Closed-Form Formulae for Many-Body Density Matrix. I. Explicit Calculations for Spinless Fermions in $d = 1$

SIEW-ANN CHEONG and C.L. HENLEY,

LASSP, Cornell U

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Motivation

- Density Matrix Renormalization Group (DMRG):
  - construct and diagonalize density matrix;
  - truncate Hilbert space.
- Analytical study of density matrix
  - algorithmic improvement (e.g. TMRG);
  - how to build symmetries of problem into the DMRG.

Density Matrices — General Definitions

- Equivalent description of QM at $T = 0$:

$$|\psi\rangle \leftrightarrow \hat{\rho} = |\psi\rangle\langle\psi| \,; \qquad \langle\psi|\hat{A}|\psi\rangle = \langle\hat{A}\rangle = \mathrm{Tr}\,\hat{\rho}\hat{A}, \tag{1}$$

  for pure states $|\psi\rangle$.

- In general, if universe is in pure state $|\Psi\rangle$, state of system is a mixed state most conveniently described by $\hat{\rho}$.

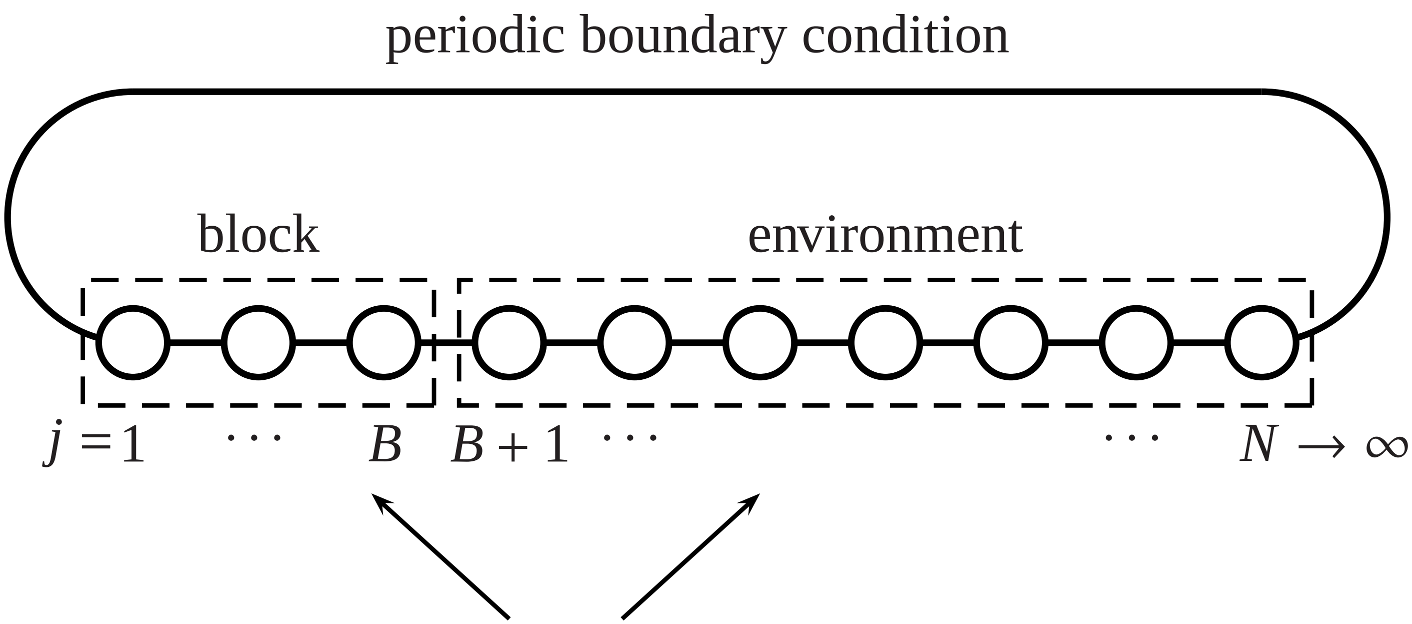
- $\hat{\rho}$ obtained from density matrix of universe $\hat{\mathscr{P}} = |\Psi\rangle\langle\Psi|$ as follows:

$$\langle\hat{A}\rangle = \mathrm{Tr}\,\hat{\mathscr{P}}\hat{A} = \mathrm{Tr}_{S,E}\,\hat{\mathscr{P}}\hat{A} = \mathrm{Tr}_S\left(\mathrm{Tr}_E\,\hat{\mathscr{P}}\right)\hat{A} \tag{2}$$

  if $\hat{A}$ acts only on system S. See that $\hat{\rho} = \mathrm{Tr}_E\,\hat{\mathscr{P}}$.

- Easy to generalize to $T > 0$.

Density Matrices — Matrix Elements



$|\Psi\rangle = \sum_{\mathbf{n}} |\mathbf{n}\rangle\, |e_{\mathbf{n}}\rangle\,;$

$|\mathbf{n}\rangle = |n_1 n_2 \cdots n_B\rangle\,,\ \ n_j = 0, 1$

$|e_{\mathbf{n}}\rangle$ unnormalized

could do d dimensions

$$\langle \hat{A}\rangle = \sum_{\mathbf{n},\mathbf{n}'} \langle e_{\mathbf{n}}|e_{\mathbf{n}'}\rangle \langle \mathbf{n}|\hat{A}|\mathbf{n}'\rangle = \sum_{\mathbf{n},\mathbf{n}'} \langle e_{\mathbf{n}}|e_{\mathbf{n}'}\rangle A_{\mathbf{n}\mathbf{n}'} = \mathrm{Tr}\,\hat{\rho}\hat{A}$$

$$\text{if} \quad \rho_{\mathbf{n}'\mathbf{n}} = \langle e_{\mathbf{n}}|e_{\mathbf{n}'}\rangle$$

Structure of $\hat{\rho}$

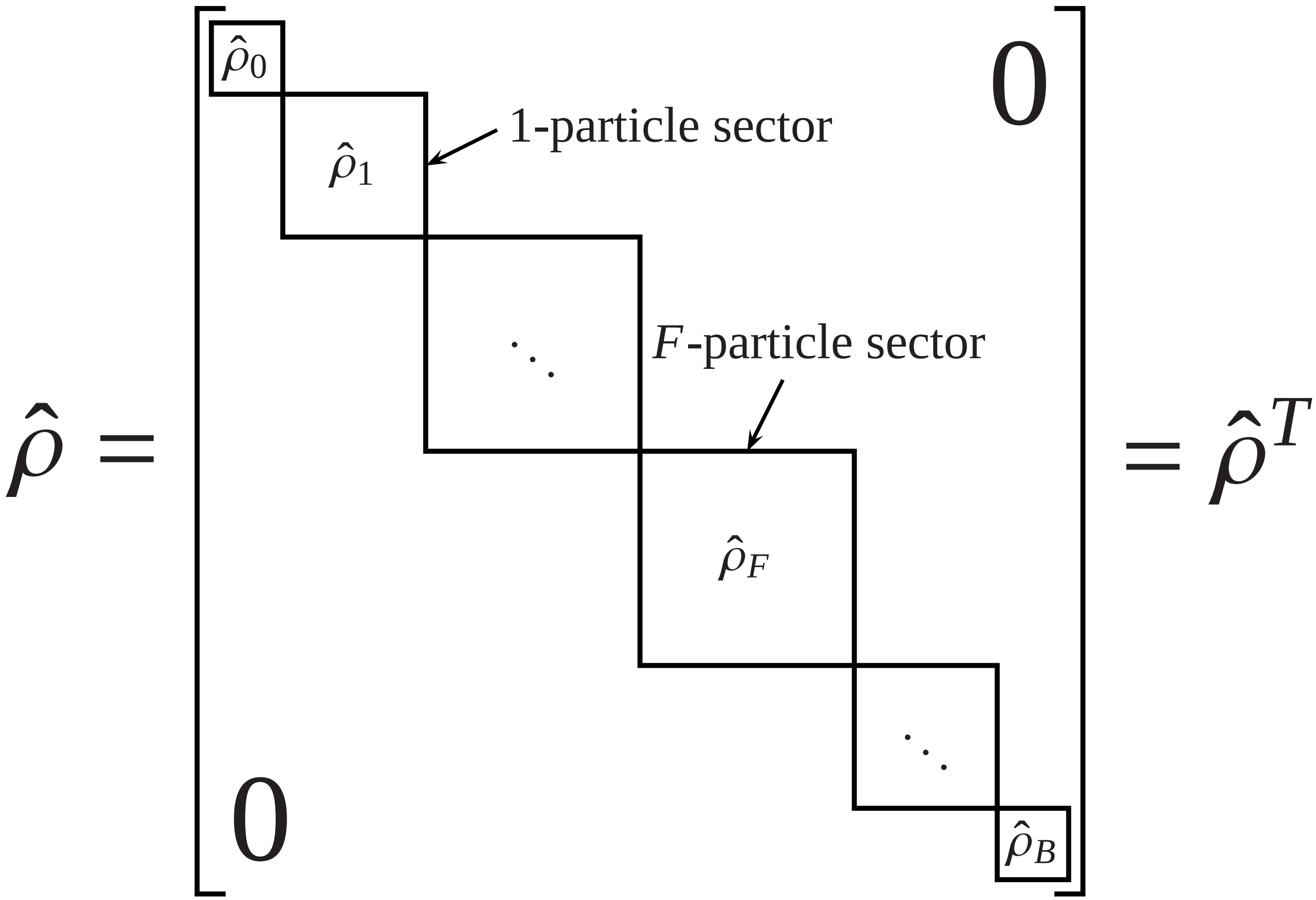
- Need to project $|\mathbf{n}\rangle$ and $|\mathbf{n}'\rangle$ to reference state $|\mathbf{0}\rangle$ to find $\langle e_{\mathbf{n}}|e_{\mathbf{n}'}\rangle$.
- Define referencing operators $K_{\mathbf{n}}$ such that $K_{\mathbf{n}}|\mathbf{n}'\rangle = \delta_{\mathbf{nn}'}|\mathbf{0}\rangle$. E.g.

$$K_{101} = c_1 c_2 c_2^\dagger c_3 \tag{3}$$

- Can check that $K_{\mathbf{n}}|\Psi\rangle = |\mathbf{0}\rangle|e_{\mathbf{n}}\rangle$, $K_{\mathbf{n}'}|\Psi\rangle = |\mathbf{0}\rangle|e_{\mathbf{n}'}\rangle$. Thus

$$\rho_{\mathbf{nn}'} = \langle\Psi|K_{\mathbf{n}'}^\dagger K_{\mathbf{n}}|\Psi\rangle\,. \tag{4}$$

- $\hat{\rho}$ real and symmetric, non-zero matrix elements of $\hat{\rho}$ in diagonal blocks corresponding to different F-particle sectors — denote by $\hat{\rho}_F$.



Closed-Form Expression for $\hat{\rho}_1$

- $\langle K^\dagger_{\mathbf{n}'} K_{\mathbf{n}} \rangle$ can be expressed as sum of $2n$-point functions $G_{\bar{i}_1 \cdots \bar{i}_n j_1 \cdots j_n}$.
- $2n$-point functions Wick factorize into sums of products of 2-point functions $G_{\bar{i}j} = \langle c^\dagger_i c_j \rangle = \sin(\pi \bar{n} |i-j|)/\pi |i-j|$ for non-interacting fermions. For example,

$$G_{\overline{123}135} = \langle c^\dagger_1 c^\dagger_2 c^\dagger_3 c_1 c_3 c_5 \rangle = (-1)^{\frac{3(3-1)}{2}} \begin{vmatrix} G_{\bar{1}1} & G_{\bar{1}3} & G_{\bar{1}5} \\ G_{\bar{2}1} & G_{\bar{2}3} & G_{\bar{2}5} \\ G_{\bar{3}1} & G_{\bar{3}3} & G_{\bar{3}5} \end{vmatrix} \quad (5)$$

  where $\bar{n}$ is filling fraction.

- 2-point functions can be organized as a *Green function matrix* $\mathscr{G}$.

$$
\mathscr{G} = \left[\begin{array}{cccc|ccc}
\multicolumn{4}{c}{\overset{\displaystyle G}{\downarrow}} & & & \\
G_{\overline{11}} & G_{\overline{12}} & \cdots & G_{\overline{1B}} & G_{\overline{1B+1}} & \cdots & G_{\overline{1N}} \\
G_{\overline{21}} & G_{\overline{22}} & \cdots & G_{\overline{2B}} & G_{\overline{2B+1}} & \cdots & G_{\overline{2N}} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
G_{\overline{B1}} & G_{\overline{B2}} & \cdots & G_{\overline{BB}} & G_{\overline{BB+1}} & \cdots & G_{\overline{BN}} \\
\hline
G_{\overline{B+11}} & G_{\overline{B+12}} & \cdots & G_{\overline{B+1B}} & G_{\overline{B+1B+1}} & \cdots & G_{\overline{B+1N}} \\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
G_{\overline{N1}} & G_{\overline{N2}} & \cdots & G_{\overline{NB}} & G_{\overline{NB+1}} & \cdots & G_{\overline{NN}}
\end{array}\right]
\begin{array}{l}
\left.\vphantom{\begin{array}{c}G\\G\\\vdots\\G\end{array}}\right\}\text{block} \\
\left.\vphantom{\begin{array}{c}G\\\vdots\\G\end{array}}\right\}\text{environment}
\end{array}
$$

$$
\underbrace{\hspace{12em}}_{\text{block}} \quad \underbrace{\hspace{10em}}_{\text{environment}}
$$

- Inspection of index structure for matrix elements of 1-particle sector $\hat{\rho}_1$ show that for system sizes $B \leq 5$,

$$\hat{\rho}_1 = G + G^2 - G\,\mathrm{Tr}\,G + G^3 - G^2\,\mathrm{Tr}\,G - \tfrac{1}{2}\left[\mathrm{Tr}\,G^2 - (\mathrm{Tr}\,G)^2\right]G + G^4 - G^3\,\mathrm{Tr}\,G - \tfrac{1}{2}\left[\mathrm{Tr}\,G^2 - (\mathrm{Tr}\,G)^2\right]G^2 - \left[\tfrac{1}{2}\,\mathrm{Tr}\,G^3 - \tfrac{1}{2}\,\mathrm{Tr}\,G\,\mathrm{Tr}\,G^2 + \tfrac{1}{6}(\mathrm{Tr}\,G)^3\right]G + \cdots . \quad (6)$$

- If we conjecture that regularity persists for $B > 5$, then series can be written as

$$\hat{\rho}_1 = G(\mathbb{1} + G + G^2 + \cdots)\exp\left[-\mathrm{Tr}(G + \tfrac{1}{2}G^2 + \tfrac{1}{3}G^3 + \cdots)\right] \quad (7)$$

which can be summed to

$$\hat{\rho}_1 = G(\mathbb{1} - G)^{-1}\det(\mathbb{1} - G). \quad (8)$$

- Proved by another method — next talk by C.L. HENLEY.

Numerical Checks

- Eigenvalues $w_{1,l}$ of $\hat{\rho}_1$ and λ_l of G related by

$$w_{1,l} = e^{-\varphi_l} \det(\mathbb{1} - G); \qquad e^{-\varphi_l} = \lambda_l (1 - \lambda_l)^{-1} \tag{9}$$

- Half-filling $\overline{n} = \frac{1}{2}$, particle-hole symmetry in $|\Psi\rangle$ — checked that the correspondences

$$\begin{aligned} \lambda_l &\leftrightarrow 1 - \lambda_l, \\ \varphi_l &\leftrightarrow -\varphi_l, \\ \log \frac{w_{1,l}}{\det(\mathbb{1} - G)} &\leftrightarrow \log \frac{\det(\mathbb{1} - G)}{w_{1,l}} \end{aligned} \tag{10}$$

reflect particle-hole symmetry.

Discussions

- Next talk by C.L. HENLEY — $\hat{\rho}$ completely determined by $\hat{\rho}_1$. Computational requirements greatly reduced from $O(e^B)$ to $O(B^2)$?
- Implications for truncation — all the art in truncating the 1-particle Hilbert space?
- Consistency amongst the truncated F-particle Hilbert spaces?