# Many-Body Fermion Density Matrix: Operator-Based Truncation Scheme

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# The Big Picture

- GOAL Ground state of infinite-sized interacting system;
- LIMITATION Numerically, can only solve finite-sized interacting system;
- Pure state (infinite system) $\Longrightarrow$ mixed state (finite subsystem) $\Longrightarrow$ natural description using density matrices; Review the use of density matrices in quantum mechanics;
- DOWN & UP Truncation & Renormalization: smaller subsystem in small system (**Q1**) $\rightarrow$ small subsystem in infinite system (**Q2**)?
  - Learning from noninteracting systems. Already know answer to **Q2**;
    - Statistical mechanics analogy: density matrix eigenstates $\leftrightarrow$ many-body energy eigenstates of noninteracting system;
    - Operator-Based Density Matrix Truncation Scheme & results for 1D free spinless fermions;
  - Cluster density matrices on 2D square lattice: Compare noninteracting and strongly interacting systems. Attempt to answer **Q1**.

# Density Matrix & Quantum Mechanics

- Quantum mechanics:

| state | wave function $|\Psi\rangle$ | density matrix (DM) $\rho$ |
|---|---|---|
| pure | ✔ | ✔ |
| mixed | ✘ | ✔ |

- If system $S$ = subsystem $A$ $(\{|a\rangle, |a'\rangle, \ldots\})$ + subsystem $B$ $(|b\rangle, |b'\rangle, \ldots\})$, state of system $\rho \to$ state of subsystem $\rho_A$:
  - Partial trace over subsystem $B$, i.e. $\rho_A = \mathrm{Tr}_B\,\rho$;
  - Expectation of referencing operators, i.e. $(\rho_A)_{aa'} = \langle K^\dagger_{a'} K_a \rangle_\rho$ [S.-A. Cheong and C. L. Henley, Phys. Rev. B **69**, 075111 (2004)].
- Applications of $\rho_A$:
  - DM-based renormalization group [S. R. White, PRL **69**, 2863 (1992); R. J. Bursill, PRB **60**, 1643 (1999)];
  - Diagnostic & extraction of important correlations [Vidal *et al*, PRL **90**, 227902 (2003)].

# DM of Free Spinless Fermions

- Free spinless fermions → Fermi sea ground state $|\Psi_F\rangle$.
- For block of $B$ sites identified as subsystem, DM found to have the structure [M.-C. Chung and I. Peschel, PRB **64**, 064412 (2001)]

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

- Relation to correlation function $G(i,j) = \langle\Psi_F|c_i^\dagger c_j|\Psi_F\rangle$, $i, j = 1, \ldots, B$, found to be [S.-A. Cheong and C. L. Henley, Phys. Rev. B **69**, 075111 (2004); I. Peschel, J. Phys. A: Math. Gen **36**, L205 (2003)]

$$\varphi_l = -\ln\left[\lambda_l(1-\lambda_l)^{-1}\right], \quad \mathbb{G}_B|\lambda_l\rangle = \lambda_l\left(f_l^\dagger|0\rangle\right), \quad (\mathbb{G}_B)_{ij} = G(i,j).$$

- A particular eigenstate of $\rho_B$ described by a set of numbers $(n_1, \ldots, n_l, \ldots, n_B)$, $n_l = 0, 1$,

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

and its weight is

$$w \propto \exp(-\Phi), \quad \Phi = \sum_{l=1}^{B} n_l \varphi_l.$$

# Statistical Mechanics Analogy

- [S.-A. Cheong and C. L. Henley, Phys. Rev. B **69**, 075112 (2004)]

| free spinless fermion | | $\rho_B$ | |
|---|---|---|---|
| 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 | $\epsilon_k$ | $\varphi_l$ | 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 | $\epsilon_F$ | $\varphi_F$ | pseudo-Fermi level |

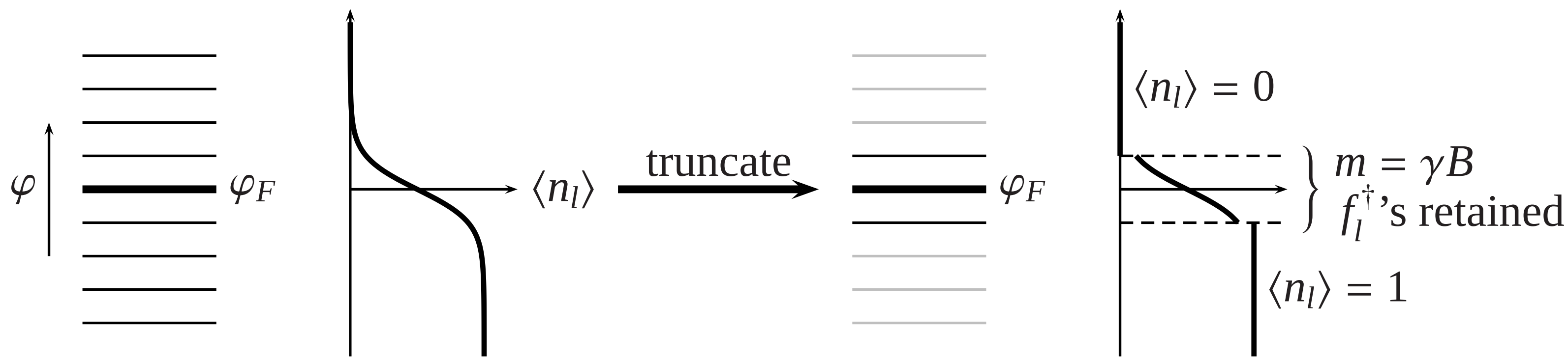
- Based on analogy, average pseudo-occupation is

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

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

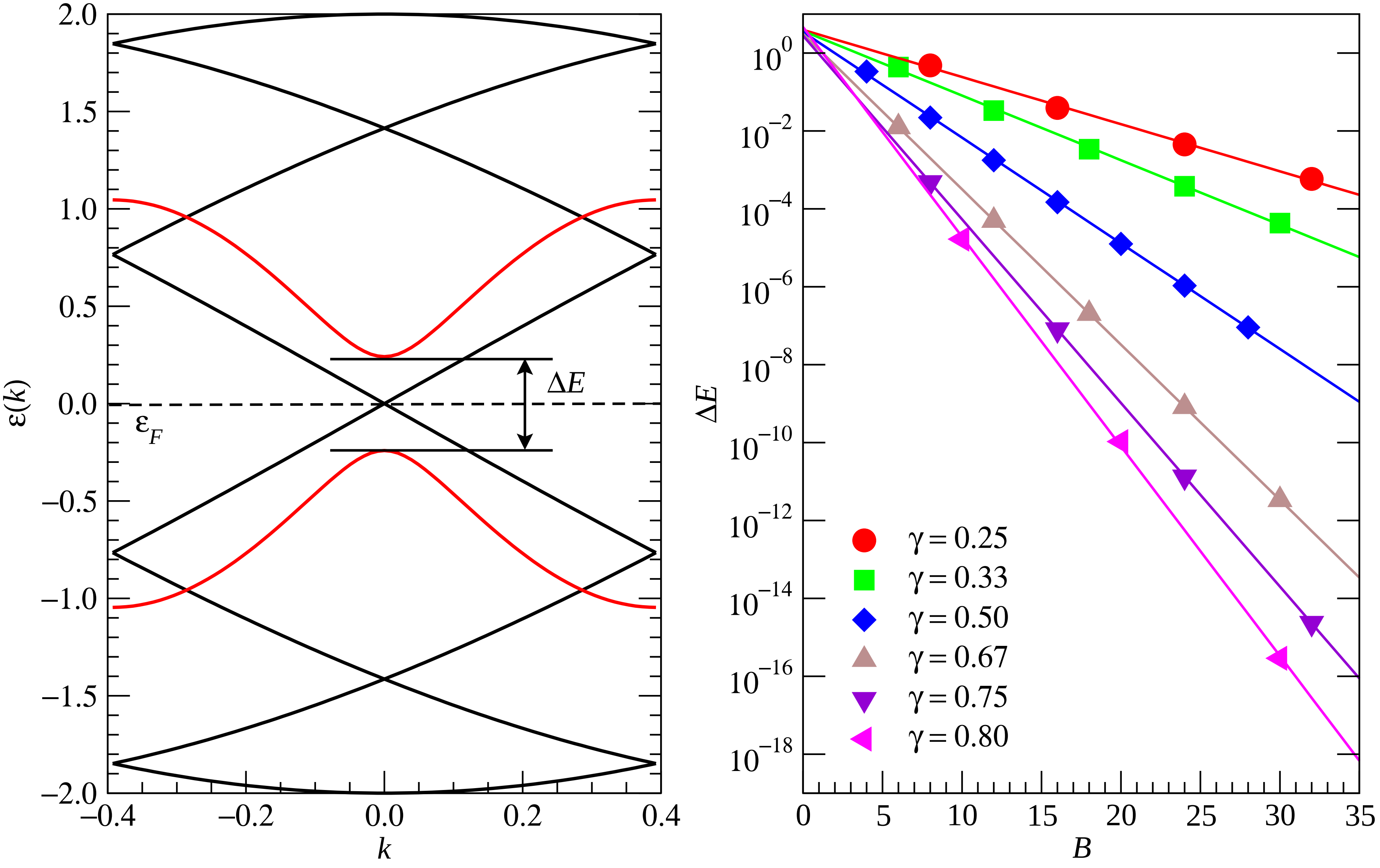
# Operator-Based DM Truncation Scheme

- 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 $\varphi_l \approx \varphi_F$:



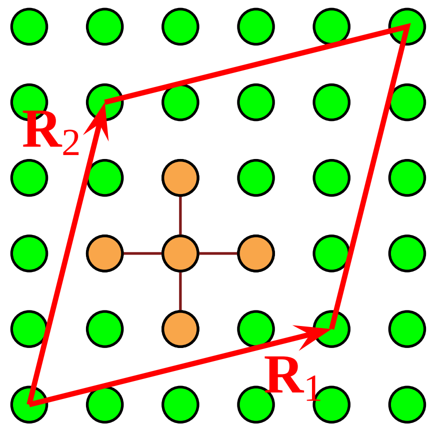

- Compare with weight-ranked truncation:
  - eigenstates with largest weights all kept;
  - some eigenstates with intermediate weights not kept, but replaced with eigenstates with slightly smaller weights;
  - eigenstates with small weights not kept.

# Results — 1D Free 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 $\rho_C$:
  - 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 and shape averaging.

# 2D Cluster DM — 1-Particle 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;
- Look at 1-particle weights: 5 of these, characterized by "angular momentum" quantum numbers $s_1$, $p_x$, $p_y$, $d$, $s_2$.
- Infinite system limit for noninteracting system, $\approx$ 200 sites for a squarish finite system;
- Small finite systems (noninteracting & interacting) of $\approx$ 20 sites, strong influence from:
  - finite size effect;
  - shell effect (most severe for $d$ state, least severe for $s_1$ state).

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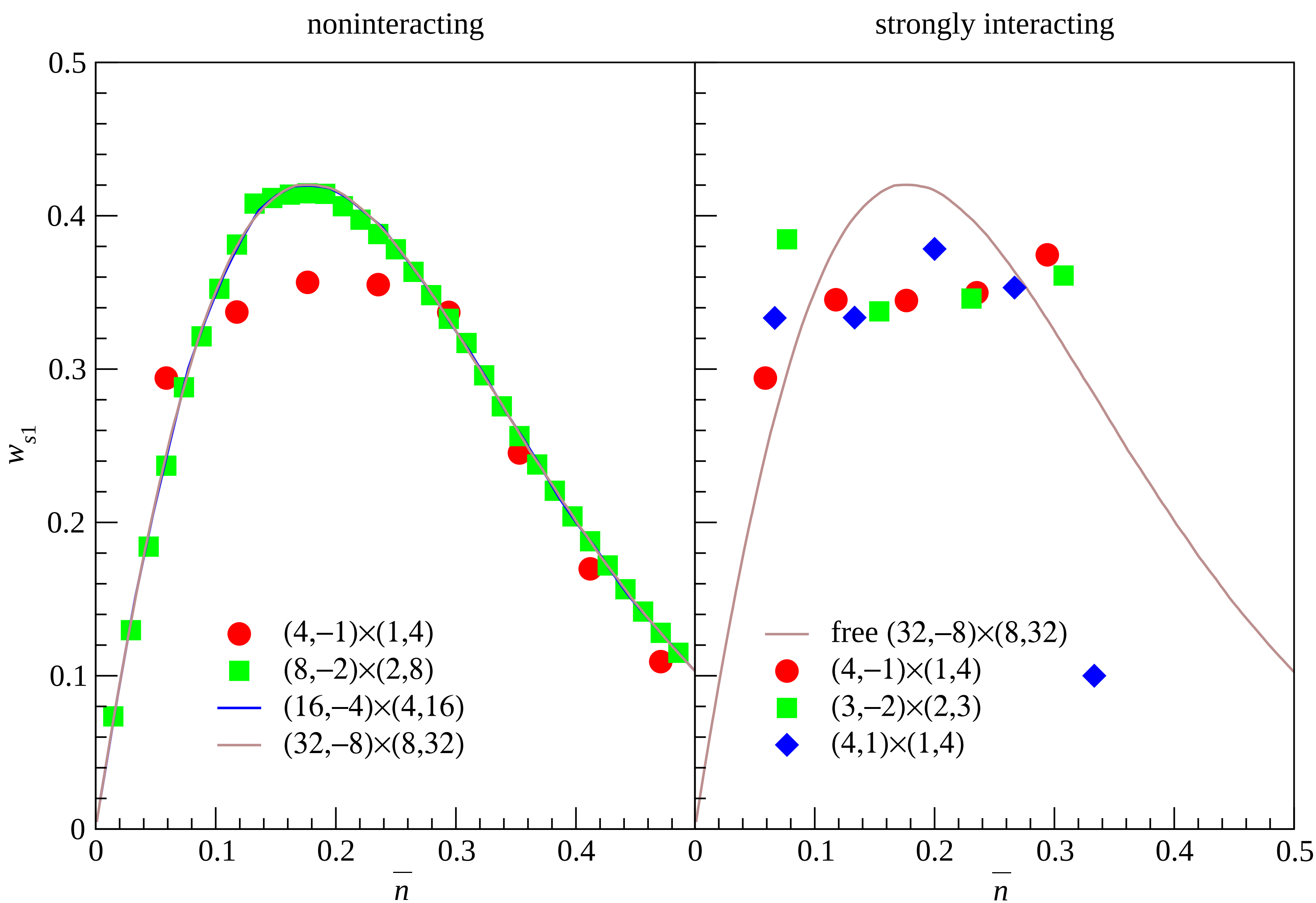

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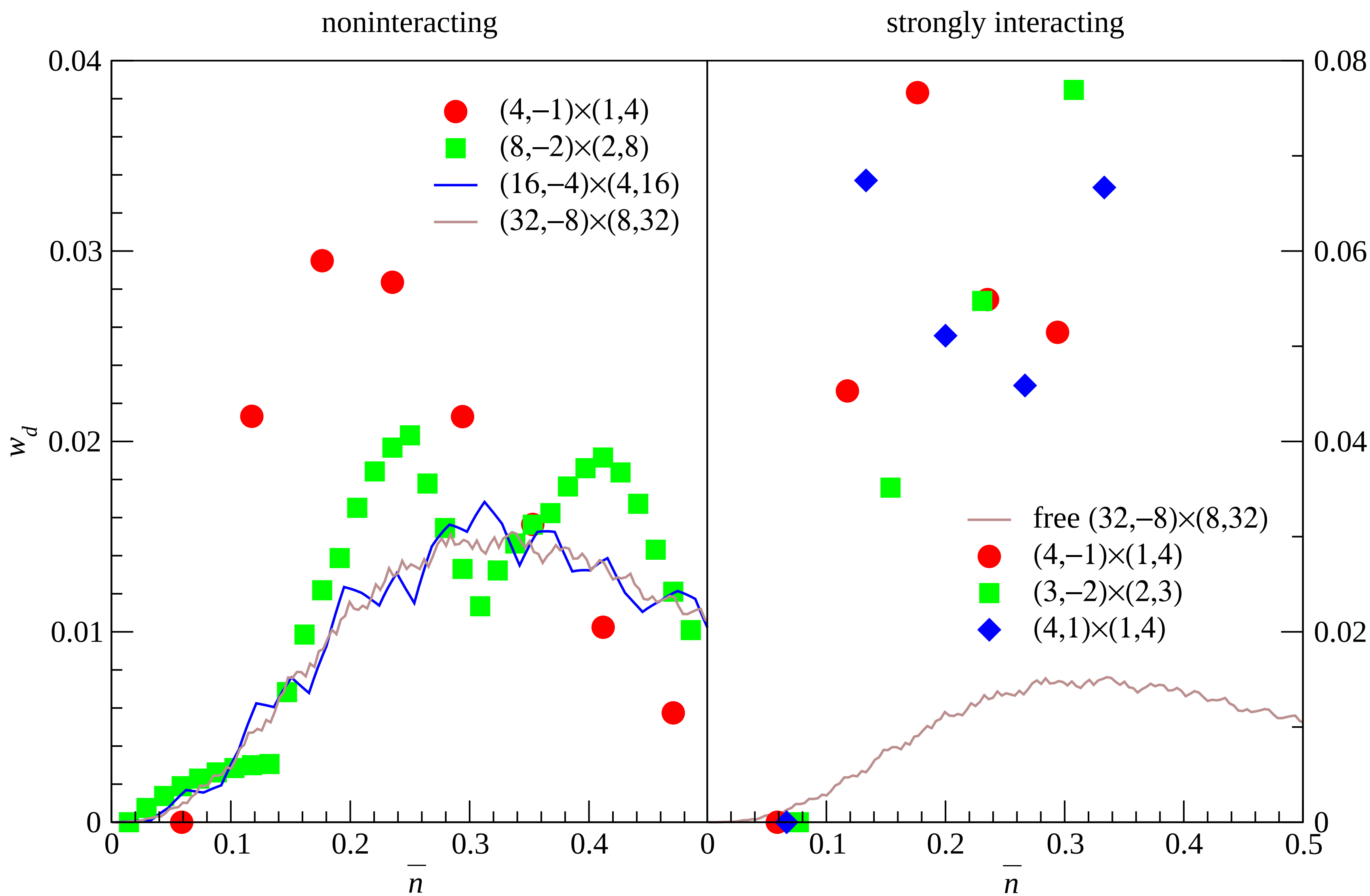

# Conclusions

- Much learnt from noninteracting spinless fermions (**Q2**):
  - 1D
    - structure of $\rho_B$;
    - Operator-Based DM Truncation Scheme;
  - 2D
    - when infinite system limit reached;
    - shell effect & its persistence;
- How much of this understanding can be applied to interacting fermions (**Q1**)?
  - finite size effect & shell effect entangled;
  - adaptation and extension of Operator-Based DM Truncation Scheme;
- Still far from eventual goal: ground state of infinite system of interacting fermions.