Many-Body Fermion Density Matrices and Pattern-Forming Cellular Automata

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Part I

Many-Body Fermion Density Matrices

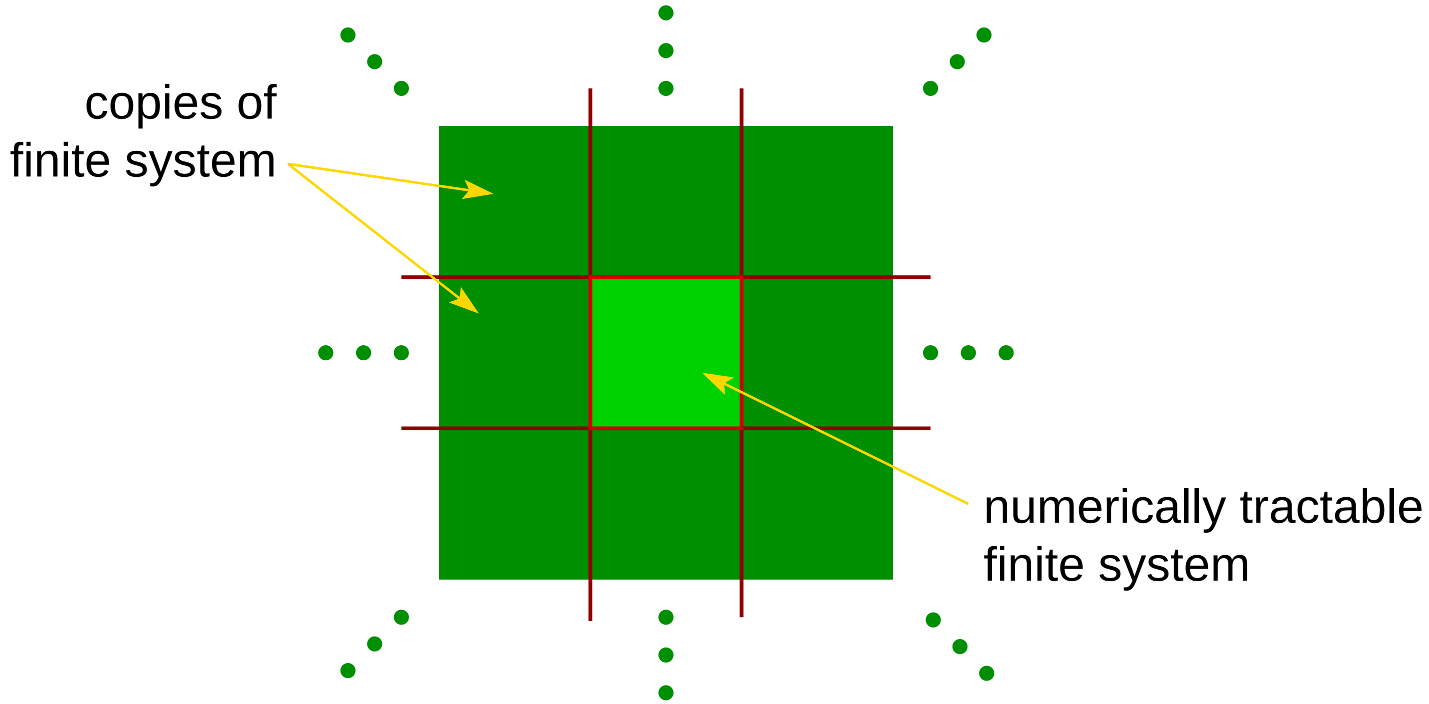
Why Numerical Methods?

- 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
  - Perbutative: 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?

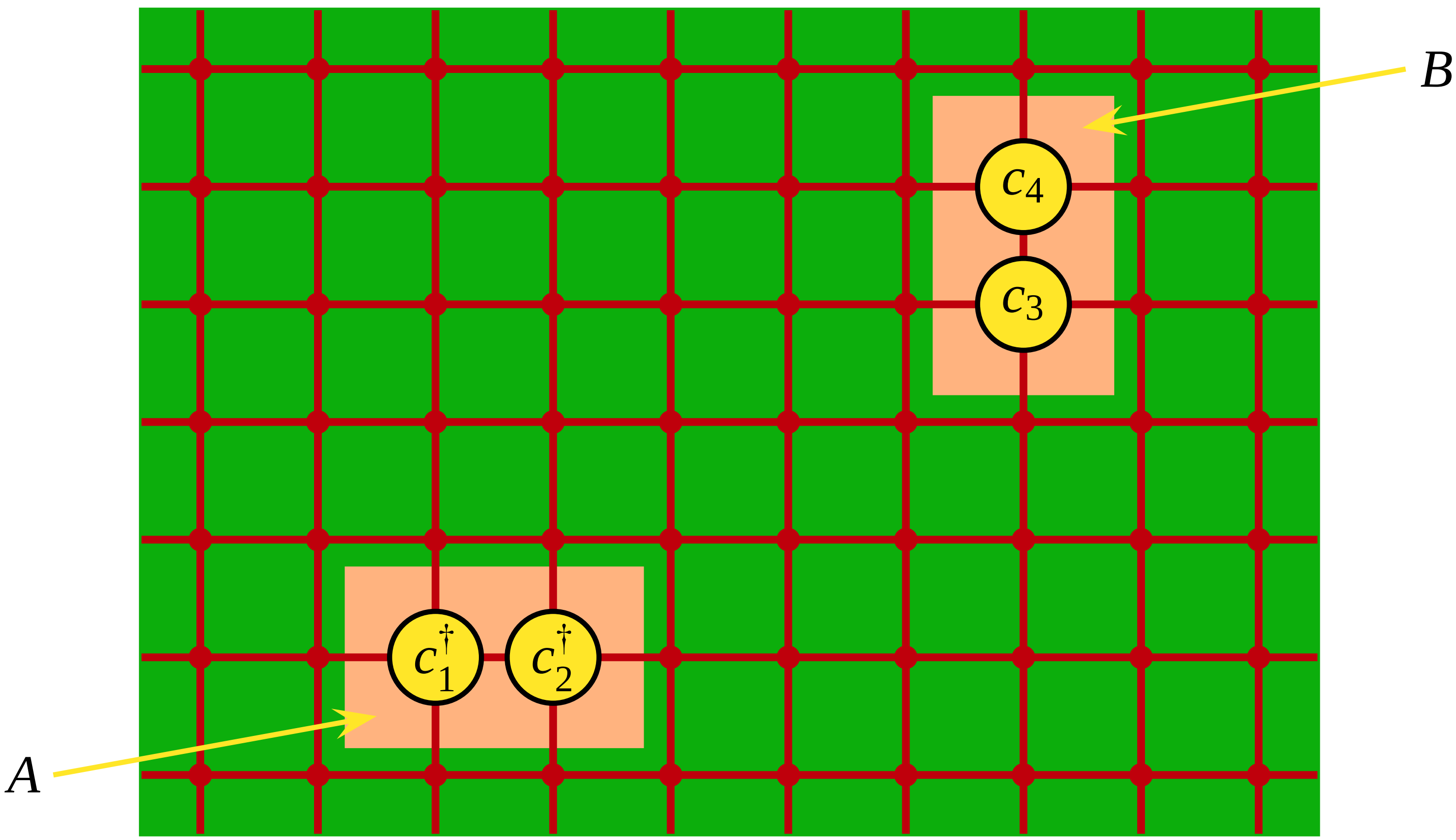
- Build up QM state of infinite system from QM states of finite subsystems.



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

Why Density Matrices?

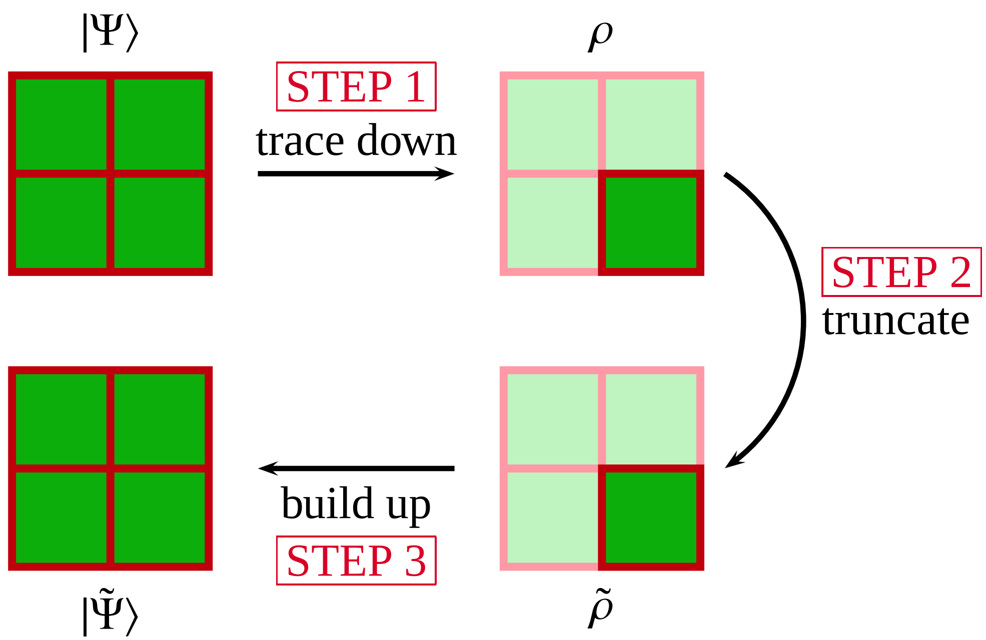
- Calculation of correlations of products of local observables.



- 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)

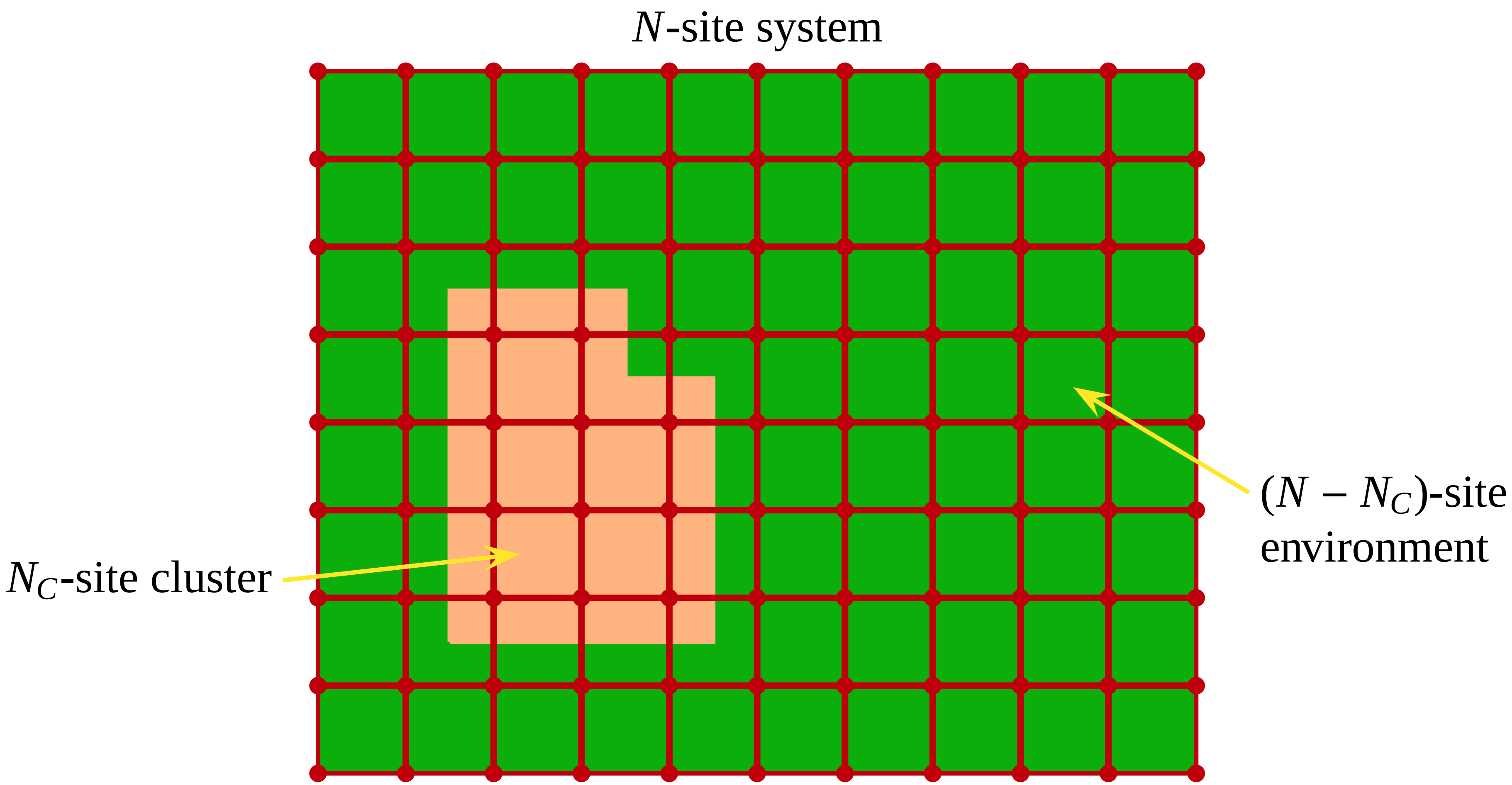
- Repeated cycles of truncation and renormalization. [S. R. White, PRL **69**, 2863 (1992); R. J. Bursill, PRB **60**, 1643 (1999)]
- Truncation naturally guided by density matrix (DM).



- 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.

Noninteracting Spinless Fermions in d Dimensions

$$H = -t \sum_{\langle \mathbf{r}_i, \mathbf{r}_j \rangle} \left[c_i^\dagger c_j + c_j^\dagger c_i \right], \qquad |\Psi_F\rangle = \text{Fermi sea ground state}$$



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)]

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

- Start from normalized grand-canonical DM of system

$$\rho_0 = \mathscr{Q}^{-1} \exp\left[-\beta(H - \mu F)\right] = \mathscr{Q}^{-1} \exp\left[\sum_{i,j} \Gamma_{i,j} c_i^\dagger c_j\right] = \mathscr{Q}^{-1} \exp\left[\sum_k \tilde{\Gamma}_{kk} \tilde{c}_k^\dagger \tilde{c}_k\right],$$

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 $\mathscr{Q}$, 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.

Exact Formula for Cluster DM

- Matrix elements of ρ_0 are

$$\langle \boldsymbol{\xi}\boldsymbol{\eta}|\rho_0|\boldsymbol{\xi}'\boldsymbol{\eta}'\rangle = \mathscr{Q}^{-1}\exp\left[\begin{pmatrix}\boldsymbol{\xi}^* & \boldsymbol{\eta}^*\end{pmatrix} e^{\Gamma}\begin{pmatrix}\boldsymbol{\xi}' \\ \boldsymbol{\eta}'\end{pmatrix}\right].$$

- 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

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

Exact Formula for Cluster DM

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

$$\begin{array}{c} G_C \\ \downarrow \end{array}$$

$$\mathscr{G} = \left[\begin{array}{cccc|ccc}
G_{\bar{1}1} & G_{\bar{1}2} & \cdots & G_{\bar{1}N_C} & G_{\bar{1}N_C+1} & \cdots & G_{\bar{1}N} \\
G_{\bar{2}1} & G_{\bar{2}2} & \cdots & G_{\bar{2}N_C} & G_{\bar{2}N_C+1} & \cdots & G_{\bar{2}N} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
G_{\overline{N_C}1} & G_{\overline{N_C}2} & \cdots & G_{\overline{N_C}N_C} & G_{\overline{N_C}N_C+1} & \cdots & G_{\overline{N_C}N} \\
\hline
G_{\overline{N_C+1}1} & G_{\overline{N_C+1}2} & \cdots & G_{\overline{N_C+1}N_C} & G_{\overline{N_C+1}N_C+1} & \cdots & G_{\overline{N_C+1}N} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
G_{\bar{N}1} & G_{\bar{N}2} & \cdots & G_{\bar{N}N_C} & G_{\bar{N}N_C+1} & \cdots & G_{\bar{N}N}
\end{array}\right]
\begin{array}{l} \left.\vphantom{\begin{array}{c}1\\1\\1\\1\end{array}}\right\}\text{block} \\ \left.\vphantom{\begin{array}{c}1\\1\\1\end{array}}\right\}\text{environment} \end{array}$$

$$\underbrace{\hphantom{G_{\bar{1}1}\;G_{\bar{1}2}\;\cdots\;G_{\bar{1}N_C}}}_{\text{block}}\qquad\underbrace{\hphantom{G_{\bar{1}N_C+1}\;\cdots\;G_{\bar{1}N}}}_{\text{environment}}$$

Exact Formula for Cluster DM

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

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

- Matrix relations

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

- 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

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

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

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

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)

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

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

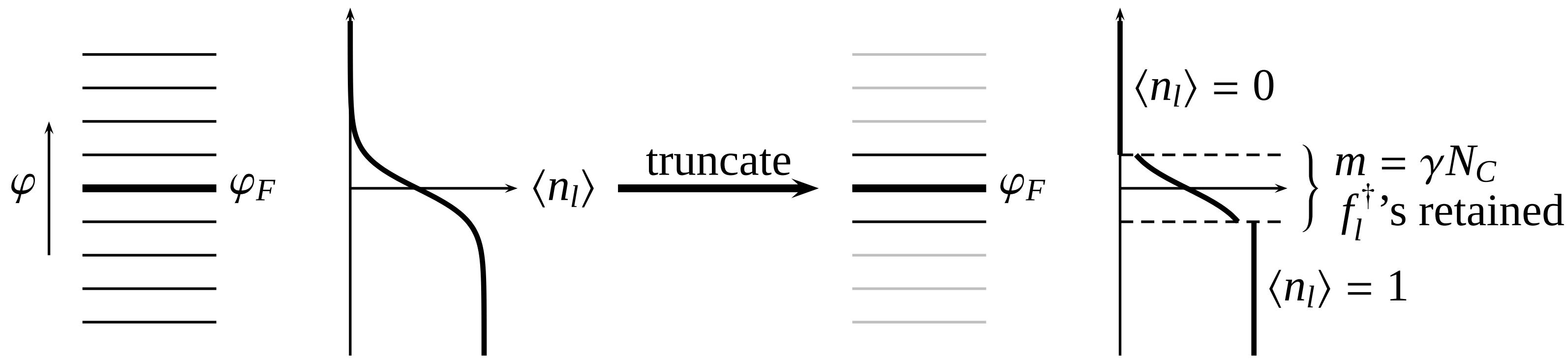
- Based on analogy, average pseudo-occupation is

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

- 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.

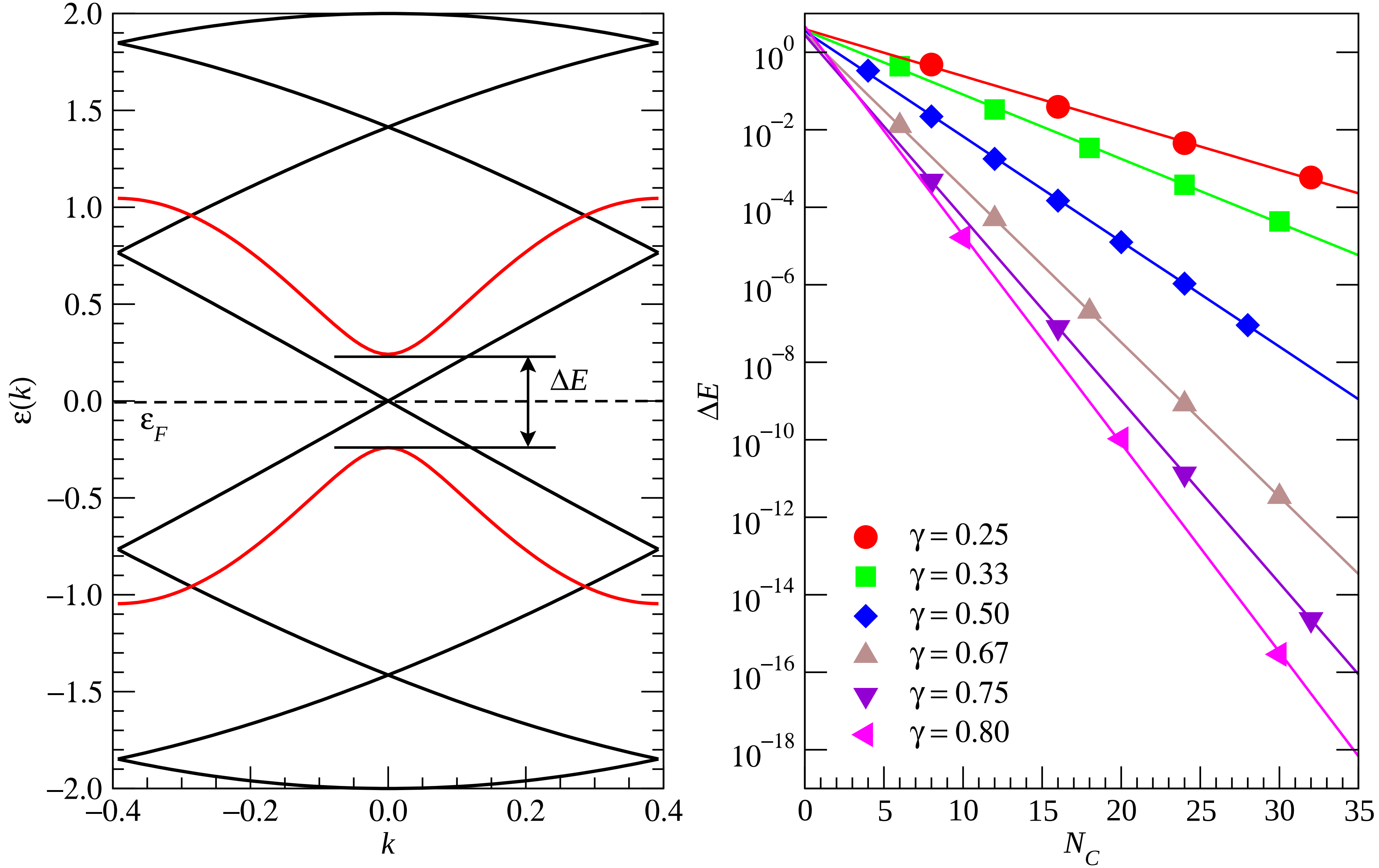
Operator-Based DM Truncation Scheme

- 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 $\varphi_l \approx \varphi_F$:



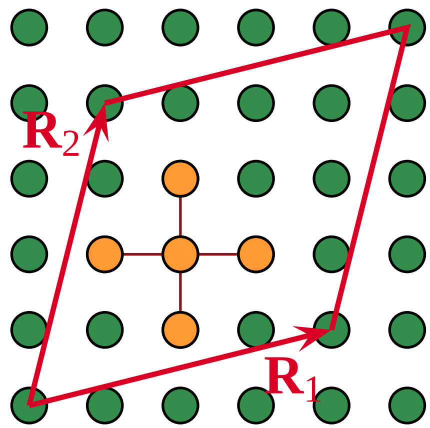
- Compare with weight-ranked truncation (used for e.g., in the DMRG):
  - eigenstates with largest weights all kept;
  - some eigenstates with intermediate weights not kept, but replaced with eigenstates with slightly smaller weights;
  - eigenstates with small weights not kept.

Results: 1D Noninteracting Spinless Fermions



Cluster DM on 2D Square Lattice

- Definition of system:

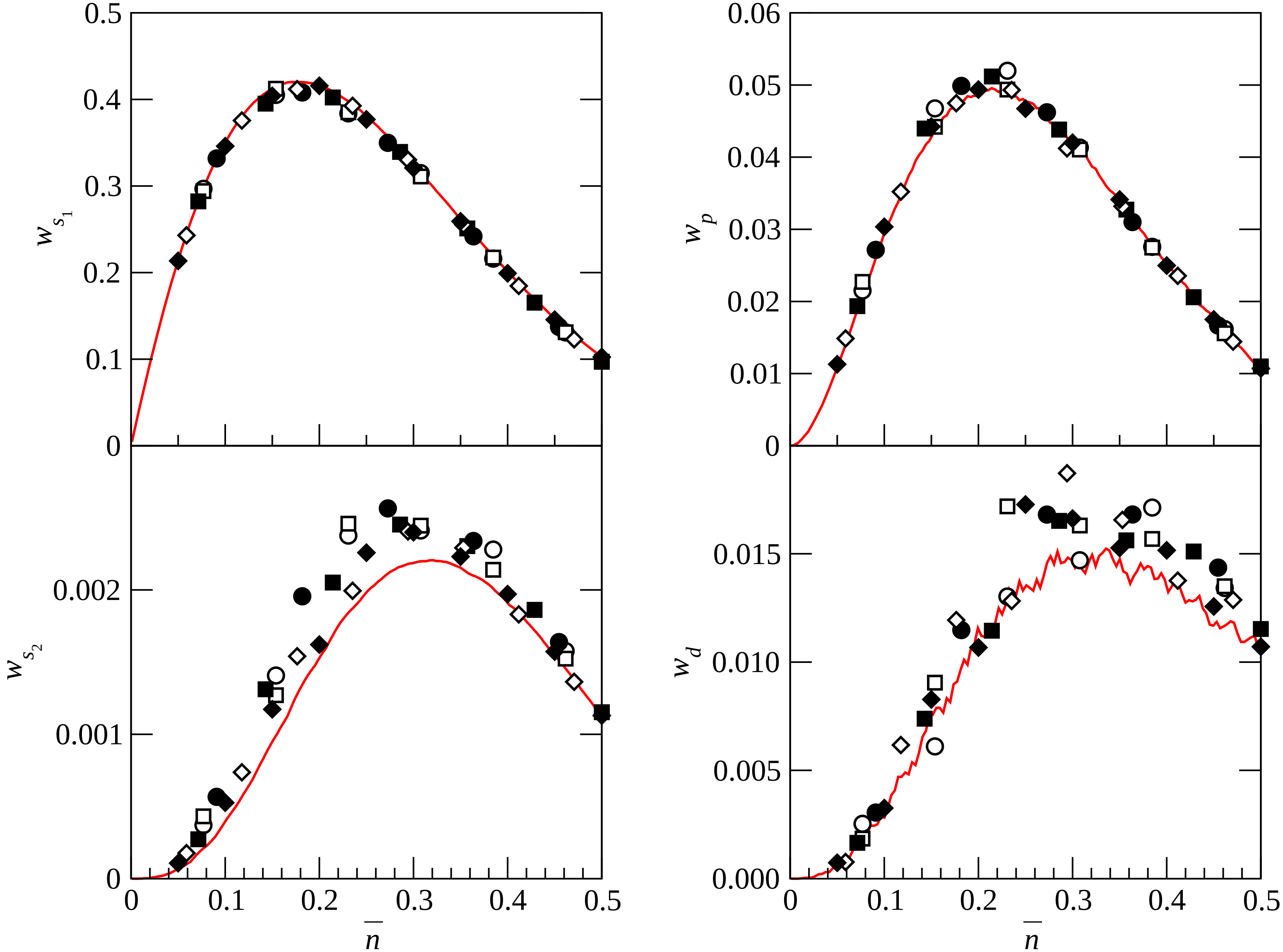


- 5-site cluster, various system sizes $N = |\mathbf{R}_1 \times \mathbf{R}_2|$.
- Computation of cluster DM ρ_C:
  - obtain ground state $|\Psi\rangle$ (exact diagonalization or otherwise);
  - $\rho_0 = |\Psi\rangle\langle\Psi| \xrightarrow[\text{trace}]{\text{partial}} \rho_C$ (care with fermion sign!);
  - translational invariance;
  - degeneracy, orientation and twist boundary conditions averaging.

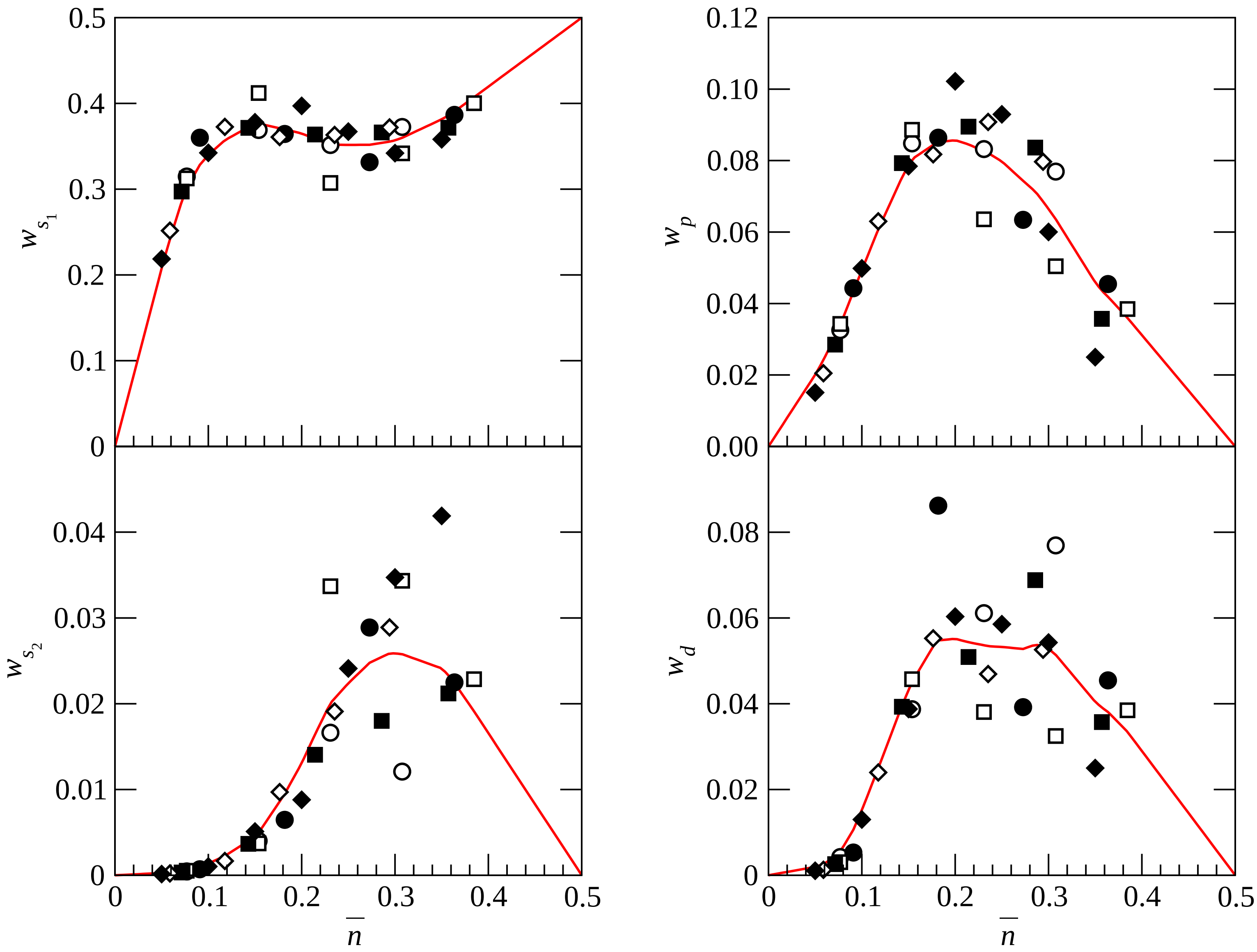
2D Cluster DM Weights

- nearest neighbor hopping (noninteracting) and nearest neighbor hopping + infinite nearest neighbor repulsion (strongly interacting);
- 0-particle weight not interesting — monotonic decreasing with filling $\bar{n}$, very similar for noninteracting and strongly interacting systems;
- 5 1-particle weights, characterized by “angular momentum” quantum numbers s_1, p_x, p_y, d, s_2.
- Infinite system limit for noninteracting system, $\sim$200 sites for a squarish finite system without twist boundary conditions averaging;
- Small finite systems (noninteracting & interacting) of $\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 averaging.

1-Particle Weights (Noninteracting)



1-Particle Weights (Strongly Interacting)



Correlation DM

- 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.

Singular Value Decomposition of Correlation DM

- Start from operator basis of referencing operators

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

- Write $\rho^c = \sum_{\mathbf{n},\mathbf{n}'} \left[(-1)^{f_{\mathbf{n}\mathbf{n}'}} \langle \mathbf{n} | \rho_{AB} | \mathbf{n}' \rangle - \langle \mathbf{l} | \rho_A | \mathbf{l}' \rangle \langle \mathbf{m} | \rho_B | \mathbf{m}' \rangle \right] K_{\mathbf{l}}^\dagger K_{\mathbf{l}'} K_{\mathbf{m}}^\dagger K_{\mathbf{m}'}$, where $|\mathbf{n}\rangle = |\mathbf{l}\rangle |\mathbf{m}\rangle$, and $K_{\mathbf{n}} = K_{\mathbf{l}} K_{\mathbf{m}}$.

- Product of referencing operators orthonormal with respect to Frobenius norm

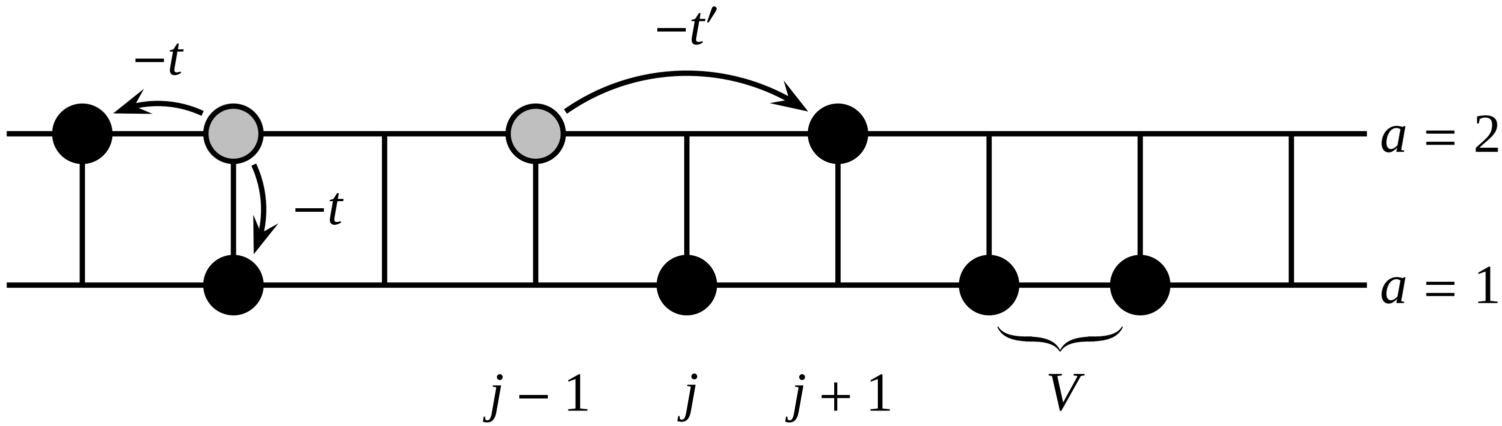
$$\mathrm{Tr}\, X_{\mathbf{l}\mathbf{l}'} X_{\mathbf{l}''\mathbf{l}'''} = \delta_{\mathbf{l}\mathbf{l}',\mathbf{l}''\mathbf{l}'''}, \quad \mathrm{Tr}\, Y_{\mathbf{m}\mathbf{m}'} Y_{\mathbf{m}''\mathbf{m}'''} = \delta_{\mathbf{m}\mathbf{m}',\mathbf{m}''\mathbf{m}'''};$$

- Numerical singular value decomposition (SVD) of coefficient matrix of ρ^c gives

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

- $X_\alpha Y_\alpha^\dagger$ and $X_\beta Y_\beta^\dagger$ represent independent quantum fluctuations on clusters A and B, i.e. can treat X_α and Y_α as order parameters.

Extended Hubbard Ladder of Spinless Fermions

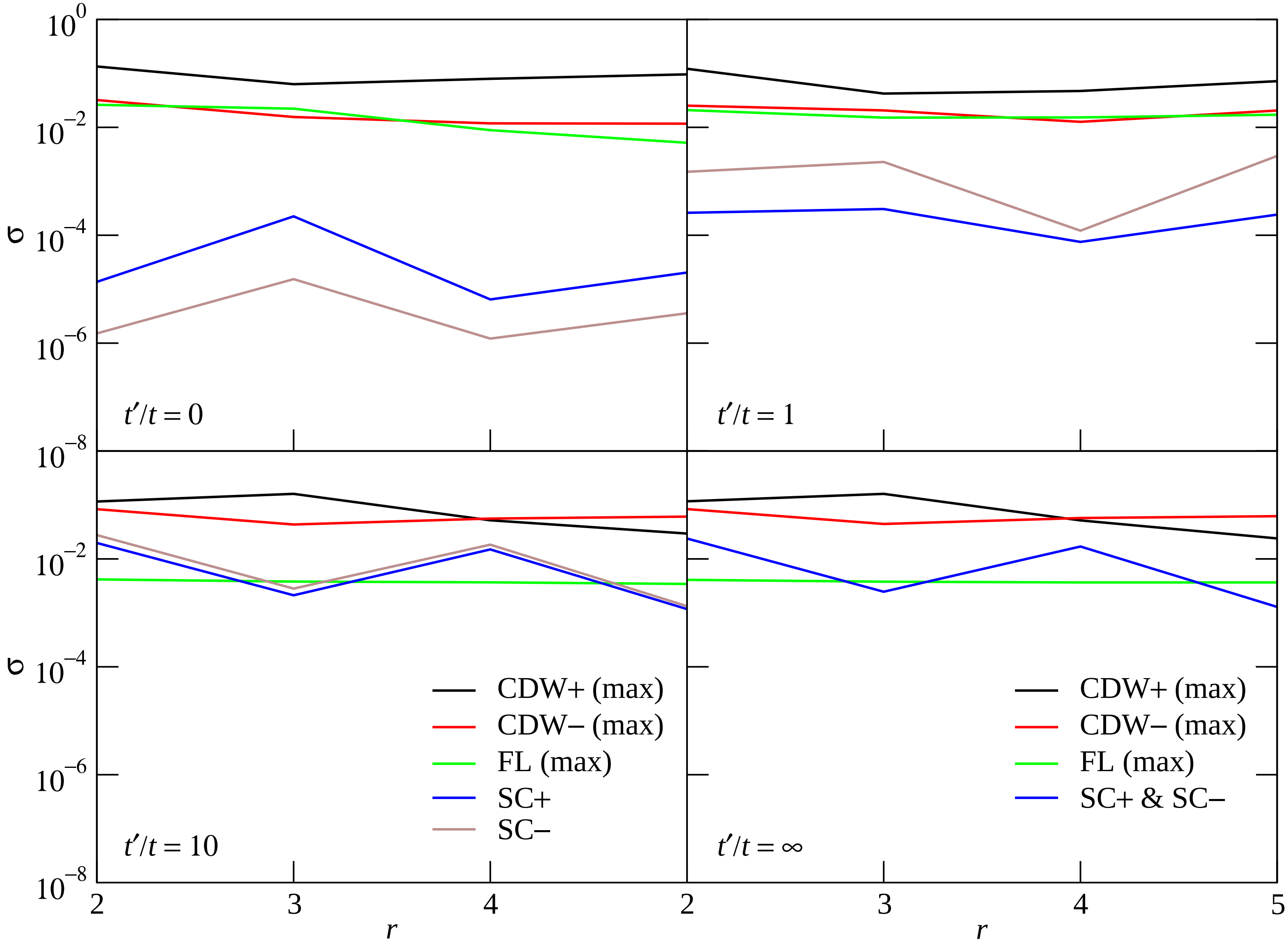


$$
\begin{aligned}
H = & -t \sum_a \sum_j \left(c^\dagger_{j,a} c_{j+1,a} + c^\dagger_{j+1,a} c_{j,a} \right) - t \sum_j \left(c^\dagger_{j,1} c_{j,2} + c^\dagger_{j,2} c_{j,1} \right) \\
& - t' \sum_j \left(c^\dagger_{j,1} n_{j+1,2} c_{j+2,1} + c^\dagger_{j+2,1} n_{j+1,2} c_{j,1} \right) \\
& - t' \sum_j \left(c^\dagger_{j,2} n_{j+1,1} c_{j+2,2} + c^\dagger_{j+2,2} n_{j+1,1} c_{j,2} \right) \\
& + V \sum_a \sum_j n_{j,a} n_{j+1,a} + V \sum_j n_{j,1} n_{j,2}
\end{aligned}
$$

Expected Order Parameters

- $V \to \infty$, no nearest-neighbor occupation, smaller Hilbert space for exact diagonalization.
- Basic physics that of spinless Luttinger liquid:
  - Power-law decay of charge density wave (CDW) and superconducting (SC) correlations;
  - CDW dominate at long distances if $K_\rho < 1$, SC dominate at long distances if $K_\rho > 1$, Fermi liquid (FL) if $K_\rho = 1$;
  - Insulator at half-filling.
- Tunable parameters in model:
  - Filling fraction $\bar{n}$: fermion fluid for $\bar{n} \gtrsim 0$, hole fluid for $\bar{n} \lesssim \frac{1}{2}$;
  - Correlated hop t' favors pairing and hence SC correlations.

Results From SVD of Correlation DM



Conclusions for Part I

- Learning from noninteracting spinless fermions:
  - Exact formula for cluster DM;
  - 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;
  - Signatures of quantum phase transitions.
- SVD of correlation DM
  - Systematic extraction of order parameters;
  - Signatures of quantum phase transitions.

Part II

Pattern-Forming Cellular Automata

Cellular Automata

- A collection of finite state machines. The state of the i^{th} machine at time t given by $s_i(t) \in \mathcal{A}$, where $\mathcal{A}$ is a finite set, also called the *alphabet*;

- A collection of neighborhoods. The neighborhood of the i^{th} machine is denoted by $\mathcal{N}_i$;

- A dynamical rule $\varphi : \mathcal{N}_i \to \mathcal{A}$, such that $s_i(t+1) = \varphi(s_j(t) \mid j \in \mathcal{N}_i)$.

Classification of CAs

- Elementary and compound CAs. Examples are Game of Life (GOL) and the Nagel-Schreckenberg model of traffic flow respectively.
- Wolfram classified all 256 1D elementary CAs (ECAs) by their dynamical properties. Types I, II and III.
- Wolfram naming convention: if the ECA is

$$\begin{array}{cccccccc} 111 & 110 & 101 & 100 & 011 & 010 & 001 & 000 \\ \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow \\ \alpha_7 & \alpha_6 & \alpha_5 & \alpha_4 & \alpha_3 & \alpha_2 & \alpha_1 & \alpha_0 \end{array}$$

  then Wolfram rule number is $\sum_{j=0}^{7} \alpha_j 2^j$.
- No known attempts at classifying ECAs of higher dimensions.

From Pattern to ECA

- In P681 Pattern Formation and Spatio-Temporal Chaos/Prof Eberhard Bodenschatz, given PDE model, find what patterns form spontaneously. Can do the same for CA models.
- Ask the inverse question instead: given a pattern, what are all the possible CAs that spontaneously generate it?
- Two parts to this question:
  - what CA rules will have given pattern as fixed point; and
  - under which CA rules is the pattern stable?

Striped Phase in 1D

- Consider striped phase in 1D:

○●○●○●○●○●○●○●○

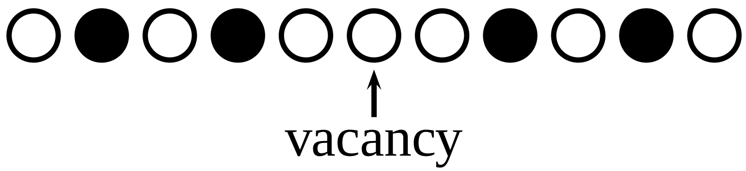
- Fixed point requirement implies the transition rules

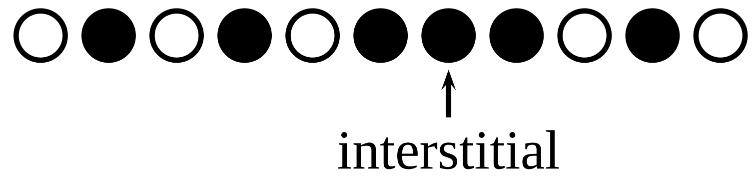
$$●○● \to ×○× \quad \text{and} \quad ○●○ \to ×●×.$$

- Does not uniquely determine ECA rule, 6 more transition rules to specify.

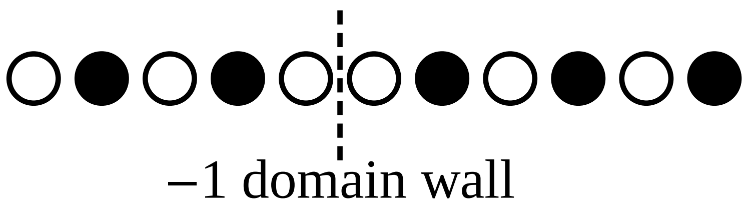
Defects in Striped Phase

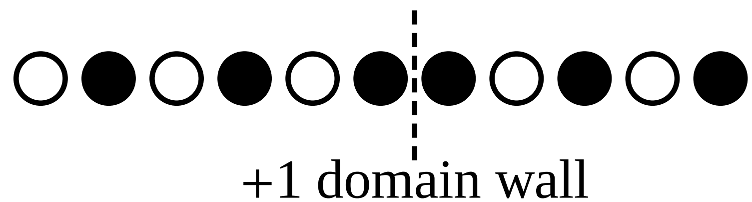
- To analyze stability of striped phase, need to investigate behaviour of departures from pattern, i.e. defects, under various ECA rules.
- Point defects:





- Domain walls:





Strips Stable in Presence of Point Defects

- Since ECA not completely specified, can choose remaining transition rules to stabilize striped phase in presence of point defects.

- Demand that isolated vacancy 'heals': implies transition rules

$$\bigcirc\bigcirc\bigcirc \rightarrow \times\bullet\times, \quad \bullet\bigcirc\bigcirc \rightarrow \times\bigcirc\times, \quad \bigcirc\bigcirc\bullet \rightarrow \times\bigcirc\times.$$

- Demand that isolated interstitial 'heals': implies transition rules

$$\bullet\bullet\bullet \rightarrow \times\bigcirc\times, \quad \bigcirc\bullet\bullet \rightarrow \times\bullet\times, \quad \bullet\bullet\bigcirc \rightarrow \times\bullet\times.$$

- ECA completely specified by requirements that: (a) striped phase is fixed point; (b) isolated vacancies 'heal'; and (c) isolated interstitials 'heal'.

Completed ECA Rule

ECA is Rule 77 in Wolfram's classification scheme:

$s_{j-1}(t)$	$s_j(t)$	$s_{j+1}(t)$	$s_j(t+1)$
0	0	0	1
0	0	1	0
0	1	0	1
0	1	1	1
1	0	0	0
1	0	1	0
1	1	0	1
1	1	1	0

Further Considerations

- **Domain Wall Dynamics.** Both ±1 domain walls stationary under Rule 77, i.e. if start from random initial configuration, all domain walls initially present will be ‘frozen in’.

- **Robustness of Striped Phase.** By modifying some transition rules in Rule 77, can test genericity of striped pattern. Found that:

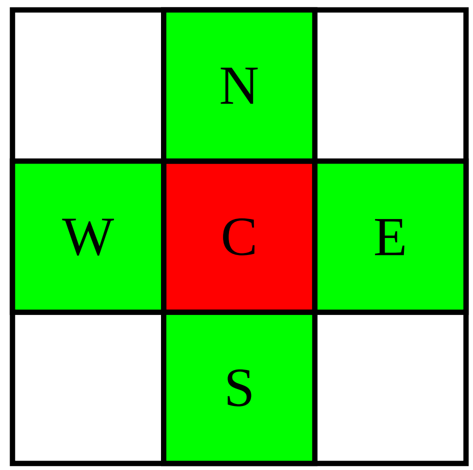
  – Striped phase *most* stable under Rule 77, but also stable under 6 other ECA rules derived from Rule 77, in which a single transition rule is modified.

  – Striped phase *marginally* stable under 4 ECA rules derived from Rule 77, in which one or two transition rules are modified.

  – Striped phase unstable once more than two transition rules are modified from Rule 77. Oscillatory phase nucleates.

2D ECAs

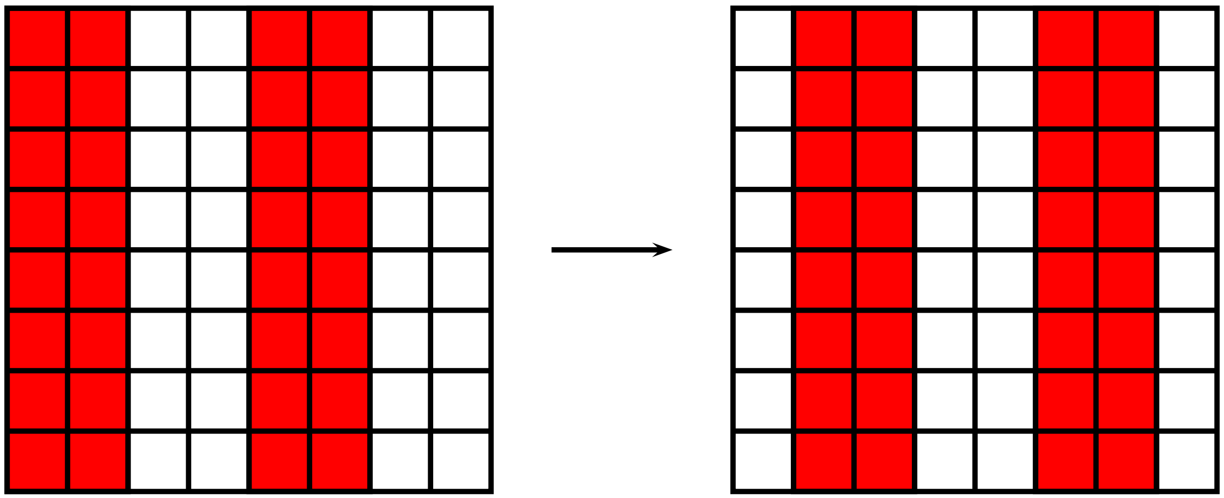
- In 1D, neighborhood simple, unless one wants to go to next nearest neighbor.
- In 2D, greater variety of neighborhoods. Simplest neighborhood for 2D CA is von Neumann (VN) neighborhood:



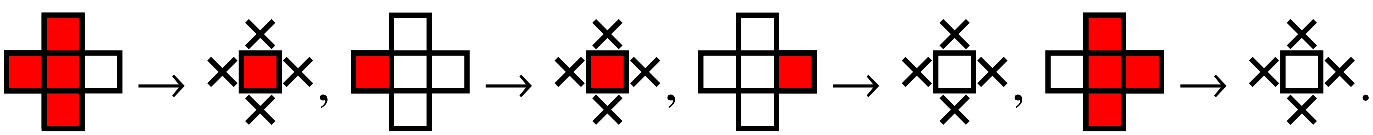
- With VN neighborhood, total of $2^5 = 32$ possible local configurations $\Longrightarrow$ total of $2^{32} = 4{,}294{,}967{,}296$ 2D ECAs.

$\lambda = 4$, $v = +1$ Traveling Wave Phase

- A traveling wave phase with $\lambda = 4$ and $v = +1$ looks like

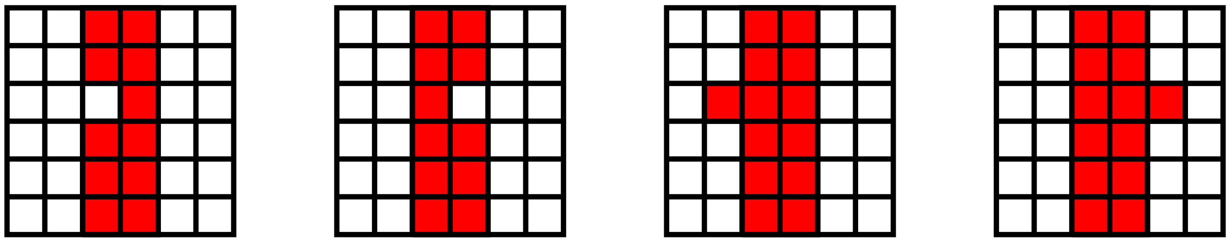


- The traveling wave transition rules are



Multiple Defect Analysis & Transition Rule Conflict

- Unlike in 1D, point defect analysis alone cannot fully specify ECA. Need to do multiple defect analysis.
- Four types of point defect:



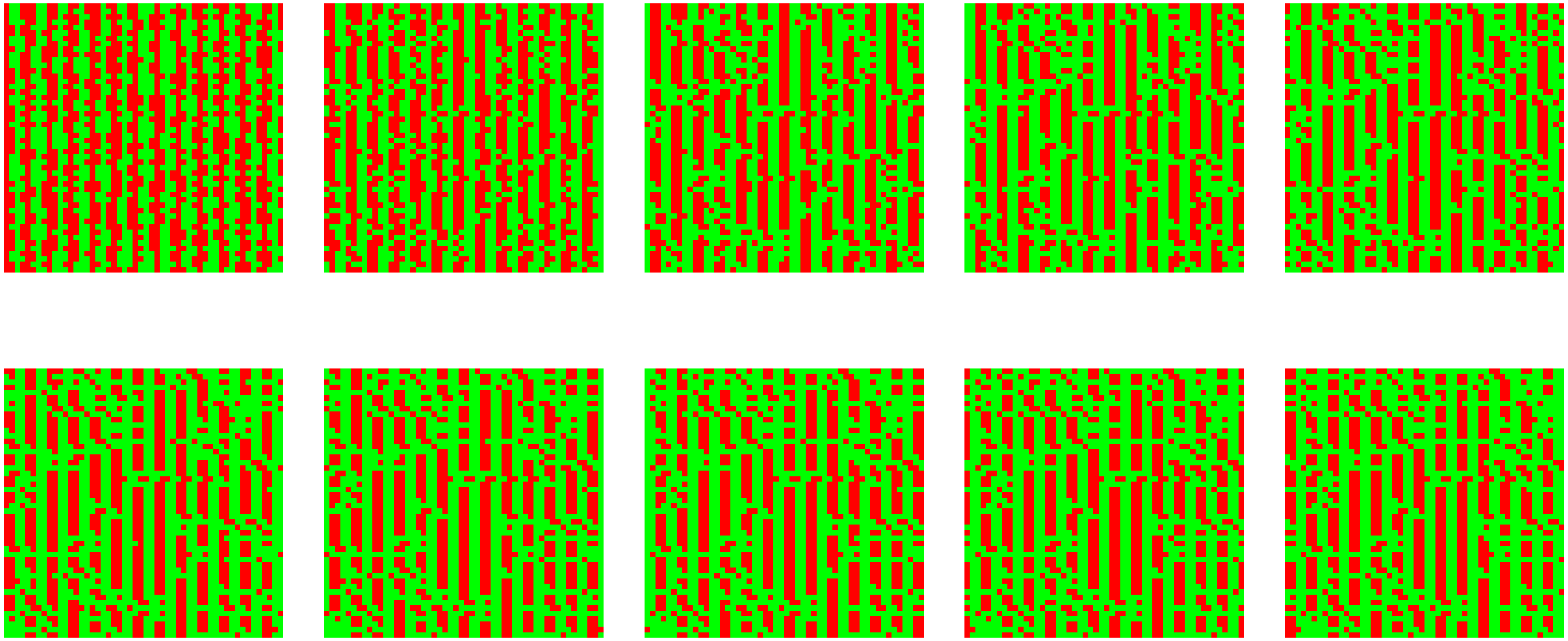
V_L V_R I_L I_R

- In this chosen pattern, transition rules implied by V_L conflicts with that implied by V_R, and transition rules implied by I_L conflicts with that implied by I_R.
- Generic problem.

Protocol for Conflict Resolution

- When transition rule implied by two configurations in conflict, give precedence to configuration with lower number of defects.
- When transition rule implied by leading edge configuration conflicts with that implied by trailing edge configuration, give precedence to trailing edge configuration.
- Can show that some multi-defect configurations whose implied transition rules are forfeited will still be 'healed'.
- Compromise necessary because traveling wave breaks left-right symmetry.
- Completed CA rule is Rule 2,383,284,874.

Simulating Rule 2,383,284,874



Compound CAs

- Some patterns cannot be achieved using ECAs because conflict resolution protocol used cannot ensure stability of desired pattern.
- What to do?
  - Use larger neighborhoods — equivalent to a restricted class of compound ECAs.
  - Use larger state space, say $s_i(t) = 0, \frac{1}{2}, 1$.
- The main idea is to increase the number of transition rules available for pattern matching.
- Another way is to compound together ECAs.
  - Enumerate all defect configurations that can be 'healed' in a few time steps.
  - For each defect configuration, find the ECA that 'heals', while acting as identity map on other configurations, other than the desired patterned configurations.

λ = 4, v = +1 Traveling Wave Phase in 1-D

config			$V_L + I_L$	$V_L + I_R$	$V_R + I_L$	$V_R + I_R$
0	0	0	1	1	0	0
0	0	1	1	1	1	1
0	1	0	0	0	1	1
0	1	1	1	1	1	1
1	0	0	0	0	0	0
1	0	1	0	1	0	1
1	1	0	0	0	0	0
1	1	1	1	0	1	0
rule			139	43	142	46

Does It Work?

- Rules 43 and 142 by themselves most readily generate the desired pattern for initial density $\rho = \frac{1}{2}$. Not good away from half-filling.
- Rules 46 and 139 less readily generate desired pattern.
- Compounding 46 + 139 or 43 + 142 does not make desired pattern any more stable.
- Reason: competing fixed points. Back to square one — need to find fixed points or limit cycles of given ECA.

Conclusions for Part II

- Standard approach to pattern formation: given model, what patterns?
- Inverse approach to pattern formation: given pattern, what models? Studied in the context of ECAs.
- Requiring that pattern be fixed point of dynamics and stable with respect to point defects completely specify 1D ECA. Notion of genericity for pattern under 'perturbations' to 1D ECA.
- For patterns in higher-dimensional ECAs, multiple defect analysis necessary.
- Generic problem of transition rule conflict, leading to reduced stability of pattern.
- Compound CAs, more transition rules for pattern matching to avoid conflicts. More transition rules $\Longrightarrow$ more fixed points and limit cycles $\Longrightarrow$ competition between fixed points.
- Try compound CAs with transition rules designed to make all but desired fixed point unstable.