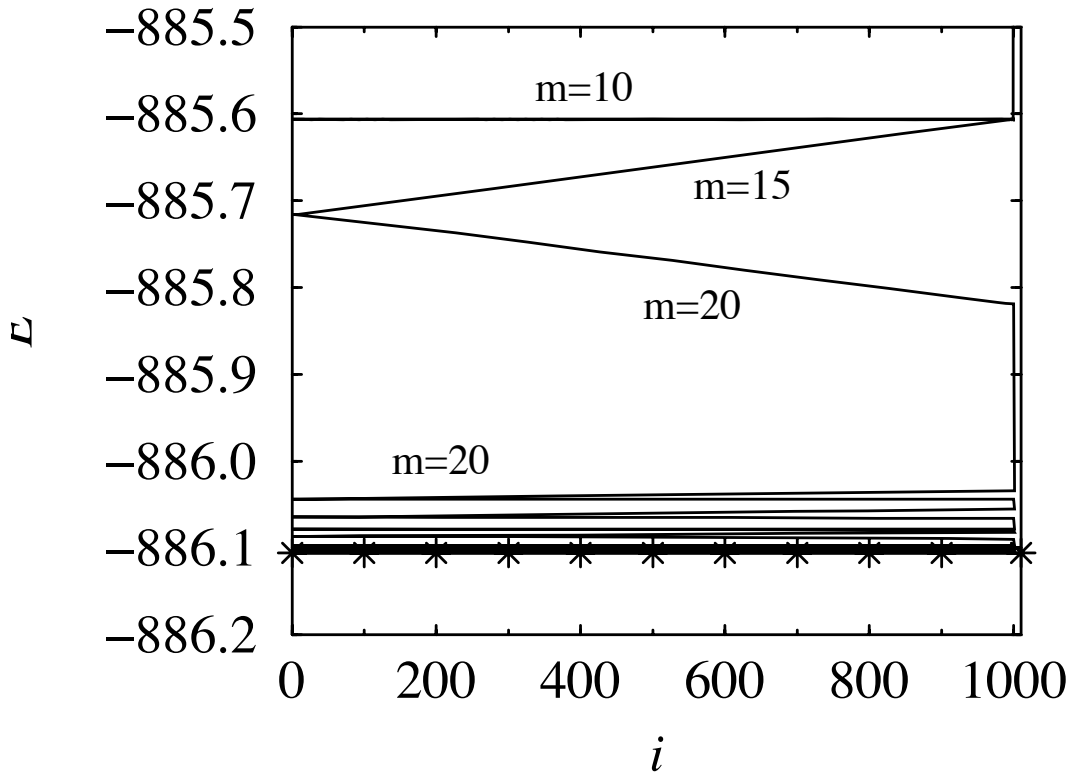
- Wavefunction = matrix product state(Ostlund & Rommer,1995)

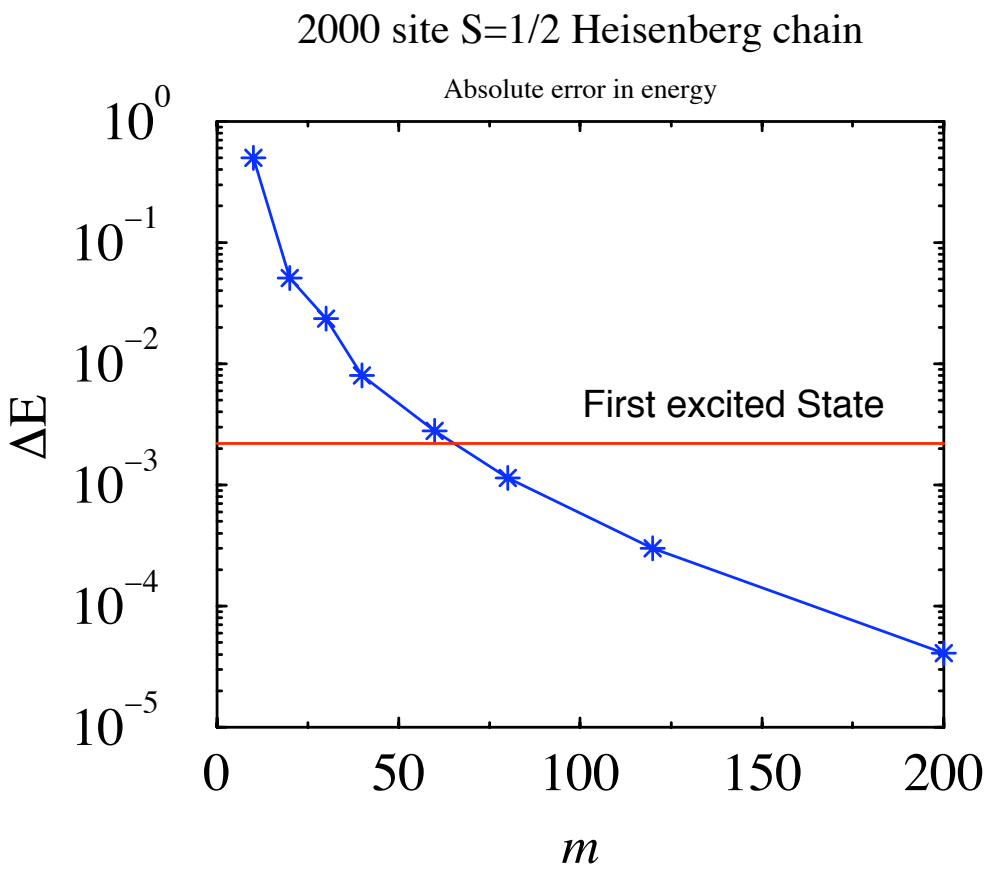
$$\psi(s_1, s_2, \ldots) = \mathrm{Tr}\{A_1^{s_1} A_2^{s_2} \ldots\}$$

- 2D: map onto chain
  - Accuracy falls of exp'ly in width

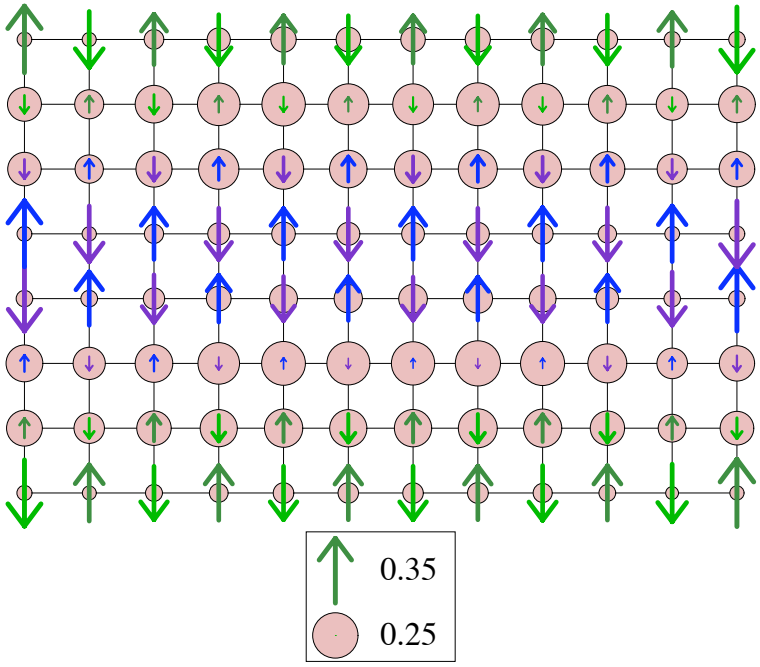


DMRG Convergence in 1D



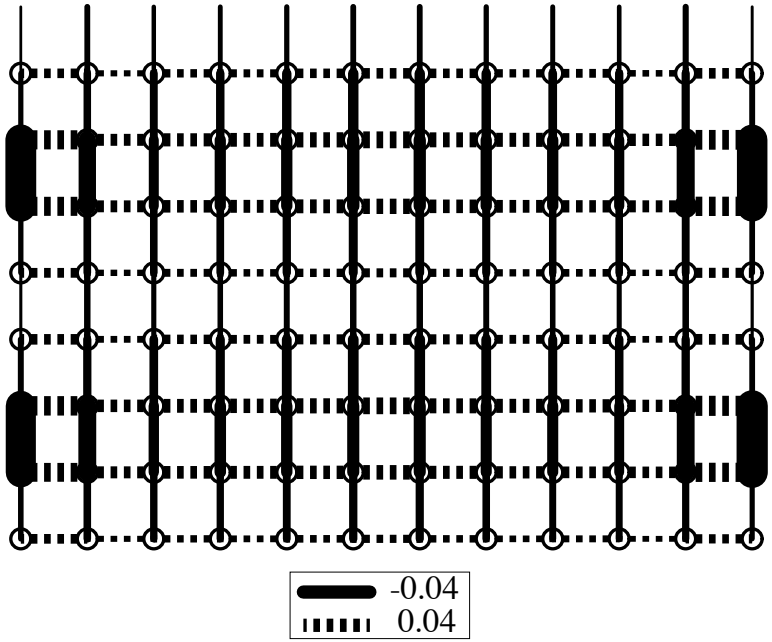


DMRG--doped "2D" systems



12 x 8 system, Vertical PBC's
Jx/t= 0.55,Jy/t=0.45, mu=1.165,doping=0.1579

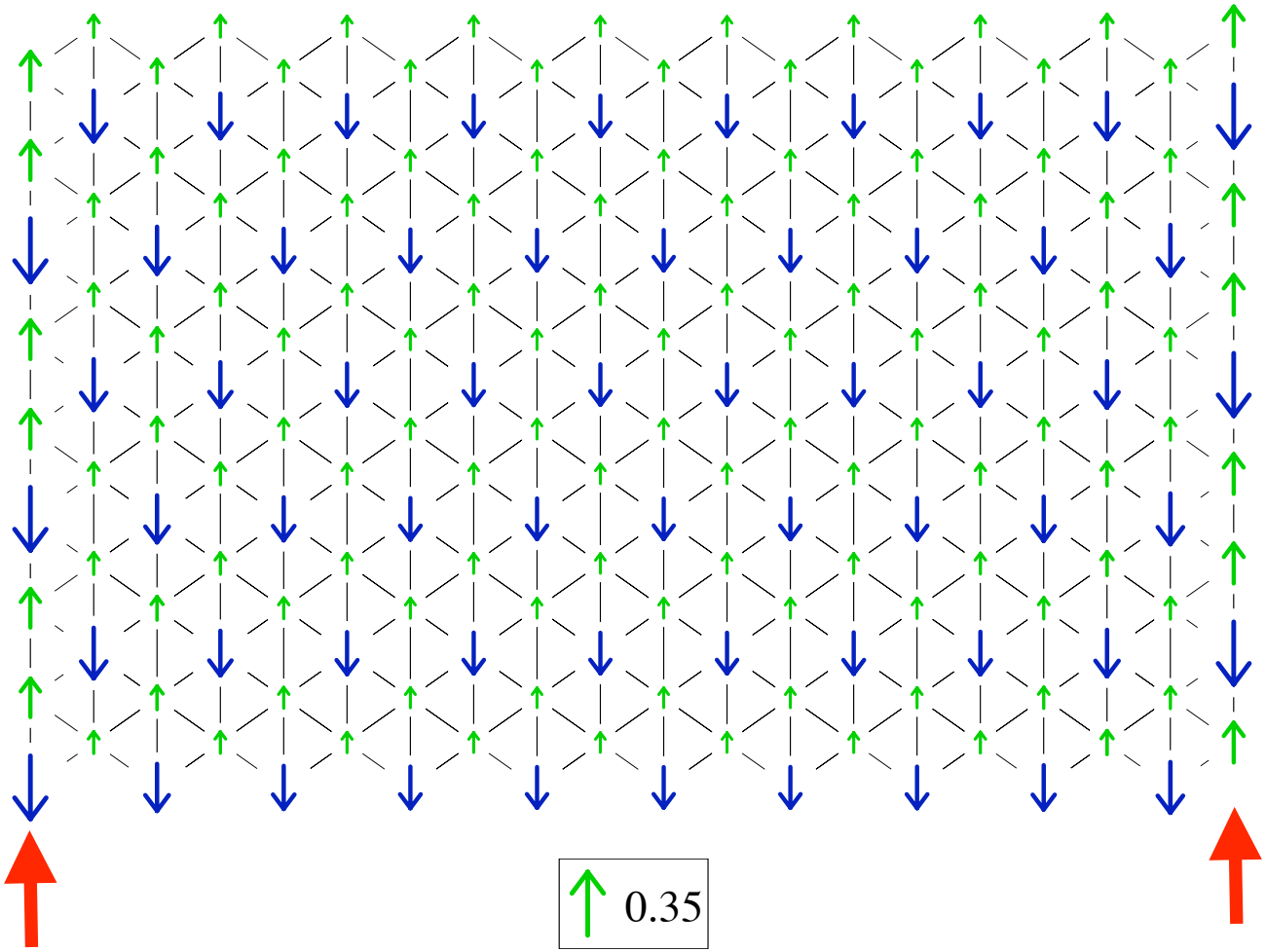
Stripes



12 x 8 system, Vertical PBC's
Jx/t= 0.55,Jy/t=0.45, mu=1.165,doping=0.1579

Local pairing along stripes

Triangular Lattice



- Only one sublattice pinned, other two rotate in a cone
- Other two have z component -M/2
- Here only have $L_y = 3, 6, 9, \ldots$

DMRG, QMC: Status as of ~2000

- 2D Unfrustrated spin systems:
  - QMC improvements (loop algorithm!) enable huge systems, high accuracy
- 2D Fermions:
  - DMRG: very accurate on ladders, accuracy falls of exp'ly with width, still useful up to ~16x8 t-J clusters
  - QMC: Improvements in methods and variational wavefunctions give excellent results
  - But: still disagreements on pairing versus stripe/CDWs in key models: materials chaos!
- Dynamics: very limited!

DMRG: New developments

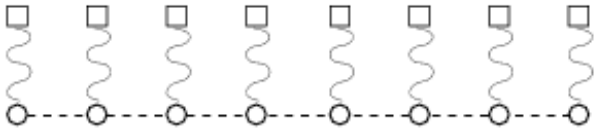
- Quantum Information: Major new ideas for DMRG!
  - Key people: Vidal, Verstraete, Cirac
  - Time evolution, even far from equilibrium
  - Finite temperature, disorder, periodic boundaries
  - New 2D "PEPS" method: linear scaling in width, all exponential scaling gone!
    - Unfortunately, on current computers, still more efficient to use older mapping to 1D DMRG.
- Why has QI been so successful?
  - They think about evolution of quantum states.
  - They introduce auxiliary systems to manage entanglement.
  - Many clever mathematical tricks.

Example of QI applied to DMRG

Ancilla and finite temperature

DMRG gets its efficiency because the basis is specialized for the state. Infinite temperature seems infinitely hard from this point of view.

Ancilla are artificial auxilliary sites paired with the real sites.



They can make a perfect heat bath (Suzuki, ..., Verstraete and Cirac). Let the state of each site-ancilla pair be a perfectly entangled state

$$|E_i\rangle = \sum_s |s\rangle|s\rangle_a$$

Then

$$|\psi\rangle = \prod_i |E_i\rangle$$

is a perfect representation of the $T = \infty$ ensemble, but requires a local DMRG basis of size $m = 1$!

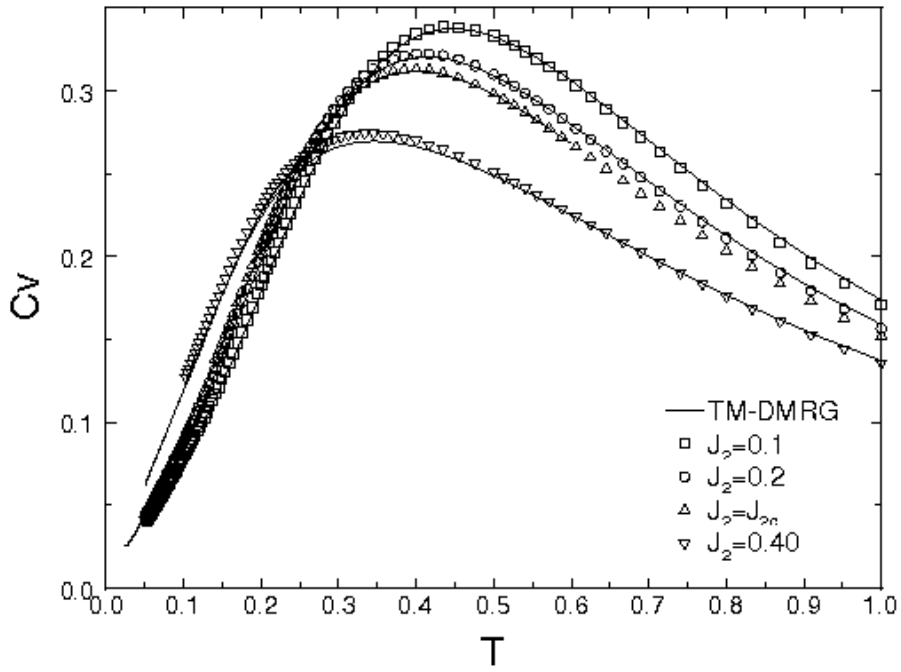
Evolve in imaginary time to get $|\psi(t)\rangle = \exp(-\beta H/2)|\psi\rangle$, then any finite temperature

β observable can be obtained:

$$< A >= \frac{\langle \psi(t)|A|\psi(t)\rangle}{\langle \psi(t)|\psi(t)\rangle}$$

The partition function, free energy, C_v, etc, as well as real-time finite temperature dynamics are easily obtained.

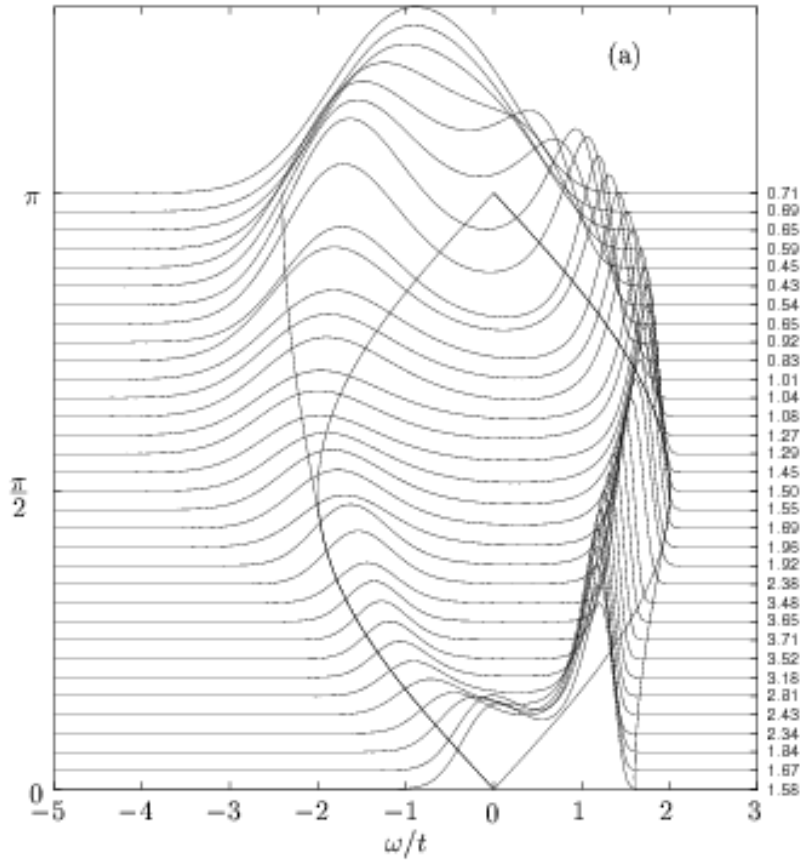
$J_1 - J_2$ Model(1D)

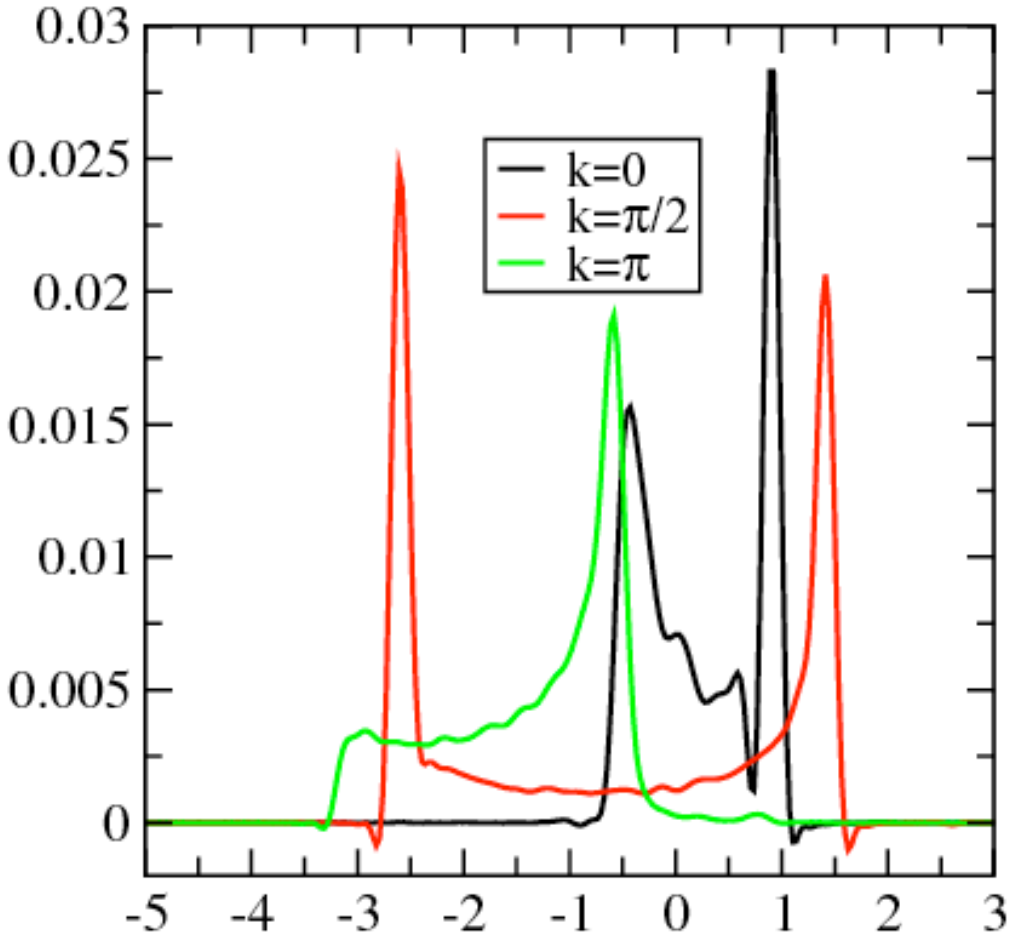


Example: dynamics from DMRG

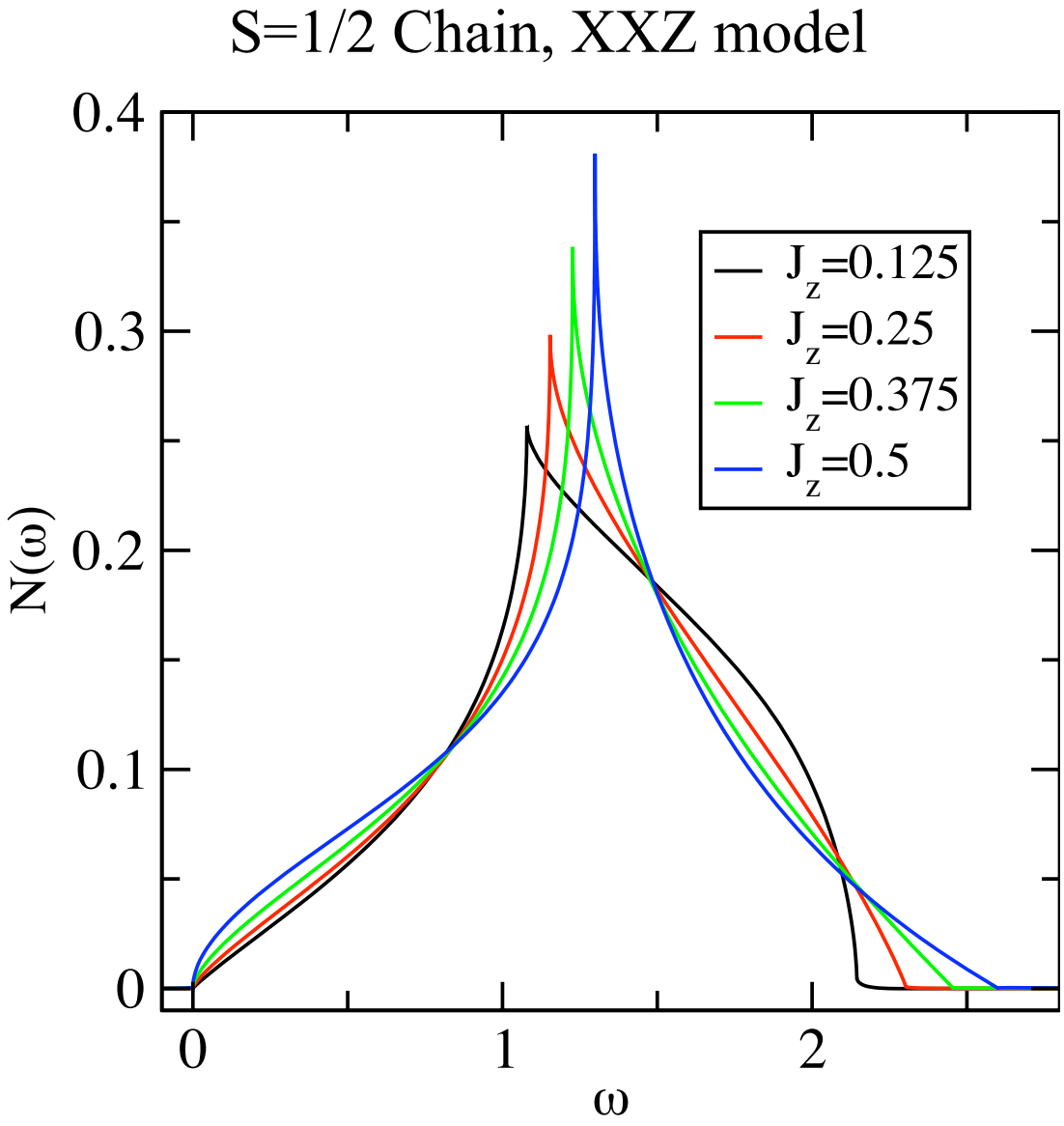
Example system: 1-d t-J model

1D t-J system, spectral weight function for adding one hole to the half-filled (undoped) system. $J = 0.4$. Left hand panel shows results of Brunner, Assaad, and Muramatsu, $L = 64$, using a special quantum Monte Carlo good for one hole and maximum entropy. Right panel is RK method, $L = 200$, $m = 300$, total time $T = 20$.





Example: dynamics for 1D systems



PEPS--True 2D DMRG?

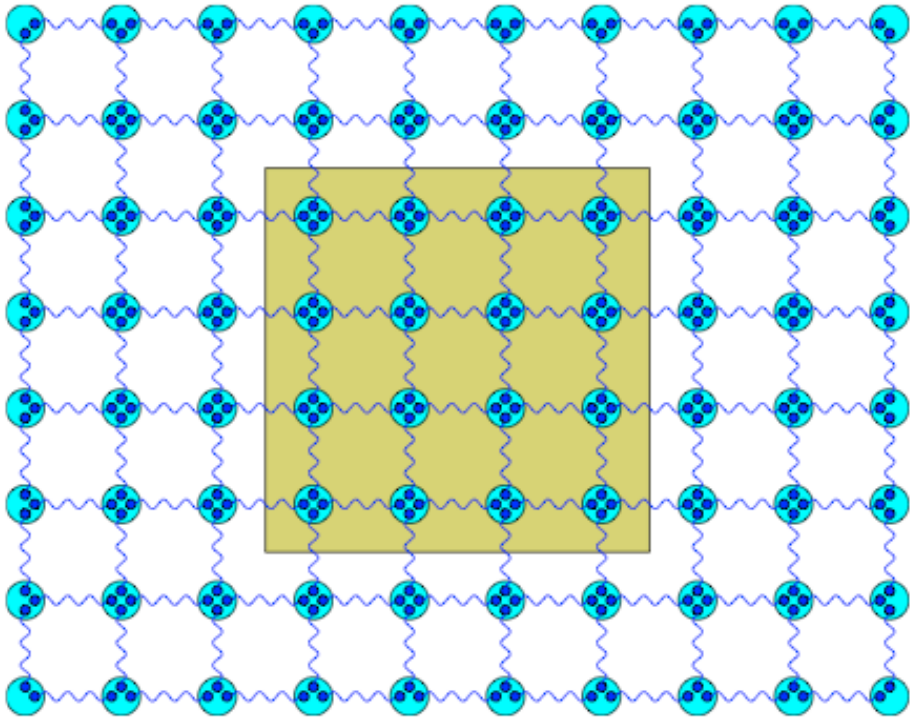
$|\psi\rangle =$

DMRG

$$\psi(s_1, \ldots s_N) = A^{s_1} \ldots A^{s_N}$$

General variational state (MPS)

Projected Entangle Pair State: wavefunction = contraction of tensor network



PEPS: prospects

- Currently, PEPS is less efficient than old-style DMRG for accessible sizes (e.g. 8x8)
- But: calculation time is not exponential (m^{10})
- In the last few months, there have been three papers combining PEPS with Monte Carlo (m^5)

Conclusions

- Algorithmic development has been the key driving force in computation for solid state physics (and other fields!)
- Quantum Information has a lot to teach us about simulations!
- Issues/Discussion:
  - Why are there so few DMRG/QMC/etc people in the US?
  - Software
    - Languages: fast production versus efficiency; freedom from bugs; large codes versus small codes; time to learn the language
    - Software libraries so you don't have to reinvent the wheel.

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