Many-Body Fermion Density Matrices

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Organization

- Motivation for thesis work:
  - Chapter 1.
- Reduced DMs of noninteracting spinless fermions:
  - Chapters 2 & 3.
- Reduced DMs of interacting spinless fermions:
  - Chapter 4.
- Correlation DM and operator singular value decomposition:
  - Chapters 5, 6, 7, & 8.
- Conclusions:
  - Chapter 9.

Overview of Chapter 1

- Why numerical methods?
- Why density matrices (DMs)?
  - Finite subsystem of larger system;
  - Correlations of products of local observables.
- Quantum renormalization group.

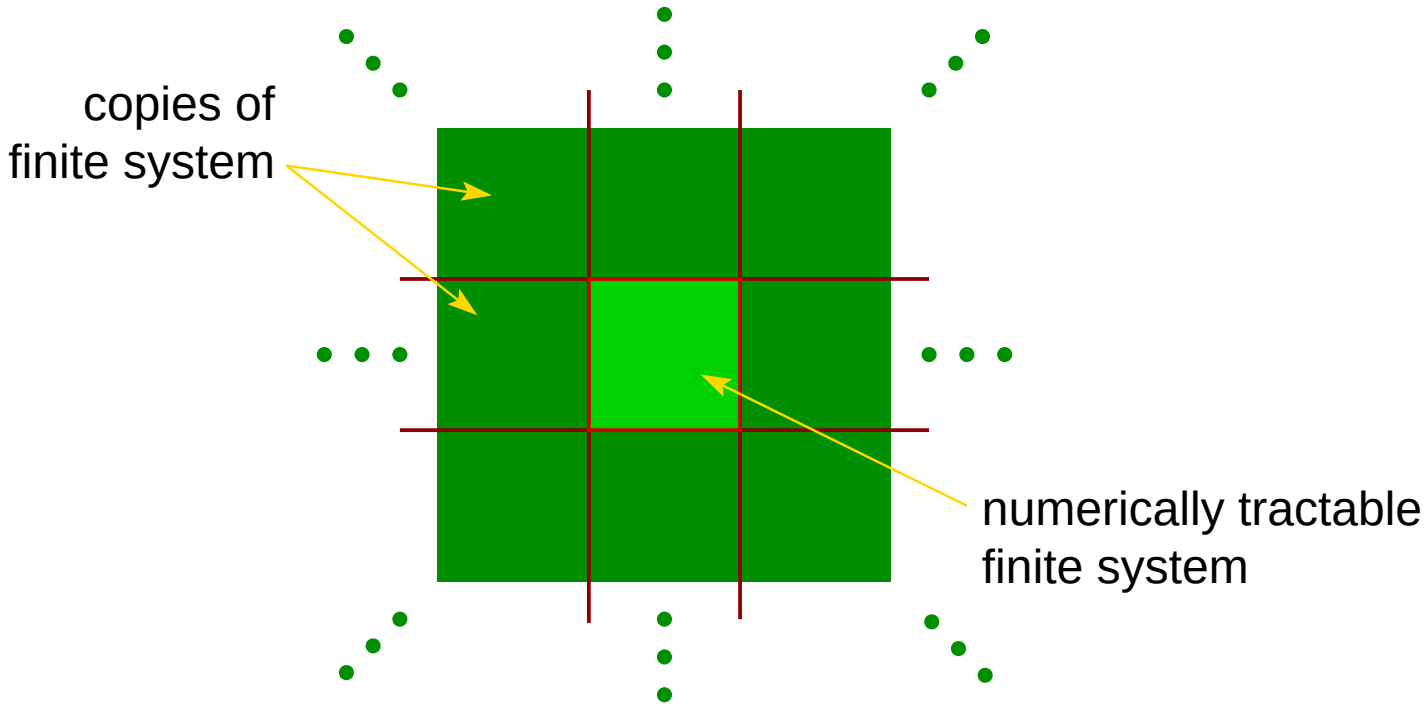
Why Numerical Methods?

- Ground-state properties (energy, correlations, $T = 0$ phase diagram) of $N \to \infty$ interacting QM degrees of freedom (spins, bosons, fermions) can be calculated from the ground-state wave function.
- Exact analytical many-body wave functions rare.
- Approximate analytical many-body wave functions
  - Perturbative: not valid over all Hamiltonian parameter(s); or
  - Variational: involve *a priori* assumptions on structure of wave function.
- Numerical methods like
  - Exact Diagonalization (ED); and/or
  - Quantum Monte Carlo (QMC)

  to obtain numerical wave functions or correlations of finite systems. Extrapolations then needed for $N \to \infty$.

Why Density Matrices?

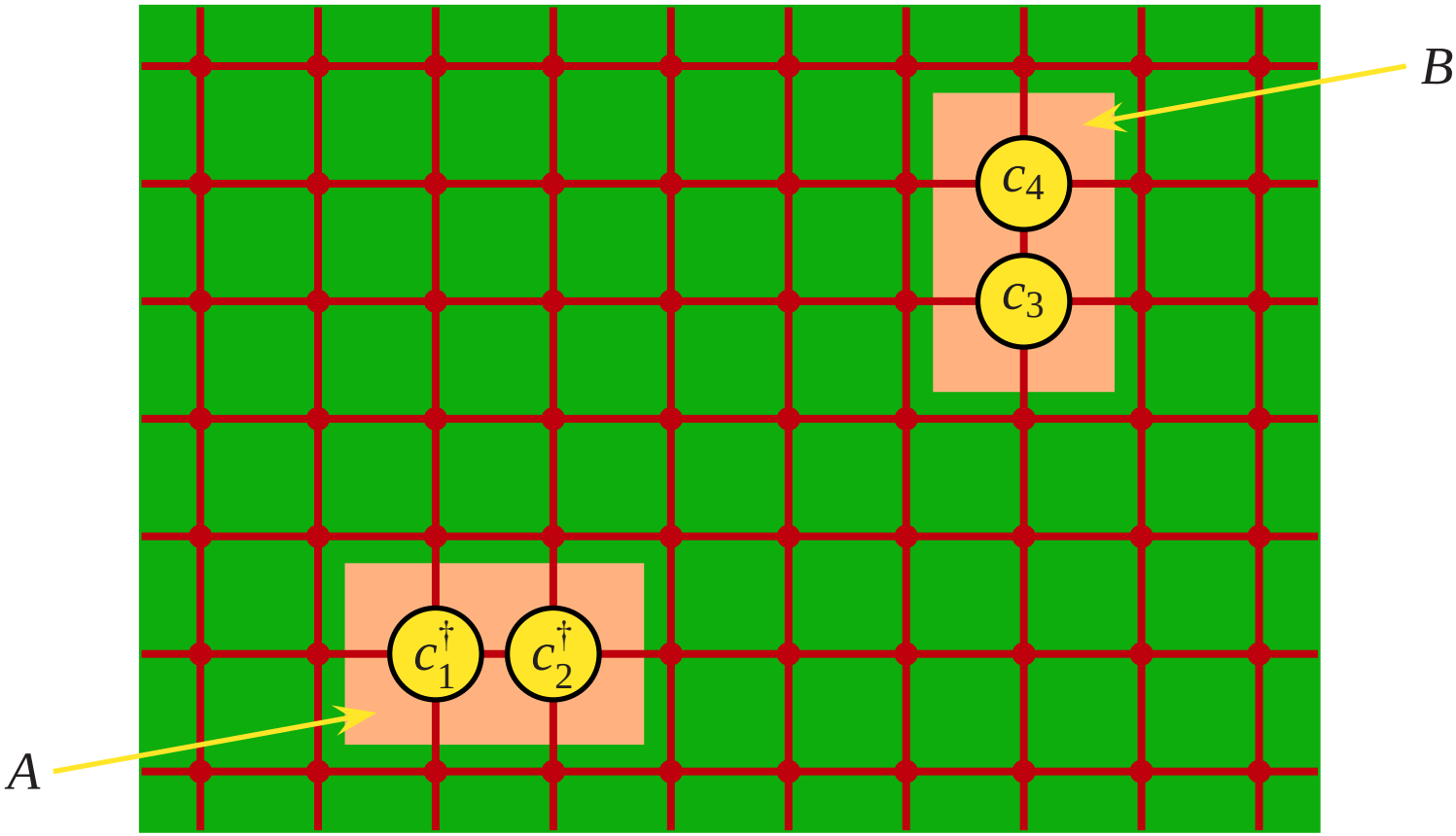
- Build up QM state of infinite system from QM states of finite subsystems.



- Pure state on infinite system $\Longrightarrow$ mixed state on finite subsystem.
  (wave function Ψ) (density matrix ρ)

Why Density Matrices?

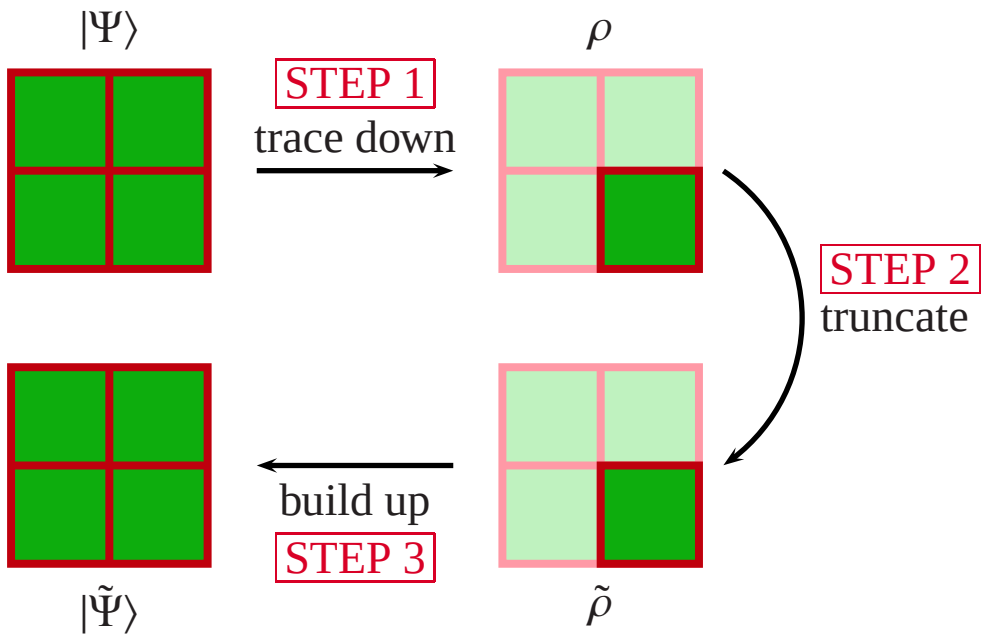
- Calculation of correlations of products of local observables.



- Expectation: $\langle\Psi|c_1^\dagger c_2^\dagger c_3 c_4|\Psi\rangle = \langle c_1^\dagger c_2^\dagger c_3 c_4\rangle = \mathrm{Tr}\,\rho_{AB} c_1^\dagger c_2^\dagger c_3 c_4.$

Quantum Renormalization Group (QRG)

- Repeated cycles of truncation and renormalization. [S. R. White, PRL **69**, 2863 (1992); R. J. Bursill, PRB **60**, 1643 (1999)]
- Truncation naturally guided by density matrix (DM).



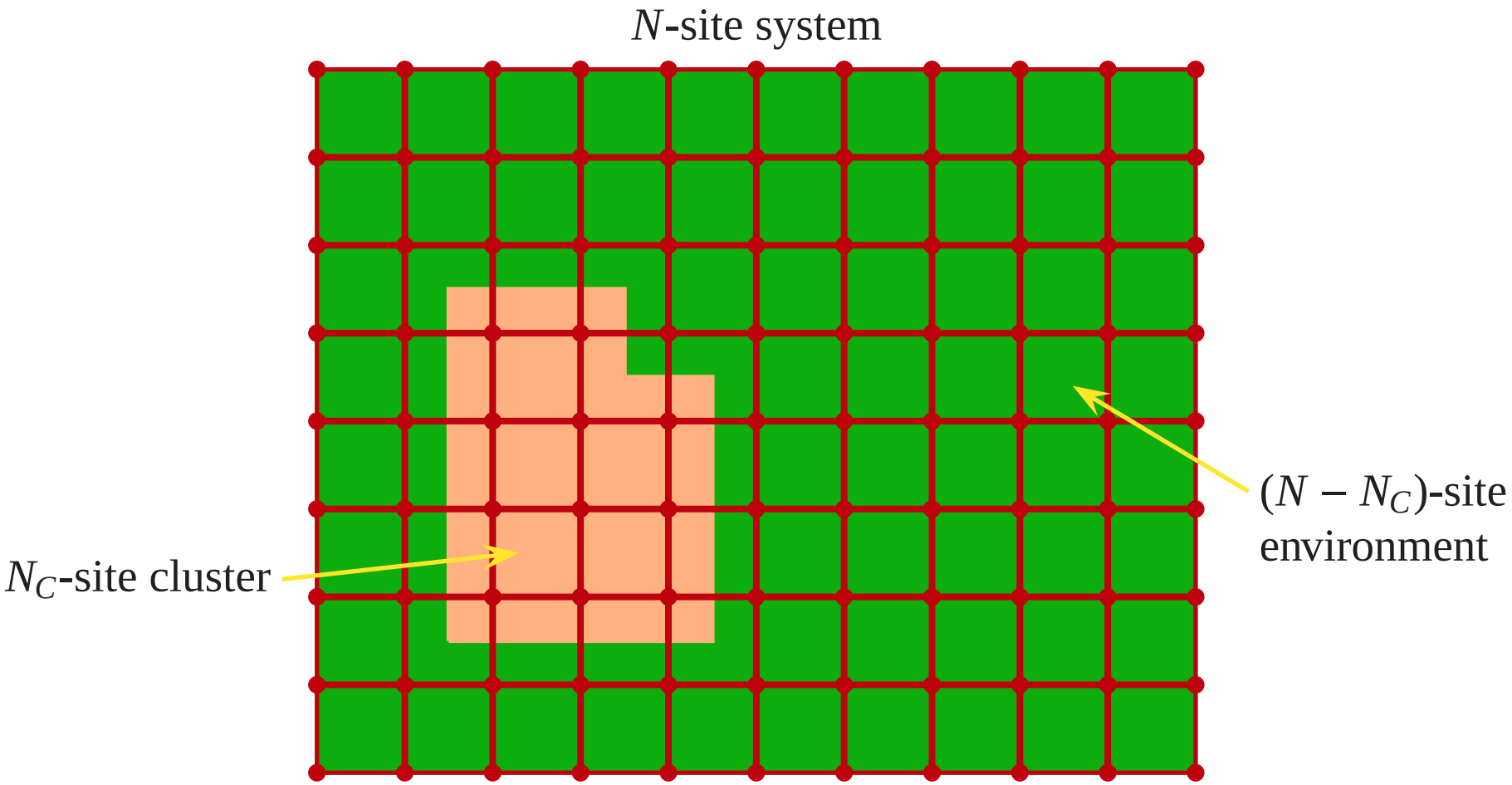
- Understanding structure of DM may lead to algorithmic improvements (e.g. Transfer-Matrix Renormalization Group (TMRG)) and better ways to build symmetries of problem into RG.

Overview of Chapters 2 & 3

- Model & system definitions.
- Exact formula for cluster DM:
  - Exact formula;
  - Cluster Green-function matrix;
  - Derivation.
- Many-body eigenstates and eigenvalues of cluster DM.
  - Scaling behaviour of cluster DM eigenvalues and eigenfunctions.
- Statistical mechanics analogy.
- Operator-based DM truncation scheme:
  - Formulation;
  - Dispersion relation calculation for 1D noninteracting spinless fermions.

Noninteracting Spinless Fermions in d Dimensions

$$H_t = -t \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} c^\dagger_{\mathbf{r}} c_{\mathbf{r}'}, \qquad |\Psi_F\rangle = \text{Fermi sea ground state}$$



Exact Formula for Cluster DM

- For cluster of N_C sites, DM found to have the structure [M.-C. Chung and I. Peschel, PRB **64**, 064412 (2001)]

$$\rho_C \propto \exp\left[-\sum_{l=1}^{N_C} \varphi_l f_l^\dagger f_l\right], \quad \{f_l, f_l^\dagger\} = 1.$$

  φ_l and f_l determined numerically.

- Exact formula for cluster DM [SAC and C. L. Henley, PRB **69**, 075111 (2004); I. Peschel, J. Phys. A: Math. Gen **36**, L205 (2003)]

$$\rho_C = \det(\mathbb{1} - G_C) \exp\left\{\sum_{i,j} \left[\log G_C (\mathbb{1} - G_C)^{-1}\right]_{ij} c_i^\dagger c_j\right\}$$

  in terms of cluster Green-function matrix G_C.

Cluster Green-Function Matrix

- Organize two-point functions $G_{\bar{i}\bar{j}} = \langle \Psi_F | c_i^\dagger c_j | \Psi_F \rangle$ into Green-function matrix $\mathscr{G}$ and cluster Green-function matrix G_C:

$$\mathscr{G} = \begin{bmatrix} \overbrace{\boxed{\begin{matrix} G_{\bar{1}\bar{1}} & G_{\bar{1}\bar{2}} & \cdots & G_{\bar{1}\bar{N}_C} \\ G_{\bar{2}\bar{1}} & G_{\bar{2}\bar{2}} & \cdots & G_{\bar{2}\bar{N}_C} \\ \vdots & \vdots & \ddots & \vdots \\ G_{\overline{N_C}1} & G_{\overline{N_C}2} & \cdots & G_{\overline{N_C}\overline{N_C}} \end{matrix}}}^{G_C} & \begin{matrix} G_{\bar{1}\bar{N}_C+1} & \cdots & G_{\bar{1}\bar{N}} \\ G_{\bar{2}\bar{N}_C+1} & \cdots & G_{\bar{2}\bar{N}} \\ \vdots & \ddots & \vdots \\ G_{\overline{N_C}\overline{N_C}+1} & \cdots & G_{\overline{N_C}\overline{N}} \end{matrix} \\ \begin{matrix} G_{\overline{N_C+1}1} & G_{\overline{N_C+1}2} & \cdots & G_{\overline{N_C+1}\overline{N_C}} \\ \vdots & \vdots & \ddots & \vdots \\ G_{\bar{N}1} & G_{\bar{N}2} & \cdots & G_{\bar{N}\bar{N}_C} \end{matrix} & \begin{matrix} G_{\overline{N_C+1}\overline{N_C}+1} & \cdots & G_{\overline{N_C+1}\overline{N}} \\ \vdots & \ddots & \vdots \\ G_{\bar{N}\bar{N}_C+1} & \cdots & G_{\bar{N}\bar{N}} \end{matrix} \end{bmatrix}$$

block (rows) / environment (rows); block (columns) / environment (columns)

Derivation of Exact Formula

- Start from normalized grand-canonical DM of system

$$\rho = \mathcal{Q}^{-1} \exp\left[-\beta(H-\mu F)\right] = \mathcal{Q}^{-1} \exp\left[\sum_{i,j} \Gamma_{i,j} c_i^\dagger c_j\right] = \mathcal{Q}^{-1} \exp\left[\sum_k \tilde{\Gamma}_{kk} \tilde{c}_k^\dagger \tilde{c}_k\right],$$

  chemical potential μ, inverse temperature β, fermion number operator $F = \sum_i c_i^\dagger c_i = \sum_k \tilde{c}_k^\dagger \tilde{c}_k$, grand-canonical partition function $\mathcal{Q}$, and coefficient matrices Γ ($\tilde{\Gamma}$ in momentum space).

- Introduce fermionic coherent states

$$|\boldsymbol{\xi\eta}\rangle = |\xi_1 \cdots \xi_{N_C}; \eta_1 \cdots \eta_{N-N_C}\rangle = \exp\left(-\sum_{i=1}^{N_C} \xi_i c_i^\dagger - \sum_{j=1}^{N-N_C} \eta_j c_j^\dagger\right)|0\rangle\,.$$

  ξ_i and η_j are anticommuting Grassman variables.

- Matrix elements of ρ are

$$\langle \boldsymbol{\xi\eta}|\rho|\boldsymbol{\xi}'\boldsymbol{\eta}'\rangle = \mathcal{Q}^{-1} \exp\left[\begin{pmatrix}\boldsymbol{\xi}^* & \boldsymbol{\eta}^*\end{pmatrix} e^{\Gamma} \begin{pmatrix}\boldsymbol{\xi}' \\ \boldsymbol{\eta}'\end{pmatrix}\right].$$

Derivation of Exact Formula

- Coefficient matrices

$$\mathbb{1} + e^{\Gamma} = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix}, \quad \left(\mathbb{1} + e^{\Gamma}\right)^{-1} = \begin{bmatrix} D & E \\ E^T & F \end{bmatrix},$$

  A and D square $N_C \times N_C$ symmetric matrices, B and E nonsquare $N_C \times (N - N_C)$ matrices, C and F square $(N - N_C) \times (N - N_C)$ symmetric matrices.

- Partial trace over environment, gaussian integration and matrix block inversion gives matrix elements of cluster DM

$$\begin{aligned} \langle \boldsymbol{\xi} | \rho_C | \boldsymbol{\xi}' \rangle &= \int d\boldsymbol{\eta}^* d\boldsymbol{\eta}\, e^{-\boldsymbol{\eta}^* \mathbb{1} \boldsymbol{\eta}}\, \langle \boldsymbol{\xi} - \boldsymbol{\eta} | \rho_0 | \boldsymbol{\xi}'\, \boldsymbol{\eta} \rangle \\ &= \det D\, \exp\left\{ \boldsymbol{\xi}^* \left[D^{-1} - \mathbb{1} \right] \boldsymbol{\xi}' \right\}. \end{aligned}$$

- Momentum space matrix elements of $\tilde{\mathscr{G}}$ and $\tilde{\Gamma}$,

$$\tilde{\mathscr{G}}_{kk} = \langle \Psi_F | \tilde{c}_k^\dagger \tilde{c}_k | \Psi_F \rangle = \frac{1}{\exp \beta(\epsilon_k - \mu) + 1}, \quad \tilde{\Gamma}_{kk} = -\beta(\epsilon_k - \mu)$$

Derivation of Exact Formula

- Matrix relations

$$e^{\tilde{\Gamma}} = \tilde{\mathcal{G}}(\mathbb{1} - \tilde{\mathcal{G}})^{-1} \implies e^{\Gamma} = \mathcal{G}(\mathbb{1} - \mathcal{G})^{-1}, \quad \mathbb{1} + e^{\Gamma} = (\mathbb{1} - \mathcal{G})^{-1}.$$

- Cluster matrix relations

$$D = \mathbb{1} - G_C, \quad D^{-1} = (\mathbb{1} - G_C)^{-1}, \quad D^{-1} - \mathbb{1} = G_C(\mathbb{1} - G_C)^{-1}.$$

- Cluster DM matrix elements

$$\langle \boldsymbol{\xi} | \rho_C | \boldsymbol{\xi}' \rangle = \det(\mathbb{1} - G_C) \exp\left[\boldsymbol{\xi}^* G_C (\mathbb{1} - G_C)^{-1} \boldsymbol{\xi}' \right].$$

- Operator form from matrix elements, using the relation

$$\langle \boldsymbol{\xi} | \exp(\boldsymbol{c}^\dagger \Gamma' \boldsymbol{c}) | \boldsymbol{\xi}' \rangle = \exp\left(\boldsymbol{\xi}^* e^{\Gamma'} \boldsymbol{\xi}' \right), \qquad \boldsymbol{c}^\dagger \Gamma' \boldsymbol{c} = \sum_i \sum_j c_i^\dagger \Gamma'_{ij} c_j.$$

Many-Body Eigenstates and Eigenvalues of Cluster DM

- Eigenstates and eigenvalues of cluster Green-function matrix

$$|\lambda_l\rangle = f_l^\dagger |0\rangle\,, \quad G_C\,|\lambda_l\rangle = \lambda_l\,|\lambda_l\rangle\,.$$

- $|\lambda_l\rangle$ simultaneous 1-particle eigenstates of ρ_C,

$$\rho_C\,|\lambda_l\rangle = \det(\mathbb{1} - G_C)\,e^{-\varphi_l}\,|\lambda_l\rangle\,, \quad \varphi_l = -\ln\left[\lambda_l(1-\lambda_l)^{-1}\right].$$

- P-particle eigenstate of ρ_C described by a set of numbers $(n_1, \ldots, n_l, \ldots, n_{N_C})$, $n_l = 0, 1$,

$$|w\rangle = f_{l_1}^\dagger f_{l_2}^\dagger \cdots f_{l_P}^\dagger |0\rangle\,, \quad n_l = \delta_{l,l_i},$$

with eigenvalue (DM weight)

$$w = \det(\mathbb{1} - G_C)\,\exp(-\Phi)\,, \quad \Phi = \sum_{l=1}^{N_C} n_l\varphi_l.$$

Scaling Behaviour of Eigenvalues & Eigenfunctions

- Approximate scaling behaviour of 1-particle pseudo-energies

$$\varphi(l, N_C, \bar{n}) \approx N_C f(\bar{n}, x), \quad x \equiv (l - l_F)/N_C, \quad l_F = \bar{n}N_C + \tfrac{1}{2}.$$

- Properties of scaling function

$$f(\bar{n}, 0) = 0, \quad f'(\bar{n}, 0) > 0, \quad f(\bar{n}, -x) = -f(1 - \bar{n}, x).$$

- Approximate scaling behaviour of pseudo-Fermi eigenfunction

$$|\chi_F(j, N_C)|^2 \approx \frac{\alpha}{N_C(\log N_C + \kappa)} g(y) \frac{\frac{1}{2}[1 - (-1)^j]}{\sin^2 \pi y}, \quad y = (j - \tfrac{1}{2})/N_C$$

  at half-filling.

- The scaling function $g(y)$ is very nearly $\sin \pi y$.

Statistical Mechanics Analogy

- [SAC and C. L. Henley, PRB **69**, 075112 (2004)]

free spinless fermion		ρ_C	
Hamiltonian	$H = \sum_k \epsilon_k \tilde{c}_k^\dagger \tilde{c}_k$	$\tilde{H} = \sum_l \varphi_l f_l^\dagger f_l$	pseudo-Hamiltonian
1-particle energy	ϵ_k	φ_l	1-particle pseudo-energy
1-particle operator	$\tilde{c}_k$	f_l	1-particle pseudo-operator
occupation number	n_k	n_l	pseudo-occupation number
total energy	$E = \sum_l n_k \epsilon_k$	$\Phi = \sum_l n_l \varphi_l$	total pseudo-energy
Fermi level	ϵ_F	φ_F	pseudo-Fermi level

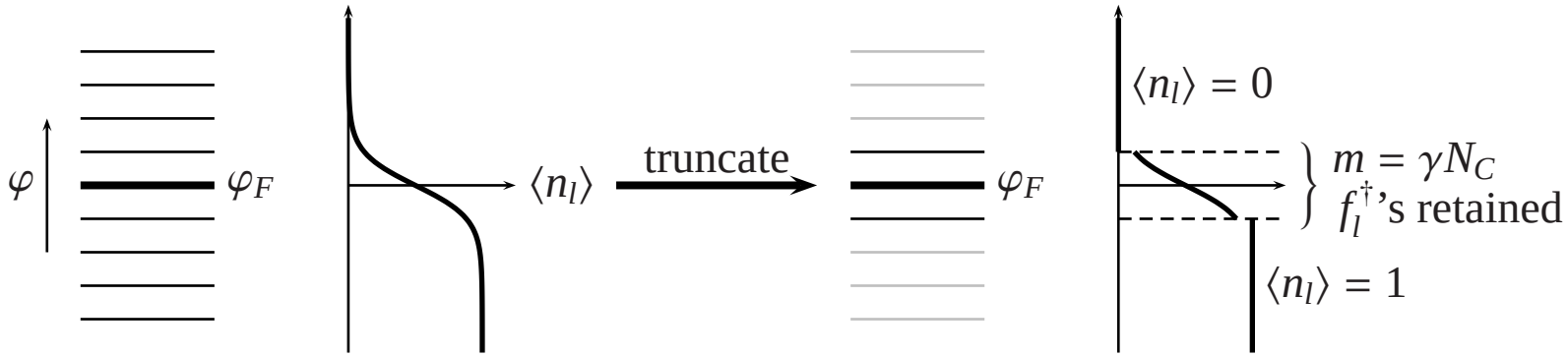
- Based on analogy, average pseudo-occupation is

$$\langle n_l \rangle = \lambda_l = \frac{1}{\exp \varphi_l + 1}.$$

- Most probable eigenstate of ρ_C has structure of Fermi sea: $\varphi_l \leq \varphi_F$ occupied, $\varphi_l > \varphi_F$ empty.
- Other eigenstates look like ‘excitations’ about Fermi sea.

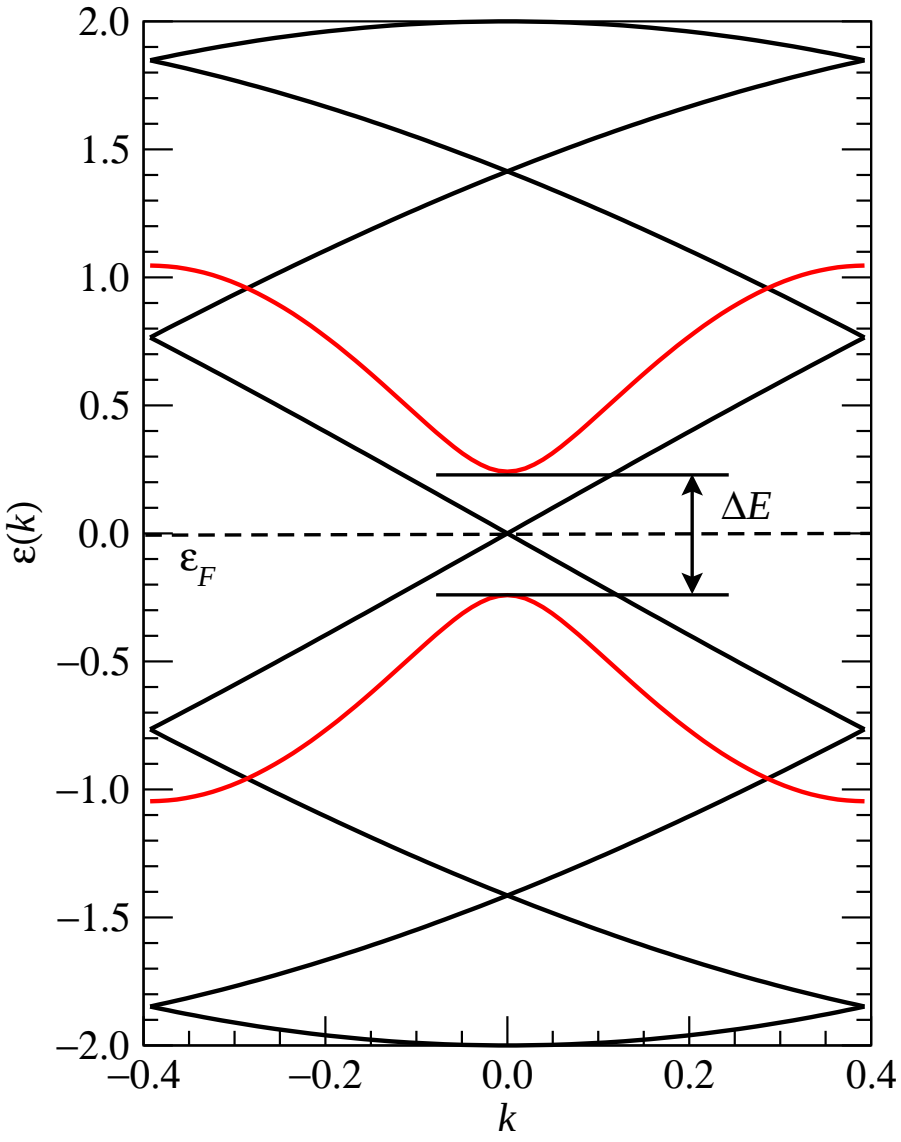
Operator-Based DM Truncation Scheme

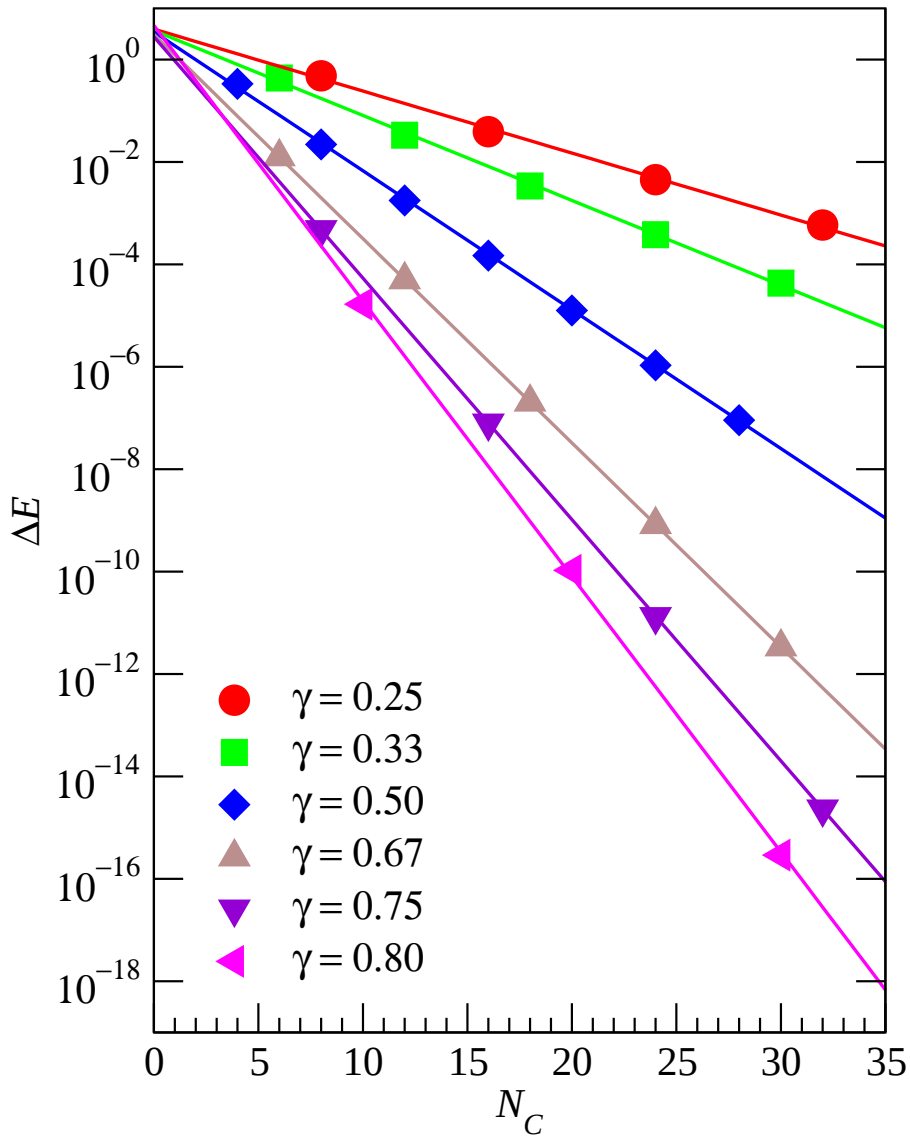
- DM eigenstates with largest weights always have $\varphi_l \ll \varphi_F$ occupied and $\varphi_l \gg \varphi_F$ empty. These differ in n_l for $\varphi_l \approx \varphi_F$;
- Keep only $f_l^\dagger$ with $\varphi_l \approx \varphi_F$:



- Compare with weight-ranked truncation (used for e.g., in the DMRG):
  - eigenstates with largest weights all kept;
  - some eigenstates with intermediate weights not kept, but replaced with eigenstates with slightly smaller weights;
  - eigenstates with small weights not kept.

Results: 1D Noninteracting Spinless Fermions



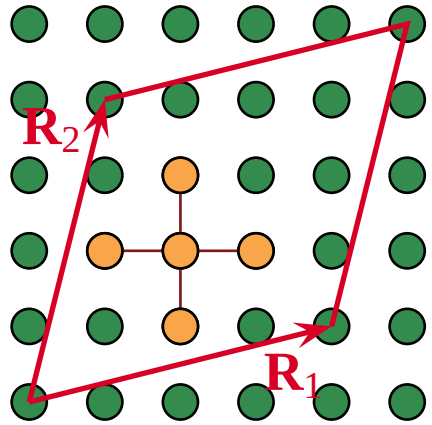


Overview of Chapter 4

- System, cluster and model definitions.
- Computation of cluster DM.
- Finite size effects and twist boundary conditions averaging.
- Comparison of cluster DM spectra:
  - Noninteracting 1-particle cluster DM weights after averaging;
  - Strongly-interacting 1-particle cluster DM weights after averaging.

System, Cluster & Model

- Various $\mathbf{R}_1 \times \mathbf{R}_2$ systems, with $N = |\mathbf{R}_1 \times \mathbf{R}_2|$ sites.



- 5-site cross-shaped cluster with same point group symmetry as square lattice; angular-momentum-like notation:

$$\text{1-particle states :} \quad |s\rangle, |p\rangle, |d\rangle, \ldots;$$
$$\text{many-particle states :} \quad |S\rangle, |P\rangle, |D\rangle, \ldots.$$

- nearest-neighbor hopping (noninteracting) and nearest-neighbor hopping + infinite nearest-neighbor repulsion (strongly-interacting);

$$H_t = -t \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} c^\dagger_{\mathbf{r}} c_{\mathbf{r}'}, \qquad H_{tV} = H_t + V \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} n_{\mathbf{r}} n_{\mathbf{r}'}.$$

Computation of Cluster DM

- obtain ground state $|\Psi\rangle = \sum_{\mathbf{n}} \Psi_{\mathbf{n}} |\mathbf{n}\rangle = \sum_{\mathbf{l}} \sum_{\mathbf{m}} (-1)^{f(\mathbf{n};\mathbf{l},\mathbf{m})} \Psi_{\mathbf{l},\mathbf{m}} |\mathbf{l}\rangle |\mathbf{m}\rangle$, where $|\mathbf{n}\rangle = (-1)^{f(\mathbf{n};\mathbf{l},\mathbf{m})} |\mathbf{l}\rangle |\mathbf{m}\rangle$, $|\mathbf{l}\rangle$, $|\mathbf{m}\rangle$ occupation number basis states of system, cluster and environment respectively:
  - noninteracting: construct finite-system Fermi-sea ground state directly;
  - strongly-interacting: ED taking advantage of translational invariance.
- $\rho = |\Psi\rangle \langle\Psi| \xrightarrow[\text{trace}]{\text{partial}} \rho_C$ (care with fermion sign $(-1)^{f(\mathbf{n};\mathbf{l},\mathbf{m})}$!) gives

$$\langle \mathbf{l} | \rho_C | \mathbf{l}' \rangle = \sum_{\mathbf{m}} \sum_{\mathbf{m}'} (-1)^{f(\mathbf{n};\mathbf{l},\mathbf{m}) + f(\mathbf{n}';\mathbf{l}',\mathbf{m}')} \Psi_{\mathbf{l},\mathbf{m}} \Psi^*_{\mathbf{l}',\mathbf{m}'} \delta_{\mathbf{m},\mathbf{m}'}.$$

- Show that ρ_C so defined gives $\langle\Psi|A|\Psi\rangle = \langle A\rangle = \mathrm{Tr}_C \rho_C A$ for observable A local to cluster.
- Average ρ_C over degenerate ground states, and orientations of system relative to cluster.

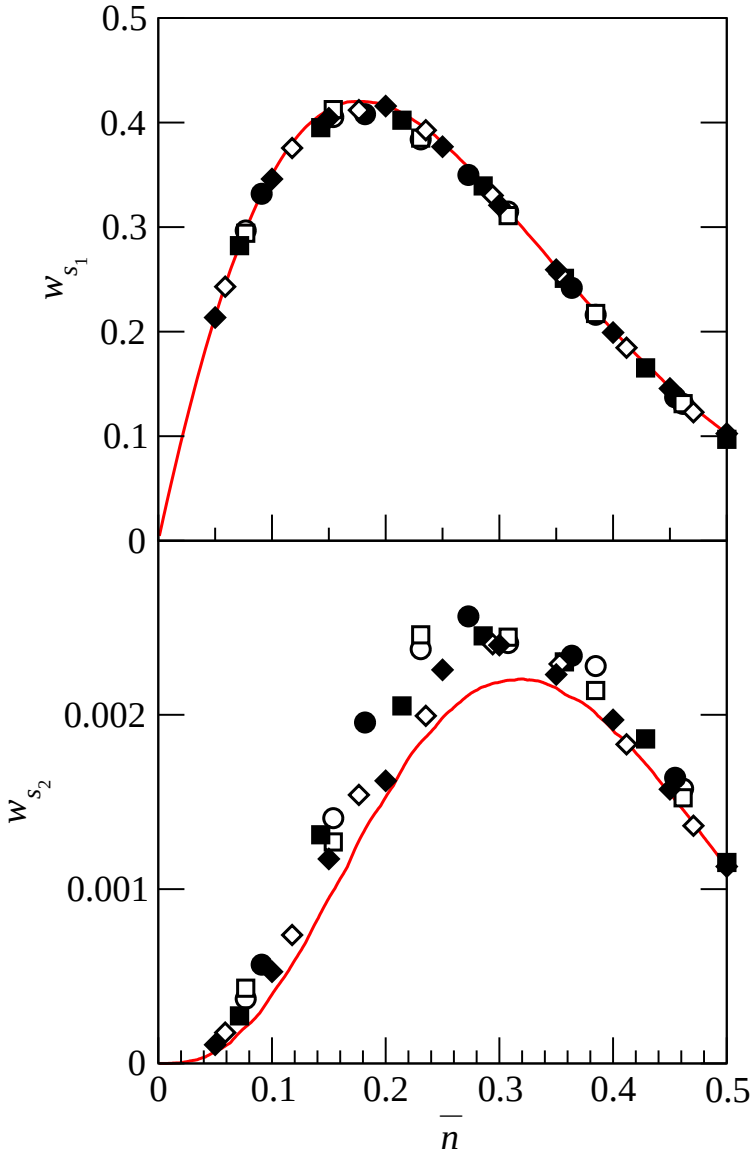
Finite Size Effects & Twist Boundary Conditions Averaging

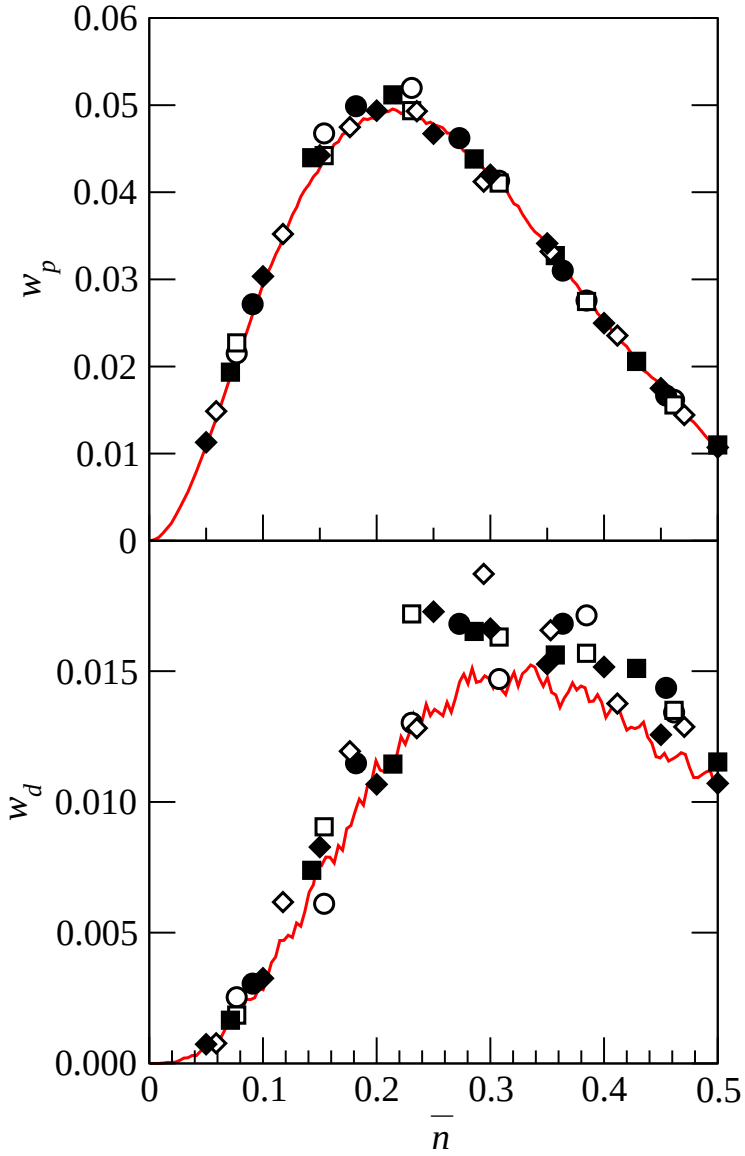
- For 'squarish' finite noninteracting systems subject to periodic boundary conditions (PBC), cluster DM spectra calculated approaches infinite-system limit when $N \sim 200$ sites.
- Small finite systems (noninteracting & strongly-interacting) of $N \sim 20$ sites, strong influence from finite size effects (most severe for d state, least severe for s_1 state) $\Longrightarrow$ require twist boundary conditions (TBC) averaging.
- In bond gauge, replace $c_{\mathbf{r}} \rightarrow e^{-\mathrm{i}\boldsymbol{\phi}\cdot\mathbf{r}} c_{\mathbf{r}}$, $c_{\mathbf{r}}^{\dagger} \rightarrow e^{\mathrm{i}\boldsymbol{\phi}\cdot\mathbf{r}} c_{\mathbf{r}}^{\dagger}$, in Hamiltonian, where $\boldsymbol{\phi} = (\phi_x, \phi_y)$ is the twist vector associated with TBC. Calculate bond-gauge ground state $|\Psi_{\mathrm{bond}}(\boldsymbol{\phi})\rangle$.
- Gauge transformation

$$\varphi : |\mathbf{n}\rangle \rightarrow e^{-\mathrm{i}\sum_{\mathbf{r}}(\boldsymbol{\phi}\cdot\mathbf{r})n_{\mathbf{r}}} |\mathbf{n}\rangle$$

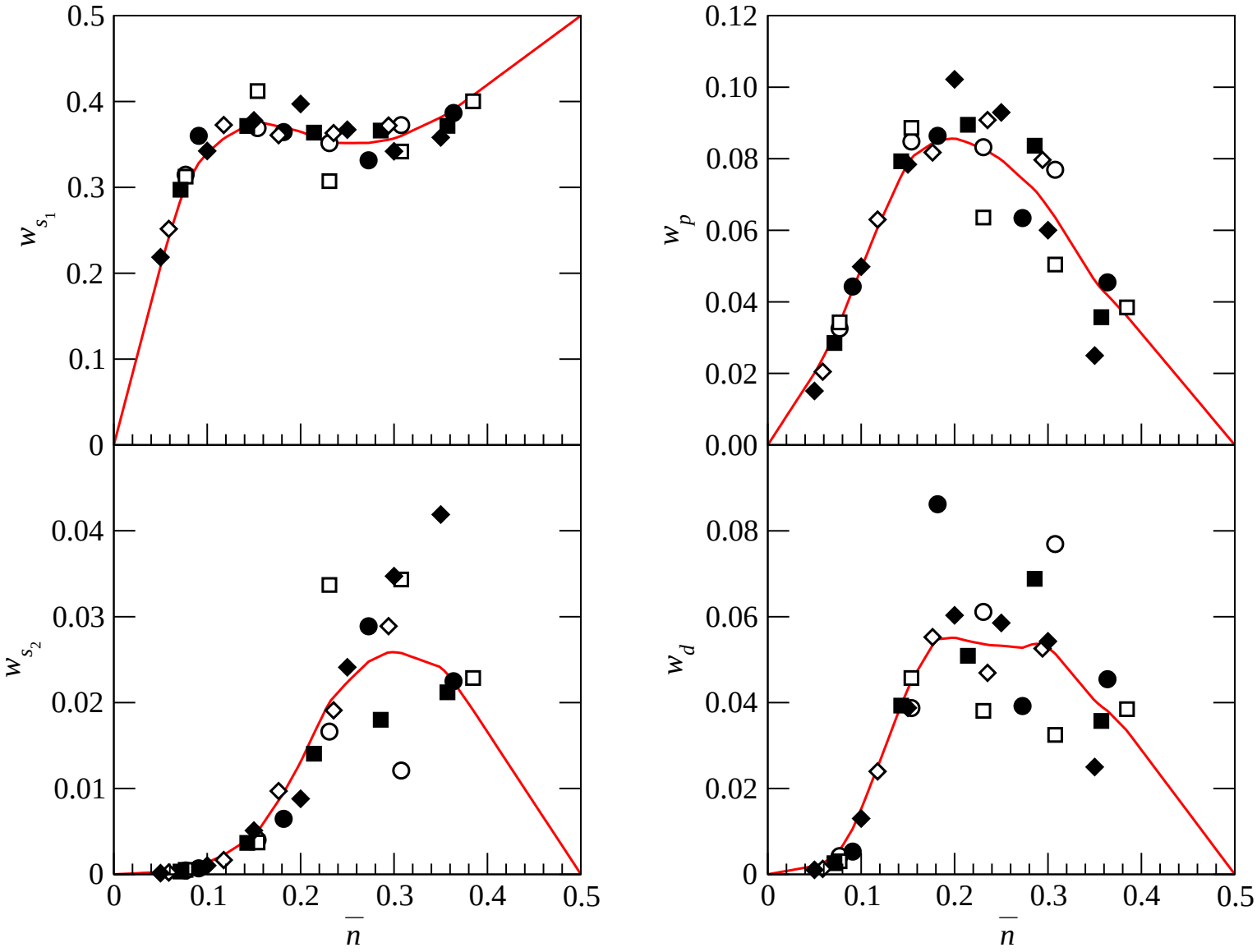
  to get boundary-gauge ground state $|\Psi_{\mathrm{boundary}}(\boldsymbol{\phi})\rangle$. Construct boundary-gauge TBC cluster DM $\rho_C(\boldsymbol{\phi})$.
- Average $\rho_C(\boldsymbol{\phi})$ over all $\boldsymbol{\phi}$ in FBZ. Best approximation to infinite-system ρ_C.

1-Particle Weights (Noninteracting)





1-Particle Weights (Strongly-Interacting)



Overview of Chapters 5, 6, 7 & 8

- Formulation (Chapters 5 & 6):
  - Definition of correlation DM, singular value decomposition (SVD), and order parameters.
  - Operator SVD starting from operator basis of referencing operators; Frobenius orthonormalization.
- Model (Chapter 7):
  - Extended Hubbard ladder of spinless fermions with correlated hops; Compare/contrast Luttinger-liquid physics of 1D interacting fermions;
  - Three limiting cases:
    - $t' \gg t_{\parallel}, t_{\perp}$;
    - $t_{\perp} \ll t_{\parallel}, t' = 0$;
    - $t_{\perp} \gg t_{\parallel}, t' = 0$.
- Numerics (Chapter 8):

Correlation DM and SVD

- Entanglement entropy $S = -\operatorname{Tr}\rho_C \log \rho_C$ as gross diagnostic of correlations. [Vidal *et al*, PRL **90**, 227902 (2003)].
- Systematic extraction of order parameters from cluster DM:
  - Disconnected clusters a at $\mathbf{r}$ and b at $\mathbf{r}'$;
  - Cluster DMs ρ^a and ρ^b, supercluster DM ρ^{ab};
  - Define correlation DM, $\rho^c = \rho^{ab} - \rho^a \otimes \rho^b$;
- Correlation DM contains all correlations between a and b — want to attribute these correlations to various order parameters. Write SVD

$$\rho^c = \sum_\alpha \sigma_\alpha X_\alpha Y_\alpha^\dagger,$$

where $X_\alpha Y_\alpha^\dagger$ and $X_\beta Y_\beta^\dagger$ represent independent quantum fluctuations on clusters a and b, i.e. X_α and Y_α are the desired order parameters.

Mechanics of SVD

- Start from operator basis of referencing operators

$$K_{\mathbf{n}} = \prod_i \left[n_i c_i + (1 - n_i) c_i c_i^\dagger \right], \quad K_{\mathbf{n}} |\mathbf{n}'\rangle = \delta_{\mathbf{n}\mathbf{n}'} |0\rangle ,$$

  for system basis states. Similarly defined for cluster and environment basis states.

- Product of referencing operators $X_{\mathbf{l}\mathbf{l}'} = K_{\mathbf{l}}^\dagger K_{\mathbf{l}'}$, $Y_{\mathbf{m}\mathbf{m}'} = K_{\mathbf{m}}^\dagger K_{\mathbf{m}'}$ orthonormal with respect to Frobenius norm

$$\mathrm{Tr}\, X_{\mathbf{l}\mathbf{l}'} X_{\mathbf{l}''\mathbf{l}'''} = \delta_{\mathbf{l}\mathbf{l}',\mathbf{l}''\mathbf{l}'''}, \quad \mathrm{Tr}\, Y_{\mathbf{m}\mathbf{m}'} Y_{\mathbf{m}''\mathbf{m}'''} = \delta_{\mathbf{m}\mathbf{m}',\mathbf{m}''\mathbf{m}'''};$$

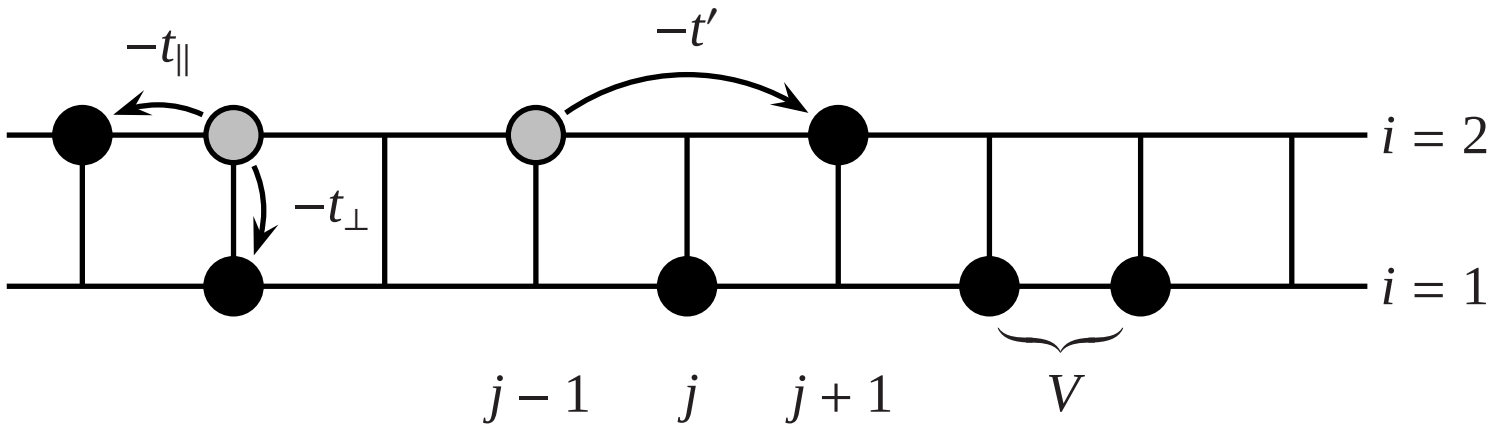
- Write

$$\rho^c = \sum_{\mathbf{n},\mathbf{n}'} \left[(-1)^{f(\mathbf{n};\mathbf{l},\mathbf{m}) + f(\mathbf{n}';\mathbf{l}',\mathbf{m}')} \langle \mathbf{n}|\rho^{ab}|\mathbf{n}'\rangle - \langle \mathbf{l}|\rho^a|\mathbf{l}'\rangle \langle \mathbf{m}|\rho^b|\mathbf{m}'\rangle \right] K_{\mathbf{l}}^\dagger K_{\mathbf{l}'} K_{\mathbf{m}}^\dagger K_{\mathbf{m}'}.$$

- Numerical singular value decompose the coefficient matrix **K** of ρ^c, whose matrix elements are

$$\mathsf{K}_{\lambda\mu} = \mathsf{K}_{\mathbf{l}\mathbf{l}',\mathbf{m}\mathbf{m}'} = (-1)^{f(\mathbf{n};\mathbf{l},\mathbf{m}) + f(\mathbf{n}';\mathbf{l}',\mathbf{m}')} \langle \mathbf{n}|\rho^{ab}|\mathbf{n}'\rangle - \langle \mathbf{l}|\rho^a|\mathbf{l}'\rangle \langle \mathbf{m}|\rho^b|\mathbf{m}'\rangle .$$

Extended Hubbard Ladder of Spinless Fermions



$$H_{t_{\parallel}t_{\perp}t'V} = -t_{\parallel}\sum_i\sum_j\left(c^{\dagger}_{i,j}c_{i,j+1} + c^{\dagger}_{i,j+1}c_{i,j}\right) - t_{\perp}\sum_j\left(c^{\dagger}_{1,j}c_{2,j} + c^{\dagger}_{2,j}c_{1,j}\right)$$
$$- t'\sum_j\left(c^{\dagger}_{1,j}n_{2,j+1}c_{1,j+2} + c^{\dagger}_{1,j+2}n_{2,j+1}c_{1,j}\right)$$
$$- t'\sum_j\left(c^{\dagger}_{2,j}n_{1,j+1}c_{2,j+2} + c^{\dagger}_{2,j+2}n_{1,j+1}c_{2,j}\right)$$
$$+ V\sum_i\sum_j n_{i,j}n_{i,j+1} + V\sum_j n_{1,j}n_{1,j}$$

$V \to \infty$, no nearest-neighbor occupation, smaller Hilbert space for ED.

Luttinger-Liquid Physics

- Tunable parameters in model:
  - Filling fraction $\overline{n}$: fermion fluid for $\overline{n} \gtrsim 0$, hole fluid for $\overline{n} \lesssim \frac{1}{2}$;
  - Nearest-neighbor hopping anisotropy $t_\perp/t_\parallel$;
  - Correlated hop $t'/t_\parallel$. Large $t'/t_\parallel$ favors pairing and hence SC.
- Three limiting cases:
  - $t' \gg t_\parallel, t_\perp$, SC dominate, FL exponential decay;
  - $t_\perp \ll t_\parallel$, $t' = 0$, FL dominant, power-law decay;
  - $t_\perp \gg t_\parallel$, $t' = 0$, true long-range CDW order at quarter-filling.
- Compare and contrast basic physics of spinless Luttinger liquid: Insulator at half-filling. Away from half-filling,
  - Power-law decay of CDW and SC correlations;
  - CDW dominate at long distances if $K_\rho < 1$, SC dominate at long distances if $K_\rho > 1$, FL if $K_\rho = 1$;

Correlated Hops Only

- In limit $t'/t_{\parallel}, t'/t_{\perp} \to \infty$, ground state of $P = 2p$ particles that of p strongly-interacting bound pairs.
- Exact infinite-ladder ground state obtained from

  bound pair $(c_{1,j}c_{2,j+1}) \to$ extended hard-core boson $(B_j) \to$
  hard-core boson $(b_j) \to$ noninteracting spinless fermion (c_j)

  sequence of maps.
- SC correlations decay as power laws,

$$\langle \Delta_j^\dagger \Delta_{j+r} \rangle = \langle B_j^\dagger B_{j+r} \rangle \sim r^{-1}, \qquad \Delta_j = \frac{1}{\sqrt{2}}(-1)^j \left(c_{1,j}c_{2,j+1} \pm c_{2,j}c_{1,j+1} \right).$$

- FL correlations decay exponentially,

$$\langle c_{i,j}^\dagger c_{i,j+r} \rangle \sim \exp\left(-r \cdot \tfrac{1}{2} \int_0^{1-\bar{n}_1} f(\bar{n}_1, x)\, dx \right),$$

  where $f(\bar{n}, x)$ is universal scaling function found in Chapter 3.

Weak Inter-Leg Hopping

- In limit $t_\perp \ll t_\parallel$, $t' = 0$, intra-leg hopping of particle on leg $i = 1$ restricted by the two particles on leg $i = 2$ closest to it, and vice versa. Hence particle on leg i will never be directly by other particles on the same leg.
- Exact infinite-ladder ground states obtained from 1D Fermi sea ground state by the staggered maps

$$c^\dagger_{j_1} c^\dagger_{j_2} \cdots c^\dagger_{j_{2p-1}} c^\dagger_{j_{2p}} \to c^\dagger_{1,j_1} c^\dagger_{2,j_2} \cdots c^\dagger_{1,j_{2p-1}} c^\dagger_{2,2p},$$
$$c^\dagger_{j_1} c^\dagger_{j_2} \cdots c^\dagger_{j_{2p-1}} c^\dagger_{j_{2p}} \to c^\dagger_{2,j_1} c^\dagger_{1,j_2} \cdots c^\dagger_{2,j_{2p-1}} c^\dagger_{1,2p}$$

- Dominant FL correlations

$$\langle c^\dagger_{\pm,j} c_{\pm,j+r} \rangle \sim r^{-1}, \qquad c_{\pm,j} = \tfrac{1}{\sqrt{2}}(c_{1,j} \pm c_{2,j}).$$

- Subdominant CDW and SC correlations

$$\langle n_j n_{j+r} \rangle \sim r^{-2}, \qquad \langle \Delta^\dagger_j \Delta_{j+r} \rangle \sim r^{-2},$$

for various n_j constructed out of $c^\dagger_{i,j} c_{i,j}$, and various Δ_j constructed out of $c_{1,j} c_{2,j+1}$ and $c_{2,j} c_{1,j+1}$.

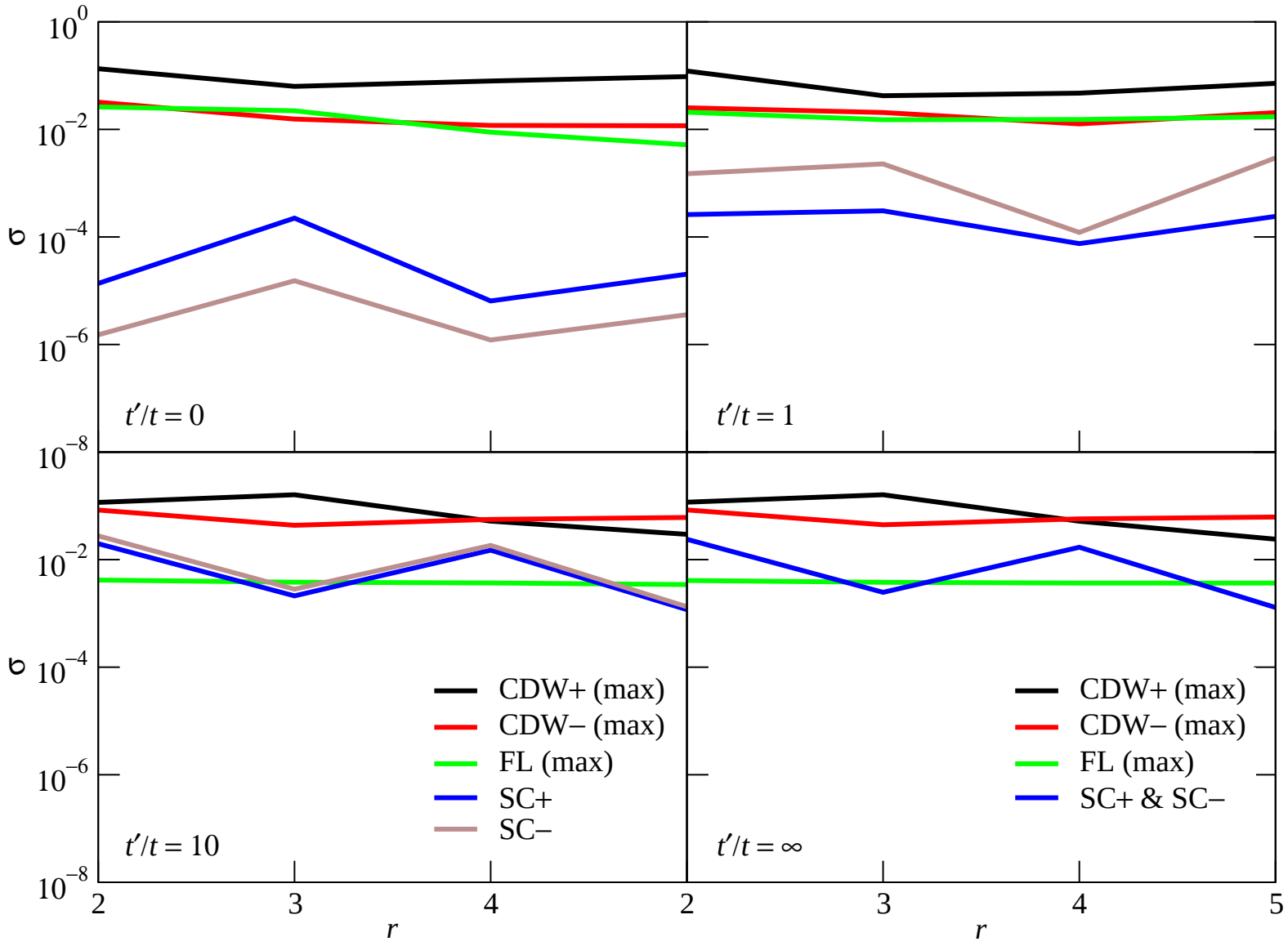
Strong Inter-Leg Hopping

- In limit $t_\perp \gg t_\parallel$, $t' = 0$, each particle very nearly in rung eigenstate. Effectively 1D gas of interacting rung-fermions with extended core, i.e. infinite nearest-neighbor repulsion.
- Can be mapped to chain of noninteracting spinless fermions,

$$C_j^\dagger N_{j+1} = 0, \quad C_j^\dagger(\mathbb{1} - N_{j+1}) \to c_j^\dagger,$$

  $C_j^\dagger$ creates extended core rung-fermions, and $c_j^\dagger$ creates spinless fermions.
- Think of leg index as 'spin projection', then intra-leg hopping $t_\parallel$ introduces only very weak exchange between rung-fermions. Essentially uncorrelated 'spin projections'.
- Slow power-law decay of CDW correlations which becomes true long-range order at quarter-filling.
- Exponential decay of FL and SC correlations, both vanishing at quarter-filling.
- Phase separation above quarter-filling.

Results From SVD of Correlation DM



Conclusions

- Learning from noninteracting spinless fermions:
  - Exact formula for cluster DM;
  - Scaling behaviour of eigenvalues and eigenfunctions;
  - Statistical mechanics analogy;
  - Operator-based DM truncation scheme;
  - When 2D infinite-system limit reached numerically;
  - Effectiveness of averaging aparatus.
- Applying to strongly-interacting spinless fermions:
  - Adaptation and extension of operator-based DM truncation scheme.
- SVD of correlation DM
  - Systematic extraction of order parameters;
  - Approximate zero-temperature phase diagram.