Diagonalization- and Numerical Renormalization-Group-based Methods for Interacting Quantum Systems

Reinhard M. Noack

Fachbereich Physik

Philipps-Universität Marburg, Germany

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Literature:

- *Density Matrix Renormalization: A New Numerical Method in Physics*, Eds. I. Peschel, X. Wang, M. Kaulke, and K. Hallberg, Springer Verlag, Berlin, June 1999.
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Outline

I. Exact Diagonalization
  (i) Introduction to interacting quantum systems
  (ii) Representation of many-body states
  (iii) Complete Diagonalization
  (iv) Iterative Diagonalization (Lanczos and Davidson)
  (v) Dynamics
  (vi) Finite temperature

II. Numerical Renormalization Group
  (i) Anderson and Kondo problems
  (ii) Numerical RG for the Kondo problem
  (iii) Numerical RG for quantum lattice problems
  (iv) Numerical RG for a noninteracting particle

III. From the NRG to the Density Matrix Renormalization Group
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IV. The DMRG in Detail
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V. Recent Developments in the DMRG

(i) Classical transfer matrices

(ii) Finite temperature

(iii) Dynamics

(iv) Quantum chemistry

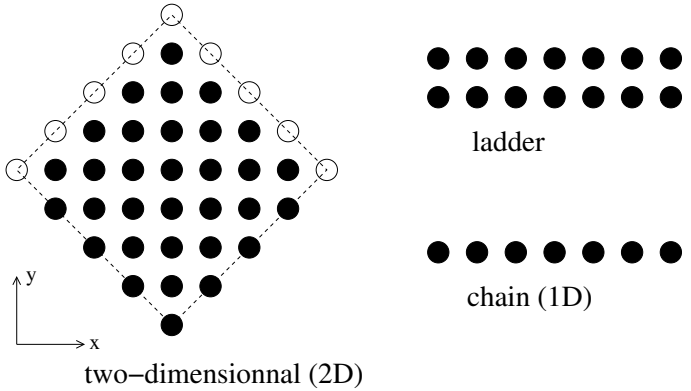
(v) Time evolution

(vi) Matrix product states

(vii) Quantum information

I. Exact Diagonalization

Direct diagonalization of Hamiltonian matrix on finite clusters



Goals

- ground state properties
- low-lying excitations
- dynamics, finite T, ...

Advantages

- almost any system can be treated
- almost any observable can be calculated
- quantum-number resolved quantities
- numerically exact (for finite cluster)

Limitation: exponential in lattice size

Largest sizes reached

- $S = 1/2$ spin models
  square lattice: $N = 40$ triangular lattice: $N = 39$, star lattice: $N = 42$
  maximum dimension of basis: 1.5 billion
- t-J models
  checkerboard lattice with 2 holes: $N = 32$
  square lattice with 2 holes: $N = 32$
  maximum dimension of basis: 2.8 billion
- Hubbard models
  square lattice at half filling: $N = 20$
  quantum dot structure: $N = 20$
  maximum dimension of basis: 3 billion
- Holstein models
  chain with $N = 14$ + phonon pseudo-sites
  maximum dimension of basis: 30 billion

I (i) Interacting Quantum Systems

Here: discrete, finite case

- system of N quantum mechanical subsystems, $\ell = 1, \ldots, N$
- finite number of basis states per subsystem

$$|\alpha_\ell\rangle \,, \qquad \alpha_\ell = 1, \ldots, s_\ell$$

- more general case: $s_\ell \to \infty$ (continuum or thermodynamic limit)

$N \to \infty$ (thermodynamic limit)

$\ell \to x$ (continuous quantum field)

Properties:

- Basis *direct product* of component basis

$$|\alpha_1, \alpha_2, \ldots, \alpha_N\rangle \equiv |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \ldots \otimes |\alpha_N\rangle$$

$\Rightarrow$ total number of states: $\prod_{\ell=1}^{N} s_\ell$

- arbitrary state in this basis

$$|\psi\rangle = \sum_{\{\alpha_\ell\}} \psi(\alpha_1, \alpha_2, \ldots, \alpha_N)\, |\alpha_1, \alpha_2, \ldots, \alpha_N\rangle$$

- behavior governed by Schrödinger equation

$$H\,|\Psi(t)\rangle = i\hbar\,\frac{\partial}{\partial t}\,|\Psi(t)\rangle \quad \text{or} \quad H\,|\psi\rangle = E\,|\psi\rangle \quad \text{(time-independent)}$$

Hamiltonians

In general, Hamiltonians can connect arbitrary numbers of subsystems

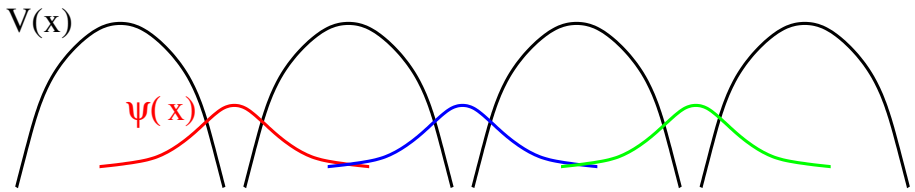
$$H = \sum_{\ell} H^{(1)}_{\ell} + \sum_{\ell,m} H^{(2)}_{\ell m} + \ldots + \sum_{\ell,m,p} H^{(4)}_{\ell mnp} + \ldots$$

- $H^{(1)}_{\ell}$ usually determines $|\alpha_\ell\rangle$
- $H^{(2)}_{\ell m}$, sometimes $H^{(4)}_{\ell mnp}$ will be important here
- $H^{(2)}_{\ell m}$ often short-ranged

Typical terms:

- tight-binding term:

$$H^{\rm tb} = -\sum_{\ell,m,\sigma} t_{\ell m}\, c^{\dagger}_{\ell,\sigma} c_{m,\sigma}$$



- localized Wannier orbitals (unfilled d- or f- orbitals in transition metals)
- states $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, $|\uparrow\downarrow\rangle$ per orbital $\rightarrow 4^N$ degrees of freedom
- overlap between near orbitals – "hopping" t_{lm} short ranged (n.n., possibly n.n.n.)

- local (Anderson) disorder

$$H_\ell^{\rm A} = \sum_\sigma \lambda_\ell \; n_{\ell,\downarrow} \quad , \qquad n_{\ell,\sigma} \equiv c^\dagger_{\ell,\sigma} c_{\ell,\sigma}$$

- Coulomb interaction between electrons $\quad H^{\rm C}_{\ell m} = \dfrac{e^2}{|\mathbf{r}_\ell - \mathbf{r}_m|}$

  screening leads to
  - on-site (Hubbard) interaction

$$H_\ell^{\rm U} = U \; n_{\ell,\uparrow} n_{\ell,\downarrow}$$

  - near-neighbor Coulomb interaction

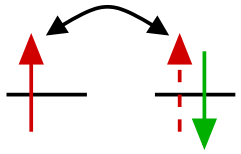
$$H^{\rm V}_{\ell m} = V \; n_\ell \; n_{\ell+\hat{\mathbf{r}}} \quad , \; (n_\ell \equiv \textstyle\sum_\sigma n_{\ell,\sigma}) \qquad \text{etc.}$$

- Spin models
  - $\mathbf{S}_i$ localized quantum mechanical spins ($S = 1/2, 1, 3/2, \ldots$)

    states $|-S\rangle \; |-S+1\rangle \ldots |S\rangle \Rightarrow (2S+1)^N$ degrees of freedom
  - Heisenberg exchange

$$H^{\rm Heis}_{\ell m} = J \; \mathbf{S}_\ell \cdot \mathbf{S}_m = J^z \; S^z_\ell S^z_m + \frac{1}{2} J^{xy} \left(S^+_\ell S^-_m + S^-_\ell \, S^+_m \right)$$

  - strong coupling limit of the Hubbard model at $n = 1$ ($S = 1/2$)



AF exchange $\rightarrow J = \frac{4t^2}{U}$

  - variations: $J^z \neq J^{xy}$ (Ising or XY anisotropy), $H^n_\ell = D(S^z_\ell)^2$ (single-ion),

$$H^{bq}_{\ell m} = J_2 \; \left(\mathbf{S}_\ell \cdot \mathbf{S}_m \right)^2 \text{ (biquadratic)}$$

- t–J model: strong-coupling limit of doped Hubbard

$$H^{tJ}_{\ell m} = \mathcal{P}\, H^{tb}_{\ell m}\, \mathcal{P} + J\, \left(\mathbf{S}_\ell \cdot \mathbf{S}_m \, - \, \frac{1}{4} n_\ell \, n_m \right)$$

  double occupancy projected out ($\mathcal{P}$) - 3 states/site

- Anderson impurity - hybridized d (or f) orbital with on-site interaction

$$H^{AI}_\ell \; = \; \varepsilon_d n^d_\ell \; + \; V \left(d^\dagger_{\ell,\sigma} c_{\ell,\sigma} + \mathrm{H.c.} \right) \; + \; U n^d_{\ell,\downarrow} n^d_{\ell,\downarrow}$$

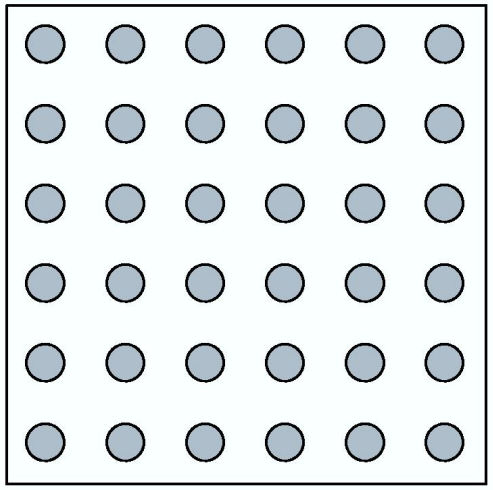
  single impurity or lattice (PAM) possible

- Kondo impurity - localized d spin $\mathbf{S}$

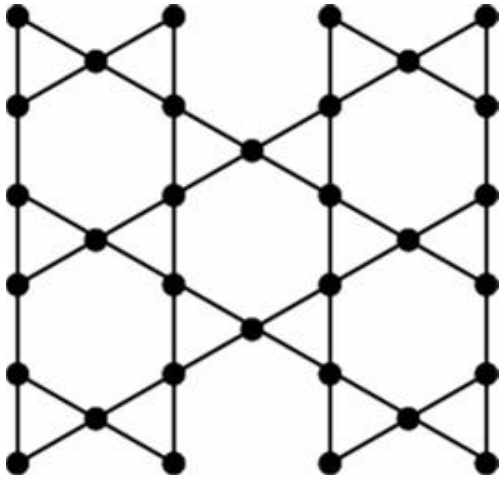
$$H^K_\ell = \frac{J_K}{2}\, \mathbf{S}_\ell \cdot \left(c^\dagger_{\ell,\alpha} \boldsymbol{\sigma}_{\alpha,\beta} c_{\ell,\beta} \right)$$

  limit of symmetric Anderson impurity at strong U

Lattices

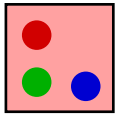


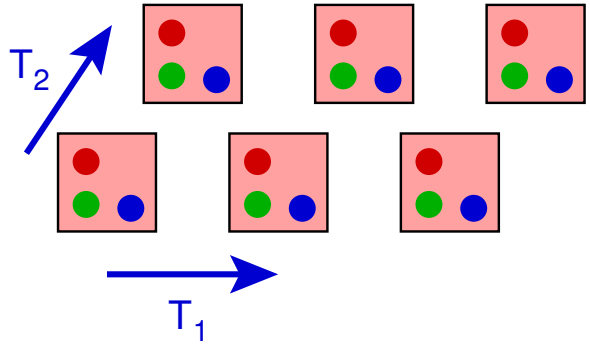
square lattice



Kagomé lattice

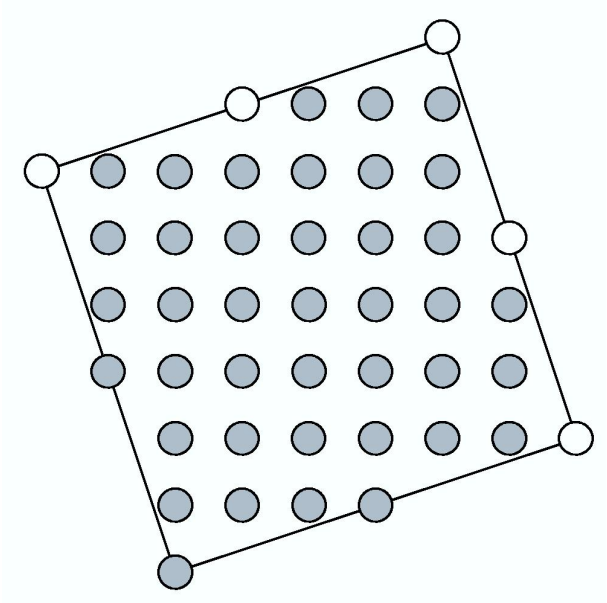
Described by

- unit cell 
- Bravais lattice: translation vectors $\mathbf{T}_1$, $\mathbf{T}_2$ (2D)



- finite lattices: finite multiples of $\mathbf{T}_1$, $\mathbf{T}_2$ and boundary conditions
  - periodic, antiperiodic
  - open
- lattice symmetries:
  - translation – multiples of Bravais lattice vector + periodic (AP) BCs
  - rotations – e.g., $\pi/2$ for a square lattice (group C_{4v})
  - reflection – about symmetry axis

Tilted clusters



40-site cluster, square lattice ($a = 1$)

$$\mathbf{T}_1 = (1, 0)\,, \;\; \mathbf{T}_2 = (0, 1)$$

Spanning vectors:

$$\mathbf{F}_1 = (6, 2)\,, \;\; \mathbf{F}_2 = (-2, 6)$$

In general,

$$\mathbf{F}_1 = (n, m)\,, \;\; \mathbf{F}_2 = (-m, n)$$
$$N = n^2 + m^2$$

translational symmetry satisfied

$\Rightarrow$ reflection/rotation symmetries become more complicated

I (ii) Representation of Many-Body States

mapping to (binary) integers:

- spin-1/2 Heisenberg:

$$|\uparrow_1\downarrow_2\ldots\uparrow_{N-1}\uparrow_N\rangle \rightarrow 1_1 0_2 \ldots 1_{N-1} 1_N$$

  spin flip = bit flip

- Hubbard

$$|N_\ell^\uparrow N_\ell^\downarrow\rangle \rightarrow N_\ell^\uparrow N_\ell^\downarrow \quad \text{or} \quad |N_\ell^e S_\ell^z\rangle$$

  with $N_\sigma = \{0, 1\}$

- other models (t–J, $S = 1$ Heisenberg, ...) more complicated

Symmetries: given group $\mathcal{G}$ with generators $\{g_p\}$

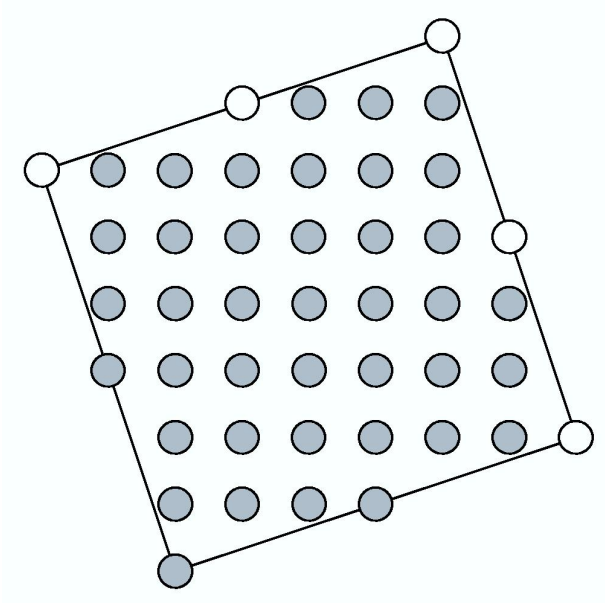
$[H, g_p] = 0 \rightarrow H$ block diagonal (Hilbert space can be divided)

- Continuous
  - conservation of particle number, S^z – U(1) $\Rightarrow$ permutations of bits
  - total spin SU(2) difficult to combine with space group
    $\Rightarrow$ spin inversion (Z_2) can be used
- Space group
  - translation: abelian local states
  - point group (reflections and rotations): non-abelian in general

$\Rightarrow$ form symmetrized linear combination of local states

Example

Reduction of Hilbert space for $S = 1/2$ Heisenberg on $\sqrt{40} \times \sqrt{40}$ cluster



- full Hilbert space: dim$= 2^{40} = 10^{12}$
- constrain to $S_z = 0$: dim$= 138 \times 10^9$
- using spin inversion: dim$= 69 \times 10^9$
- utilizing all 40 translations: dim$= 1.7 \times 10^9$
- using all 4 rotations: dim$= 430,909,650$

I (iii) Complete Diagonalization

To solve $H\,|\psi\rangle = E\,|\psi\rangle$ (H real, symmetric)

Method (*Numerical Recipes*, Ch. 11)

1. Householder transformation - reduction to tridiagonal form T
   - $\approx 2n^3/3$ operations ($4n^3/3$ with eigenvectors)
2. Diagonalization of a tridiagonal matrix
   - roots of secular equation: inefficient
   - QL (QR) algorithm - factorization $T = Q\,L$,
     Q orthogonal, L lower triangular
     $\approx 30n^2$ operations ($\approx 3n^3$ with eigenvectors)

Useful for:

- Simple problems, testing
- Matrix H dense
- Many eigenstates required

But

- H must be stored
- entire matrix must be diagonalized

I (iv) Iterative Diagonalization

Idea: project H onto a cleverly chosen subspace of dimension $M \ll N$

$\Rightarrow$ good convergence of extremal eigenstates

Methods

- Power method $|v_n\rangle = H^n|v_0\rangle$
  - conceptually simple, but converges poorly
  - needs only two vectors, $|v_n\rangle$ & $|v_{n-1}\rangle$
- Lanczos: orthogonal vectors in Krylov subspace (spanned by $\{|v_n\rangle\}$)
  - simple to implement
  - memory efficient - only 3 vectors needed at once
  - works well for sparse, short-range H
- Davidson: subspace expanded by diagonal approximation to inverse iteration
  - higher-order convergence than Lanczos (usually)
  - implementation more complicated
  - works best for diagonally-dominated H
- Jacobi-Davidson: generalization of Davidson
  - nontrivial problem-specific preconditioner (approximation to inverse)
  - can be applied to generalized eigenvalue problem

$$A\,|x\rangle = \lambda\, B\,|x\rangle \qquad (A,\, B \text{ general, complex matrices})$$

Lanczos Algorithm

0) choose $|u_0\rangle$ (random vector, $|\tilde{\psi}_0\rangle$ from last iteration, ...)

1) form $|u_{n+1}\rangle = H\ |u_n\rangle - a_n|u_n\rangle - b_n^2\ |u_{n-1}\rangle$

   where $a_n = \frac{\langle u_n|H|u_n\rangle}{\langle u_n|u_n\rangle}$ and $b_n^2 = \frac{\langle u_n|u_n\rangle}{\langle u_{n-1}|u_{n-1}\rangle}$

2) Is $\langle u_{n+1}|u_{n+1}\rangle < \varepsilon$?

   yes: do 4) then stop

   no: continue

3) repeat starting with 1) until $n = M$ (maximum dimension)

4) diagonalize $\langle u_i|H|u_j\rangle$ (tridiagonal) using QL algorithm

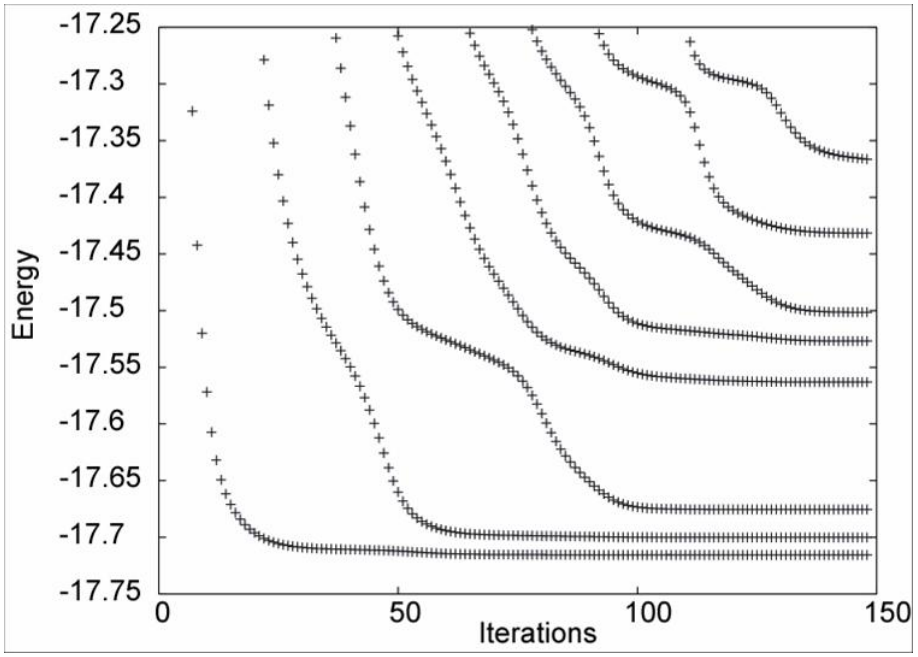
   diagonal elements $\mathbf{D} = (a_0, a_1, \ldots, a_n)$,

   off-diagonal elements $\mathbf{O} = (b_1, b_2, \ldots, b_n)$

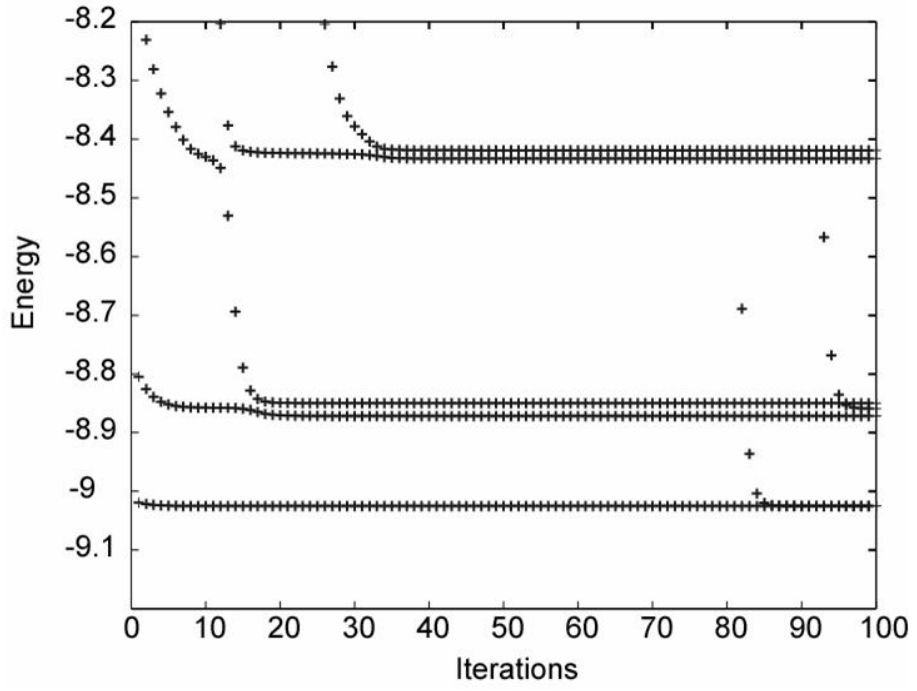
   $\Rightarrow$ eigenvalue $\tilde{E}_0$, eigenvector $|\tilde{\psi}_0\rangle$

5) repeat starting with 0), setting $|u_0\rangle = |\tilde{\psi}_0\rangle$

Convergence of Lanczos Algorithm



- eigenvalues converge starting with extremal ones
- excited states can get "stuck" for a while

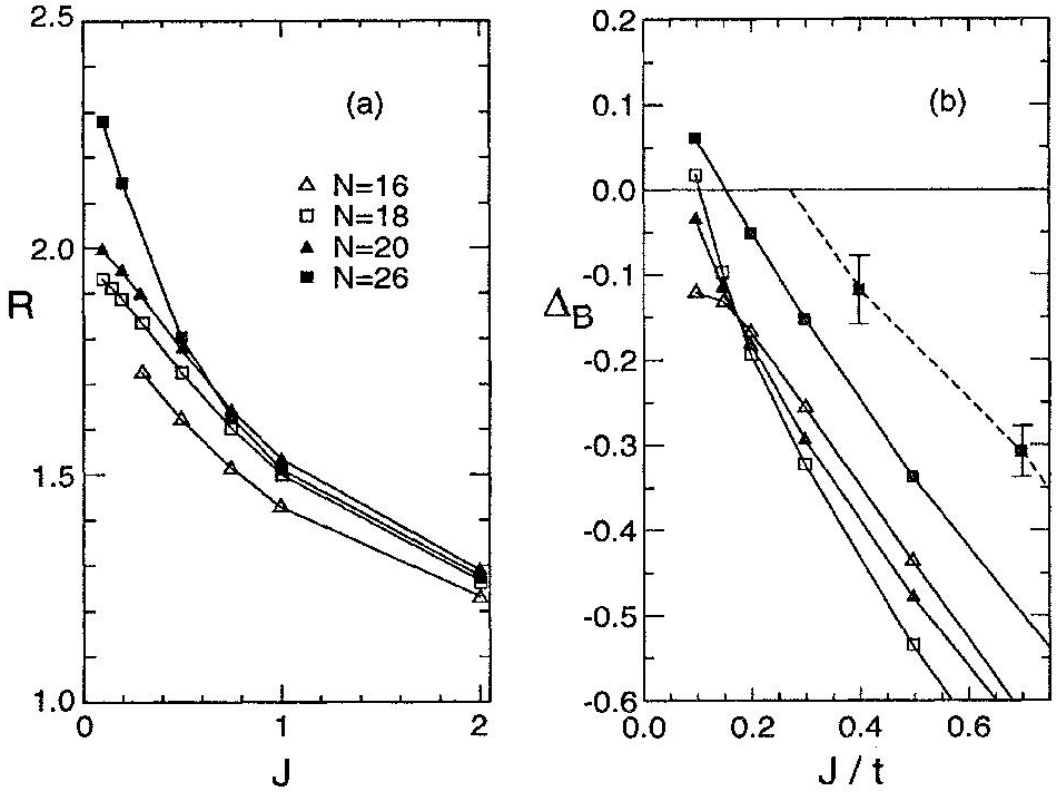


at longer times:

- true eigenvalus converged
- spurious or "ghost" eigenvalues produced
- multiplicity of eigenstates increases

Example: 2D t-J Model

Binding of 2 holes



R: average hole-hole distance
Δ_B: binding energy

(Poiblanc, Riera, & Dagotto, 1993)

- holes closer than two lattice spacings
- pair binding for $J > J_c$, but large finite-size effects

$\Rightarrow$ Does binding persist for larger lattices and constant doping (more holes)?

I (v) Dynamics with Exact Diagonalization

Time-dependent correlation functions

$$C(t) = -i\langle\psi_0|A(t)\ A^\dagger(0)|\psi_0\rangle$$

Fourier transform to frequency space (retarded)

$$\tilde{C}(\omega + i\eta) = \langle\psi_0|\, A\ (\omega + i\eta - H + E_0)^{-1}\ A^\dagger\,|\psi_0\rangle \qquad \text{(resolvent)}$$

Spectral function

$$I(\omega) = -\frac{1}{\pi}\lim_{\eta\to 0^+} \mathrm{Im}\,\tilde{C}(\omega + i\eta)$$

Examples from theory and experiment

name	notation	operators	experiment
single-particle spectral weight	$A(\mathbf{k},\omega)$	$A = c_{\mathbf{k},\sigma}$	photoemission
structure factor	$S_{zz}(\mathbf{q},\omega)$	$A = S^z_{\mathbf{q}}$	neutron scattering
optical conductivity	$\sigma_{xx}(\omega)$	$A = j_x$	optics
4-spin correlation	$R(\omega)$	$\sum_{\mathbf{k}} R_{\mathbf{k}}\, \mathbf{S}_{\mathbf{k}} \cdot \mathbf{S}_{-\mathbf{k}}$	Raman scattering

Methods

Krylov space method (continued fraction)

restart Lanzcos procedure with

$$|u_0\rangle = \frac{1}{\sqrt{\langle\psi_0| A\ A^\dagger |\psi_0\rangle}} A^\dagger |\psi_0\rangle$$

In this Lanczos basis,

$$\tilde{C}(z = \omega + i\eta + E_0) = \cfrac{\langle\psi_0| A\ A^\dagger |\psi_0\rangle}{z - a_1 - \cfrac{b_2^2}{z - a_2 - \cfrac{b_3^2}{z - a_3 - \ldots}}}$$

Interpretation:

- calculation of eigenvector not needed
- consider Lehmann representation of spectral function

$$I(\omega) = \sum_n |\langle\psi_n|A^\dagger|\psi_0\rangle|^2\, \delta(\omega - E_n + E_0)$$

  $\Rightarrow$ poles and weights of $\tilde{C}(z)$ determine $I(\omega)$
- weight decreases with $n \rightarrow$ truncate after M steps
- spectrum discrete $\rightarrow$ finite broadening η

Correction vector method (Soos & Ramasesha, 1984)

Calculate vectors

$$|\phi_0\rangle = A^\dagger |\psi_0\rangle \ , \qquad |\phi_1\rangle = (\omega + i\eta - H + E_0)^{-1} \ |\phi_0\rangle$$

directly, then

$$I(\omega) = \frac{1}{\pi} \, \mathrm{Im} \, \langle \phi_0 | \phi_1 \rangle$$

Advantages:

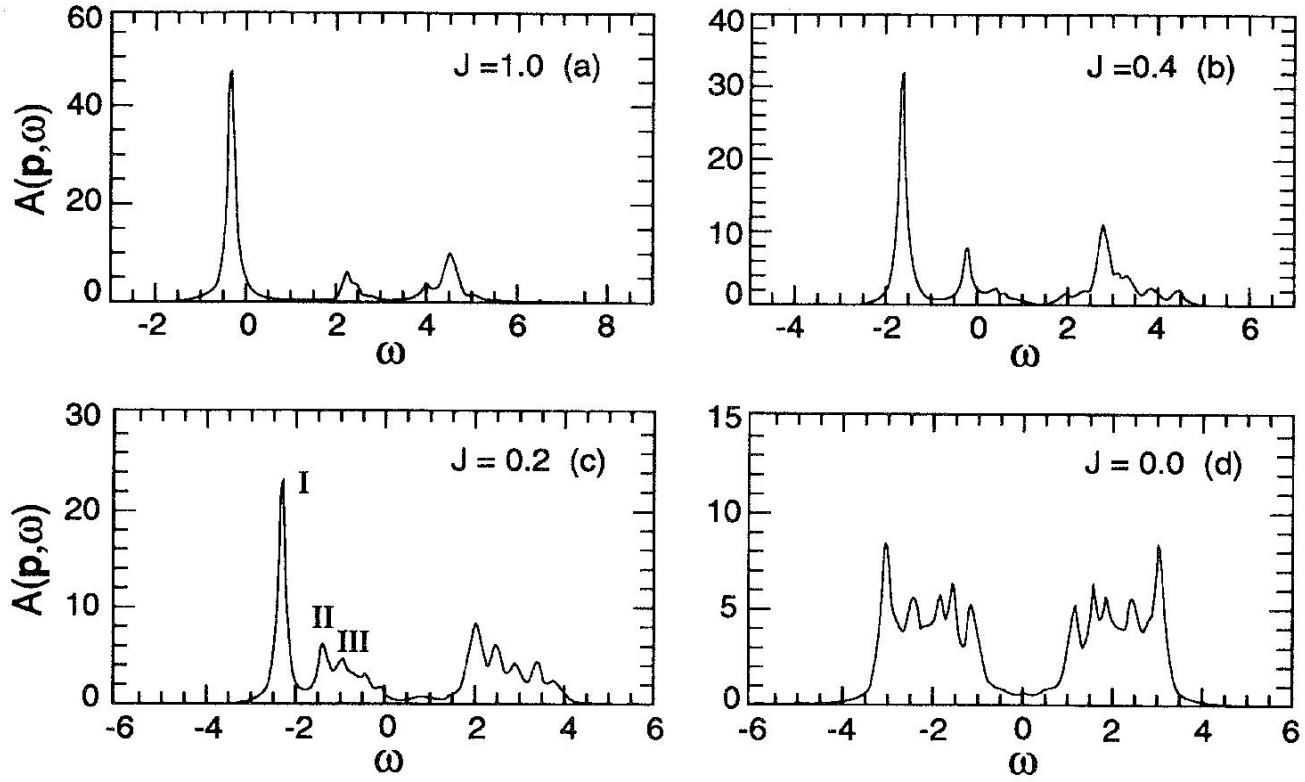
- spectral weight calculated exactly for a given range
- nonlinear spectral functions computed by higher order correction vectors
- can be run in conjunction with Davidson algorithm

Disadvantage: system $(H - z)|\phi_1\rangle = |\phi_0\rangle$ must be solved for each ω desired

Example: Dynamics in 2D t-J Model

Single-particle spectral weight $A(\mathbf{k}, \omega)$ at $\mathbf{k} = \mathbf{k}_F = (\pi/2, \pi/2)$ for one hole

4×4 lattice (Dagotto, Joynt, Moreo, Bacci, & Gagliano, 1993)



Does a single quasiparticle propagate in an antiferromagnet?

- strongly localized hole with string exitations at $J/t = 1.0$
- quasiparticle peak remains until $J/t = 0.4$
- "lump" with pseudogap at $J/t = 0.2$
- pseudogap due to finite-size effects at $J/t = 0$ (symmetric in ω)

I (vi) Finite Temperature with Exact Diagonalization

To calculate finite-T properties in orthonormal basis $|n\rangle$

$$\langle A\rangle = \frac{1}{Z}\sum_{n}^{N}\langle n|Ae^{-\beta H}|n\rangle\ , \qquad Z = \sum_{n}^{N}\langle n|e^{-\beta H}|n\rangle\ ,$$

Problem: expensive to calculate for all $|n\rangle$

Idea: stochastic sampling of Krylov space (Jaklic & Prelovsek, 1994)

$$\langle A\rangle \approx \frac{1}{Z}\sum_{s}\frac{N_s}{R}\sum_{r}^{R}\sum_{m}^{M} e^{-\beta\varepsilon_m^{(r)}}\langle r|\Psi_m^{(r)}\rangle\langle\Psi_m^{(r)}|A|r\rangle$$

where

$$Z \approx \sum_{s}\frac{N_s}{R}\sum_{r}^{R}\sum_{m}^{M} e^{-\beta\varepsilon_m^{(r)}}\left|\langle r|\Psi_m^{(r)}\rangle\right|^2$$

- $\sum_s$ over symmetry sectors of dimension N_s
- $\sum_r$ average over R random starting vectors $|\Psi_0^{(r)}\rangle$
- $\sum_m$ Lanczos propagation of starting vectors: $|\Psi_m^{(r)}\rangle$ at step m

$\Rightarrow$ useful if convergence good when $M \ll N_s$ and $R \ll N_s$

Properties

- related to high-T expansion – $T \to \infty$ limit correct
- high to medium T properties in thermodynamic limit
- low-temperature limit correct (on finite lattice), up to sampling error

  reduction of (large) sampling error: (Aichhorn *et al.*, 2003)

  start with:

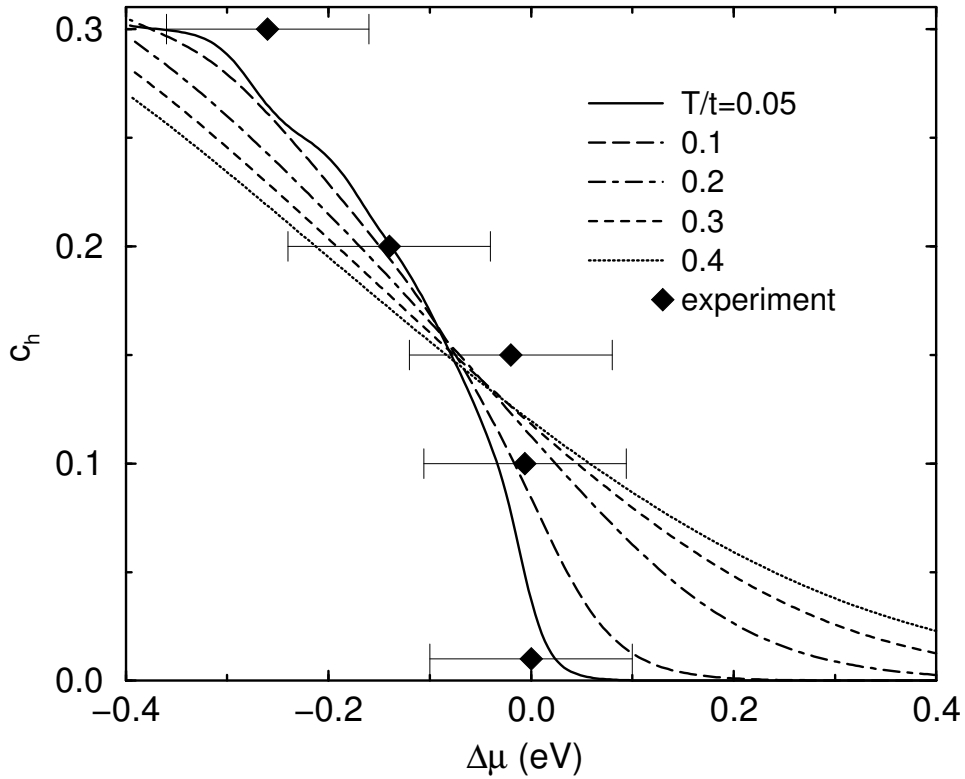
$$\langle A \rangle = \frac{1}{Z} \sum_{n}^{N} \langle n | e^{-\beta H/2} \, A \, e^{-\beta H/2} | n \rangle \ ,$$

  $\Rightarrow$ twofold insertion of Lanczos basis $\rightarrow$ smaller fluctuations at low T
- can calculate
  - thermodynamic properties: specific heat, entropy, static susceptibility, ...
  - static correlation functions
  - dynamics: $A(\mathbf{k}, \omega)$, $S_{zz}(\mathbf{q}, \omega)$, $\sigma_{xx}(\omega)$, ...

Example: t-J Model at finite T

Hole concentration $c_h(=x)$ vs. chemical potential shift $\Delta\mu = \mu_h - \mu_h^0$

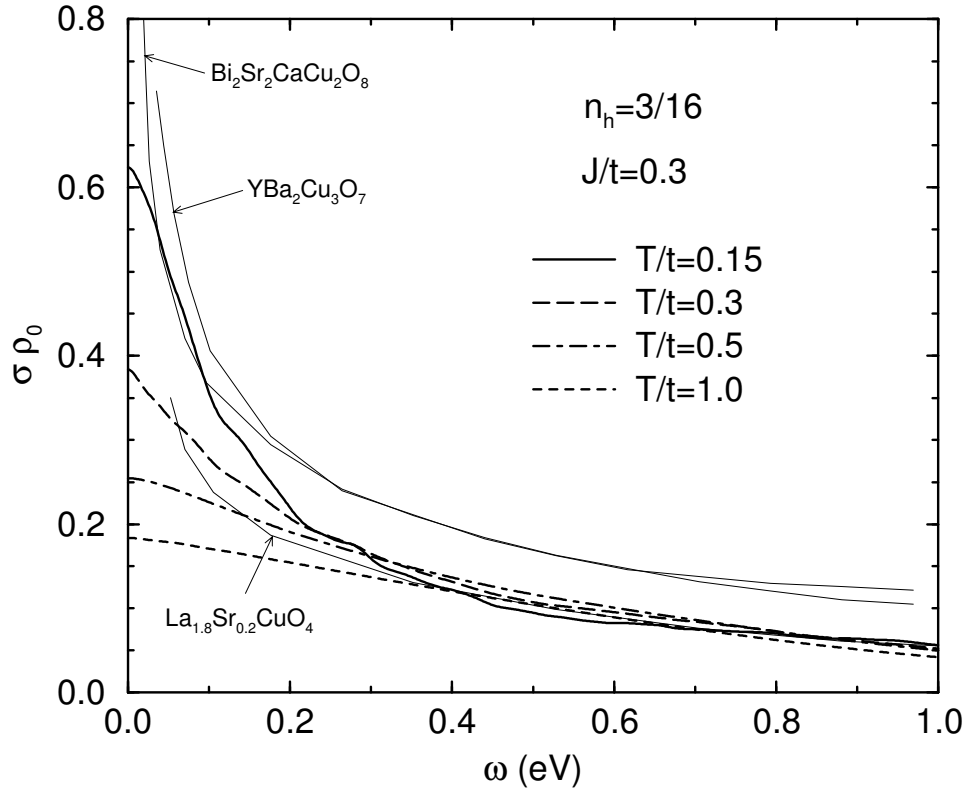
2D t-J model, 16, 18, 20 sites, $t/J = 0.3$, $t = 0.4$eV



(Jaklic & Prelovsek, 1998)

- experimental results for LSCO from photoemission shift (Ino *et al.*, 1997)
- holes only when $\mu < \mu_h^0 \approx -1.99t$ as $T \to 0$
- compressibility finite $\Rightarrow$ no phase separation

Optical conductivity compared with various cuprates at intermediate doping



(Jaklic & Prelovsek, 1998)

- Cuprates measured at $T < 200$K, c_h somewhat uncertain
- high-T falloff slower for materials – transitions to higher excited states?
- experimental curves:
  - LCSO, $c_h \sim x = 0.2$ (Uchida *et al.*, 1991)
  - BISCCO, $c_h \sim 0.23$ (Romero *et al.*, 1992)
  - YBCO, $c_h \sim 0.23$ (Battlogg *et al.*, 1994)

Discussion: Exact Diagonalization

- Method conceptually straightforward, numerically exact
- Iterative diagonalization allows the treatment of surprisingly large matrices
- Efficient implementation using symmetries useful
- System sizes nevertheless strongly restricted
- Extensions to basic method can calculate
  - dynamical correlation functions
  - finite temperature properties
- Not mentioned here, but also possible:
  calculation of full time evolution of quantum state with Lanczos

$\Rightarrow$ Benchmark for other methods, useful when other methods fail

II (i) Anderson and Kondo Problem

Problem: one localized impurity in a noninteracting electron gas

Single Impurity Anderson Model (SIAM)

$$H^{AI} = \varepsilon_d\, n^d_\ell + U n^d_{\ell,\downarrow} n^d_{\ell,\downarrow} + \sum_{\mathbf{k},\sigma} \left(V_{\mathbf{k},d}\, c^\dagger_{\mathbf{k},\sigma} d_{\mathbf{k},\sigma} + \text{H.c.} \right) + \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$$

- general scattering $V_{\mathbf{k},d}$ between impurity and band
- Coulomb interaction on d-site only
- usual simplifications:
  - isotropic scattering: $V_{\mathbf{k},d} \Rightarrow V_{k,d}$, $c_{\mathbf{k},\sigma} \Rightarrow c_{k,l=m=0,\sigma}$ (s-wave)
  - symmetric: $\varepsilon_d = -U/2$
  - constant or semi-elliptical density of states

Mapping onto semi-infinite chain

$$\tilde{H}^{AI} = \varepsilon_d\, n^d_\ell + U n^d_{\ell,\downarrow} n^d_{\ell,\downarrow} + V \sum_{\mathbf{k},\sigma} \left(f^\dagger_{0,\sigma} d_\sigma + \text{H.c.} \right) + \sum_{n=0,\sigma}^{\infty} \left[\epsilon_n\, f^\dagger_{n,\sigma} f_{n,\sigma} + \lambda_n \left(f^\dagger_{n,\sigma} f_{n+1,\sigma} + \text{H.c.} \right) \right]$$

obtained through Lanczos tridiagonalization of $\sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}}\, c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma}$

where $V\, f^\dagger_{0,\sigma} = \sum_k V_{kd}\, c_{k,\sigma}$ and $V^2 = \sum_k |V_{kd}|^2$

Kondo model

$$H^K = J_K\,\mathbf{S}_d\cdot\mathbf{s}_0 + \sum_{\mathbf{k},\sigma}\varepsilon_{\mathbf{k}}\,c^\dagger_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma} \quad \text{with} \quad \mathbf{s}_0 = f^\dagger_{0,\sigma}\vec{\sigma}_{\sigma\mu}f_{0,\mu}\,, \quad f_{0,\sigma} = \textstyle\sum_k c_{k,\sigma}$$

- strong-coupling limit ($U \gg V^2$) of symmetric, isoptropic H^{AI} (Schrieffer-Wolff transformation)
- local, isotropic coupling of spin to band

Mapping to a linear chain model via

1. Lanczos tridiagonalization
2. constant density of states ρ_0
3. logarithmic discretization of conduction band

$$\tilde{H}^K = \frac{1}{2}(1+\Lambda^{-1})\sum_{n=0}^{\infty}\Lambda^{-n/2}\left(f^\dagger_{n,\sigma}f_{n+1,\sigma} + \text{H.c.}\right) + 2J_K\,\rho_0\,f^\dagger_{0,\sigma}\vec{\sigma}_{\sigma\mu}f_{0,\mu}$$

where the Lanczos coefficients $\epsilon_n = 0$ and $\lambda_n \approx \frac{1}{2}(1+\Lambda^{-1})\Lambda^{-n/2}$, $n \gg 1$

$\Rightarrow$ "hopping" falls off exponentially!

Related models

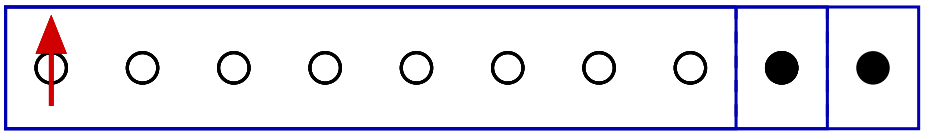
- anisotropic Kondo model $\mathbf{S}_d\cdot\mathbf{s}_0 \rightarrow S^z_d s^z_0 + \frac{\alpha}{2}(S^+_d s^-_0 + S^-_d s^+_0)$
- Ohmic two-state system
- generalized Anderson impurity model (DMFT)

II (ii) Numerical Renormalization Group for Kondo Problem

(Wilson, 1974)

Idea: Numerically integrate out degrees of freedom $\longrightarrow$ low-energy properties

Kondo problem $\longrightarrow$ 1D quantum lattice model (4^N degrees of freedom)



- isolate finite system
- diagonalize numerically
- keep m lowest energy eigenstates
- add a site
- iterate

Assumption: low-energy states most important for low-energy behavior of larger system

$\Rightarrow$ powerful method for impurity problems (Kondo, Anderson, ...)

Why does it work so well?

- Each system size corresponds to a lower energy scale
- Each RG step can be justified perturbatively (Λ^{-1} is a small parameter)
- substantial portion $(1/4)$ of Hilbert space is kept at each step

Calculation of observables with the NRG

Effective Hamiltonian for a given size associate with energy scale

$$\bar{H}_N \equiv H_N/D_N \quad , \qquad D_N = \tfrac{1}{2}(1+\Lambda^{-1})\,\Lambda^{-(N-1)/2} \quad \text{(lowest scale)}$$

- RG flow - fixed point defined by $R[H^*] = H^*$
  numerically: range $N_1 \le N \le N_2$ in which $\bar{E}_p^N \approx \bar{E}_p$ (independent of N)
  $\Rightarrow$ identify fixed points and crossover energy scales
- thermodynamic quantities
  effective partition function at scale D_N

$$Z_N(T) \equiv \mathrm{Tr}\; e^{-H_N/k_BT} = \sum_p e^{-E_p^N/k_BT}$$

  valid at $k_BT = k_BT_N \approx D_N$

  other quantitites can be formed from the partition function

  e.g., impurity suceptibility for Anderson model

$$\chi_{\mathrm{imp}}(T) = \frac{(g\mu_B)^2}{k_BT}\left[\frac{1}{Z}\,\mathrm{Tr}(S_z^{\mathrm{tot}})^2 e^{-H/k_BT} - \frac{1}{Z_c}\,\mathrm{Tr}(S_{z,c}^{\mathrm{tot}})^2 e^{-H_c/k_BT}\right]$$

- dynamical quantities ($T = 0$)
  e.g., impurity spectral function:

$$A(\omega) = -\frac{1}{\pi} \operatorname{Im} G(\omega + i\eta) \qquad \text{where } G(t) = -i\langle\psi_0| T\, d(t) d^\dagger(0) |\psi_0\rangle$$

  At finite N,

$$A_N(\omega) = \frac{1}{Z_N} \sum_p \left|\langle p|d_\sigma^\dagger|0\rangle\right|^2 \delta(\omega - E_p + E_0) + \left|\langle 0|d_\sigma^\dagger|p\rangle\right|^2 \delta(\omega + E_p - E_0)$$

  $A_N(\omega) \approx A(\omega)$ when $\omega \approx \omega_N \equiv k_B T_N$

  $\Rightarrow$ dynamics can be performed at the current RG energy scale

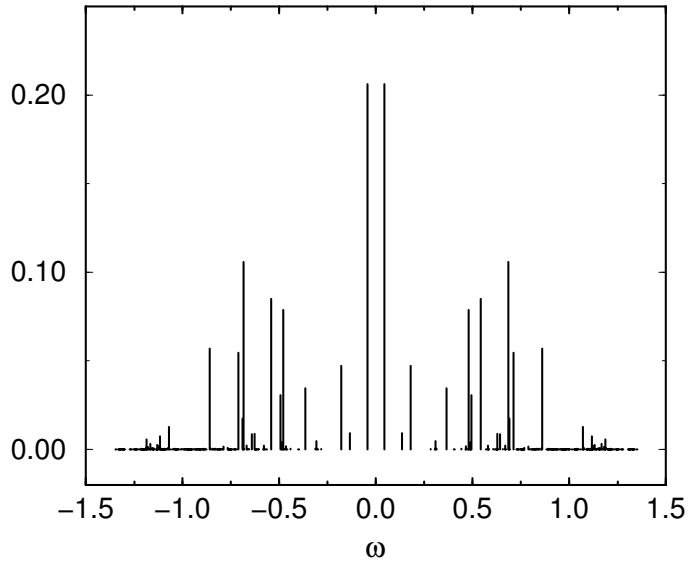
  - energy summation gives sum of δ-functions
  - broadening needed to get a continuous spectrum

- dynamical properties at finite-T similar (appropriate T, ω)

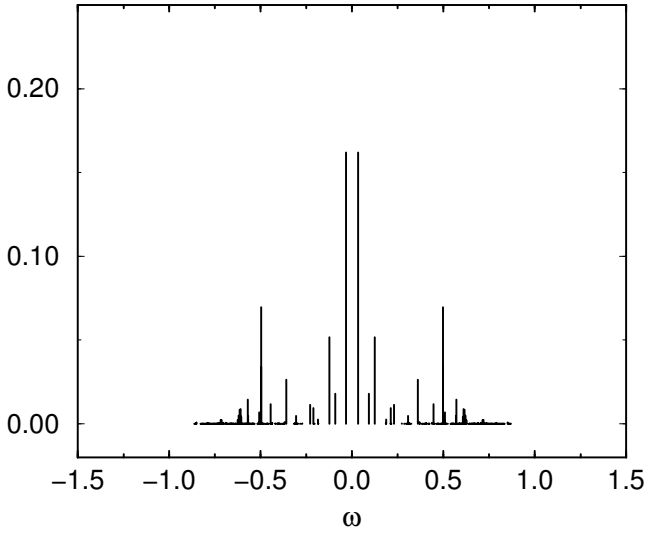
  $\Rightarrow$ transport properties

Dynamics at finite N (SIAM) (Bulla, 2000)

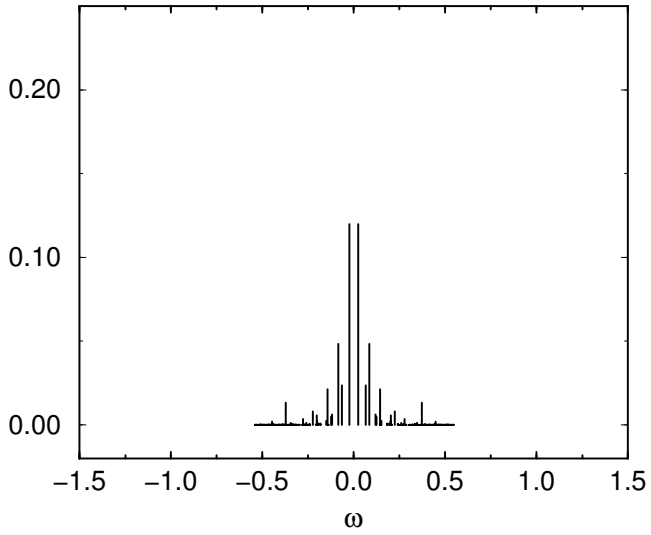
$N = 14$



$N = 16$



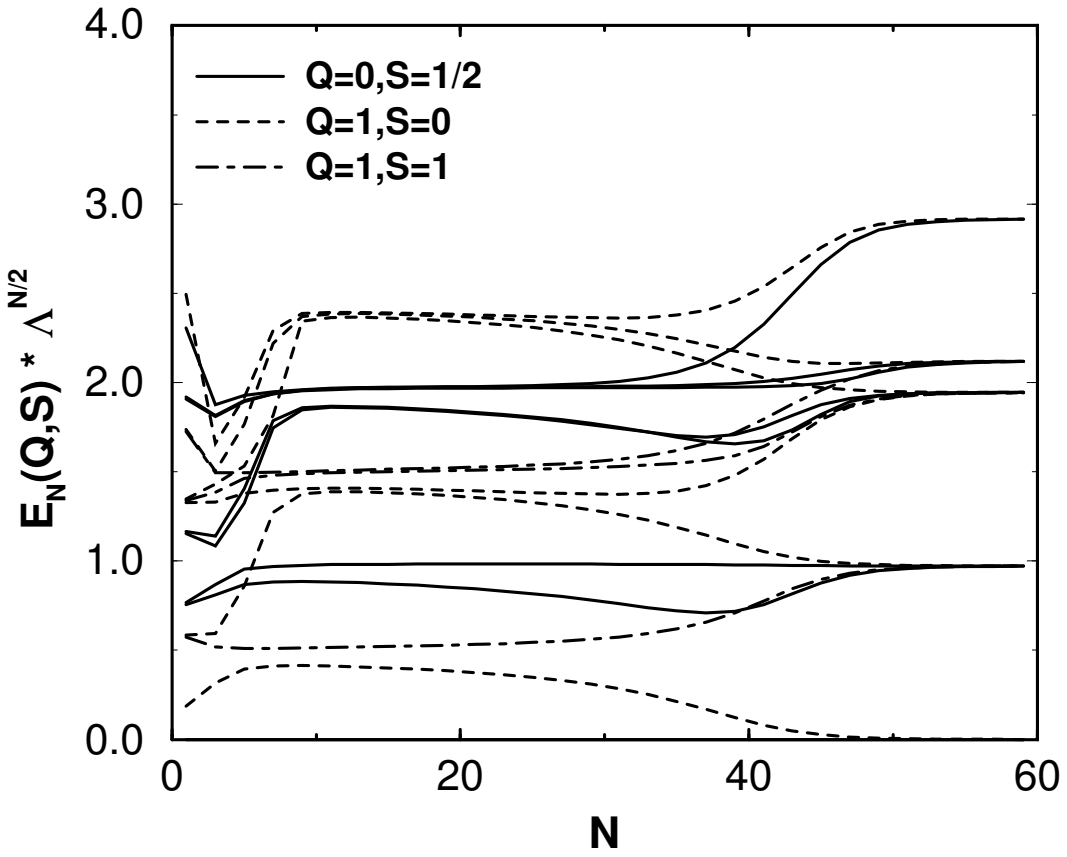
$N = 18$



Physics of the Kondo Problem

Flow of coupling constants

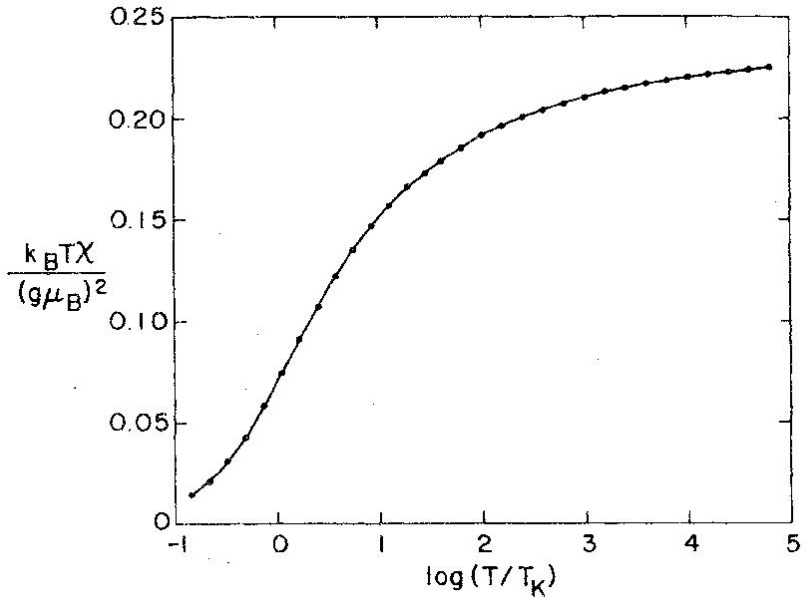
(SIAM, $\varepsilon_d = -0.2$, $U = 0.4$, $\Delta = \frac{1}{2}\pi V^2 N(E_f) = 0.015$)



(Bulla, 2000)

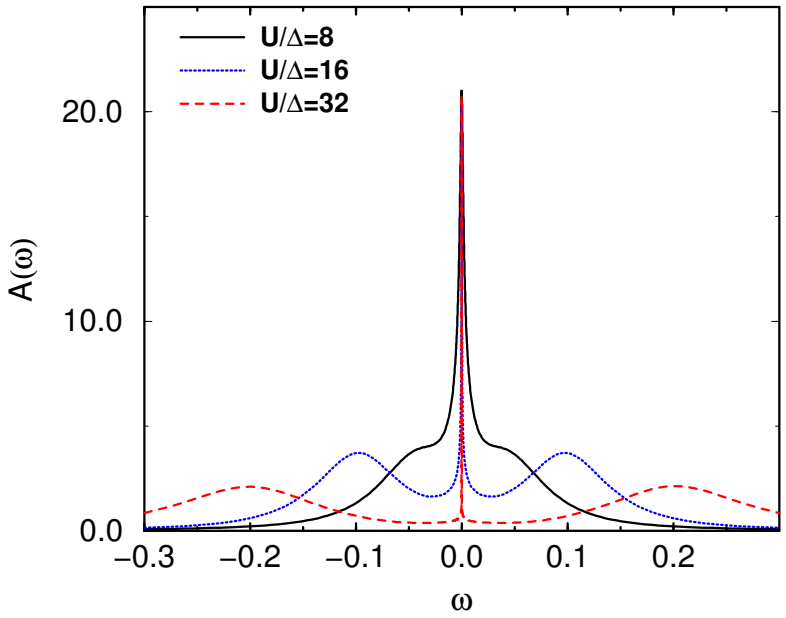
- Crossover to local moment behavior at $N \approx 5 \Rightarrow$ unstable fixed point
- Crossover to screening behavior at energy scale $k_B T_K$
  $\Rightarrow$ stable low-T fixed point

Susceptibility universal on Kondo scale $\Rightarrow$ universal value at $T = 0$



(Krishna-murthy, Wilkins, & Wilson, 1980)

Quasiparticle peak at Fermi energy in SIAM



(Bulla, 2000)

Application to other quantum lattice models unsuccessful:

- 1D Hubbard model (Bray & Chui, 1979)

  lattice size $L = 2, 4, 8, 16$

  10% error in E_0 after 4 steps $\Rightarrow$ $L = 16$

- 1D Heisenberg model (Xiang & Gehring, 1992)

  $S = 1$, $L = 18$ sites, OBCs: 3% error in E_0

- 2D Anderson localization (Lee, 1979)

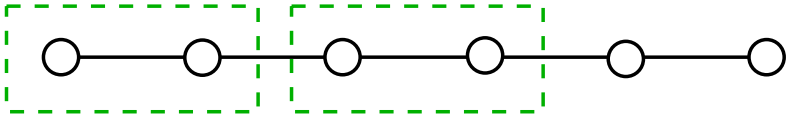
  Found a localization transition in 2D

  (scaling theory: no transition, 2D critical dimension)

$\Rightarrow$ separation of energy scales not applicable

Single-Particle Problem

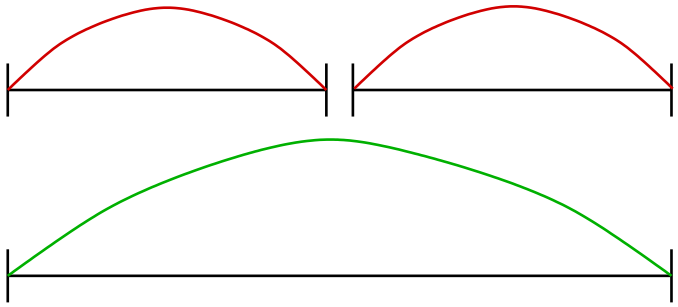
Wilson procedure for particle on a tight-binding lattice (Wilson, 1985)



$$H = \left(\begin{array}{cc|cc} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ \hline 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 \end{array}\right) \longrightarrow -\frac{\partial^2}{\partial x^2} + \text{fixed BCs}$$

(equivalent to modes of a string with fixed ends)

Putting two "blocks" together



$\Rightarrow$ treatment of boundaries critical

Test calculation:

State	Exact	NRG	
E_0	2.351×10^{-6}	1.9207×10^{-2}	10 blockings (2048 sites)
E_1	9.403×10^{-6}	1.9209×10^{-2}	8 states kept
E_2	2.116×10^{-5}	1.9714×10^{-2}	

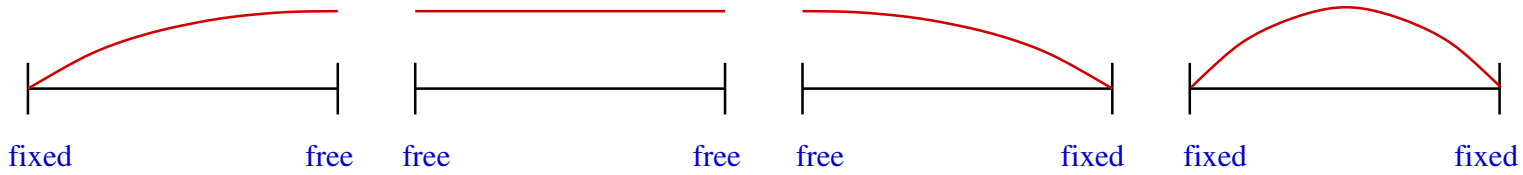
Discussion: Numerical RG

- Iterative diagonalization scheme - effort per step remains constant as system grows
- Truncation carried out by transforming to the basis of m lowest energy eigenstates
- Degrees of freedom added by adding site
- NRG works well for impurity problems because of exponential separation of energy scales on effective chain model
- Thermodynamics, dynamical correlations, and transport properties can be calculated
- NRG becomes inaccurate quickly for quantum lattice models such as Hubbard and Heisenberg chains
- Origin of problem can be understood for single particle on a tight-binding chain – treatment of boundaries as blocks are put together

$\Rightarrow$ Very useful for the right problem, but can fail badly

III (i) Better Methods for the Noninteracting Particle

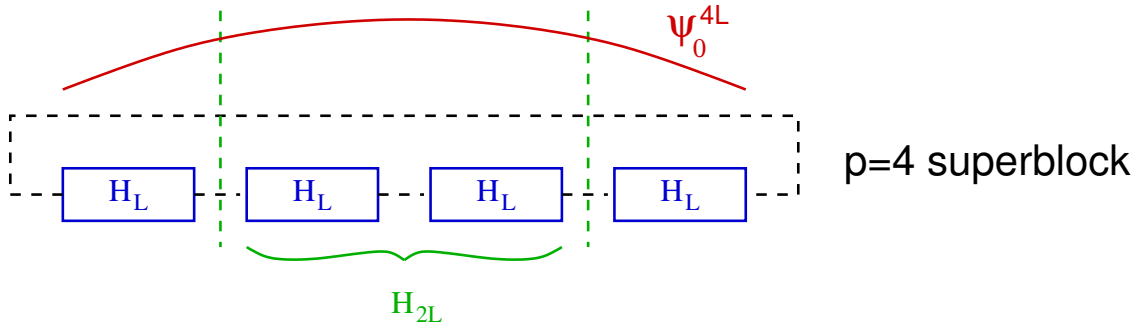
Combinations of BCs technique (White & Noack, 1992)



- Diagonalize H_L with different combinations of BCs
- Use orthogonalized set of states as new basis
- Energies accurate to 10 digits (2 states/BC, 10 iterations)

$\Rightarrow$ Not easy to generalize to interacting systems

Superblock technique



Idea: Fluctuations in additional blocks allow general behavior at boundaries

- Diagonalize superblock of p blocks
- Project wavefunctions onto size $2L$ block, orthogonalize
- Exact as $p \to \infty$

$\Rightarrow$ Projection is no longer trivial for interacting systems

Review: entanglement in quantum mechanics

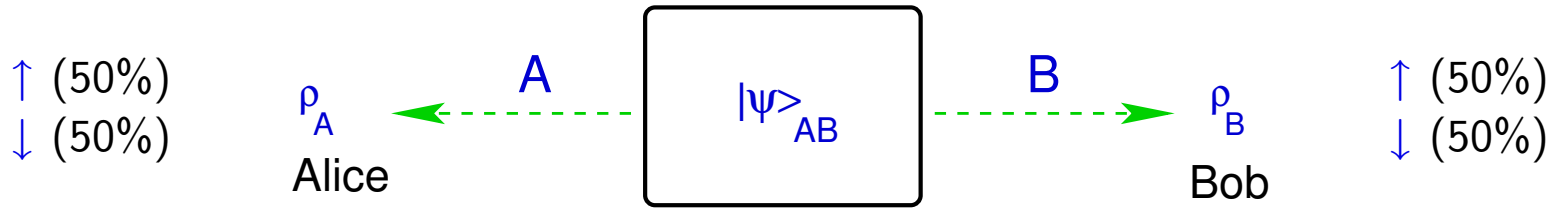
system made up of $S = \frac{1}{2}$ spins A, B

$$|\uparrow\uparrow\rangle \equiv |\uparrow\rangle_A \otimes |\uparrow\rangle_B \qquad \text{(or } |\downarrow\downarrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle\text{)}$$

superposition:

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$$

Measurements:



measurements correlated: A $\uparrow \Rightarrow$ B $\uparrow$ with 100% probability

$\Rightarrow$ state (maximally) entangled!

Einstein, Podolsky, Rosen (1935): "spooky action-at-a-distance"
(spukhafte Fernwirkung)

Schrödinger (1935): entanglement *essential* property of quantum mechanics!

More complete description: density matrices

density matrix describes part of system

$$\rho_A = \mathrm{Tr}_B \, |\psi\rangle \langle\psi| = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \qquad \text{(similar for } \rho_B\text{)}$$

$\Rightarrow$ mixed state

Schmidt decomposition

$$|\psi\rangle_{AB} = \sum_\alpha \sqrt{w_\alpha} \, |\phi_\alpha\rangle_A \, |\chi_\alpha\rangle_B = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)$$

$|\phi_\alpha\rangle_A$: eigenstate of ρ_A, $|\chi_\alpha\rangle_B$: eigenstate of ρ_B

w_α: common eigenvalues

Schmidt number: number of $w_\alpha \neq 0$

$= 1$: $|\psi\rangle = |\phi_0\rangle_A \, |\chi_0\rangle_B$ e.g., $= |\uparrow\uparrow\rangle$ not entangled

> 1: A and B entangled

Relationship to Quantum Information

relabeling:

$$|\downarrow\rangle \equiv |0\rangle, \quad |\uparrow\rangle \equiv |1\rangle \;\Rightarrow\; \text{qubit}$$

Is information contained in a pair of qubits?

quantum information content: von Neumann entropy

$$S(\rho) = -\mathrm{Tr}\ \rho\ \log \rho$$

examples:

- $|\psi\rangle = |\phi\rangle|\chi\rangle$: $S(\rho_A) = 0 \Rightarrow$ classical
- $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle|1\rangle + |0\rangle|0\rangle\right)$: $S(\rho_A) = 1 \Rightarrow$ entangled qubits

entanglement: mutual quantum information

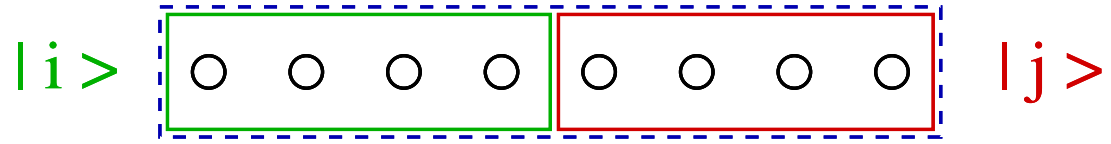
classical analog: Shannon entropy – information content in a message

Applications of entanglement

- quantum data compression
- quantum cryptography
- quantum teleportation
- quantum computing

III (ii) Density-Matrix Projection

What can be learned from dividing a many-body system?



- For the state $|\psi_0\rangle$ of the system (or approximation)
- reduced density matrix of subsystem ("system block")

$$\rho = \mathrm{Tr}_{|j\rangle}\ |\psi_0\rangle\,\langle\psi_0|$$

trace over states of the "environment block"

Properties:

- eigenstates $|\phi_\alpha\rangle$ form a complete basis for system block
- eigenvalues w_α
  - weight of a state
  - entanglement/mutual quantum information

$$S(\rho) = -\mathrm{Tr}_{|j\rangle}\,(\rho \log \rho) = -\sum_\alpha w_\alpha \log w_\alpha$$

- optimal approximation: sum over m eigenstates with the largest w_α

$$|\psi_0\rangle \approx \sum_{\alpha}^{m < \dim(\alpha)} \sqrt{w_\alpha}\,|\phi_\alpha\rangle\,|\chi_\alpha\rangle \qquad \text{(Schmidt decomposition)}$$

Density Matrix Renormalization Group (White, 1992)

Goal: ground-state properties of a 1D quantum lattice model

Density-matrix projection

- diagonalization (e.g., Lanczos) of a finite lattice $\Rightarrow |\psi_0\rangle$
- division of system
- reduction of the system block basis via density matrix $\Rightarrow m$ states
- Properties:
  - variational, ground state properties (numerically) on a finite lattice
  - very exact for 1D models with "open" boundary conditions
  - energies, local quantities most accurate
  - correlation functions (somewhat) less accurate

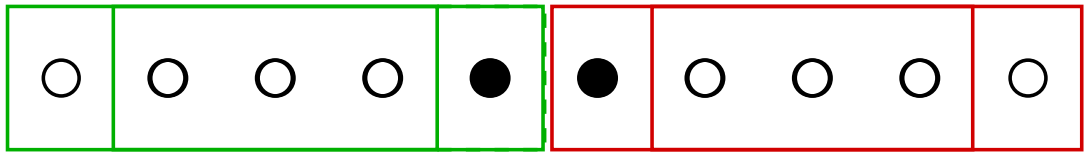
Buildup of system (RG)

- add one site at a time $\Rightarrow$ fewest possible degrees of freedom at once
- need to choose environment block
  possibilities:
  - one or more "exact" sites
  - reflection of system block
  - stored block from a previous step

III (iv) DMRG Algorithms

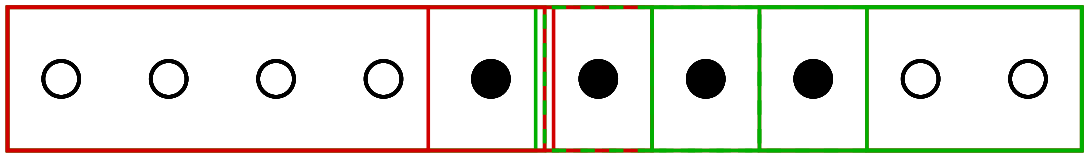
2 ways of building up superblock, depending on choice of the environment block

Infinite System Algorithm



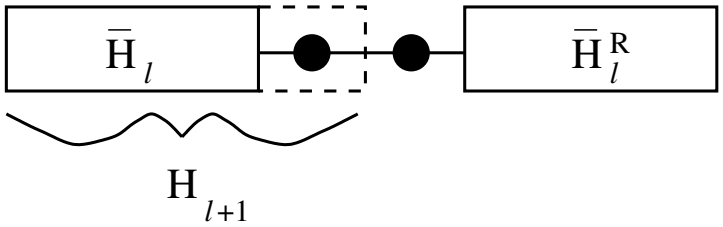
- environment block: reflection of the system block
- superblock grows by 2 lattice sites per iteration

Finite System Algorithm



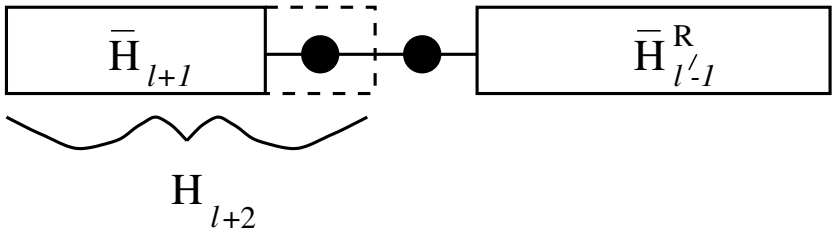
- starting point: infinite system method
- size of superblock stays the same environment block shrinks
- "zipping" back and forth $\Rightarrow$ iterative convergence
- environment block stored from previous iteration

Infinite System Algorithm in Detail



1. Form a superblock containing L sites which is small enough to be exactly diagonalized.
2. Diagonalize the superblock Hamiltonian $H_L^{\rm super}$ numerically, obtaining *only* the ground state eigenvalue and eigenvector $|\psi\rangle$ using the Lanczos or Davidson algorithm.
3. Form the reduced density matrix $\rho_{ii'}$ for the new system block from $|\psi\rangle$ using $\rho_{ii'} = \sum_j \psi^*_{ij}\psi_{i'j}$. Note that $\ell' = \ell = L/2 - 1$.
4. Diagonalize $\rho_{ii'}$ with a dense matrix diagonalization routine to obtain the m eigenvectors with the largest eigenvalues.
5. Construct $H_{\ell+1}$ and other operators in the new system block and transform them to the reduced density matrix eigenbasis using $\bar{H}_{\ell+1} = O_L^\dagger H_{\ell+1} O_L$, $\bar{A}_{\ell+1} = O_L^\dagger A_{\ell+1} O_L$, etc., where the columns of O_L contain the m highest eigenvectors of $\rho_{ii'}$, and $A_{\ell+1}$ is an operator in the system block.
6. Form a superblock of size $L+2$ using $\bar{H}_{\ell+1}$, two single sites and $\bar{H}^R_{\ell+1}$.
7. Repeat starting with step 2, substituting $H^{\rm super}_{L+2}$ for $H^{\rm super}_L$.

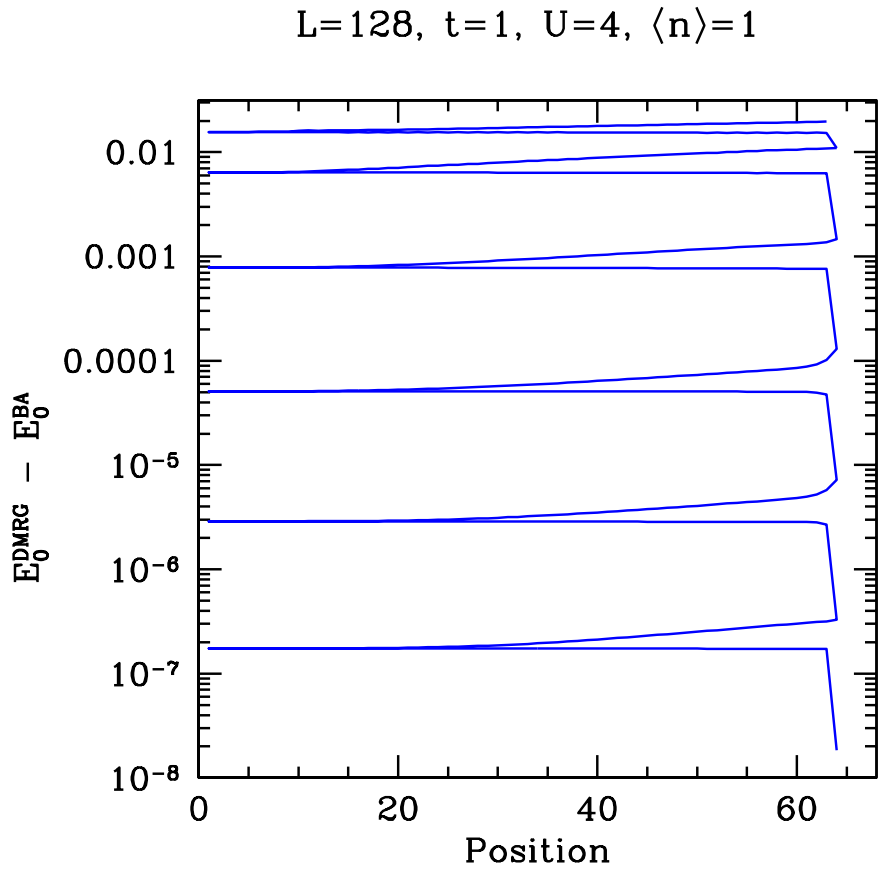
Finite System Algorithm in Detail



0. Carry out the infinite system algorithm until the superblock reaches size L, storing $\bar{H}_\ell$ and the operators needed to connect the blocks at each step.
1. Carry out steps 3-5 of the infinite system algorithm to obtain $\bar{H}_{\ell+1}$. Store it. (Now $\ell \neq \ell'$.)
2. Form a superblock of size L using $\bar{H}_{\ell+1}$, two single sites and $\bar{H}^R_{\ell'-1}$. The superblock configuration shown above where $\ell' = L - \ell - 2$.
3. Repeat steps 1-2 until $\ell = L - 3$ (i.e. $\ell' = 1$). This is the *left to right* phase of the algorithm.
4. Carry out steps 3-5 of the infinite system algorithm, reversing the roles of $\bar{H}_\ell$ and $\bar{H}^R_{\ell'}$, i.e. switch directions to build up the right block and obtain $\bar{H}^R_{\ell'+1}$. Store it.
5. Form a superblock of size L using $\bar{H}_{\ell-1}$, two single sites and $\bar{H}^R_{\ell'+1}$.
6. Repeat steps 4-5 until $\ell = 1$. This is the *right to left* phase of the algorithm.
7. Repeat starting with step 1.

Convergence of the DMRG

Comparison with exact solution (Bethe ansatz):
1D Hubbard model, 128 sites, open BCs



- finite system algorithm, 6 iterations
- $m = 50$ to 800 states kept
- reflection symmetry at center used
- CPU time: ca. 6 hours on a 1.2 MHz Athlon

$\Rightarrow$ energy exact to 10 decimal places!

Applications: spin chains (XY, Heisenberg, biquadratic, $S = 1/2, 1, 3/2, 2, \ldots$), 1D Hubbard-like models (plain, extended, ionic, Peierls-, ...)

What can be done with the DMRG?

What is it? Approximate diagonalization on a finite lattice

- Variational
- Large systems (up to 1000 sites)
- Accuracy comparable to exact diagonalization (in many cases)
- No problems with frustration or fermions
- What can be calculated?
  - Ground-state properties: gaps, correlation functions, susceptibilities
  - Dynamics of a quantum system
  - Finite temperature (high and low temperature)
  - Classical systems at finite temperature
  - Time evolution of a quantum system

Limitations

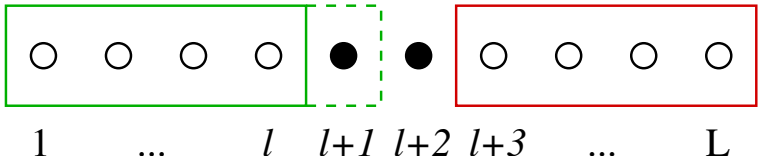
- Convergence depends on details of system
  - dimensionality (1D best)
  - boundary conditions (open BCs best)
  - range of Hamiltonian (short-range best)
- Efficient program can be complicated

Single-Particle Problem Revisited

More DMRG-like algorithm for single-particle problem

$$H_{ij} = 2\,\delta_{ij} - \delta_{i,i+1} - \delta_{i,i-1}$$

Divide the system into 4 parts:



Use *one* basis state per block ($m = 1$) so that

$$\psi_j = \begin{cases} a_1 L_j & j \le \ell \\ a_2 & j = \ell + 1 \\ a_3 & j = \ell + 2 \\ a_4 R_j & j \ge \ell + 3 \end{cases}$$

Hamiltonian matrix element between ψ and ψ':

$$\langle\psi|H|\psi'\rangle = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}^T \begin{pmatrix} H_{11} & T_{12} & 0 & 0 \\ T_{12} & 2 & -1 & 0 \\ 0 & -1 & 2 & T_{34} \\ 0 & 0 & T_{34} & H_{44} \end{pmatrix} \begin{pmatrix} a'_1 \\ a'_2 \\ a'_3 \\ a'_4 \end{pmatrix}$$

where

$$H_{11} = \langle L|H|L\rangle, \qquad H_{44} = \langle R|H|R\rangle$$
$$T_{12} = \langle L|H|l+1\rangle = -L_\ell, \qquad T_{34} = \langle l+2|H|R\rangle = -R_{\ell+3}$$

Algorithm to find the ground state

Given $L(\ell)$ and $R(\ell+3)$ – left and right bases at step ℓ

- Iteratively improve $\{L(\ell)\}$ by getting improved $L(\ell+1)$, given $L(\ell)$ and $R(\ell+3)$ (left to right)
- Then improve $\{R(\ell)\}$, given $L(\ell)$ and $R(\ell+3)$ (right to left)

Basic left to right step

- Diagonalize H (4×4 matrix) to get ground state (a_1, a_2, a_3, a_4)
- Normalize a_1 and a_2 as $a_1' = a_1/N$, $a_2' = a_2/N$, $N = \sqrt{a_1^2 + a_2^2}$
- New basis state is then $$L(\ell+1)' = \begin{pmatrix} a_1' L(\ell)_1 \\ \vdots \\ a_1' L(\ell)_\ell \\ a_2' \end{pmatrix}$$
- New Hamiltonian matrix element is
$$\langle L(\ell+1)'|H|L(\ell+1)'\rangle = {a_1'}^2 \langle L(\ell)|H|L(\ell)\rangle + 2{a_2'}^2 - 2a_1'a_2' L(\ell)_\ell$$

If $L(\ell)$ and $R(\ell+3)$ were pieces of exact ground state, this would be exact $\Rightarrow$ energy cannot increase.

Since we add degrees of freedom when $\ell \to \ell+1$, energy will decrease if state is not exact ground state.

Initialization (infinite system procedure)

- Start with $L = 4$ to get $L(2)$
- Reflect $L(2)$ to get $R(5) \Rightarrow L = 6$
- Increase L by 2 until desired size is reached

Implementation in C++

(Uses "MatrixRef" matrix library by S.R.W. and R.M.N.)

C++ can use natural "objects" such as blocks:

(file pbox.h)

```
class Block
    {
public:
    Real H11;
    Real L_inner;

    Block()     // Default: construct a one-site block
        : H11(2.0), L_inner(1.0) { }
    Block Reflect() const { return *this; }
    };
```

- `H11` and `L_inner` are real numbers containing H_{11} (H_{44}) and L_ℓ ($R_{\ell+3}$) for left (right) blocks
- `Block()` (the default constructor) defines that
  `Block S;`
  will create a block consisting of a single site
- `Reflect()` interchanges left and right blocks, i.e.
  `Block R = L.Reflect();` (actually just returns itself)

Now define the collection of blocks making up the system:

```
class WaveFunction;

class System
    {
public:
    const Block& b1;
    const Block& b2;
    const Block& b3;
    const Block& b4;

    System(const Block& bb1,const Block&bb2,
                const Block&bb3, const Block&bb4)
        : b1(bb1), b2(bb2), b3(bb3), b4(bb4) { }

    Real GetGroundState(WaveFunction& p);
    };
```

- `b1, b2, b3, b4` are *references* to four blocks
- The statement
  `System S(leftblock,siteblock,siteblock,rightblock);`
  creates a system of four blocks
- GetGroundState returns the ground state energy and ground state wavefunction `p` (will be defined later, in "pbox.cc")

Still need to define a WaveFunction:

```
class WaveFunction
    {
public:
    Vector v;
    WaveFunction() : v(4) {}
    };
```

just a vector of length 4, `Vector` is from MatrixRef library

Definition of GetGroundState: (file pbox.cc)

```
Real System::GetGroundState(WaveFunction& p)
    {
    Matrix H(4,4), evecs(4,4);
    Vector evals(4);
    H = 0.0;
    H(1,1) = b1.H11;
    H(2,2) = b2.H11;
    H(3,3) = b3.H11;
    H(4,4) = b4.H11;
    H(1,2) = H(2,1) = -b1.L_inner;
    H(2,3) = H(3,2) = -1.0;
    H(3,4) = H(4,3) = -b4.L_inner;
    EigenValues(H,evals,evecs);
    p.v = evecs.Column(1);
    if(p.v.sumels() < 0.0) p.v *= -1.0;
    Real energy = evals(1);
    return energy;
    }
```

- Forms the 4×4 matrix H as defined previously
- Diagonalizes H using `EigenValues` from MatrixRef
- Puts lowest eigenvector in `p`
- Return value is lowest eigenvalue

The density matrix for the noninteracting system involves just a_1 and a_2 (a_4 and a_3 for right block):

```
enum LR {Left, Right};
class DensityMatrix
    {
public:
    Real a,b;
    DensityMatrix(const WaveFunction& psi,LR lr) {
        if(lr == Left)
            { a = psi.v(1); b = psi.v(2); }
        else
            { a = psi.v(4); b = psi.v(3); }
        }
    Vector NewBasis() {
        Vector res(2);
        Real norm = sqrt(a*a+b*b);
        res(1) = a / norm;
        res(2) = b / norm;
        return res;
        }
    };
```

- An `enum` takes on a finite set of values, `LR`: left/right flag
- `NewBasis()` defines the new basis by normalizing `a`, `b`

This new basis can be used to form a new (left) block:

```
Block NewLeft(const Block& b1, const Block& b2, const Vector& bas)
    {
    Block res;
    res.H11 = bas(1) * bas(1) * b1.H11 + 2 * bas(2) * bas(2)
        - 2 * bas(1) * bas(2) * b1.L_inner;
    res.L_inner = bas(2);
    return res;
    }
```

There is a similar routine `NewRight` for right blocks

We are now ready to define the main program: (file dmrgpb.cc)

First read in length, # of sweeps, and initialize array of blocks:

```
int main()
    {
    Block siteblock;
    cerr << "Input length, number of iterations: ";
    int i, length, nsweeps;
    cin >> length >> nsweeps;
    cout << "length, nsweeps = " << length SP nsweeps << endl;
    cout << "Exact energy = " << exacten(length) << endl;
    exlen = length;
    Array1<Block> allblocks(length);
    WaveFunction psi;
    Real energy;
```

- `cout`, `cerr` statements are C++ "print", `cin` reads in variables, `SP` is macro printing one space
- `Array1<Block>` defines 1D array of `Block`s

Next, do "warmup" sweep, building from 4 sites to full size:

```
// Warmup sweep
    allblocks[1] = siteblock;
    for(i = 1; i < length/2; i++)
        {
        Block rightblock = allblocks(i).Reflect();

        System S(allblocks(i),siteblock,siteblock,rightblock);

        energy = S.GetGroundState(psi);
        cout << i+1 SP psi.v(2) SP energy SP 0 << endl;

        DensityMatrix rho(psi,Left);
        Vector basis = rho.NewBasis();

        allblocks[i+1] = NewLeft(allblocks(i),siteblock,basis);
        }
```

- Print step #, g.s. energy, wave function at ℓ $(= i + 1)$, iteration # $(= 0$ for warmup) at each step

Now do "finite system" iterations:

```
// Finite System sweeps
    for(int swp = 1; swp <= nsweeps; swp++)
        {
// We assume reflection symmetry:
        allblocks[length/2 + 2] = allblocks(length/2 - 1).Reflect();
        cout << endl;

// Right to left
        for(i = length/2+2; i > 3; i--)
            {
            System S(allblocks(i-3),siteblock,siteblock,allblocks(i));
            energy = S.GetGroundState(psi);
            cout << i-1 SP psi.v(3) SP energy SP swp - 0.5 << endl;

            DensityMatrix rho(psi,Right);
            Vector basis = rho.NewBasis();

            allblocks[i-1] = NewRight(siteblock,allblocks(i),basis);
            }
```

- Start at symmetric configuration, use reflection symmetry

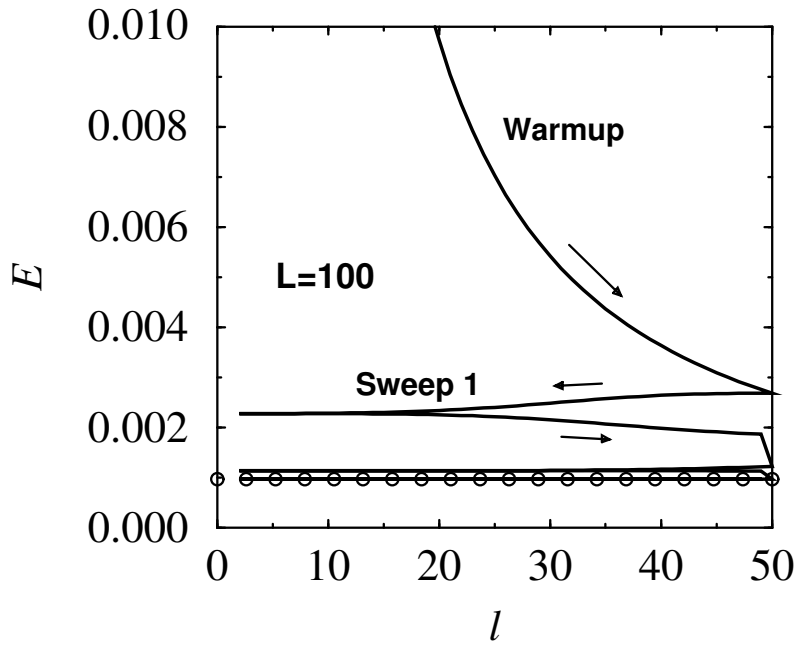
left to right half sweep analogous

```
// Left to right
        cout << endl << 1 SP psi.v(1) SP energy SP swp << endl;
        for(i = 1; i < length/2-1; i++)
            {
            System S(allblocks(i),siteblock,siteblock,allblocks(i+3));
            energy = S.GetGroundState(psi);
            cout << i+1 SP psi.v(2) SP energy SP swp << endl;

            DensityMatrix rho(psi,Left);
            Vector basis = rho.NewBasis();

            allblocks[i+1] = NewLeft(allblocks(i),siteblock,basis);
            }
        }
    return 0;
    }
```

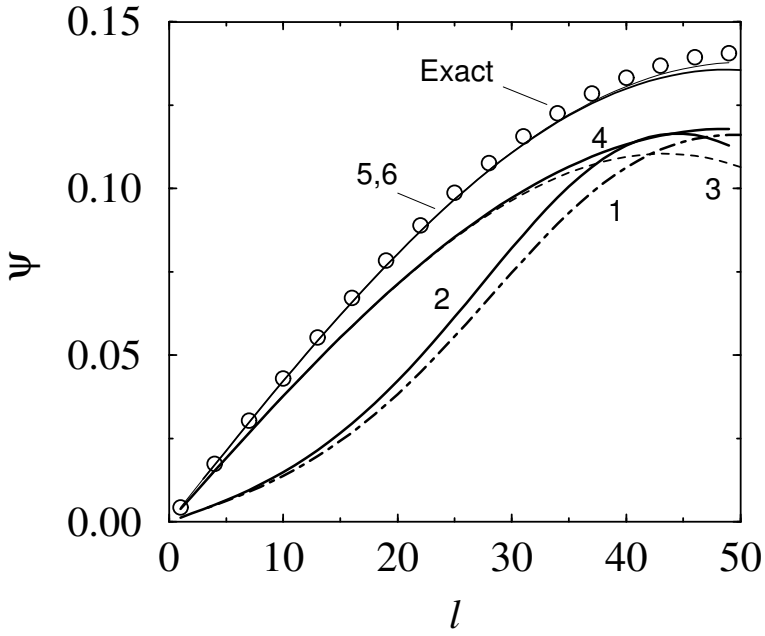
Behavior

$L = 100$, 6 finite-system sweeps

Ground-state energy:



Wavefunction:



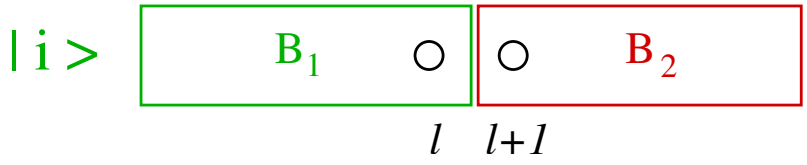
$\Rightarrow$ near machine accuracy by diagonalizing only 4×4 matrix

IV (i) Programming Details

Concrete example: nearest-neighbor Heisenberg exchange

$$\mathbf{S}_\ell \cdot \mathbf{S}_{\ell+1} = S^z_\ell S^z_{\ell+1} + \frac{1}{2}\left(S^+_\ell S^-_{\ell+1} + S^-_\ell S^+_{\ell+1}\right)$$

- Putting 2 blocks together



$$[H_{12}]_{ii';jj'} = [H_1]_{ii'}\,\delta_{jj'} \;+\; \delta_{ii'}\,[H_2]_{jj'} \;+\; \left[S^z_\ell\right]_{ii'}\left[S^z_{\ell+1}\right]_{jj'} + \frac{1}{2}\left(\left[S^+_\ell\right]_{ii'}\left[S^-_{\ell+1}\right]_{jj'} + \left[S^-_\ell\right]_{ii'}\left[S^+_{\ell+1}\right]_{jj'}\right)$$

- Transforming operators:

  Transformation matrix $O_{ij;\alpha}$ composed of m basis vectors u^α_{ij} with $\alpha = 1, \ldots, m$ (usually density matrix eigenvectors)

  Operator $A_{ij;i'j'}$ transformed via

$$A_{\alpha\alpha'} = \sum_{i,j,i',j'} O_{ij;\alpha} A_{ij;i'j'} O_{i'j';\alpha'}$$

  Dimension of A: $(m_1 m_2) \times (m_1 m_2) \rightarrow m \times m$

  Typically: B_1 left or right block, B_2: added site

Efficiency

- Efficient multiplication of $H^{super}|\psi\rangle$ (needed for Lanczos ED)
  - could construct (sparse) matrix for H^{super} $\Rightarrow$ inefficent
  - instead generate terms from block operators

    H for two block system can be written

    $$[H]_{ij;i'j'} = \sum_{\nu} A^{\nu}_{ii'} B^{\nu}_{jj'}$$

    (ν sum over all combinations of block operators in H)

    $H\psi$ becomes

    $$\sum_{i'j'} [H]_{ij;i'j'}\, \psi^{\nu}_{i'j'} = \sum_{\nu} \sum_{i'} A^{\nu}_{ii'} \sum_{j'} B^{\nu}_{jj'} \psi_{i'j'}.$$

    Do j' sum then i' as sequence of 2 matrix–matrix products

    $\Rightarrow$ Reduces CPU as well as memory for most systems
  - Computational cost: CPU $\sim Lm^3$ Memory $\sim m^2$

Efficiency (2)

- Using quantum numbers
  - Abelian quantum numbers like S^z and $N_{\rm ferm}$ good in any subsystem
    $\Rightarrow$ any basis can be partitioned by quantum number
    $\Rightarrow$ all operators consist of rectangular blocks that map between definite quantum numbers
  - Can store operators as collections of (dense) matrices, lists of quantum number pairs $\Rightarrow$ C++ convenient
  - Above operations then have loops over quantum numbers
  - Nonabelian quantum numbers (e.g., $\mathbf{S^2}$) also possible, but more complicated
- Writing to disk

  Information not used in current step can be written to disk
  e.g., previously generated blocks in finite size algorithm

IV (ii) Measurements

- given state ψ_{ij} on two-block system
  - single-site expectation value $\langle\psi|S^z_\ell|\psi\rangle$

$$\langle\psi|S^z_\ell|\psi\rangle = \sum_{i,i',j} \psi^*_{ij}\,[S^z_\ell]_{ii'}\,\psi_{i'j}$$

  - correlation functions such as $\langle\psi|S^z_\ell S^z_m|\psi\rangle$
    - ℓ and m on different blocks:

$$\langle\psi|S^z_\ell S^z_m|\psi\rangle = \sum_{i,i',j,j'} \psi^*_{ij}\,[S^z_\ell]_{ii'}[S^z_m]_{jj'}\,\psi_{i'j'}$$

    - ℓ and m on the *same* block:
      Incorrect for approximate ψ_{ij}:

$$\langle\psi|S^z_\ell S^z_m|\psi\rangle \approx \sum_{i,i',i'',j} \psi^*_{ij}\,[S^z_\ell]_{ii'}[S^z_m]_{i'i''}\,\psi_{i''j}$$

      Reason: sum over i' should run over complete set of states, but it doesn't
      Correct:

$$\langle\psi|S^z_\ell S^z_m|\psi\rangle = \sum_{i,i',j} \psi^*_{ij}\,[S^z_\ell S^z_m]_{ii'}\,\psi_{i'j}$$

General Rule: Compound operators internal to a block must be accumulated as the calculation proceeds

Almost all equal–time correlation functions can be generated like this

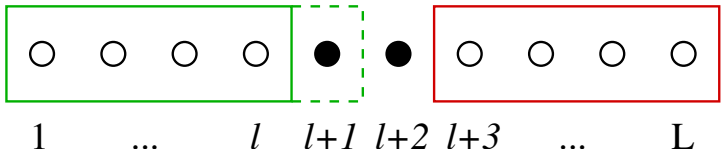
IV (iii) Wavefunction Transformations

$H^{super}\psi_T^k$ for Lanczos or Davidson costly (e.g., 40-100 steps)

Can be reduced if ψ_T^0 is a good guess for ψ_0

Good Guess: Use ψ_0 obtained from previous finite system step

$\Rightarrow$ must transform ψ_0 obtained from step ℓ to $\ell+1$ basis



Basis: $|\alpha_\ell s_{\ell+1} s_{\ell+2} \beta_{\ell+3}\rangle = |\alpha_\ell\rangle \otimes |s_{\ell+1}\rangle \otimes |s_{\ell+2}\rangle \otimes |\beta_{\ell+3}\rangle$

Transform to: $|\alpha_{\ell+1} s_{\ell+2} s_{\ell+3} \beta_{\ell+4}\rangle$

Transformation of left basis:

$$|\alpha_{\ell+1}\rangle = \sum_{s_{\ell+1},\alpha_\ell} L^{\ell+1}[s_{\ell+1}]_{\alpha_{\ell+1},\alpha_\ell} |\alpha_\ell\rangle \otimes |s_{\ell+1}\rangle.$$

where $L^{l+1}[s_{l+1}]_{\alpha_{l+1},\alpha_\ell} = u^{\alpha_{l+1}}_{s_{l+1}\alpha_\ell}$ (u^α_{ij} new basis vectors)

Similarly for right basis

$$|\beta_{\ell+3}\rangle = \sum_{s_{\ell+3},\beta_{l+4}} R^{\ell+3}[s_{\ell+3}]_{\beta_{\ell+3},\beta_{\ell+4}} |s_{\ell+3}\rangle \otimes |\beta_{\ell+4}\rangle$$

Superblock wavefunction:

$$|\psi\rangle = \sum_{\alpha_\ell s_{\ell+1} s_{\ell+2} \beta_{\ell+3}} \psi(\alpha_\ell s_{\ell+1} s_{\ell+2} \beta_{\ell+3}) |\alpha_\ell s_{\ell+1} s_{\ell+2} \beta_{\ell+3}\rangle$$

Since there is a truncation, must approximate

$$\sum_{\alpha_{\ell+1}} |\alpha_{\ell+1}\rangle\langle\alpha_{\ell+1}| \approx 1$$

New wavefunction:

$$\psi(\alpha_{\ell+1}s_{\ell+2}s_{\ell+3}\beta_{\ell+4}) \approx$$
$$\sum_{\alpha_\ell s_{\ell+1}\beta_{\ell+3}} L^{\ell+1}[s_{\ell+1}]_{\alpha_{\ell+1},\alpha_\ell}\psi(\alpha_\ell s_{\ell+1}s_{\ell+2}\beta_{\ell+3})R^{\ell+3}[s_{\ell+3}]_{\beta_{\ell+3},\beta_{\ell+4}}$$

Perform in two steps:

1. intermediate result:

$$\psi(\alpha_{\ell+1}s_{\ell+2}\beta_{\ell+3}) = \sum_{\alpha_\ell s_{\ell+1}} L^{\ell+1}[s_{\ell+1}]_{\alpha_{\ell+1},\alpha_\ell}\psi(\alpha_\ell s_{\ell+1}s_{\ell+2}\beta_{\ell+3})$$

2. then form

$$\psi(\alpha_{\ell+1}s_{\ell+2}s_{\ell+3}\beta_{\ell+4}) = \sum_{\beta_{\ell+3}} \psi(\alpha_{\ell+1}s_{\ell+2}\beta_{\ell+3})R^{\ell+3}[s_{\ell+3}]_{\beta_{\ell+3},\beta_{\ell+4}}$$

- Analogous transformation is used in right to left steps
- Transformation relatively inexpensive in CPU and memory
- Since ψ_T^0 is physically close to ψ_0, Davidson convergence criterium can be relaxed without converging to wrong state
- All transformations can be stored on disk
  $\Rightarrow$ arbitrary operators can be reconstructed *after* final ψ_0 is obtained, at end

$\Rightarrow$ Number of $H\psi_T^k$ steps can be greatly reduced

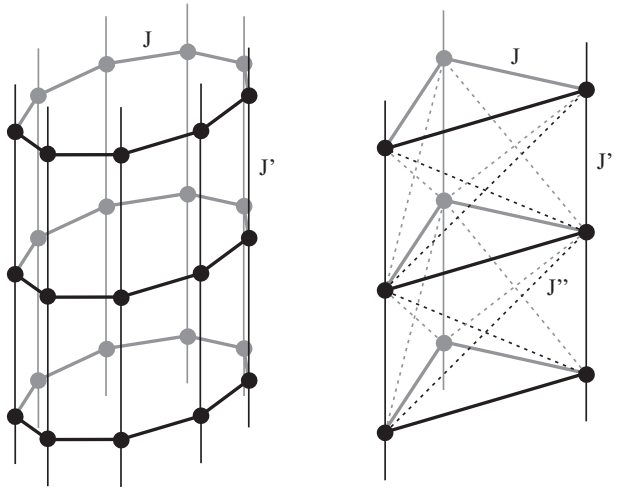
Application: Vanotubes

(Luscher, Noack, Misguich, Kotov, Mila, cond-mat/0405131)

$Na_2V_3O_7$

V^{4+}: $S = \frac{1}{2}$

spin tubes with $J \gg J'$



effective 3-chain model

Ring with odd number of $S = \frac{1}{2}$ spins: 4-fold degenerate

$$H_{\text{eff}} = K \sum_{r=1}^{N-1} \boldsymbol{S}_r \cdot \boldsymbol{S}_{r+1} \left(1 + \alpha \left(\tau_r^+ \tau_{r+1}^- + \tau_r^- \tau_{r+1}^+\right)\right)$$

$\boldsymbol{S}_r$: spin, τ_r chirality on a ring: $S = \frac{1}{2}$ pseudospin

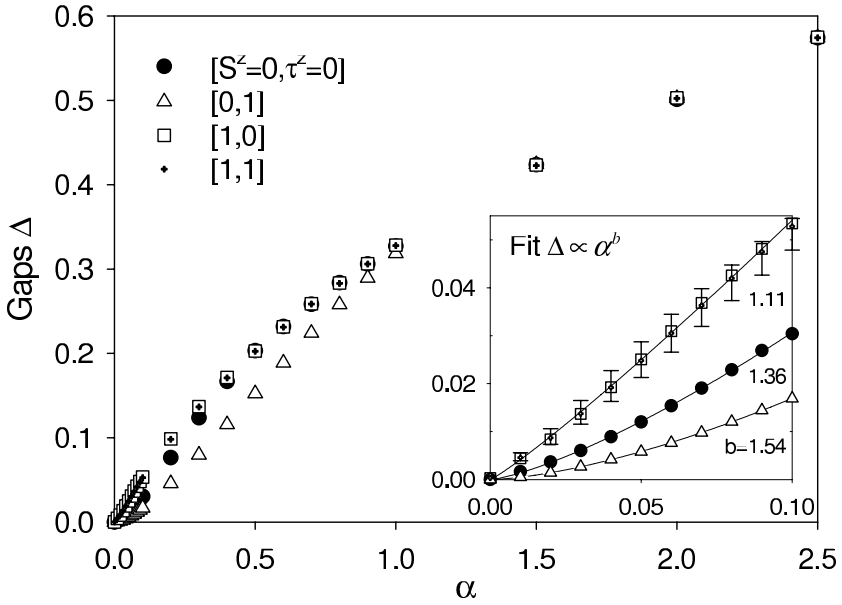
strong ring coupling: $\alpha \geq 4$ (3 legs, $J'' = 0$)

Bosonization (Schulz 1996), DMRG (Kawano & Takahashi, 1997): spin gap

Experiment (susceptibility, NMR): no spin gap (Gavilano *et al.*, 2003)

$\Rightarrow$ effect of frustration? $\alpha \ll 4$

spin and chirality gaps
in $[S^z, \tau^z]$ sectors



$\Rightarrow$ chirality excitation [0,1]
lowest for $\alpha < 1$

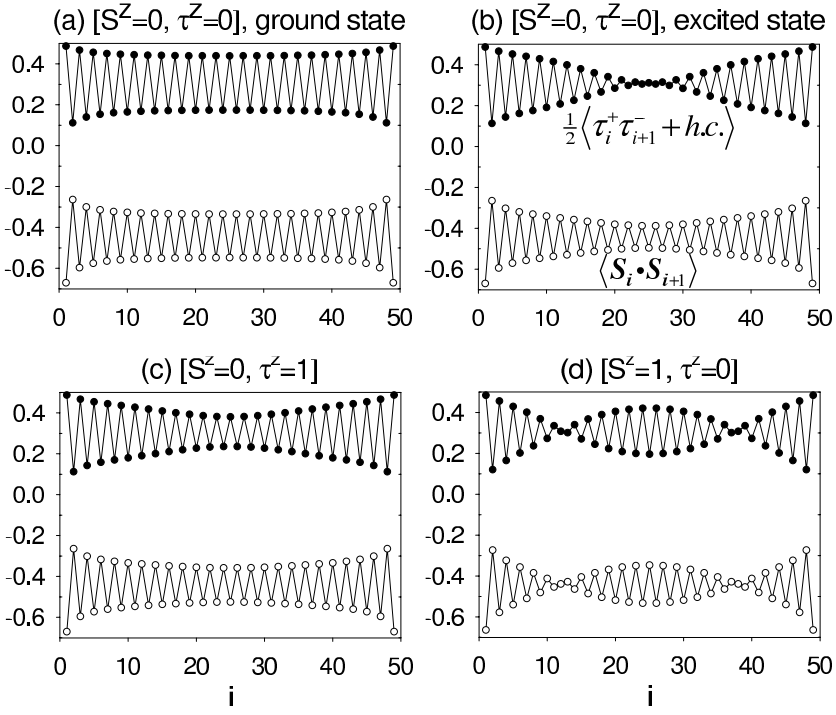
$\Rightarrow$ gaps vanish as $\alpha \to 0$

$\alpha = 0.1$

character of the states:

$\langle\psi_n|\tau_i^+\tau_{i+1}^- + \tau_i^-\tau_{i+1}^+|\psi_n\rangle$

$\langle\psi_n|\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}|\psi_n\rangle$



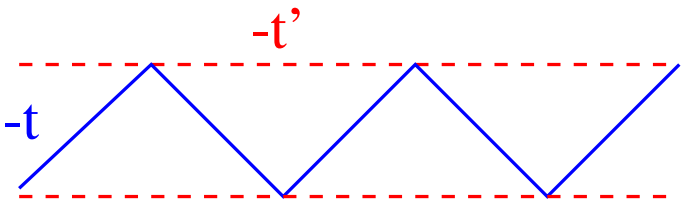
[0,0]: dimerized

[0,1]: bound soliton pair

[1,0]: free solitons

Application: frustrated Hubbard chain

t-t'-U Hubbard chain:



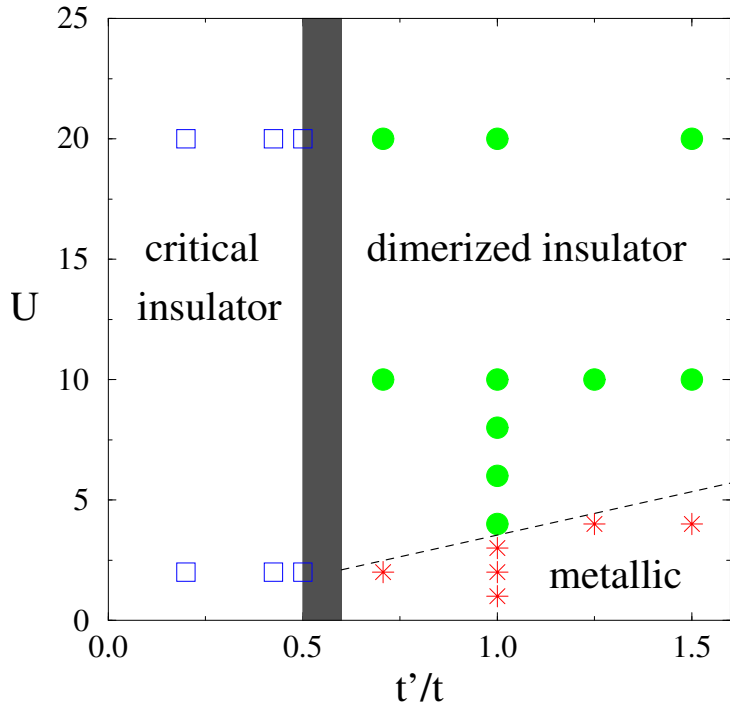
$$H = -\sum_{i,\sigma}(t\ c^\dagger_{i\sigma}c_{i+1\sigma}\ +\ t'\ c^\dagger_{i\sigma}c_{i+2\sigma} + \text{h.c.}) + \ U\ \sum_i n_{i\uparrow}n_{i\downarrow}$$

Dispersion: $\varepsilon(k) = -2t\cos k - 2t'\cos 2k \qquad (t = 1)$

Ground–state phase diagram, $n = 1$:
(Daul and Noack, 1999)

Behavior as a function of U:

- $t' < 0.5$: 1D Hubbard, $U_c = 0$
  $\Delta_s = 0$, $\Delta_c > 0$
- $t' > 0.5$: Mott–Hubbard transition at $U_c > 0$
  $\Delta_s > 0$, $\Delta_c = 0 \rightarrow \Delta_c > 0$



Quantum Critical Behavior

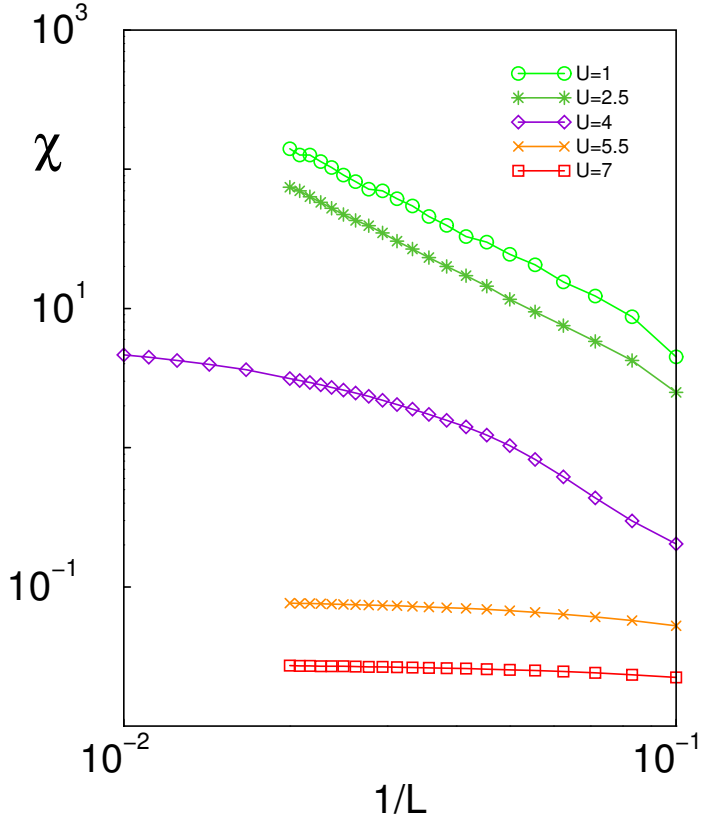
(Aebischer, Baeriswyl, & Noack, 2001)

Metal-Insulator transition as a function of U

Electric susceptibility:

$$\chi = \left.\frac{\partial \langle \mathcal{P} \rangle}{\partial E}\right|_{E=0} = -\frac{1}{L}\left.\frac{\partial^2 E_0(E)}{\partial E^2}\right|_{E=0} \approx \frac{1}{LE}\sum_i x_i \, \langle n_i \rangle$$

Finite-size scaling:

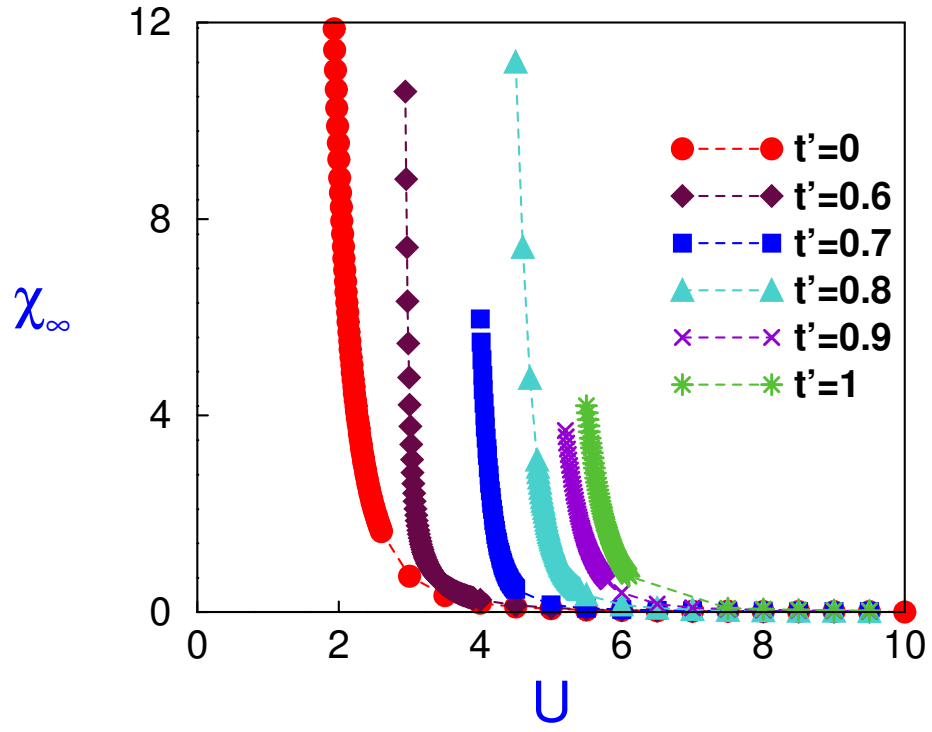


metal
$\chi \sim L^2$

critical

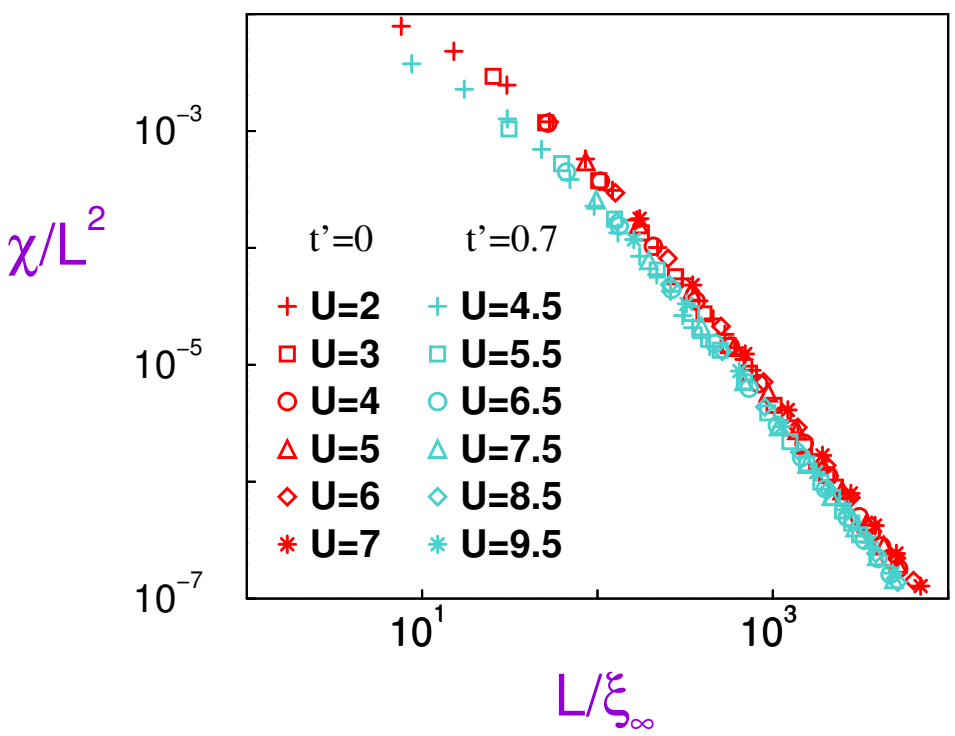
insulator:
$\chi \longrightarrow$ const.

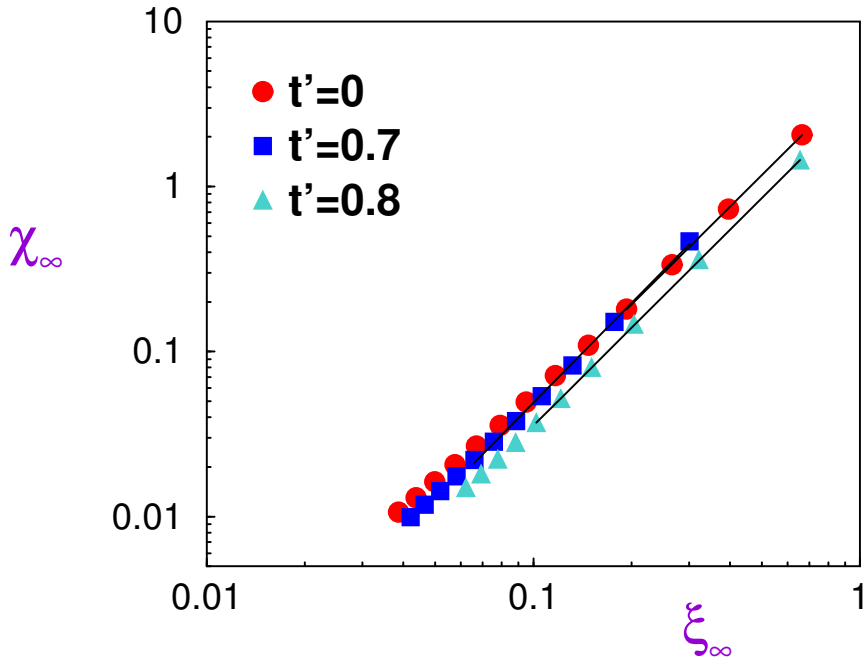
Extrapolated value:



Form: $\chi_\infty \propto \exp\left(\frac{4\pi}{U - U_c}\right)$

Scaling Analysis





$\Rightarrow \chi_\infty \propto \xi_\infty^2$

finite-size scaling: $\frac{\chi}{L^2} = C(t')\Phi(L/\xi_\infty)$

(Privman & M.E. Fisher, 1984)

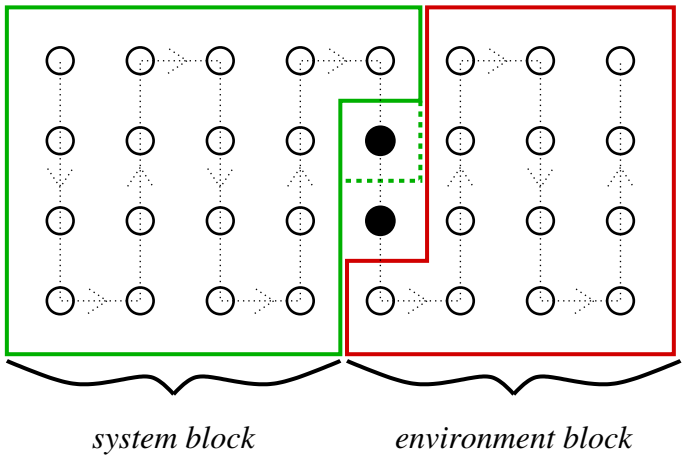
hyperscaling: $\chi_\infty \sim \xi_\infty^{2+z-d}$

(Kim & Weichman, 1991)

Further work: doping ($n < 1$) $\Rightarrow$ itinerant ferromagnetism at large U/t!

IV (iv) Extensions – 2D and Fermion Systems

(Noack, White, Scalapino, 1994)



- 1D algorithm "folded" into 2D
- finite system algorithm necessary

- convergence depends strongly on width of system
  $\Rightarrow$ exponential in width for spinless fermions (Liang & Pang 1994)

Applications:

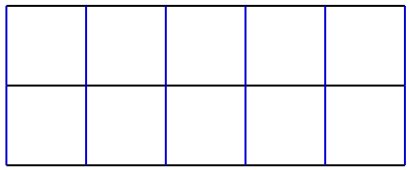
- Heisenberg, Hubbard and t–J–ladders; 2D t–J–model
  $SrCu_2O_3$, $Sr_2Cu_3O_5$, $Sr_{14-x}Ca_xCu_{24}O_{41-\delta}$
  NaV_2O_5, CaV_2O_5, high–T_c superconductors
- Kondo lattice model, periodic Anderson model
  heavy fermion systems ($CeAl_3$, UPt_3)
- Quantum Hall systems (Shibata & Yoshioka, 2001)

Spin Chains and Ladders

(White, Noack & Scalapino, 1994)

Heisenberg model on $n_c = 1, 2, 3, 4$ chains

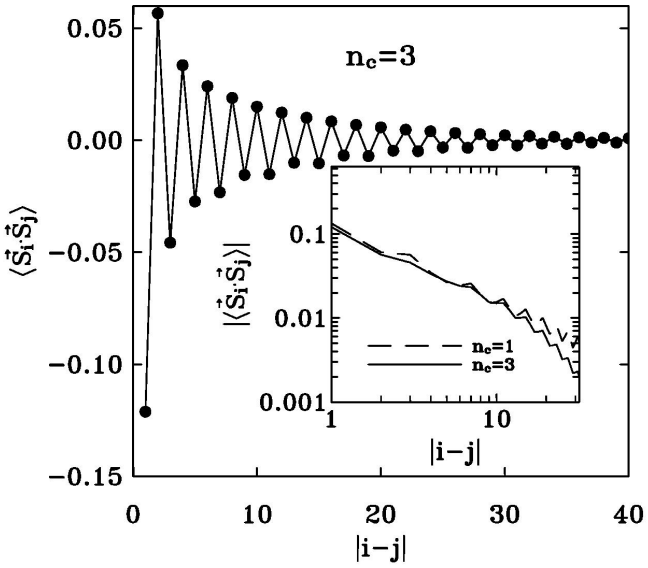
$$H = J_{\parallel} \sum_{j=i+\hat{x}} \mathbf{S}_j \cdot \mathbf{S}_i + J_{\perp} \sum_{j=i+\hat{y}} \mathbf{S}_j \cdot \mathbf{S}_i$$



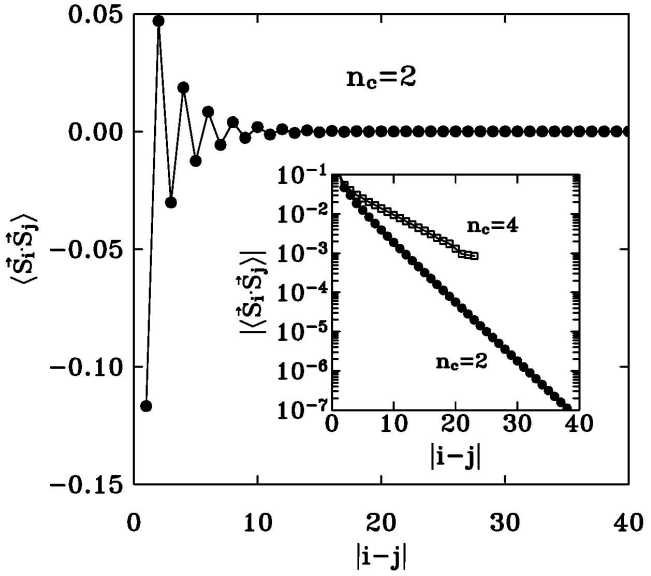
$n_c = 3$

$n_c = 2$

Spin-spin correlation functions



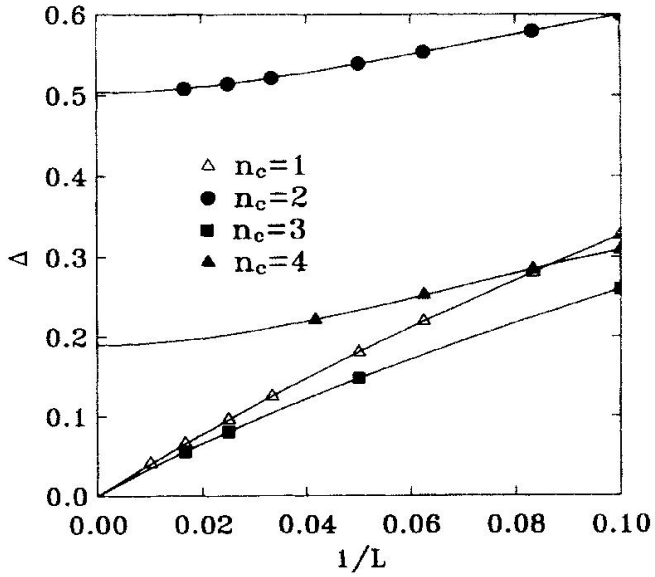
power law – critical



exponentially decaying – disordered

Spin excitations

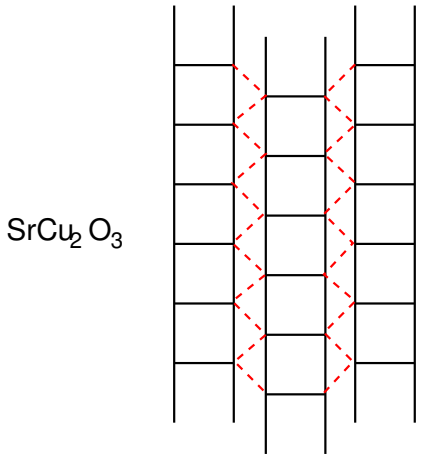
$$\Delta = E_0(S=1,L) - E_0(S=0,L)$$



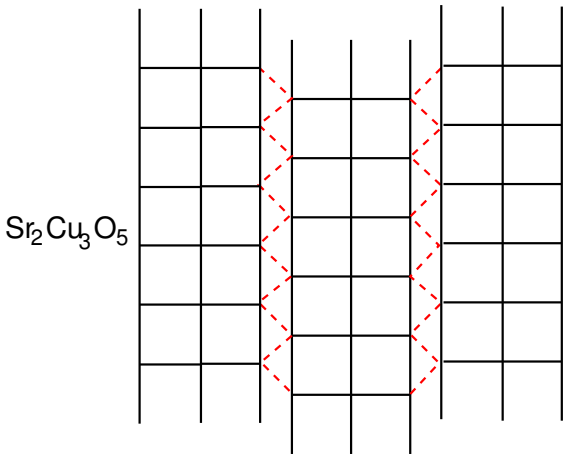
- $\Delta = 0$, n_c odd
- $\Delta > 0$, n_c even
- $J_\perp \gg J_\parallel$ limit:
  $n_c = 2$: rung $S = 0$ singlet
  $n_c = 3$: rung effective spin-1/2

$\Rightarrow$ Quantum effect – Haldane gap

Spin ladder materials



spin gap

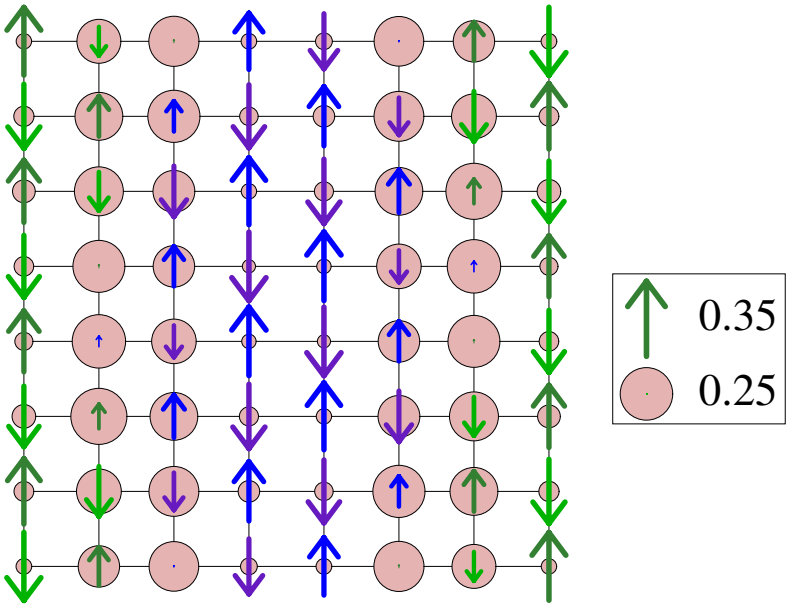


no spin gap

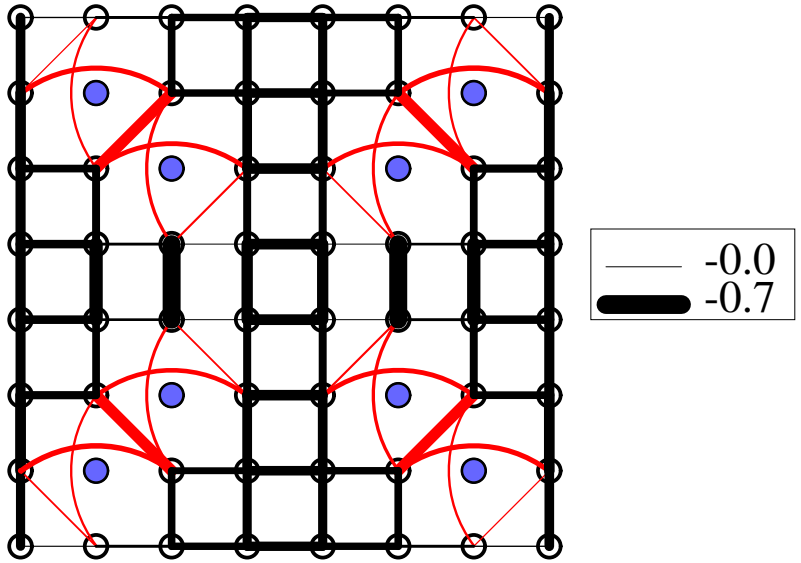
2D t–J Model (White & Scalapino, 1998)

Stripe formation - high-T_c?

- 16×8 lattice (cylinder)
- doping $x = 1/8$
- circles: charge density
  arrows: spin density
- domain walls: π-phase, 1/2-filled, bond centered
- site-centered, diagonal walls also possible



- 8×8 cylinder, 8 holes
- blue circles: most probable hole position
- lines: AF exchange strength



General conclusions:

- stripes w/o long-range Coulomb
- competition with $d_{x^2-y^2}$ pairing
- stripes "evaporate" with t'
  (sign $\longrightarrow$ electron-doping)

Hubbard Model in Momentum Space

(Xiang, 1996; Nishino, Jeckelmann, Gebhard & Noack, 2002)

$$H = \sum_{k\sigma} \varepsilon_k \, c^\dagger_{k\sigma} c_{k\sigma} + \frac{U}{N} \sum_{pkq} c^\dagger_{p-q\uparrow} c^\dagger_{k+q\downarrow} c_{k\downarrow} c_{p\uparrow}$$

Method: choose a 1D path in k-space, similar to 2D algorithm in real space

- advantages
  - convergence only weakly dependent on dimensionality (enters only in ε_k)
  - method exact in weak coupling
  - momentum is a conserved quantity
- disadvantages: interaction non-local
  - convergence poor at large U/t
  - bookkeeping for the interaction terms

$\Rightarrow$ more accurate than real-space DMRG for sufficiently small U

2D square lattice, periodic BCs: $U/t \approx 8$

- current research: more general models

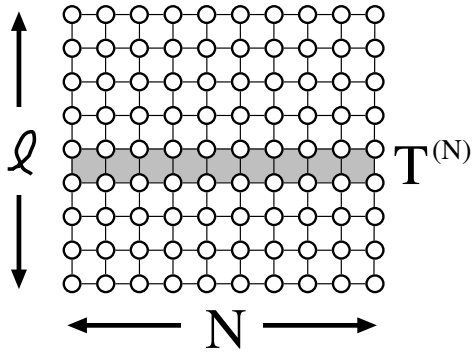
$$\sum_{pkq} V_{\sigma\sigma'}(q) \, c^\dagger_{p-q\sigma} c^\dagger_{k+q\sigma'} c_{k\sigma'} c_{p\sigma}$$

V (i) Classical Transfer Matrices

1D Quantum Systems closely related to 2D classical systems

Row Transfer Matrix (Nishino, 1995)

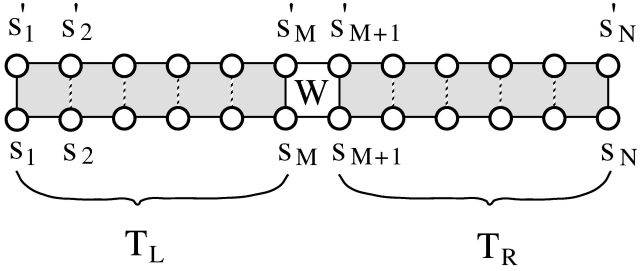
Ising model on a cylinder (periodic in ℓ)



Row transfer matrix $T^{(N)}(\mathbf{s}'|\mathbf{s})$
has dimension 2^N

$\Rightarrow$ Treat $T^{(N)}$ using DMRG

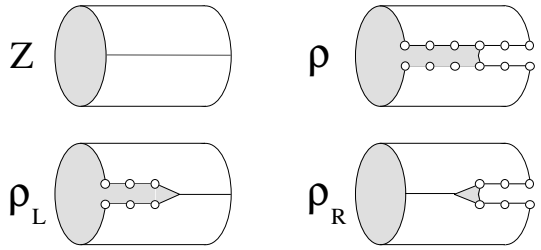
Can divide into two parts:



$$T^{(N)}(\mathbf{s}'|\mathbf{s}) = T_L(\mathbf{s'_L}|\mathbf{s_L}) W(s'_M s'_{M+1}|s_M s_{M+1}) T_R(\mathbf{s'_R}|\mathbf{s_R})$$

Partition function:

$$Z = \mathrm{Tr}\rho = \mathrm{Tr}(T^{(N)})^{\ell} = \sum_{\alpha} \lambda_{\alpha}^{\ell}$$



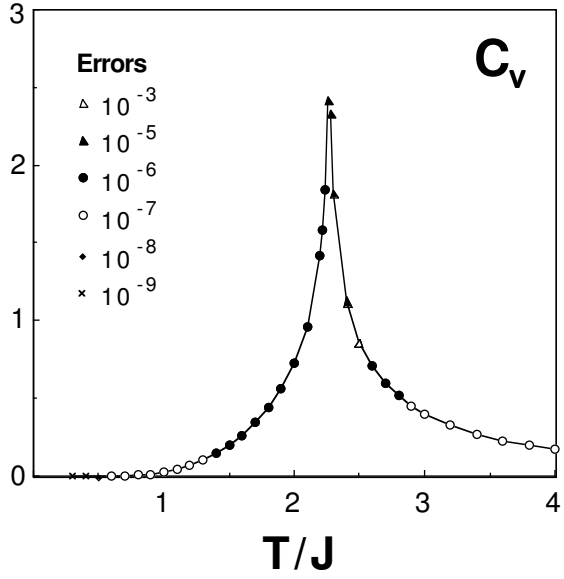
For $\ell >> N$, only largest eigenvalue λ_1^{ℓ} is important $\Rightarrow$ Use DMRG to obtain λ_1^{ℓ}

Can define reduced transfer matrices ρ_L, ρ_R

Both infinite and finite system algorithms can be used

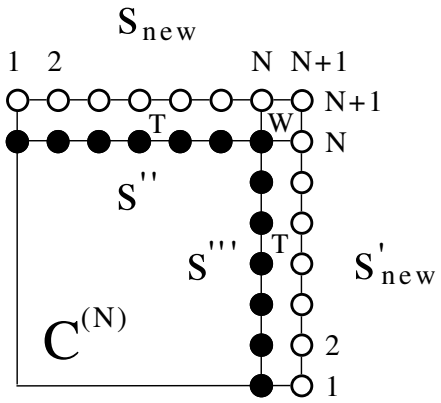
Example: (Nishino, 1995)

Specific heat for the 2D Ising model



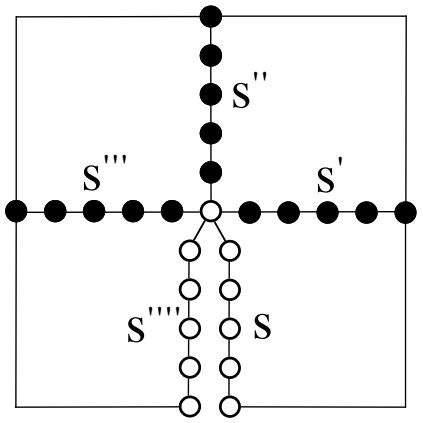
Corner Transfer Matrix: (Nishino and Okunishi, 1996)

Can also treat Corner Transfer Matrix (Baxter, 1968)



Variational partition function fourth power of C.T.M.

$$Z^{(2N-1)} = \mathrm{Tr}\rho_c \approx \mathrm{Tr}\left(\tilde{C}_c^{(N)}\right)^4 = \sum_{\nu=1}^{m} \alpha_\nu^4$$



Baxter treated $N \to \infty$ limit variationally

$\Rightarrow$ Equivalent to infinite system algorithm (Okunishi, 1996)

However, $\tilde{C}_c^{(N)}$ need not be explicitly diagonalized!

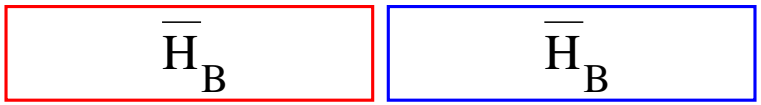
V (ii) Finite Temperature

Simplest idea: Use Boltmann weight $e^{-\beta E_\alpha}$ to weight target states $|\psi^\alpha\rangle$ in mixed density matrix:

$$\rho_{ii'} = \sum_\alpha e^{-\beta E_\alpha} \sum_j \psi^\alpha_{ij} \psi^{\alpha\,*}_{i'j}$$

Refinement: (Moukouri and Caron, 1996)

Target $M \sim 10$ – 30 states with weight $1/M$, project to smaller Hilbert space by forming



$\Rightarrow$ *Fully* diagonalize H_{BB}, calculate Boltzmann sum

$$\langle A \rangle = \sum_\gamma e^{-\beta E_\gamma} \langle \psi^\gamma_{BB} | A | \psi^\gamma_{BB} \rangle$$

Idea: Basis of $\bar{H}_B$ good description of *all* states

Advantages

- Straightforward extension of original DMRG
- Most accurate at low T (on finite system)

Disadvantages

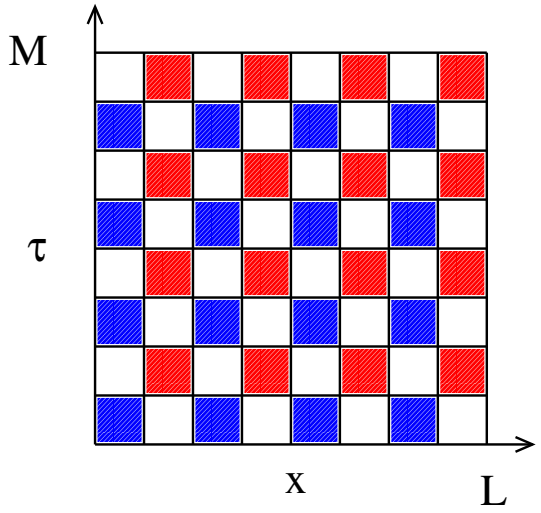
- Finite–size effects (largest at small T)
- Not clear whether high–T limit converges

Transfer Matrix DMRG (TMRG)

(Bursill *et al.*, 1996)
(Wang and Xiang, 1997)

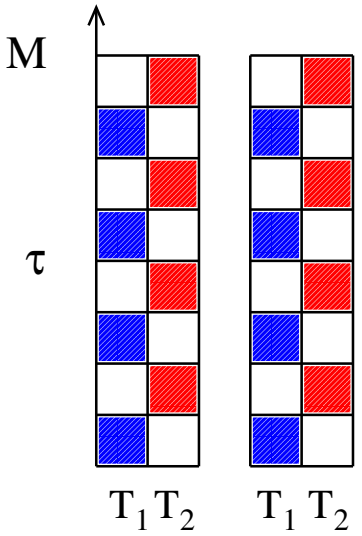
Idea: Treat quantum system as $1+1$ dimensional classical system using Trotter–Suzuki (checkerboard) decomposition

$$Z = \mathrm{Tr}\; e^{-\beta H} = \mathrm{Tr}(e^{-\Delta\tau H_{\mathrm{odd}}} e^{-\Delta\tau H_{\mathrm{even}}})^{M/2} + \mathcal{O}(\Delta\tau^2)$$



Transfer Matrix in *space* direction:

$$Z_M^{\infty} = \lim_{L\to\infty} \mathrm{Tr}\,(T_1 T_2)^{L/2}$$



Obtain partition function for *infinite* system at finite T

Free energy related to largest eigenvalue of transfer matrix

$$F = -\lim_{\Delta\tau \to 0} \frac{\ln \lambda_{\max}}{2\beta}$$

$\Rightarrow$ Use DMRG to obtain $\lambda_{\max}$

Advantages

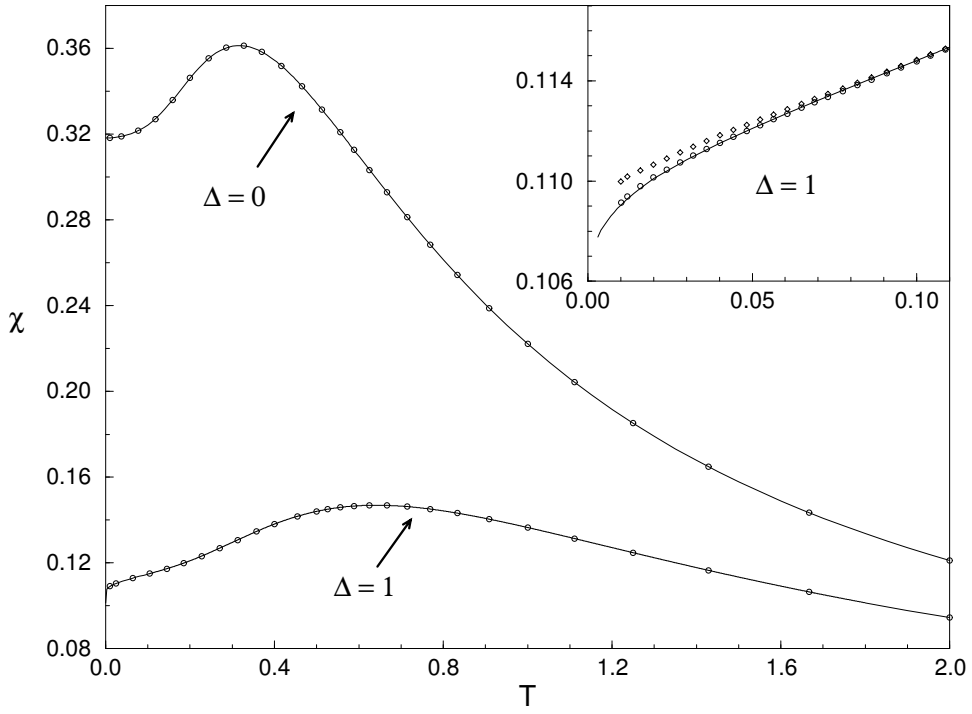
- In thermodynamic limit – calculates properties of infinite system
- Exact at high T
- Can calculate thermodynamic properties easily
- τ–dependence available for local dynamics
  - Must analytically continue $i\omega_m \longrightarrow \omega + i\delta$ (Maximum Entropy)
  - Spatial (or k) dependence more difficult

Disadvantages

- Technical difficulties – $(T_1 T_2)$, ρ not symmetric in general
- Must extrapolate to $\Delta\tau \to 0$
- Lower temperature more difficult – "size" $\Longleftrightarrow T$
- Longer distance correlation functions more difficult

Example (Wang and Xiang, 1997)

Wang et al Fig. 3



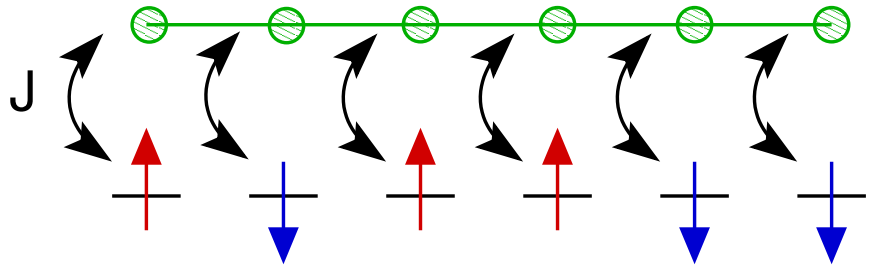
Spin Susceptibility for the spin–1/2 XY ($\Delta = 0$) and Heisenberg chains

1D Kondo Lattice Model

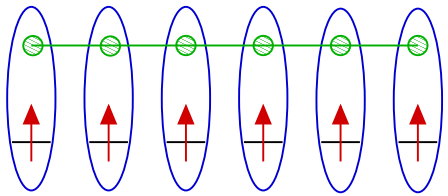
(Shibata & Tsunetsugu, 1999)

Hamiltonian

$$H = -t\sum_{i,\sigma}\left(c^{\dagger}_{i,\sigma}c_{i+1,\sigma} + \text{h.c.}\right) + \frac{J}{2}\sum_{i}\mathbf{S}_i \cdot \left(c^{\dagger}_{i,\alpha}\boldsymbol{\sigma}_{\alpha,\beta}c_{i,\beta}\right)$$

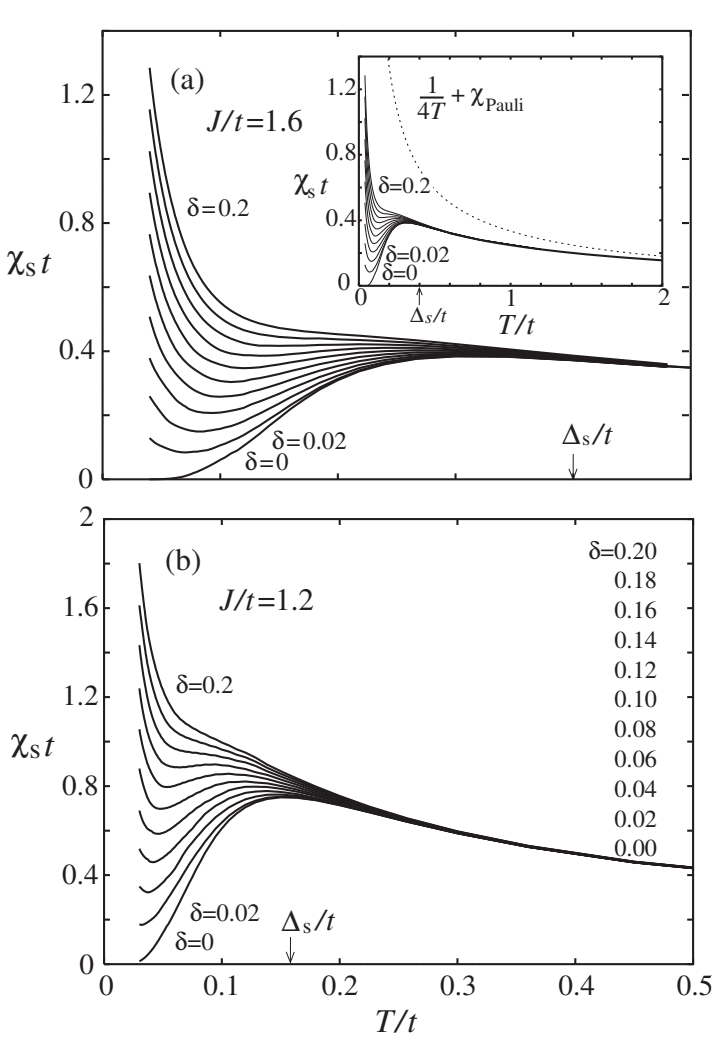


- Single 1D conduction band
- Localized spin-1/2 impurity at each site
- Half-filling ($\langle n\rangle = 1$): Kondo insulator: localized singlets $\Delta_c > \Delta_s > 0$



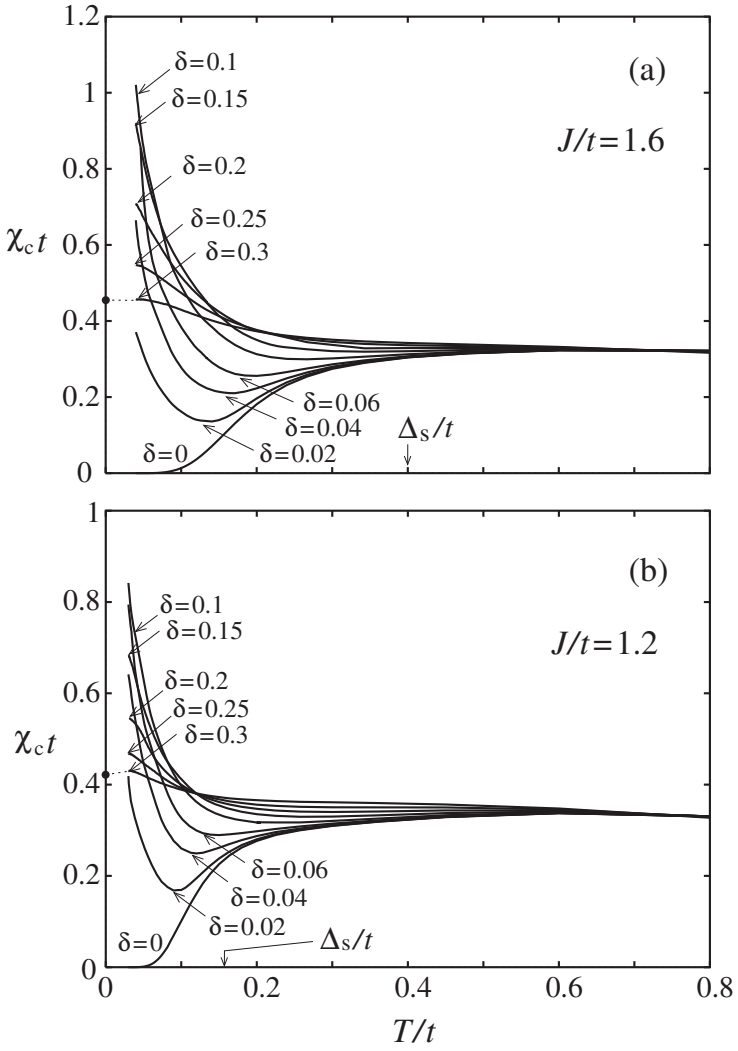
- doping ($\langle n\rangle = 1-\delta$): crossover to metallic behavior (RKKY Luttinger liquid)

Spin susceptibility



- high T: $\chi_s = \chi_{\rm Pauli} + \chi_{\rm Curie}$
- low T, $\delta = 0$: spin gap
- low T, $\delta > 0$: crossover to metal

Charge susceptibility



- high T: free electron behavior
- low T, $\delta = 0$: charge gap
- low T, $\delta = 0$: crossover to metal

V (iii) Dynamics of a Quantum System

dynamical correlation function

$$G(\mathbf{k},\omega) = \langle\psi_0|A_{\mathbf{k}}^{\dagger}(\omega + i\eta - H)^{-1}A_{\mathbf{k}}|\psi_0\rangle$$

additional density-matrix eigenstates must be "targetted":

- Lanczos vector method (Hallberg, 1995)
  target vectors: Krylov basis
  $$|\psi_0\rangle,\ A_{\mathbf{k}}|\psi_0\rangle,\ HA_{\mathbf{k}}|\psi_0\rangle,\ H^2A_{\mathbf{k}}|\psi_0\rangle,\ \ldots$$
- correction vector method: (White & Kühner, 1999)
  target vectors:
  $$|\psi_0\rangle,\ A_{\mathbf{k}}|\psi_0\rangle,\ (\omega + i\eta - H)^{-1}A_{\mathbf{k}}|\psi_0\rangle$$
  $\Rightarrow$ more accurate, but more costly: different run for each ω
- minimization method (Jeckelmann, 2002)
  correction vector minimizes functional
  $$W_{A,\eta}(\omega,\psi) = \langle\psi|(E_0 + \omega - H)^2 + \eta^2)|\psi\rangle\ +\ \eta\langle A|\psi\rangle\ +\ \eta\langle\psi|A\rangle$$
  to get spectral weight
  $$W_{A_{\mathbf{k}},\eta}(\omega,\psi_{\min}) = -\pi\eta\,\mathrm{Im}\,G(\mathbf{k},\omega)$$
  $\Rightarrow$ mimimization more stable and efficient than matrix inversion

Example: Single-Particle Spectral Weight for Hubbard Chain

(Benthien, Gebhard, & Jeckelmann, 2004)

1D Hubbard model (open BCs)

$$H = -t \sum_{\ell=1,\sigma}^{L-1} \left(c^\dagger_{\ell,\sigma} c_{\ell+1,\sigma} + c^\dagger_{\ell+1,\sigma} c_{\ell,\sigma} \right) + U \sum_{\ell=1}^{L} n_{\ell,\uparrow} n_{\ell,\downarrow}$$

Single-particle spectral weight for holes (photoemission)

$$A(k,\omega) = \frac{1}{\pi} \operatorname{Im} \langle \psi_0 | \, c^\dagger_{k,\sigma} \, \frac{1}{H + \omega - E_0 + i\eta} \, c_{k,\sigma} \, | \psi_0 \rangle$$

where $c_{k,\sigma} = \frac{1}{\sqrt{L}} \sum_\ell e^{ik\ell} \, c_{\ell,\sigma}$ (assumes periodic BCs)

Problem: open BCs

Solution: use particle-in-a-box states

$$c_{k,\sigma} = \sqrt{\tfrac{2}{L+1}} \sum_\ell \, \sin(k\ell) \, c_{\ell,\sigma}$$

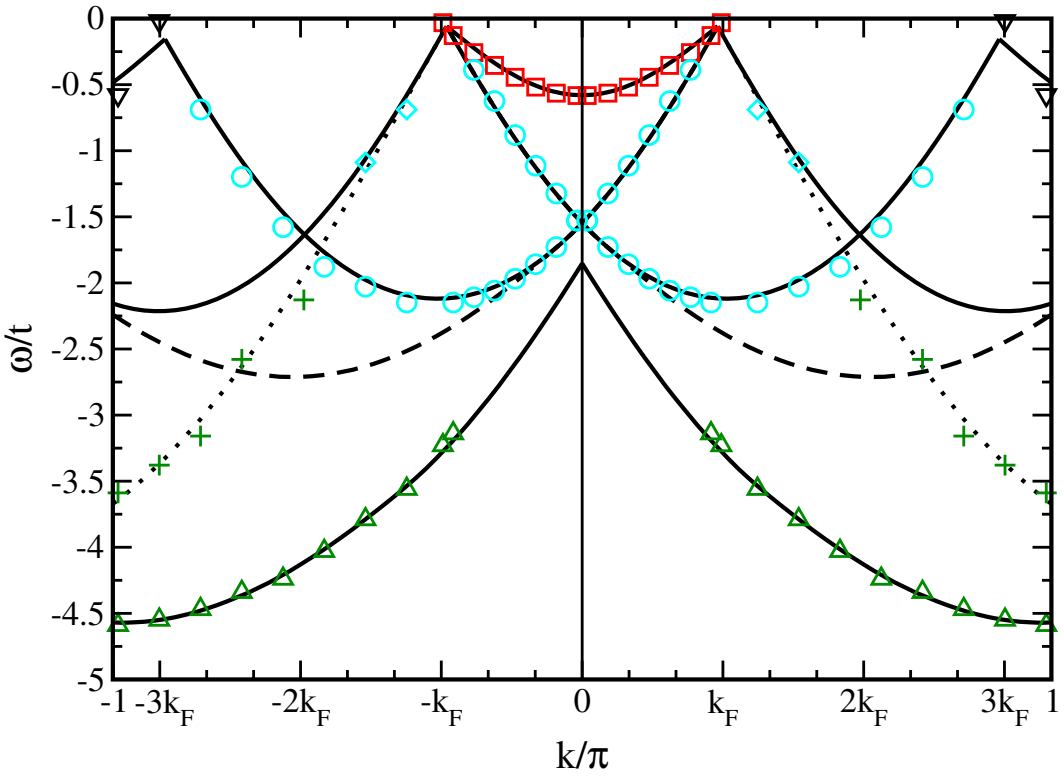
$\Rightarrow$ What does $A(k,\omega)$ look like in a Luttinger liquid?

(Spin-charge separation, no fermionic quasiparticle, ...)

Comparison with Bethe Ansatz

Bethe Ansatz: dispersion of specific excitations (no spectral weight)

$n = N_e/L = 0.6, U/t = 4.9, L = 90$



lines: Bethe Ansatz

□ spinon band

○ ◇ holon band

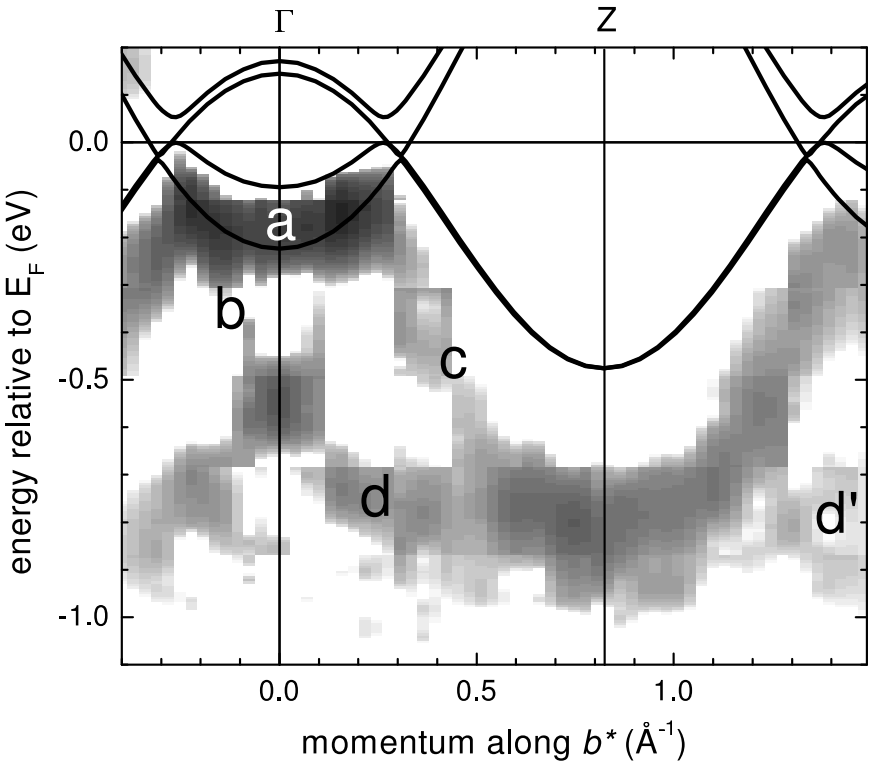
\+ lowest $4k_F$ charge excitation

△ lowest $4k_F$-singlet charge excitation + one spinon

$\Rightarrow$ excellent agreement with Bethe Ansatz dispersion

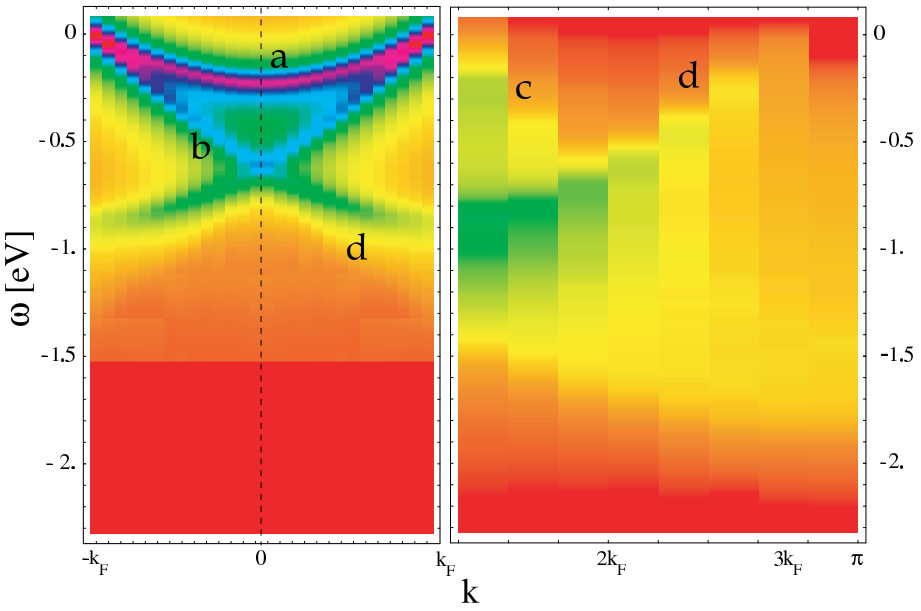
Comparison with ARPES on TTF-TCNQ

ARPES



(Sing *et al.*, *2003*)

DDMRG



V (iv) Quantum Chemistry

(White & Martin, 1999)

$$H = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + \frac{1}{2} \sum_{i,j,k,l} G_{ijkl} \sum_{\sigma,\sigma'} c^\dagger_{i\sigma} c^\dagger_{j\sigma'} c_{k\sigma'} c_{l\sigma}.$$

- $c^\dagger_{i\sigma}$ creates electron in molecular orbital i (N orbitals)
- t_{ij} single-electron integral of molecular orbitals i and j
- G_{ijkl} two-electron integral (Coulomb repulsion)

  $\Rightarrow$ exact diagonalization: "full CI"

- Method: similar to momentum-space, 2D methods
- Computational cost: $(N^4 m^2 + N^3 m^3)$
- Applications
  - H_2O (White & Martin, 1998)
  - CH_4, HHeH (Daul, Ciofini, Daul, & White, 2000)
  - Be_2, N_2, HF (Mitrushenkov et al., 2001)
  - CH_2, F_2, LiF (Legeza, Röder, & Hess, 2002; 2003)

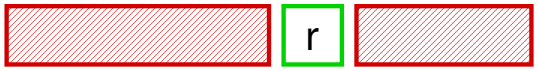
    ionic-neutral crossing in LiF: potential to 10^{-6}, dipole moment to 10^{-5}
  - Ne, H_2O, N_2, C_2H_4, H_2-chains (Chan & Head-Gordon, 2002)

  $\Rightarrow$ energies compare well to full CI (up to 6 digits of accuracy)

Site Ordering Problem

Which orbitals should be placed near one another?

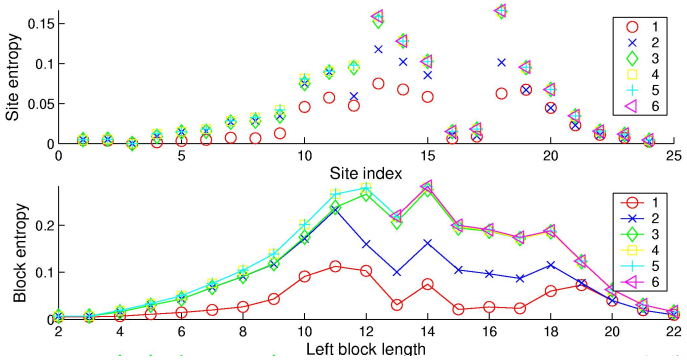
- single-site Density Matrix ρ_p (Legeza & Solyom, ...)



$\Rightarrow S(\rho_p)$: influence of site p

site entropy $S(\rho_p)$

block entropy $S(\rho_A)$



H_2O molecule

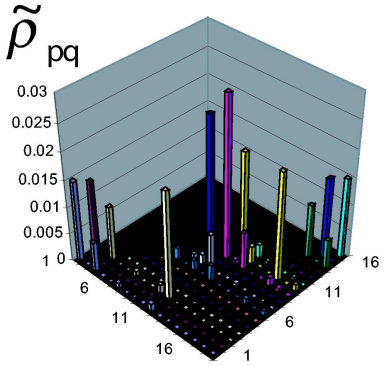
- two-site density matrix $\rho_{p,q}$ (Rissler, White & RMN, ...)

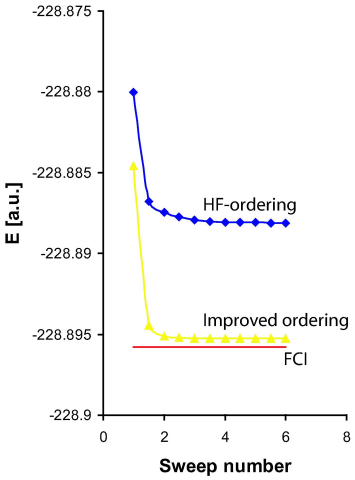
$\Rightarrow$ effective interaction between p and q

Fluorine

18 orbitals

$m = 200$





V (v) Time Evolution

Time evolution of a state in quantum mechanics

$$|\psi(t)\rangle = e^{-iHt}\,|\psi(0)\rangle$$

typically: $H = H_0 + H_1\,\Theta(t)\,,$ $|\psi(0)\rangle = |\psi_0\rangle$ or $A^\dagger\,|\psi_0\rangle$

DMRG approaches:

- Runge-Kutta integration of $|\psi_0\rangle_{\rm DMRG}$ (Cazallila & Marston, 2002)
  $\Rightarrow$ only good for small times t
- division of e^{-iHt} into 2-site terms
  (White & Feiguin, 2004; Daley, *et al.*, 2004)
  Trotter-Suzuki decomposition, 2-site parts exactly applied $\Rightarrow$ quantum gates
- expansion of e^{-iHt} in Krylov basis (Schmitteckert, cond-mat/0403759)
  (Manmana, Muramatsu & Noack, ...)
  multi-target method – optimal targetting under development

Applications: tunnel current between Luttinger liquids,
transport current in a quantum dot
Bose-Hubbard model: Bose-Einstein condensation, atom traps

V (vi) Matrix Product States

DMRG changes the state of the system block in 2 steps:

1. blocking (add a site to a block)

$$|\alpha\rangle_\ell \otimes |s_\ell\rangle \rightarrow |\beta'_{\ell+1}\rangle$$

2. truncation (in density matrix eigenbasis)

$$|\beta_{\ell+1}\rangle = u^{\beta}_{\beta'} |\beta'_{\ell+1}\rangle$$

Both steps can be combined (as in wavefunction transformations)

$$|\beta_{\ell+1}\rangle = \sum_{s_\ell,\alpha} A^s_{\beta\alpha} |\alpha_\ell\rangle \otimes |s_\ell\rangle$$

$A^s_{\beta\alpha}$ is a matrix which maps from α_ℓ to $\beta_{\ell+1}$

The DMRG wavefunction can be written as a sum of such products

(Ostlund & Rommer, 1995)

$$|\psi_{\rm MPS}\rangle = \sum_{\{s_\ell\}} {\rm Tr}\left\{ A^{s_1} A^{s_2} A^{s_3} \ldots A^{s_L} \right\} |s_1, s_2, \ldots, s_L\rangle$$

The A^{s_ℓ} are $m \times m$ matrices, except for A_1 & A_L which are m-element *vectors*

This is a special case of a *matrix product state*

The DMRG is a variational calculation in the space of such states

Features

- Any state can be described as a MPS (with dimension of A^{s_ℓ} large enough)
- Some states are very compactly described:
  - Neél state $|\uparrow\downarrow\uparrow\downarrow\uparrow\ldots\rangle$
  - Bell state $|\uparrow\uparrow\uparrow\ldots\rangle \pm |\downarrow\downarrow\downarrow\ldots\rangle$
  - AKLT state: product of singlets to describe spin-1 chain

  $\Rightarrow 2 \times 2$ matrices
- Matrix product states can be variationally optimized using different methods
  - power method $H^n|\psi_{\rm MPS}\rangle$
  - imaginary time evolution $e^{\Theta H}|\psi_{\rm MPS}\rangle$
  - Lanczos
  - DMRG – very efficient, but complicated
- an arbitrary operator X can be evaluated directly in terms of matrix products

$\Rightarrow$ Calculations with matrix product states generalize DMRG

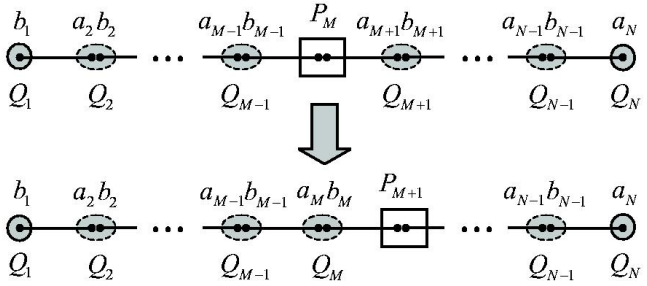
Are other MPS's better than the DMRG state for particular problems?

Answer: yes (almost certainly)

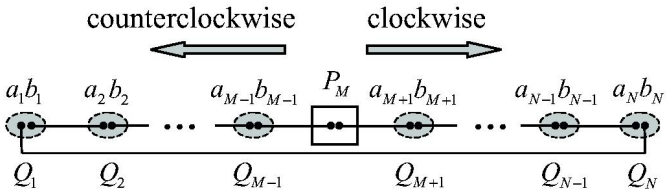
Better Matrix Product-like States

Periodic boundary conditions (Verstraete, Porras & Cirac, c-m/0404706)

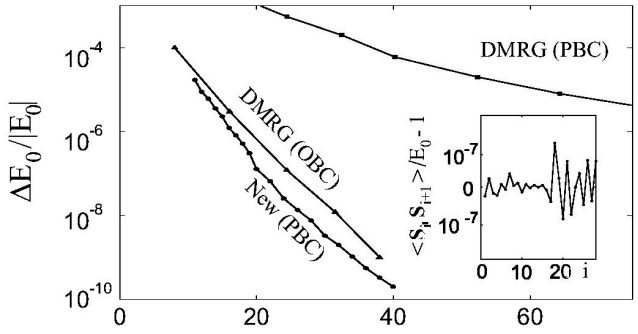
DMRG



New Method



Results: $L = 28$ Heisenberg chain



Questions:

- computational cost - matrices no longer sparse
- optimal minimization algorithms?

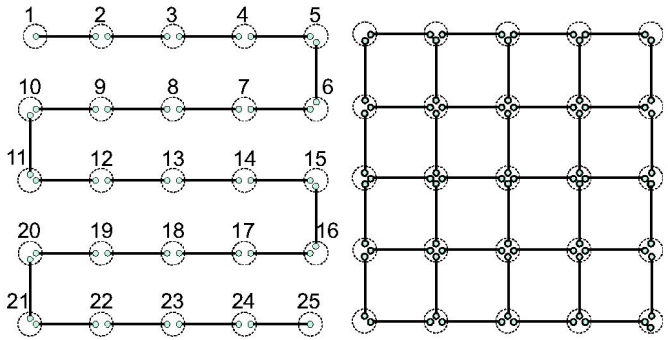
Application to other systems

- Finite temperature or dissipation

  (Verstraete, García-Ripoll & Cirac, cond-mat/0406426)

- 2D systems

  (Verstraete, & Cirac, cond-mat/0407066)



Entanglement in all 4 directions $\Rightarrow$ Tensor product states needed!

DMRG and Quantum Information

Application of Quantum Information in the DMRG

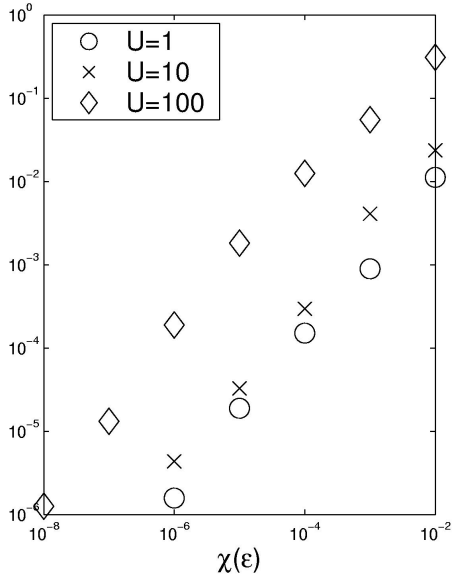
- entanglement (von Neumann) entropy $S_A = -\mathrm{Tr}\,\rho_A \ln \rho_A = S_B$

Error in E_0

vs.

Change in ρ_A after truncation

1D Hubbard model, $L = 80$
(Legeza & Solyom, 2004)



$\Rightarrow$ How does ρ_A depend on characteristics of system?

Applications of the DMRG in Quantum Information Theory

- decoherence
  $\Rightarrow$ DMRG simulation of entanglement with environment
- foundations of quantum information theory
  example: bounds on information content of a noisy chanel

Discussion: DMRG

- DMRG is now a "standard method" for 1D+ spin and fermion systems
- Basic algorithm can still be improved, for example through better use of symmetries (S^2, lattice symmetries, ...)
- Biggest challenge: more efficient extension to 2D+ or 3D+ (classical systems) lattices
- Currently under development:
  - more general models in momentum space
  - quantum chemistry: more realistic systems
  - dynamics of quantum systems: efficiency can be improved, many possibilities for applications
  - transfer matrices: improved dynamics, more systems
  - non-equilibrium systems: new field!
- Exciting new ideas (from Quantum Information Theory)
  - Matrix and tensor product states $\Rightarrow$ generalizations of DMRG

    Prospects for
    - periodic boundary conditions
    - 2D systems
    - finite temperature, dissipative systems