Matrix Product Ansatz-II

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Q1. *Two species particles:* Consider two different kind of particles (A and B) on a periodic 1D lattice. The particles evolve using the following particle conserving dynamics

$$A0 \underset{q}{\overset{p}{\rightleftharpoons}} 0A; \quad B0 \underset{\beta}{\overset{\alpha}{\rightleftharpoons}} 0B \tag{1}$$

(a) Assume a matrix-product state for the system where particles A, B and vacancy 0 are represented by matrices $\mathbb{A}, \mathbb{B}$ and $\mathbb{O}$ respectively. Obtain the matrix-algebra for $\mathbb{A}, \mathbb{B}, \mathbb{O}$ using auxiliaries $\tilde{\mathbb{A}}, \tilde{\mathbb{B}}, \tilde{\mathbb{O}}$.

(b) Show that scalar auxiliaries $\tilde{\mathbb{A}} = 0 = \tilde{\mathbb{B}}, \tilde{\mathbb{O}} = \omega$ reduces the matrix algebra to

$$p\mathbb{A}\mathbb{O} - q\mathbb{O}\mathbb{A} = \omega\mathbb{A}; \quad \alpha\mathbb{B}\mathbb{O} - \beta\mathbb{O}\mathbb{B} = \omega\mathbb{B}; \tag{2}$$

(c) Why should the matrix algebra depend on an auxiliary ω which arbitrary? How do you assume that the steady state probabilities are independent of ω? What about uniqueness of steady state ?

Ans: If $\mathbb{A}, \mathbb{B}$ solves the above algebra, clearly $a\mathbb{A}, b\mathbb{B}$ are also solutions (a, b being nonzero scalars). Thus with the choice $a = b = \omega$ we could have gotten $p\mathbb{A}\mathbb{O} - q\mathbb{O}\mathbb{A} = \mathbb{A}; \quad \alpha\mathbb{B}\mathbb{O} - \beta\mathbb{O}\mathbb{B} = \mathbb{B};$

(d) If the partition function of a system of size L having $N_{A,B}$ number of A, B particles is Q_{N_A,N_B} show that the grand partition function $Z(x, y)$ with fugacities x, y that controls the density of A, B particles is

$$\begin{aligned} Z(x,y) &= \sum_{N_A=0}^{\infty} \sum_{N_B=0}^{\infty} x^{N_A} y^{N_B} Q_{N_A,N_B} \\ &= Tr[(x\mathbb{A} + y\mathbb{B} + \mathbb{O})^L]. \end{aligned} \tag{3}$$

Q2. Two particles: Consider the system described above, with only two particles: one of each kind. One can then use a representation where $\mathbb{A}^2 = 0 = \mathbb{B}^2$ (why ?).

(a) Find 2×2 non commuting matrices $\mathbb{A}, \mathbb{B}$ that satisfy $\mathbb{A}^2 = 0 = \mathbb{B}^2$. Use them in Eq. (2) to get $\mathbb{O}$. One of the representation is given below - find another one.

$$\begin{aligned} \mathbb{A} &= |1\rangle\langle 2| = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \mathbb{B} = |2\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \\ \mathbb{O} &= \frac{\omega}{\alpha p - \beta q} \begin{pmatrix} p+\beta & 0 \\ 0 & q+\alpha \end{pmatrix} \end{aligned} \tag{4}$$

Note: These matrices works for an ensemble where $N_A = N_B$ and A and B particles are placed alternately. This is because the dynamics of the system will will never bring two As or Bs as neighbours.

(b) Calculate the partition function

$$\equiv Q_L = \sum_{k=0}^{L-2} Tr[\mathbb{A}\mathbb{O}^{L-2-k}\mathbb{B}\mathbb{O}^k] \tag{5}$$

(c) A special case (B diffuses and A drifts): Take $\alpha = \psi = \beta$ and show that the matrix $\mathbb{O}$ can be written as $\mathbb{O} = \begin{pmatrix} \gamma & 0 \\ 0 & 1 \end{pmatrix}$ mith $\gamma = \frac{p+\psi}{q+\psi}$, if you choose $\omega = \psi\frac{p-q}{q+\psi}$. Verify (using Eq. (5))that the partition function is

$$Q_L = \sum_{k=0}^{L-1} \gamma^k = \frac{\gamma^L - 1}{\gamma - 1} \tag{6}$$

(d) Prove that in the steady state current

$$\begin{aligned} J_A &= \langle pA0\rangle - q\langle 0A\rangle = \frac{Q_{L-1}}{Q_L} \\ &\simeq \frac{\omega}{\gamma} = \frac{\psi}{p+\psi}(p-q), \end{aligned} \tag{7}$$

where thermodynamic limit $L \to \infty$ is used in 2nd line. Note that, the B particle which only diffuses, generates a current because of A. In absence of particle exchange ($AB \rightleftharpoons BA$) hard core repulsion for current of $J_B = \psi(\langle B0\rangle - \langle 0B\rangle)$ to be same as J_A. Calculate J_B and explicitly verify that $J_A = J = J_B$

Q. *Negative differential mobility (NDM):* Consider a particle subjected to a potential $V(x) = -\epsilon x$, with $\epsilon > 0$. When it moves forward (backward) by one unit the its energy is decreased (increased) by ε amount. To obey detailed balance locally, the rate of forward and backward move of the particle must be related by $\frac{\text{forward}-\text{rate}}{\text{backward}-\text{rate}} = e^{\epsilon}$.

Now, the rates of A particle in Eq. (1), moving to right (left) neighbour can be set as $p = 1$ ($q = e^{-\epsilon}$ which corresponds to an applied local field ϵ on the lattice.

(a) Show that when ψ is independent of ϵ, the conductivity $\sigma = \frac{dJ}{d\varepsilon} = \frac{\psi}{1+\psi}$, when ε is small.

(b) If the rate of diffusion of B depends on ε, then show that $\frac{dJ}{d\varepsilon}$ can become negative for large ε, if $\frac{d\psi}{d\varepsilon} < 0$.

(c) As an example take $\psi = \frac{1}{7}1 + \varepsilon$. Show that in this case the differential mobility $\frac{dJ}{d\varepsilon}$ becomes negative when

ε is increased beyond a threshold value $\varepsilon^* = 1.50524$ determined form $e^{\varepsilon^*} = 3 + \varepsilon^*$.

Note: This is a basic mechanism how, in an interacting particle system the driven modes/particles excites non-driven modes and generates NDM "move less by pushing more." For more details see [AK Chatterjee, U. Basu, PKM PRE **97**, 052137 (2018)].

Q3. *Driven Dimers:* Dimers occupy two consecutive sites on a lattice. Biased diffusion of dimers on a periodic one dimensional lattice is described by the dynamics

$$110 \underset{q}{\overset{p}{\rightleftharpoons}} 011 \tag{8}$$

where $n_i = 1$ represents if site i is occupied by a dimer, else $n_i = 0$. Ifthere are M dimers in the system then $\sum_{i=0}^{L} n_i = 2M$; we define the monomer density as $\rho = \frac{2M}{L}$.

(a) Find out how many ways M dimers can be placed on a periodic 1D lattice having L sites.

(b) Verify that matrices $\mathbb{D}, \mathbb{E}$ representing site vriables $n_i = 1, 0$ respectively gives rise to the following matrix algebra.

$$p\mathbb{D}\mathbb{D}\mathbb{E} - q\mathbb{E}\mathbb{D}\mathbb{D} = \tilde{\mathbb{E}}\tilde{\mathbb{D}}\mathbb{D} - \mathbb{E}\tilde{\mathbb{D}}\tilde{\mathbb{D}} = -(\tilde{\mathbb{D}}\tilde{\mathbb{D}}\mathbb{E} - \mathbb{D}\tilde{\mathbb{D}}\tilde{\mathbb{E}}) \tag{9}$$

$$\tilde{\mathbb{E}}\tilde{\mathbb{E}}\mathbb{E} - \mathbb{E}\tilde{\mathbb{E}}\tilde{\mathbb{E}} = 0 = \tilde{\mathbb{D}}\tilde{\mathbb{D}}\mathbb{D} - \mathbb{D}\tilde{\mathbb{D}}\tilde{\mathbb{D}} \tag{10}$$

$$\tilde{\mathbb{E}}\tilde{\mathbb{E}}\mathbb{D} - \mathbb{E}\tilde{\mathbb{E}}\tilde{\mathbb{D}} = 0 = \tilde{\mathbb{E}}\tilde{\mathbb{D}}\mathbb{E} - \mathbb{E}\tilde{\mathbb{D}}\tilde{\mathbb{E}} \tag{11}$$

Here we have used a different cancellation scheme (replacing two of matrices by auxiliary matrices). Show that this cancellation scheme too cancels the residual term from site i with a term in site $i+1$.

(c) Verify that the algebra becomes simple when $\tilde{\mathbb{E}} = 0$,

$$p\mathbb{D}\mathbb{D}\mathbb{E} - q\mathbb{E}\mathbb{D}\mathbb{D} = -\mathbb{E}\tilde{\mathbb{D}}^2 = -\tilde{\mathbb{D}}^2\mathbb{E} \text{ and } [\tilde{\mathbb{D}}^2, \mathbb{D}] = 0. \tag{12}$$

(d) At this stage, it is good to think of matrices which satisfy $\mathbb{E}\mathbb{D}^{2k+1}\mathbb{E} = 0$ but $\mathbb{E}\mathbb{D}^{2k}\mathbb{E} \neq 0$ (why?). Show that $\mathbb{D} = \sigma_x$ and $E = |1\rangle\langle 1|$ are the two-dimensional matrices that satisfy above conditions. They naturally obey Eq. (12) when $\tilde{\mathbb{D}} = \sqrt{q-p}$. (Does it matter, that $\tilde{\mathbb{D}}$ is a complex number when $q < p$?).

(d) Partition function: With a fugacity z that contorls the average number of vacant sites $N_0 = L - 2M$, or their density $\rho_0 = \frac{N_0}{L}$, we getthe partition function is $Z = Tr[(\mathbb{T})^L]$ where $\mathbb{T} = \mathbb{D} + z\mathbb{E}$. Show that $|e_\pm\rangle = \frac{1}{\sqrt{1+\lambda_\pm^2}}\begin{pmatrix}\lambda_\pm \\ 1\end{pmatrix}$ are the normalized eigenvectors of T with eigenvalues $\lambda_\pm = \frac{1}{2}(z \pm \sqrt{z^2+4})$.

(e) Show that

$$\rho_0 = z\frac{d}{dz}\ln(\lambda_+) = \frac{z}{\sqrt{z^2+4}} => z = \frac{2\rho_0}{\sqrt{1-\rho_0}}$$

$$J = \frac{z}{Tr[\mathbb{T}^L]} Tr[(p\mathbb{D}^2\mathbb{E} - q\mathbb{E}\mathbb{D}^2)\mathbb{T}^{L-3}] \tag{13}$$

$$= (p-q)z\frac{Tr[\mathbb{E}\mathbb{T}^{L-3}]}{Tr[\mathbb{T}^L]} = \frac{(p-q)z}{\lambda_+(1+\lambda_+^2)}$$

$$= (p-q)\frac{\rho_0(1-\rho_0)}{1+\rho_0} = (p-q)\frac{\rho(1-\rho)}{2-\rho} \tag{14}$$

Note: For further studies look at Phase-coexistence in a system having monomers 1s and dimers 2s with the following dynamics [AK Chatterjee, B Daga, PKM, PRE **94**, 012121 (2016).]

$$10 \xrightarrow{v} 01; \quad 20 \xrightarrow{v} 02; \quad 211 \underset{1}{\overset{1}{\rightleftharpoons}} 121 \tag{15}$$

The last step represents reconstitution dynamics of dimers and monomers. You may look at Ref. [S. Gupta, M. Barma, U. Basu and PKM, PRE **84**, 041102 (2011)] to look at S=steady state correlation properties of diffusing k-mers on a lattice (formally known as the Tonks Gas [L. Tonks, Phys Rev. **50**, 955 (1936)])

Q5. *Active-absorbing phase-transition:* Consider the following dynamics for particles on an 1D periodic lattice,

$$110 \xrightarrow{1} 101 \tag{16}$$

The dynamics separates particles when they are close by. In other wards particles move forward only when assisted by another particle. The process is refereed to as assisted exclusion process (AEP). The particle number N and thus $\rho = \frac{N}{L}$ is conserved.

(a) Convince yourself that the dynamics of AEP is same as the four-site dynamics

$$1100 \xrightarrow{1} 1010 \tag{17}$$

$$1101 \xrightarrow{1} 1011 \tag{18}$$

where dynamics (17) destroy '11' and '00' whereas (17) keeps '11' conserved. Use these arguments prove the following statements.
(i) Consecutive 1s (i.e., 11s) will disappear from the system if $\rho < \frac{1}{2}$. In absence of 11s neither of dynamics (17) or (18) can run; thus the system will reach an inactive (or absorbing) state.
(ii) Consecutive 1s (i.e., 11s) will disappear from the system if $\rho \geq \frac{1}{2}$. In absence of 00s dynamics (17) will not apply but (18) can go on. Thus a transition from absorbing to active state occurs her at $\rho_c = \frac{1}{2}$.

(b) MPA in active state. The active state is characterized by $\mathbb{E}^2 = 0$ and by the dynamics (18). Show that the matrix algebra for (18) is

$$\mathbb{D}\mathbb{D}\mathbb{E}\mathbb{D} = \mathbb{D}\tilde{\mathbb{E}}\mathbb{D}\mathbb{D} - \mathbb{D}\mathbb{E}\tilde{\mathbb{D}}\mathbb{D} = -(\mathbb{D}\tilde{\mathbb{D}}\mathbb{E}\mathbb{D} - \mathbb{D}\mathbb{D}\tilde{\mathbb{E}}\mathbb{D})$$

$$[\mathbb{D}, \tilde{\mathbb{D}}] = 0 = [\mathbb{E}, \tilde{\mathbb{E}}] \tag{19}$$

(c) Show that a scalar choice of auxiliaries $\tilde{\mathbb{D}} = -1, \tilde{\mathbb{E}} = 0$ leads to a condition $D = \mathbb{DED}$ which can be solved by a matrix $\mathbb{D}$ that obey $\mathbb{D}^2 = \mathbb{D}$. A simple representation is $\mathbb{D} = |1\rangle\langle 2| + |2\rangle\langle 2|$.

Note: As expected (why?) the algebra does not impose any condition $\mathbb{E}$. We must take $\mathbb{E}$ so that $\mathbb{E}^2 = 0$. A simple choice is $\mathbb{E} = |2\rangle\langle 1|$. Can you find another representation for $\mathbb{D}, \mathbb{E}$?

(d) The partition function is now $Z = Tr[\mathbb{T}^L]$ with $T = z\mathbb{D} + \mathbb{E}$. Show that the density-fugacity relation is

$$\rho == \frac{1}{2}\left(1 + \sqrt{\frac{z}{4+z}}\right); \quad z = \frac{(2\rho-1)^2}{\rho(1-\rho)} \tag{20}$$

Note: The variation of z in the range $(0, \infty)$ leads to density variation $\frac{1}{2} \le \rho \le 1$. The minimum density in the active state is $\rho_c = \frac{1}{2}$.

(e) It is evident from (16) that $\langle 110\rangle$ in the steady state is a measure of activity; let us denote it ρ_a. For any nonzero value of ρ_a, some particles in the system are able to move (the system is then active). Show that

$$\rho_a = z^2 \frac{Tr[\mathbb{DDET}^{L-3}]}{Tr[\mathbb{T}^L]} = \frac{1}{\rho}(2\rho-1)(1-\rho) \tag{21}$$

(f) ρ_a acts as the order parameter of the active-absorbing phase transition. Near the critical point $\rho_c = \frac{1}{2}$, $\rho_a \sim (\rho - \rho_c)^\beta$. Find the critical exponent β for this transition. *Further reading:* U. Basu and PKM, PRE **79**, 041143 (2009).

Resources:

1. Exact solution of a 1D asymmetric exclusion model using a matrix formulation, B. Derrida, M. R. Evans, V. Hakim, V. Pasquier, J. Phys. A Math. Gen. **26**, 1493 (1993).

2.*Nonequilibrium Steady States of Matrix Product Form: A Solver's Guide*, R. A. Blythe, M. R. Evans, J. Phys. A Math. Theor. **40** R333-R441(2007)