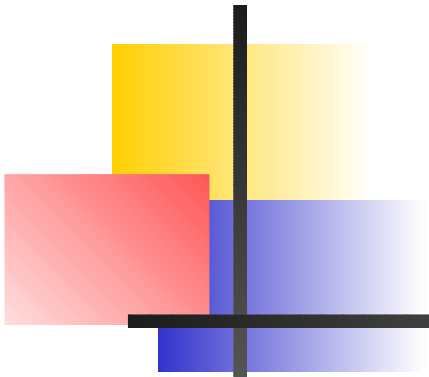
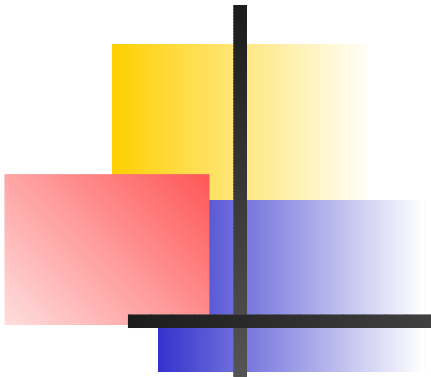


Section I

Exact diagonalisations and Lanczos methods

Comparison with other methods



Outline

1. Power method & Lanczos algorithm: how to get started
2. Finite size scaling: a simple example – 1D chain of correlated fermions
3. How to implement it on a computer
4. Dynamical correlations
5. Comparison with other methods
   - DMRG method (basic notions)
   - Stochastic methods (see R. Scalettar's Course)

Some references

-*Exact diag:* "Simulations of pure and doped low-dimensional spin-1/2 systems", N. Laflorencie and D. Poilblanc, Chapter 5, *Quantum Magnetism*, Lecture Notes in Physics, Ed. U. Schollwöck et al., Spinger (2004)

-*DMRG:* Review by R.M. Noack in *"Lectures on The Physics of Highly Correlated Electron Systems IX"*, AIP Conf. Proceedings Vol.789 (2004).

Some lattice models to study

Hubbard model (metal & insulator phases)

$$H_U = H_K + \sum_{\mathbf{i},\mathbf{j}} V_{\mathbf{ij}} n_{\mathbf{i}} n_{\mathbf{j}}$$

$$H_K = \sum_{\mathbf{i},\mathbf{j},s} t_{\mathbf{ij}}\, c^{\dagger}_{\mathbf{i},s} c_{\mathbf{j},s}$$

Typically $V_{\mathbf{ij}}$ restricted to on-site repulsion (Hubbard U term) and nearest neighbor V

Strong coupling limits

- Heisenberg model (insulator at half-filling)

$$H_J = \sum_{\mathbf{i},\mathbf{j}} J_{\mathbf{ij}}\, \mathbf{S_i} \cdot \mathbf{S_j}$$

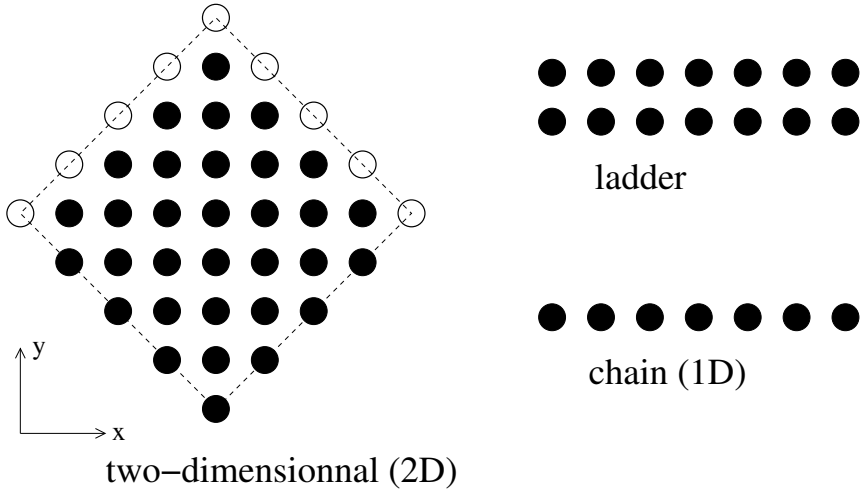
- Strong coupling: t-J

$$\begin{aligned} H_{t-J} &= H_J + \mathcal{P} H_K \mathcal{P}, \\ H_K &= \sum_{\mathbf{i},\mathbf{j},s} t_{\mathbf{ij}}\, c^{\dagger}_{\mathbf{i},s} c_{\mathbf{j},s} \end{aligned}$$

$\mathcal{P}$ Gutzwiller projector: $\mathcal{P} = \prod_i (1 - n_{i\uparrow} n_{i\downarrow})$

Finite size clusters

→ Computation on finite size clusters



- Correlated lattice models
- Goals: ⇒ ground state properties
- ⇒ low energy excitations

The simple power method

H^n acts as a projector on the GS for $n \to \infty$

$$|\Phi_n\rangle = (H - \lambda)^n |\Phi_0 > ,$$

Then:

$$\langle \Phi_n | H | \Phi_n \rangle / \langle \Phi_n | \Phi_n \rangle \to E_{\rm GS}$$

The Lanczos algorithm

Build a tri-diagonal matrix

$$
\begin{aligned}
H|\Phi_1\rangle &= e_1|\Phi_1\rangle + b_2|\Phi_2\rangle, \\
&\vdots \\
H|\Phi_n\rangle &= e_n|\Phi_n\rangle + b_{n+1}|\Phi_{n+1}\rangle \\
&+ b_n|\Phi_{n-1}\rangle
\end{aligned}
$$

Recurrent procedure:

$$e_n = \langle\Phi_n|H|\Phi_n\rangle$$

$$|\phi_{n+1}\rangle = H|\Phi_n\rangle - e_n|\Phi_n\rangle - b_n|\Phi_{n-1}\rangle$$

References

- C. Lanczos, J. Res. Natl. Bur. Stand. **45**, 255 (1950)
- J.C. Bonner and M.E. Fisher, Phys. Rev. **135**, 640 (1964)
- J. Oitmaa and D.D. Betts, Can. J. Phys. **56**, 897 (1978)

Use of symmetries

Goal: Block-diagonalize the H matrix

$$J_{\mathbf{xy}} = J(\mathbf{x}-\mathbf{y})$$

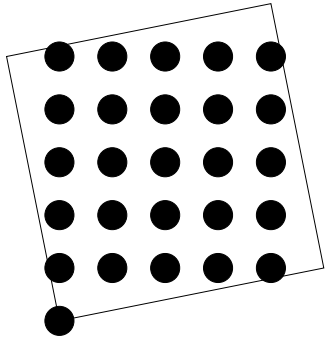
and

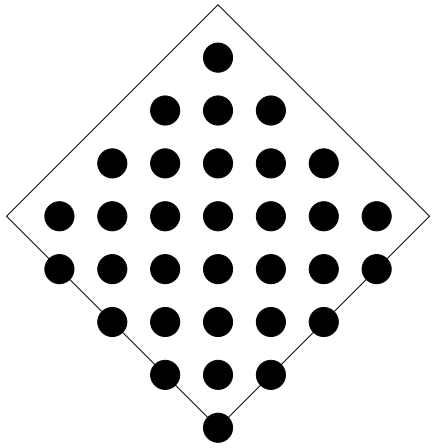
$$\forall g_P \in \mathcal{G}_P, \quad J(g_P(\mathbf{r})) = J(\mathbf{r}).$$

Space Group: $\mathcal{G} = \mathcal{G}_P \otimes \mathcal{T}$

- Transl. group: $\mathcal{T} = \{t_p\}$, $p = 1, ..., N$
- Point group: $\mathcal{G}_P = C_{4v}$ (square lattice)

A simple example: the 2D t-J model





N=26 **N=32**

$N_h \,/\, \sqrt{N} \times \sqrt{N}$	Hilbert space for $S_Z = S_Z^{\min}$	Symmetry group	Reduced HS
$1 \,/\, 4 \times 4$	102 960	T_{16}	6 435
$1 \,/\, \sqrt{26} \times \sqrt{26}$	135 207 800	T_{26}	5 200 300
$1 \,/\, \sqrt{32} \times \sqrt{32}$	9 617 286 240	$T_{32} \otimes C_{4v}$	37 596 701*
$4 \,/\, \sqrt{26} \times \sqrt{26}$	10 546 208 400	$T_{26} \otimes C_4 \otimes I_2$	50 717 244

Use of "Block theorem"

$$\mathbf{K} = \sum_\mu n_\mu \mathbf{K}_\mu \, ,$$

where $\mathbf{K}_\mu$ reciprocal lattice vectors

$$\mathbf{K}_\mu = \frac{2\pi}{N} \mathbf{T}_\mu \wedge \mathbf{e}_z$$

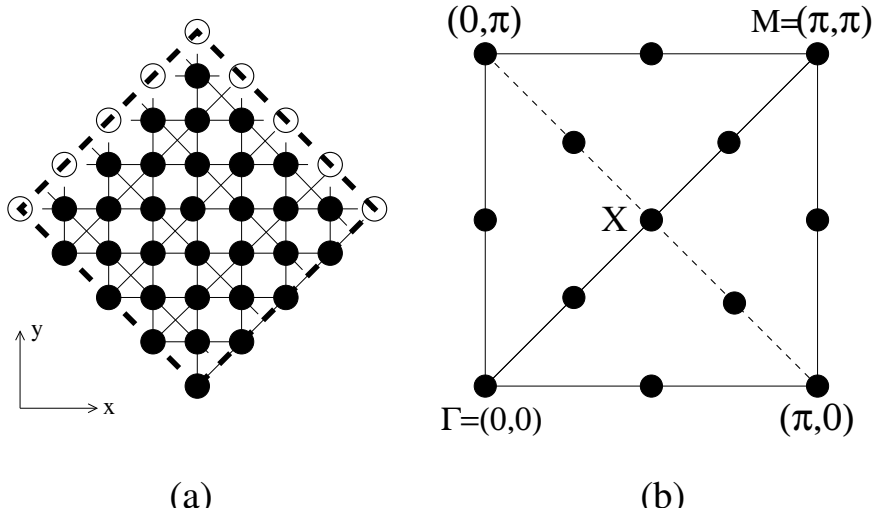
$\mathcal{G}^P_{\mathbf{K}}$, little group of $\mathbf{K}$ ($\mathcal{G}^P_{\mathbf{K}} \subset \mathcal{G}_P$), containing g_P such that

$$g_P(\mathbf{K}) = \mathbf{K} \, .$$

The relevant subgroup of $\mathcal{G}$:

$$\mathcal{G}_{\mathbf{K}} = \mathcal{G}^P_{\mathbf{K}} \otimes \mathcal{T} \, .$$

Example: the checkerboard lattice



(a) (b)

. $N = 32$ sites "checkerboard" cluster

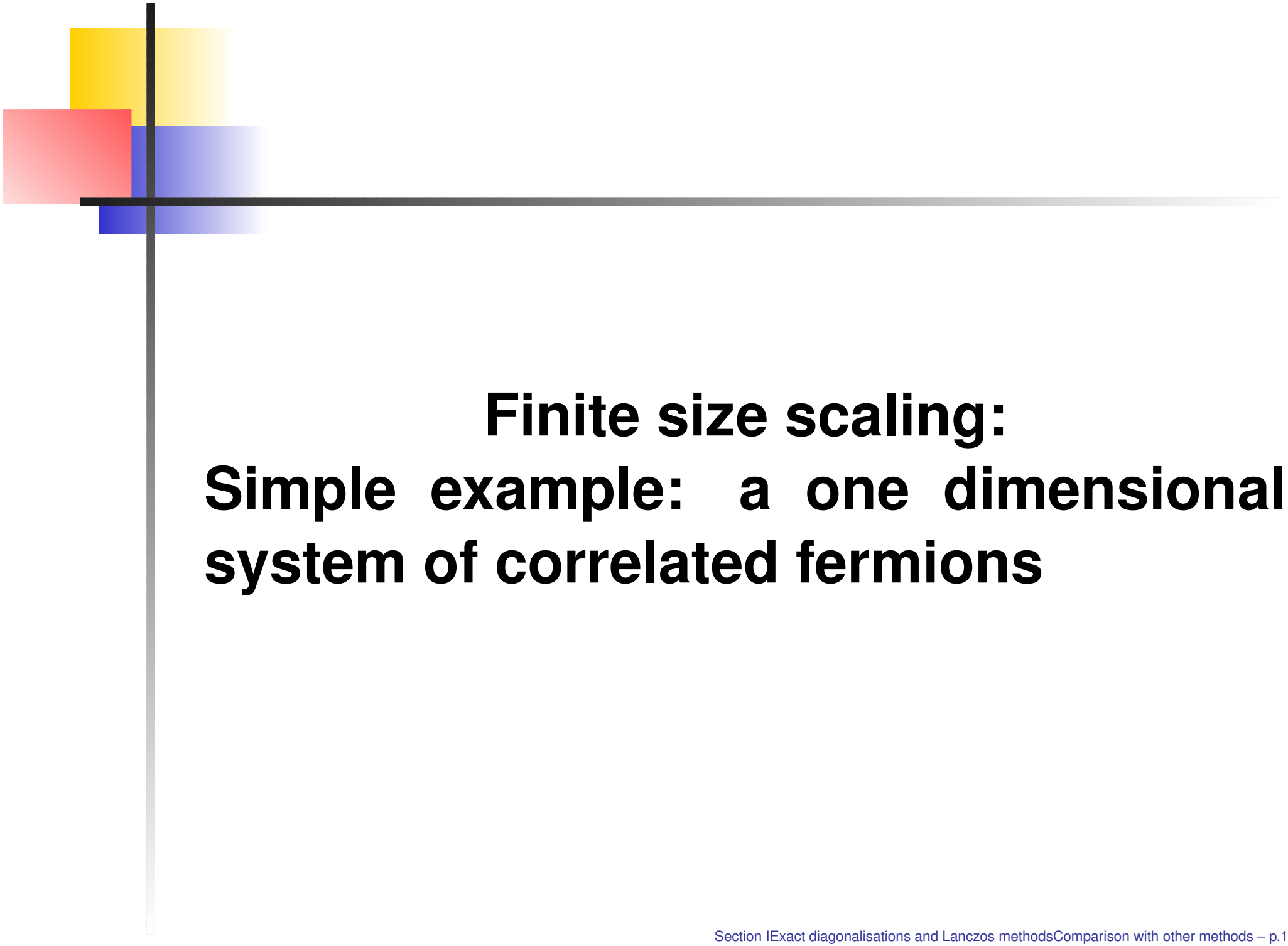
- $\mathbf{K} = (0, 0)$ or (π, π): $\mathcal{G}_{\mathbf{K}} = C_{4\mathrm{v}} \otimes \mathcal{T}_{16}$
- $\mathbf{K} = (0, \pi)$ or $(\pi, 0)$: $\mathcal{G}_{\mathbf{K}} = C_{2\mathrm{v}} \otimes \mathcal{T}_{16}$
- $\mathbf{K} = (\pi/2, \pi/2)$: $\mathcal{G}_{\mathbf{K}} = C_{\mathrm{v}} \otimes \mathcal{T}_{16}$

Change boundary conditions

- translation vectors of the form
$\mathbf{T}_\mu = (0, ..., 0, L_\mu, 0, ..., 0)$

- flux Φ (in unit of the flux quantum) through one hole of d-dimensional torus
$\longrightarrow$ twist in the boundary conditions along direction $\mathbf{e}_\mu$:

$$t_{\mathbf{xy}}\, c^\dagger_{\mathbf{x},s} c_{\mathbf{y},s} \rightarrow t_{\mathbf{xy}}\, c^\dagger_{\mathbf{x},s} c_{\mathbf{y},s} \exp\left(2i\pi \frac{\Phi}{L_\mu} (\mathbf{x} - \mathbf{y}) \cdot \mathbf{e}_\mu\right)$$



Finite size scaling: Simple example: a one dimensional system of correlated fermions

1D correlated fermions: Hubbard chain

1D systems: spin and charge collective modes with velocities u_ρ and u_σ

Density of state: $N(\omega) \sim |\omega|^\alpha$

α and K_ρ non-universal exponents:

$$\alpha = \frac{1}{4}(K_\rho + \frac{1}{K_\rho} - 2)$$

Practical formula: $\pi D = 2 u_\rho K_\rho$

$\rightarrow u_\rho$ and D obtained on finite systems:

- "Drude weight": $D = \frac{\partial^2 (E_0/L)}{\partial \phi^2}$ where $\phi = 2\pi \frac{\Phi}{L}$.
- Velocity u_ρ: ΔE between $k = 0$ and $k = 2\pi/L$ eigen-states

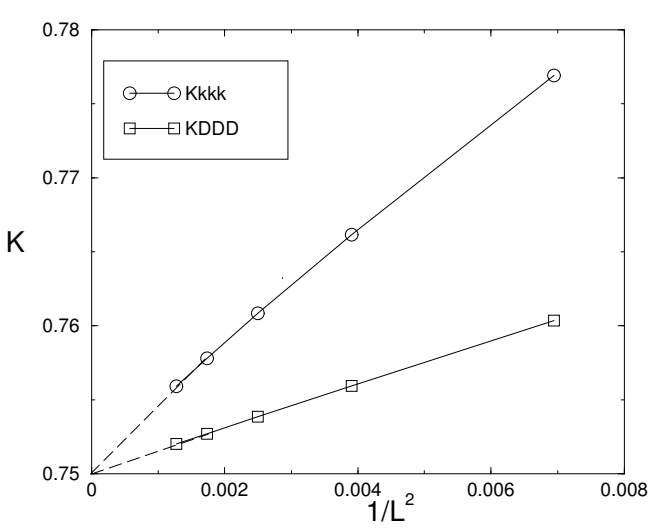
Finite size in 1D

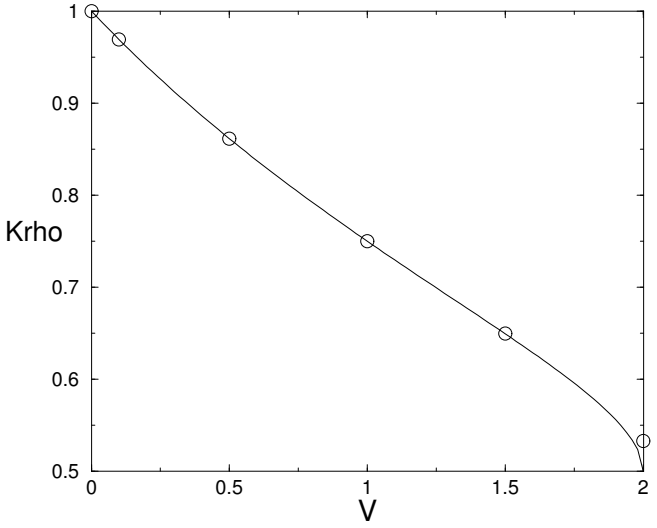
- conformal invariance implies: $\frac{\pi}{2}\frac{u_\rho}{K_\rho} = \frac{1}{\kappa}$
- compressibility $\kappa^{-1} = \frac{1}{2}\frac{\partial^2(E_0/L)}{\partial n^2}$ computed numerically
  $\longrightarrow$ check consistency of LL picture
- finite size scaling of GS energy:
  $\frac{E_0(L)}{L} = e_\infty - \frac{\pi(u_\rho+u_\sigma)}{6L^2}c + \mathcal{O}(1/L^2)$
- central charge c given by symmetry
  spin velocity u_σ calculated independently.

Results & comparison with BA

Spinless fermion chain (t-V model) exactly solvable by Bethe-Ansatz ($n = 1/2$)

Note: periodic boundary conditions used





S. Capponi, Thèse 1999 (Toulouse)

Partial summary

Advantages

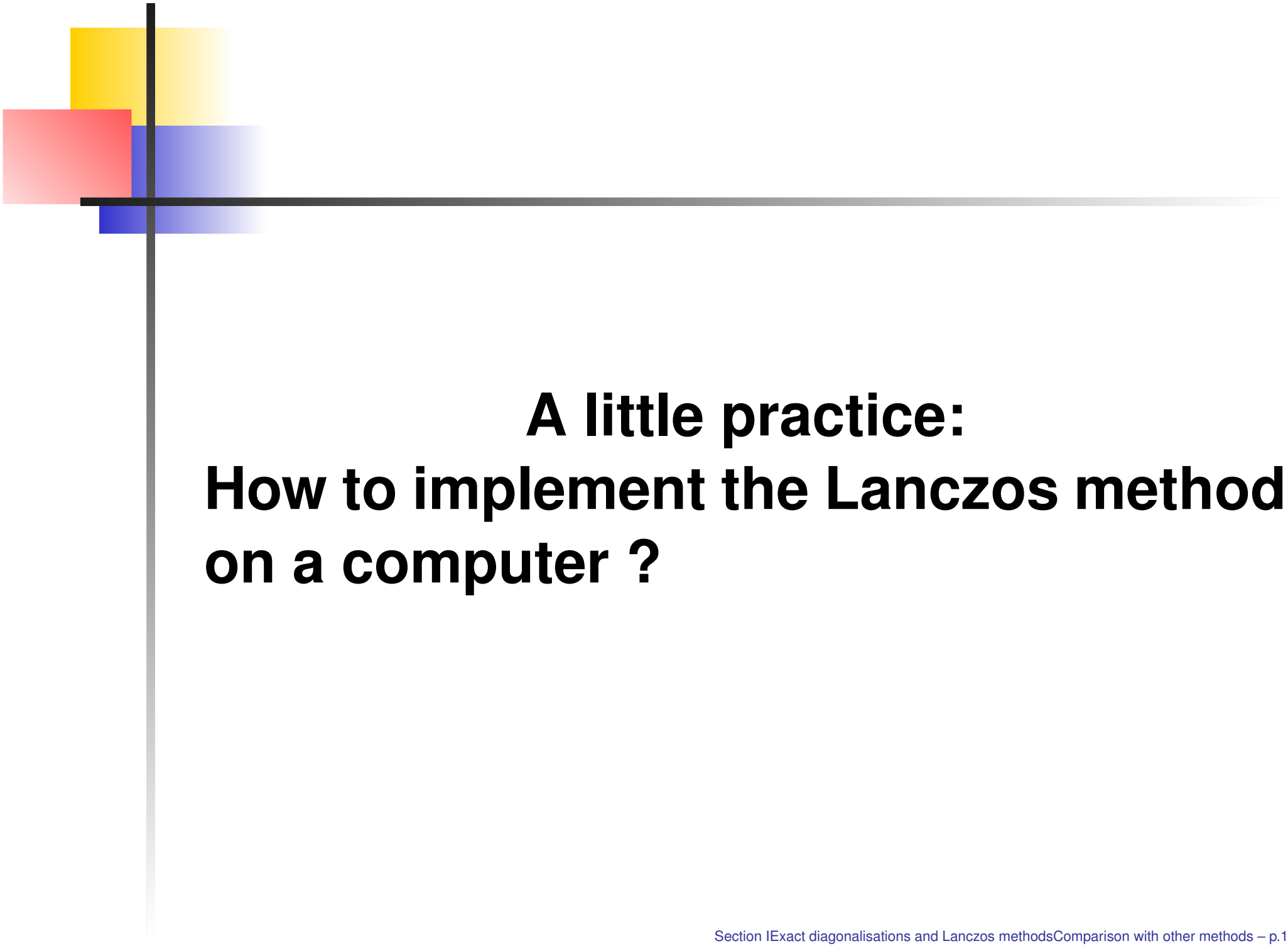
- **Non-perturbative** method !!
- Comparisons to experiments:
  - Fits $\longrightarrow$ microscopic parameters
  - Structure factors (ordering, etc...)
  - Thermodynamics
  - Spectroscopies (ARPES, INS, $\sigma(\omega)$,...)

Versatile method !

Extensions to many models - e.g. models with phonons

Limitations

- Small clusters !!
- Simple models (with few degree of freedom/ / site)



A little practice: How to implement the Lanczos method on a computer ?

The Hilbert space

P^N states $\propto \exp N$!!

- Hubbard $\rightarrow P = 4$; $\emptyset, \uparrow, \downarrow, \uparrow\downarrow$
- Heisenberg: $\rightarrow P = 2$; $\uparrow, \downarrow$
- t-J: $\rightarrow P = 3$; $\emptyset, \uparrow, \downarrow$

Digital coding: $|c\rangle = |s_1, ..., s_i, ..., s_N\rangle \Rightarrow$ 1 integer

Heisenberg: $N(|c\rangle) = \sum_1^N 2^{i-1}\sigma_i$, with $\sigma_i = 0, 1$

t-J: $N(|c\rangle) = \sum_1^N 2^{2(i-1)}\sigma_i$

with $\sigma_i = 0$="00", 1="01", 2="10"

N=4 states: $|\uparrow, \emptyset, \uparrow, \downarrow\rangle = 0_{64}...0_9 0_8 1_7 1_6 0_5 0_4 0_3 1_2 0_1$

The irreducible representations

- .Symmetry sector: $l = (\mathbf{K}, \tau_{\mathbf{K}})$
  $\tau_{\mathbf{K}}$ irreducible representations (IR) of $\mathcal{G}^P_{\mathbf{K}}$
- ."symmetric" state $|\alpha\rangle \equiv |\alpha\rangle\{|c\rangle\}$:
  $\sum_{g_P \in \mathcal{G}^P_{\mathbf{K}}, t \in \mathcal{T}} e(\tau_{\mathbf{K}}, g_P) \exp(i\mathbf{K} \cdot \mathbf{T}_t) (g_P\, t)(|c\rangle)$,
  where $e(\tau_{\mathbf{K}}, g_P)$ = characters of IR $\tau_{\mathbf{K}}$
- $\Rightarrow$ keep only one state $|r\rangle = R(|c\rangle)$
  among related states $(g_P\, t)(|c\rangle)$
- .Convenient choice: *smallest* integer
  $N(|c\rangle)$ i.e. $N(|r\rangle) = \min_{g \in \mathcal{G}_{\mathbf{K}}} \{N(g(|c\rangle))\}$
- Set of all representatives $\mathcal{A}_l = \{|r\rangle\}$
  $\Rightarrow$ Hilbert space reduced by card$(\mathcal{G}_{\mathbf{K}})$

How to construct "representatives"

.The simplest case: Hubbard-like models

$$|c\rangle = |c(\uparrow)\rangle \otimes |c(\downarrow)\rangle$$

$$N(|c\rangle) = N'(|c(\uparrow)\rangle) \times 2^N + N'(|c(\downarrow)\rangle)$$

.Minimisation of $N(g(|c\rangle))$ over $g \in \mathcal{G}_{\mathbf{K}}$:

1. generate all $\uparrow$ spins configs $\longrightarrow |r(\uparrow)\rangle$ kept,
2. store $\mathcal{E}_{\mathbf{K}}[|r(\uparrow)\rangle] \subset \mathcal{G}_{\mathbf{K}}$ / $|r(\uparrow)\rangle$ invariant,
3. construct full set of configs as $|r(\uparrow)\rangle \otimes |c(\downarrow)\rangle$,
4. apply all elts of $\mathcal{E}_{\mathbf{K}}[|r(\uparrow)\rangle]$ to $\downarrow$ part,
5. only retain $|c(\downarrow)\rangle$ such:
   $\forall g' \in \mathcal{E}_{\mathbf{K}}[r(\uparrow)\rangle] \;\; N'(|c(\downarrow)\rangle) \leq N'[g'(|c(\downarrow)\rangle)]$.

Hamiltonian matrix

.Problem reduces to $H|r_\gamma\rangle \propto \sum_{\beta=1}^{\beta_{max}} (-1)^{\theta_{\gamma,\beta}} |c_{\gamma,\beta}\rangle$

- fermionic commutation relations $\longrightarrow (-1)^{\theta_{\gamma,\beta}}$
- $\beta_{max} \sim N \longrightarrow$ small "connectivity" in configuration space $\longrightarrow$ sparse matrix

How to calculate $|r_{\gamma,\beta}\rangle_f = R\{|c_{\gamma,\beta}(\uparrow)\rangle \otimes |c_{\gamma,\beta}(\downarrow)\rangle\}$?

$\Rightarrow$ apply all symmetries of $\mathcal{G}_{\mathbf{K}}$ to $|c_{\gamma,\beta}(\uparrow)\rangle$:

1. tabulate R : $|c(\uparrow)\rangle \longmapsto |r(\uparrow)\rangle$
2. store $\mathcal{R}_{\mathbf{K}}[(|c(\uparrow)\rangle] = \{g \in \mathcal{G}_{\mathbf{K}}; g((|c(\uparrow)\rangle) = |r(\uparrow)\rangle\}$

$\Rightarrow$ apply symmetries $\mathcal{R}_{\mathbf{K}}[|c_{\gamma,\beta}(\uparrow)\rangle]$ to $|c_{\gamma,\beta}(\downarrow)\rangle$

Worry about phase factors !

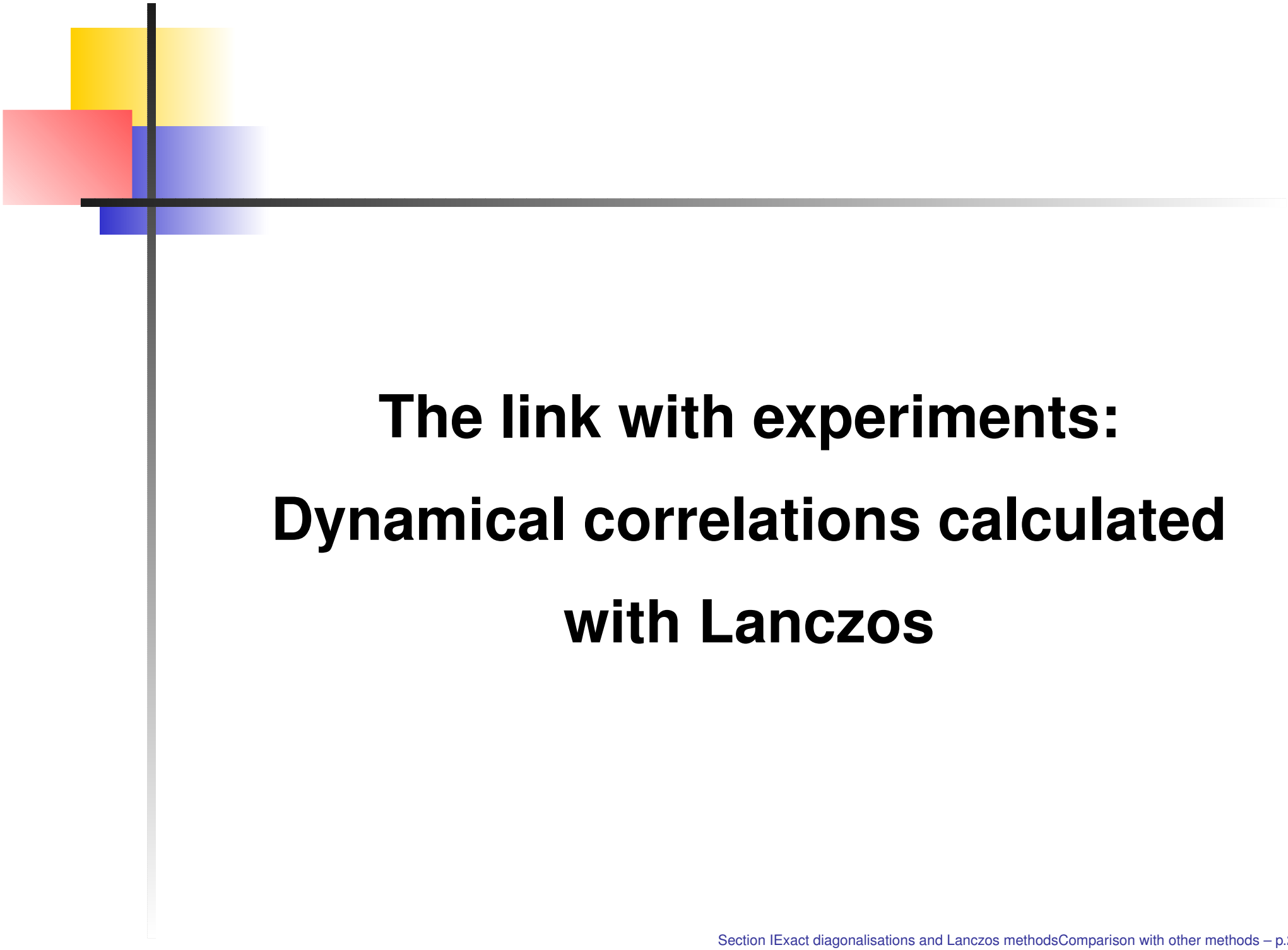
Transf. "generated states $\Rightarrow$ representatives" involves phases:

$$\lambda_{\gamma,\beta} = (-1)^{\theta_{\gamma,\beta}} e(\tau_{\mathbf{K}}, g_P(g^*_{\gamma,\beta})) \exp\left(i\mathbf{K}\cdot\mathbf{T}(g^*_{\gamma,\beta})\right)$$

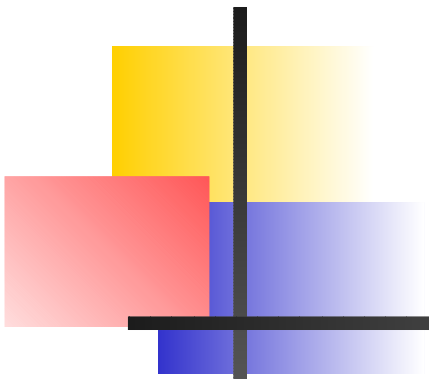
$g^*_{\gamma,\beta} \in \mathcal{R}_{\mathbf{K}}[|c_{\gamma,\beta}(\uparrow)\rangle]$ defined by $|r_{\gamma,\beta}\rangle_f = g^*_{\gamma,\beta}(|c_{\gamma,\beta}\rangle)$

$\Rightarrow$ store $\lambda_{\gamma,\beta}$ (in integer form) $+ N\{|r_{\gamma,\beta}\rangle_f\} \rightarrow$ 64-bit integers

Exemple: Hilbert space of 10^{10} (10 billions) states / ~ 128 symmetries $\rightarrow$ Reduced Hilbert space of 10^8 (100 millions) $\times \sim 40$ images per state =4 Gw i.e. 32 Gb.



The link with experiments: Dynamical correlations calculated with Lanczos



Computing Dynamics Correlations - Outline

1. The continued-fraction method
2. Experimentally accessible fluctuations
3. The convergence of the method

Dynamical correlations

Time-dependent correlations

$$C(t) = \langle \Psi_0 | A(t) A^\dagger(0) | \Psi_0 \rangle$$

Fourier transform $\Rightarrow$ frequency space: $z = \omega + i\epsilon$

$$\tilde{C}(z) = \langle \Psi_0 | A \frac{1}{z - H + E_0} A^\dagger | \Psi_0 \rangle$$

$$\Downarrow$$

Spectral function

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

Construct "initial state"

$A^\dagger$ is applied to GS to construct a new orthogonal state:

$$|\tilde{\Phi}_1\rangle = \frac{1}{(\langle\Psi_0|AA^\dagger|\Psi_0\rangle)^{1/2}} A^\dagger|\Psi_0\rangle$$

1. matrix elements of $A^\dagger$ calculated as for H
2. $A^\dagger$ connects $\neq$ symmetry sectors $\rightarrow$ construct both Hilbert subspaces

$$\Rightarrow \quad \tilde{C}(z) = \langle\Psi_0|AA^\dagger|\Psi_0\rangle\langle\tilde{\Phi}_1|(z' - H)^{-1}|\tilde{\Phi}_1\rangle$$

where $z' = z + E_0$.

second Lanczos iterative procedure

Starting with $|\tilde{\Phi}_1\rangle$ as an initial state:

$$z' - H = \begin{pmatrix} z' - \tilde{e}_1 & -\tilde{b}_2 & \dots & 0 \\ -\tilde{b}_2 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -\tilde{b}_M \\ 0 & \dots & -\tilde{b}_M & z' - \tilde{e}_M \end{pmatrix} \quad (1)$$

$\rightarrow$ matrix expressed in the new basis $\{|\tilde{\Phi}_n\rangle\}$ with new choice $|\Phi_1\rangle = |\tilde{\Phi}_1\rangle$.

Recurrence relations

Straightforwardly:

$$\tilde{C}(z) = \langle \Psi_0 | A A^\dagger | \Psi_0 \rangle \, \frac{D_2}{D_1} \, ,$$

where D_n is defined as $D_n = \det \Delta_n$
Δ_n is the $(M - n + 1) \times (M - n + 1)$ matrix:

$$\Delta_n = \begin{pmatrix} z' - \tilde{e}_n & -\tilde{b}_{n+1} & \dots & 0 \\ -\tilde{b}_{n+1} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -\tilde{b}_M \\ 0 & \dots & -\tilde{b}_M & z' - \tilde{e}_M \end{pmatrix} \tag{2}$$

"Practical" formula

Determinants D_n (for a given z) calculated recursively:

$$D_n = (z' - \tilde{e}_n) D_{n+1} - \tilde{b}_{n+1}^2 D_{n+2}$$

for $1 \leq n \leq M - 2$.

Basic formula !! $\Rightarrow$ spectral weight computed from knowledge of tridiagonal matrix.

$$(D_M, D_{M-1}) \rightarrow D_{M-2} \rightarrow \ldots \rightarrow D_2 \rightarrow D_1$$

Some "re-writing"

- Continued-fraction:

$$\tilde{C}(z) = \cfrac{\langle \Psi_0 | A A^\dagger | \Psi_0 \rangle}{z + E_0 - \tilde{e}_1 - \cfrac{\tilde{b}_2^2}{z + E_0 - \tilde{e}_2 - \cfrac{\tilde{b}_3^2}{z + E_0 - \tilde{e}_3 - \ldots}}}$$

- Physical meaning:

$$I(\omega) = \sum_m |\langle \Psi_m | A^\dagger | \Psi_0 \rangle|^2 \delta(\omega - E_m + E_0)$$

1. poles and weights $\rightarrow$ dynamics of $A^\dagger$
2. symmetry of $A^\dagger \rightarrow |\Psi_m\rangle \in$ one IR of symmetry group
   $\rightarrow$ well defined quantum number & selection rules
3. ! calculation of eigen-states/vectors not required !

Physical Quantities

Correlations	Notations	Operators	Experimen
Green function	$A(\mathbf{k},\omega)$	$A = c_{\mathbf{k},\sigma}$	ARPES
Structure factors	$S\mathbf{q},\omega)$	$A = S^z_{\mathbf{q}}$	INS
Conductivity	$\sigma(\omega)$	$A = j_x$	Optics
4-spin corr.	$R(\omega)$	$\sum_{\mathbf{k}} R_{\mathbf{k}} \mathbf{S}_{\mathbf{k}} \cdot \mathbf{S}_{-\mathbf{k}}$	Raman

Dynamical correlations from experiment and theory

-ARPES="Angular Resolved Photoemission Spectro."

-INS="Inelastic Neutron Scattering experiments"

-Raman="Two-magnon Raman scattering"

Problems of convergence ?

A priori, should worry about:

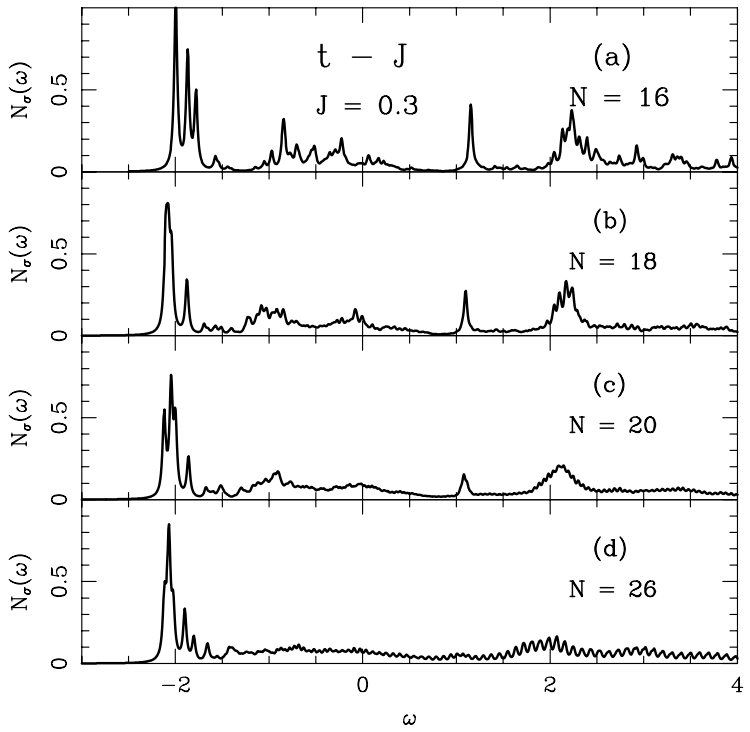
1. role of M, the # of Lanczos iterations ?
2. role of the imaginary part ϵ in $z = \omega + i\epsilon$?
3. role of system size ?

In fact, numerically EXACT results for a given system size

Convergence with size

Ex.: single hole in a 2D antiferromagnet

Local density of state: $N(\omega) = \sum_{\mathbf{k}} A(\mathbf{k}, \omega)$



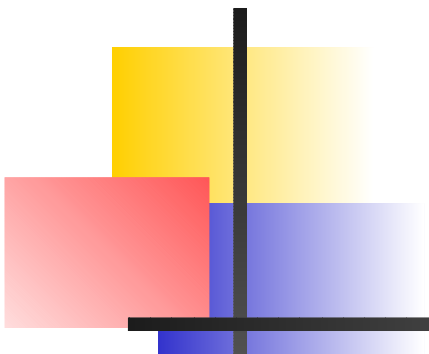
$|\Psi_0\rangle$ = Heisenberg GS

$A = c_{i\sigma}$: hole creation

Use of 2D "tilted" clusters: $N = n^2 + m^2$

$$\mathbf{T}_1 = (n, m)$$
$$\mathbf{T}_2 = (-m, n)$$
$$|\mathbf{T}_1| = |\mathbf{T}_2| \;\&$$
$$\mathbf{T}_1 \cdot \mathbf{T}_2 = 0$$

D.P. et al., PRB (1993)



Other numerical methods:

CORE method – Density Matrix Renormalisation Group (DMRG) – Quantum Monte Carlo (QMC)

Comparison with Lanczos

COntractor REnormalisation

CORE method (Auerbach et al., Capponi et al.)

1. "Macrosites" (= rungs, plaquettes, etc...) $\longrightarrow$ < degrees of freedom
2. construct effective H with longer-range & m-body interactions

DMRG (basics)

Numerical RG (Kondo problem):

K.G. Wilson, Rev. Mod. Phys **47**, 773 (1975)

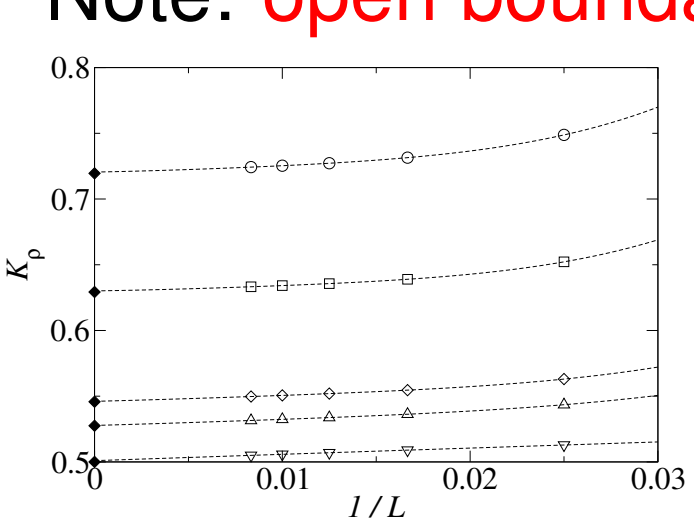
Density Matrix approach: S.R. White, PRL **69**, 2863 (1992)

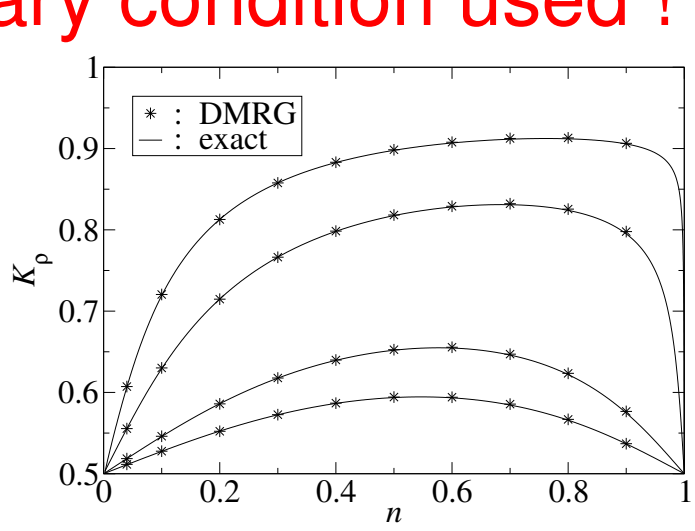
- 1. Start with block B and construct "super-block"
  B-site$_1$-site$_2$-B
- 2. Diag. super-block Hamiltonian $\Rightarrow \Psi(i_1, i_2, i_3, i_4)$
- 3. Calculate reduced density matrix,
  $\rho(i_1, i_2, i'_1, i'_2) = \sum_{i_3, i_4} \Psi(i_1, i_2, i_3, i_4)\Psi(i'_1, i'_2, i_3, i_4)$
  keep m eigenvectors of maximum weights
- 4. Re-write all operators in new truncated basis;
  B $\Rightarrow$ B'=B-site $\Rightarrow$ step 1.

Results & comparison with BA

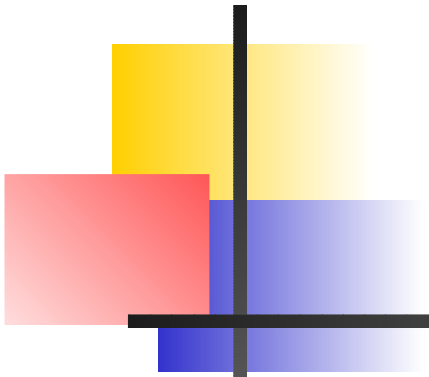
Hubbard chain exactly solvable by Bethe-Ansatz ($U = 1, 2, 6, 10, \infty$).

Note: open boundary condition used !





S. Ejima et al., Europhys. Lett., 70, 492 (2005)



Quantum Monte Carlo methods (basics)

1. Metropolis algorithm
2. World-line algorithms
3. Continuous-time & SSE
4. Determinantal MC (fermions)

Monte Carlo method

"Non-local updates for QMC simulations", M. Troyer et al., p.156 in "The Monte Carlo Method in the Physical Sciences", AIP Conf. Proc., Vol. 690 (2003)

- Monte Carlo: iterative stochastic procedure in configuration space
- Metropolis algorithm to sample probability distrib. $p(i)$:

$$P(i \rightarrow j) = \min[1, \frac{p(j)}{p(i)}]$$

Metropolis, Rosenbluth, Rosenbluth, Teller & Teller (1953)

Quantum Monte Carlo

Generalization of MC to Quantum systems

$\rightarrow$ Trotter-Susuki formula:

M. Susuki, Prog. Theor. Phys. **56**, 1454 (1976)

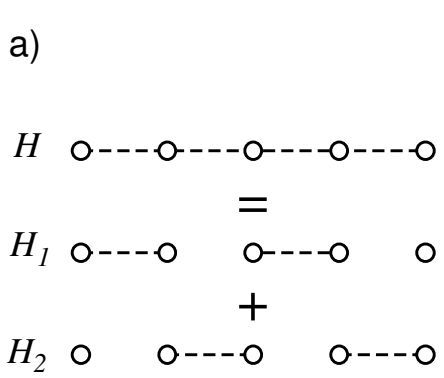
$$
\begin{aligned}
Z &= Tr[\exp(-\frac{\beta}{M}(H_1+H_2))]^M \\
&= Tr\ [\exp(-\frac{\beta}{M}H_1)\exp(-\frac{\beta}{M}H_2)]^M + O(1/M^2) \\
&= \sum \langle\Psi_1|e^{-\frac{\beta}{M}H_1}|\Psi_2\rangle ... \langle\Psi_{2M}|e^{-\frac{\beta}{M}H_2}|\Psi_1\rangle
\end{aligned}
$$

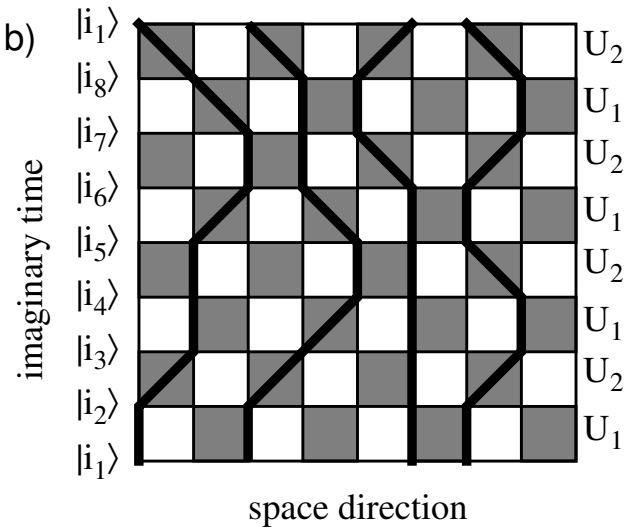
Quantum spins in d dimensions $\Rightarrow$ classical problem in d+1 dimensions

World-line representations

$\longrightarrow$ Evolution in imaginary time:
time step $\Delta\tau = \beta/M$

Example: quantum spin chain





Continuous-time and SSE

- Continuous time limit: $\Delta\tau \Rightarrow 0$, $M \Rightarrow \infty$

  $\Rightarrow$ No systematic error! (Prokof'ev et al. (1996))

- Stochastic Series Expansions (Sandvik (1991))

  $\Rightarrow$ Taylor expansion of Z

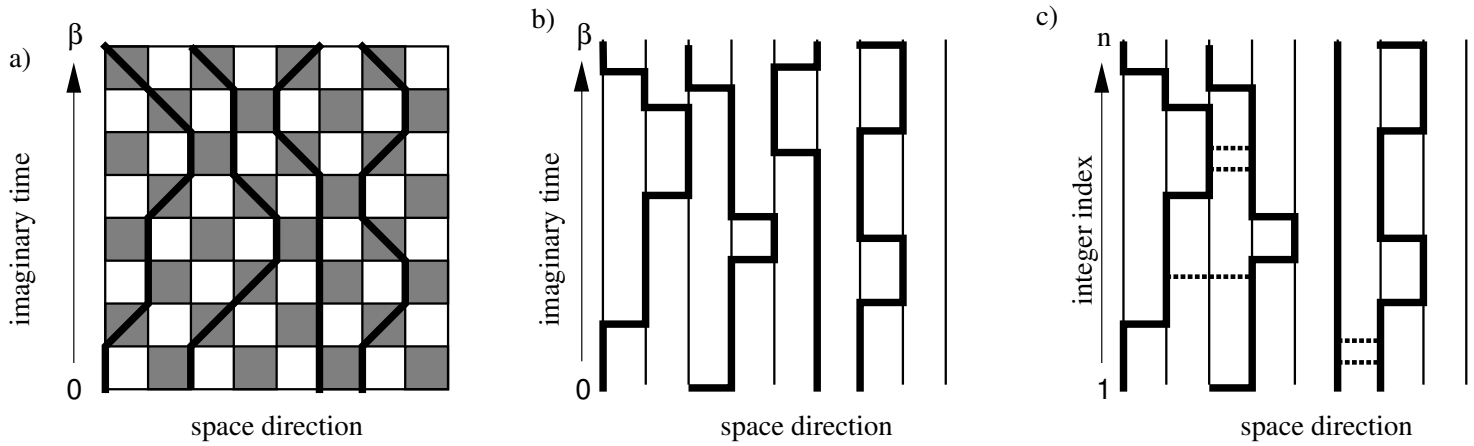
$$Z = \ Tr \ \ \exp\left(-\beta H\right) = \sum_n \frac{\beta^n}{n!} Tr(-H)^n$$

$$= \sum_n \frac{\beta^n}{n!} \ \sum \ \left\langle \Psi_1 \right| - H_{b_1} \left| \Psi_2 \right> \ldots$$

$$\ldots \ \ < \Psi_n \left| - H_{b_n} \right| \Psi_1 >$$

World-line representations (II)

Comparison between discrete, continuous time and SSE QMC methods:



How to simulate fermions ?

Fermionic case - J.H. Hirsch, 1985

Hubbard-Stratonovich transformation

Idea: (i) use Trotter formula for "decoupling" K (kin.) & V (int.)
(ii) decouple interaction term
(iii) integrate out fermionic variables

$$e^{-\Delta\tau U n_{i,\uparrow} n_{i,\downarrow}} \propto \sum_{s=\pm 1} e^{-\Delta\tau s_{i,l} \lambda (n_{i,\uparrow} - n_{i,\downarrow})}$$

$$Z = \sum_{s=\pm 1} \det M^{+}(s) \det M^{-}(s)$$

Conclusions

Lanczos (ED)

- $T = 0$ unbiased computation
- Static & **dynamical** correlations
- Access to quantum # & symmetries
- Versatile method: frustration, long range inter., 1D, 2D. etc...
- Limited to small clusters $\longrightarrow$ Finite size effects
- Possible ext. $\Rightarrow$ effective hamiltonians (CORE)

QMC

- Can reach Large systems
- Max Ent techniques for dynamics
- Finite T method (mostly)
- To beat "critical slowing down" $\longrightarrow$ Loop algorithms
- When frustration or doping ($n \neq 1/2$) Minus sign problem

DMRG

- Can reach Large systems
- $T = 0$ methods
- New developments for excited states and/or time-dependent quantities
- Very accurate in 1D (or quasi-1D) (frustration & doping possible) but problem when $\longrightarrow$ 2D