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Phase Transition and Shock in a One-Dimensional Reaction-Diffusion Model

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Abstract: *There is a one-dimensional model in which particles undergo many different reactions such as diffusion, coagulation and decoagulation. One boundary of chain is open to particles' entry and exit. The aim is inspecting different phases in parameters space of model, probing phase transition point, and calculating quantities like density distribution function in each phase, particles' flow and particles' correlation functions in each site of lattice. To solve these kind of problems, different approaches such as mean field approximation, bethe's Ansatz, vacant sites formalism and computer simulation have extended but here matrix product Ansatz way was used to solve the model. Results have revealed high density and low density phases for model for particles' density of course with a constraint on parameters. A traveling shock is seen that moves in the body of lattice before attaching to steady state, too.*

Keywords: *phase transition, reaction diffusion, bethe Ansatz, matrix product Ansatz, many particles systems, non-equilibrium models*

INTRODUCTION

Stochastic Systems are evolutioned and transformed from one configuration to the other but finally reach to steady state. Phase transitions between different phases are often seen in stochastic reaction diffusion systems. These have abrupt and too changes called first order phase transitions while physical quantities in higher order phase transitions have smooth changes. Phase transitions discussion is the most important aim in this research.

Literature review

Much of many particles systems in the nature belong to non-equilibrium and one-dimensional reaction diffusion systems which have been solved using modelling (Jafarpour et al., 2009; Mondal & Mallik, K, 2008; Mallick.k et al., 1999; Crampe et al., 2016). For example, to solve auto cellular models of traffic flow of vehicles in streets and moving peoples, stochastic systems have been used (Evans et al., 1998; Li et al., 2015; Perkins et al., 2014; Zeraati et al., 2013). The simple diffusion models are appropriate to discuss synetic of biopolymerization (Sharma & Chowdhury, 2011; Tobias, 2016; Sanchez et al., 2016).
These stochastic many particles models can be used to explain the distribution of votes among candidates. How do views of candidates influence other people's views (Dietrich, 2001; Dietrich & de Oliveira, 2002). Foraging behavior of group animals that live in fixed colonies like ants, bees and so on as an important problem in ecology have studied using non-equilibrium models (Lixiang et al., 2014; Couzin, 2005; Liang et al., 2012, Chen et al., 2011). Fluctuations of heat flux in the stochastic systems using stochastic modelling have been discussed (Brunet et al., 2010). These non-equilibrium and one-dimensional models show interesting collective behaviors such as phase transition while are not seen in equilibrium systems, thus are observed by researchers in physics and the other fields (Sasamoto et al., 2000; Schutz, 2001).

Problem

Suppose a one-dimensional lattice (chain) in which classical particles can diffuse in its bulk toward left and right, also if two particles encounter to each other, they will be converted to a single particle (coagulation). Furthermore, a single particle can be split to two particles (decoagulation). If site 1 (the left site) is empty ($\emptyset$), particles can enter it by rate α . Also If it is full (A), can become vacant by rate β. Therefore, we have in the left boundary:

$$\emptyset \to A \text{ , by rate } \alpha \text{ و } A \to \emptyset \text{ by rate } \beta \quad ,(1)$$

Time evolution operator (Hamiltonian operator) is defined in form of Bra and Ket:

$$\frac{d}{dt}|P(t)\rangle = H|P(t)> \quad ,(2)$$

In which $|P(t)>$ vector is in system configurations space and H is a stochastic matrixe with $2^L \times 2^L$ dimensions and is similar to hamiltonian in the schrodinger's wave function that gives us correspondent eigenvectors to eigenvalues. H elements are transition rates between different system configurations. Due to conservation of probability, sum of elements which are on each column of H matrix should be zero. H matrix has below form:

$$H = H^{(l)} + \left(\sum_{j=l}^{L-1} h_{j,j+1}\right) + H^{(L)}$$

$$H^{(1)} = h^{(1)} \otimes I^{\otimes(L-1)} \quad , \quad H^{(L)} = I^{\otimes(L-1)} \otimes h^{(L)}$$

$$h_{j,j+1} = I^{\otimes(j-1)} \otimes h \otimes I^{\otimes(L-j-1)} \quad ,(3)$$

In which $h^{(1)}$ and $h^{(L)}$ are 2×2 matrices and states site 1 and site tail (L) respectively, I is 2×2 identity matrix and h is a 4×4 matrix that showes mutual and dual site interactions in the chain bulk. In long time finally system reach to steady state and $\frac{d}{dt}|P(t)\rangle = 0$.

Using this equation , $H|P(t)\rangle = 0$, (4)

Therefore, the vector correspondent to eigenvalue zero give us system's steady state. Using (3) time evolution operator can be written as below:

$$H^{(l)} = h^{(1)} \otimes I^{\otimes(L-1)} \quad , H = \left(\sum_{j=l}^{L-1} h_{j,j+1}\right) + H^{(l)}$$

$$h_{j,j+1} = I^{\otimes(j-1)} \otimes h \otimes I^{\otimes(L-j-1)} \quad , \quad (5)$$

Now $H^{(1)}$ can be deleted because right boundary of the system is closed. Now h and $h^{(1)}$ operators in the basis of $(\phi\phi, \phi A, A\phi, AA)$ have forms of :

$$h = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & q(1+\Delta) & -q^{-1} & -q^{-1} \\ 0 & -q & q^{-1}(1+\Delta) & -q \\ 0 & -\Delta q & -\Delta q^{-1} & q+q^{-1} \end{bmatrix} ,(6)$$

$$h^{(1)} = \begin{pmatrix} \alpha & -\beta \\ -\alpha & \beta \end{pmatrix} \quad ,(7)$$

Exact Solve

Infact, Matrix product Ansatz way is eigenvector equation for zero energy state. To solve (4) steady state weights are:

$$f_L(s_1, \dots, S_l) = < W| \prod_{i=1}^{L} (S_i D + (1 - S_i)E)|V > ,(8)$$

Therefore, weights are given from product L square matrices by D and E and two Linear $< W|$ and column $|V>$ vector. If arbitrary site i occupied by one particle, S_i is equal 1 and related matrix for this position is D. If arbitrary site i is vacant, S_i is equal zero and related matrix for this position is E. It can be proved that matrices and vectors which fulfill algebra below then (4) is fulfilled and steady state is obtained:

$$\begin{cases} h\left[\begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix}\right] = \begin{pmatrix} \bar{E} \\ \bar{D} \end{pmatrix} \otimes \begin{pmatrix} E \\ D \end{pmatrix} - \begin{pmatrix} E \\ D \end{pmatrix} \otimes \begin{pmatrix} \bar{E} \\ \bar{D} \end{pmatrix} \\ < W| h^{(1)} \begin{pmatrix} E \\ D \end{pmatrix} = -< W| \begin{pmatrix} \bar{E} \\ \bar{D} \end{pmatrix} \\ h^{(L)} \begin{pmatrix} E \\ D \end{pmatrix} |V> = \begin{pmatrix} \bar{E} \\ \bar{D} \end{pmatrix} |V> \quad , \qquad (9) \end{cases}$$

Here $\overline{E}$ and $\overline{D}$ in (9) are auxiliary matrices.

Useful quantities

The particles' density function in arbitrary site i in steady state is:

$$< S_i >_L = \frac{\sum_{S_1=0,1} \dots \sum_{S_L=0,1} S_i f_L(S_1 \dots\dots S_L)}{z_L} \quad ,(10)$$

And binomial correlation functions $< S_i S_j >_L$ states the probably of synchronous presence of particles in sites i and j in steady state is defined in form of:

$$< S_i S_j >_L = \frac{\sum_{S_1=0,1} \dots \sum_{S_L=0,1} S_i S_j f_L(S_1 \dots\dots S_L)}{z_L} \quad ,(12)$$

Particles' Current in the steady state in arbitrary site i is useful for our discussion. It is defined as:

$$J = < S_i(1 - S_{i+1}) > \quad , \qquad (13)$$

In these equations, z_L is a normalization factor and is similar to partition function in statistical mechanic. It can be given by adding all of the system configurations. Then:

$$z_L = \sum_{S_1=0,1} \dots \sum_{S_L=0,1} f_L(S_1 \dots\dots S_L) \quad ,(14)$$

Now new operator C = D + E is defined and our quantities are rewritten to follow matrix forms:

$$< S_i >_L = \frac{<W|\, C^{i-1} D\, C^{L-1} \,|\, V>}{<W|\, C^L \,|\, V>} \quad ,(15)$$

$$< S_i S_j >_L = \frac{< W|\, C^{i-1} D\, C^{i-j-1} \, DC^{L-j} \,|\, V >}{< W|\, C^L \,|\, V >} \quad ,(16)$$

$$J = \frac{<W|\, C^{i-1} D\, E\, C^{L-i-1} \,|\, V>}{<W|\, C^L \,|\, V>} \quad ,(17)$$

Finally, m-point correlation function using vectors and matrices have new form (18):

$$< S_{k_1}, \dots, S_{k_m} >_L$$

$$= \frac{< W|C^{k_1-1} D\, C^{k_2-k_1-1} \, D \dots C^{L-k_m}|V >}{< W|\, C^L \,|\, V >} \quad ,(18)$$

Now using relations (9), (5), (6) and (7) the algebra of model is obtained:

$$[C, \bar{C}] = 0 \quad , \quad [E, \bar{E}] = 0$$

$$\bar{E}C - E\bar{C} = (q + q\Delta + q^{-1})EC - q(1+\Delta)E^2 - q^{-1}C^2$$

$$\bar{C}E - C\bar{E} = (q^{-1} + q^{-1}\Delta + q)CE - q^{-1}(1+\Delta)E^2 - qC^2$$

$$< W|\big((\alpha+\beta)E + \bar{E} - \beta C\big) = 0$$

$$, < W|\bar{C} = 0 \;, \bar{E}|V> = 0 \;, \bar{C}|V> = 0 \quad ,(19)$$

and $C = D + E$ and $\bar{C} = \bar{D} + \bar{E}$. The last work is finding representations for (19) algebra.

Algebraic representation

One of the limited dimension representations comes in follow form, but in case $q^2 \neq 1 + \Delta$:

$$c = \begin{bmatrix} 1+\Delta & 0 \\ 0 & q^2 \end{bmatrix} \quad , \quad \bar{c} = 0 \;,$$

$$E = \begin{bmatrix} 1 & \lambda \\ 0 & q^2 \end{bmatrix} \quad , \quad \bar{E} = \begin{bmatrix} \frac{q^2 - 1}{q}\Delta & -\frac{\Delta}{q}\lambda \\ 0 & 0 \end{bmatrix}$$

$$|\mathrm{V}> = \begin{bmatrix} \frac{\lambda}{q^2 - 1} \\ 1 \end{bmatrix} \qquad ,$$

$$< \mathrm{W}| = \begin{bmatrix} \frac{q\Delta(q^2 - q\beta - 1)}{\lambda(\beta\Delta - \beta - q\Delta)} \ , & 1 \end{bmatrix} , (20)$$

In the upper relations, λ is a free parameter with constraint:

$\alpha = (q^{-1} - q + \beta)\Delta \quad , (21)$

For other values, we do not have any representation. A possible representation form for case $q^2 = 1 + \Delta$ is:

$$c = \begin{bmatrix} 1 & \lambda \\ 0 & 1 \end{bmatrix} \quad , \quad \bar{c} = 0 \ ,$$

$$E = \begin{bmatrix} \frac{1}{q^2} & \lambda \\ 0 & 1 \end{bmatrix} \quad , \quad \bar{E} = \begin{bmatrix} \frac{(q^2 - 1)^2}{q^3} & -\frac{q^2 - 1}{q}\lambda \\ 0 & 0 \end{bmatrix}$$

$$|\mathrm{V}> = \begin{bmatrix} \frac{q^2 \lambda}{q^2 - 1} \\ 1 \end{bmatrix} \qquad ,$$

$$< \mathrm{W}| = \begin{bmatrix} -\frac{q^3 - \beta q^2 - 2q + q^{-1} + \beta}{\lambda(q^3 - \beta q^2 - q + \beta)} & 1 \end{bmatrix} , (22)$$

Results and Conclusions

Using equation (15) and representation (20), particles' density in arbitrary site i in steady state is prepared:

$$< \mathrm{S}_i >_L = \frac{\Delta(1+\Delta)^{-1}(1-q^2+q\beta)\left(\Delta(1+\Delta)^L q^{2i} - (q^2-1)(1+\Delta)^i q^{2L}\right) q^{-2i+1}}{q\Delta(q^2-1)\left(q^{2L} - (1+\Delta)^L\right) + \beta\left(\Delta q^2 (1+\Delta)^L - q^{2L}(q^2-1)(1+\Delta)\right)} \quad , (23)$$

It is found that in thermodynamic limit $\to \infty$, the system has two different phases for density. In low density phase $(q^2 > 1 + \Delta)$:

$$< \mathrm{S}_i >_L = \frac{q^2 \alpha}{(1+\Delta)(\beta(1+\Delta) - q\Delta)} \left(\frac{q^2}{1+\Delta}\right)^{-i} \quad , (24)$$

In this phase density of particles in the bulk chain and right side is constant and is equal to zero approximately but at the left side, it is high and gradually is vanished by characteristic length ξ .

$$\xi^{-1} = \left| \ln \frac{q^2}{1 + \Delta} \right| \qquad , \ (25)$$

In the high density phase $(q^2 < 1 + \Delta)$, $< \mathrm{S}_i >_L$ is given by :

$$< \mathrm{S}_i >_L = \frac{\Delta}{1+\Delta} - \frac{q^2-1}{1+\Delta} \left(\frac{q^2}{1+\Delta}\right)^{L-i} \quad , \quad (26)$$

Here density of particles in the bulk chain and left side is constant and approximately is equal to $\frac{\Delta}{1+\Delta}$ but in the right side, goes toward zero. Using (15) and (22), density in thermodynamic limit $\to \infty$, for case $q^2 = 1 + \Delta$ is obtained in form:

$< \mathrm{S}(x) > = \frac{\Delta}{1+\Delta}(1 - x)$, (26) while $x = \frac{i}{L}$, $0 < \mathrm{x} < 1$.

Using (16), binomial correlation functions $< S_i S_j >_L$ and matrix forms and vectors are obtained:

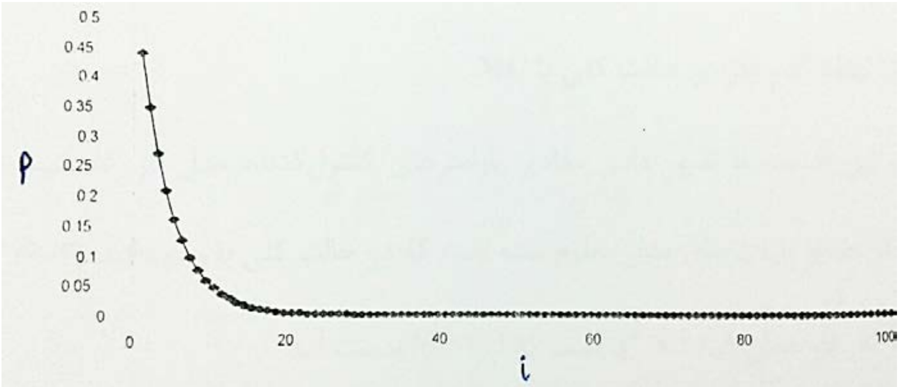
$$< S_i S_j >_L =$$

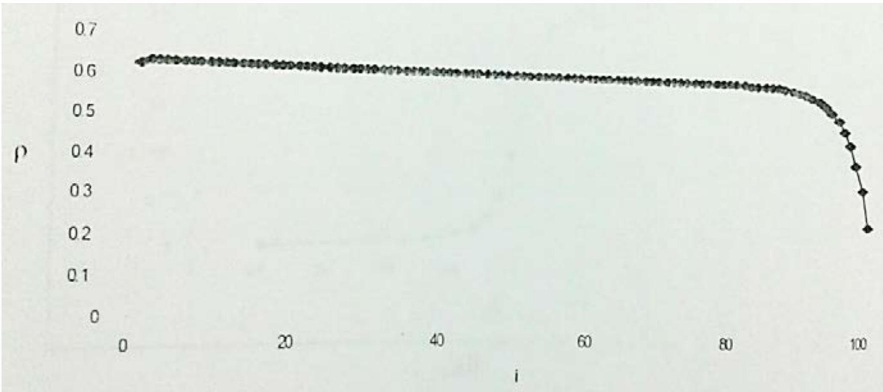
$$\frac{q\,\Delta^2(q^2-q\beta-1)}{Z_L(\beta+\beta\Delta-\Delta q)}\left[\frac{\Delta(1+\Delta)^{L-2}}{q^2-1}-q^{2(L-j)}\,(1+\Delta^{j-2})\right] \quad ,(27)$$

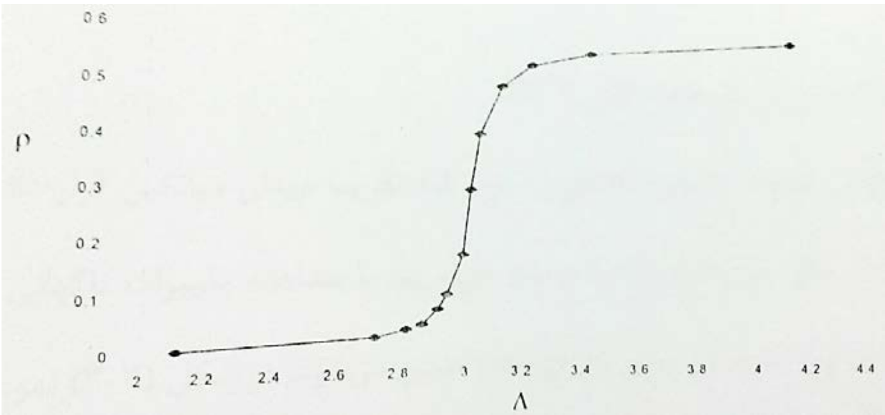
That

$$Z_L = q^{2\,L}+\frac{\Delta q(q^2-q\beta-1)(1+\ \Delta)^L}{(q^2-1)(\beta+\beta\Delta-q\Delta)} \quad ,(28)$$

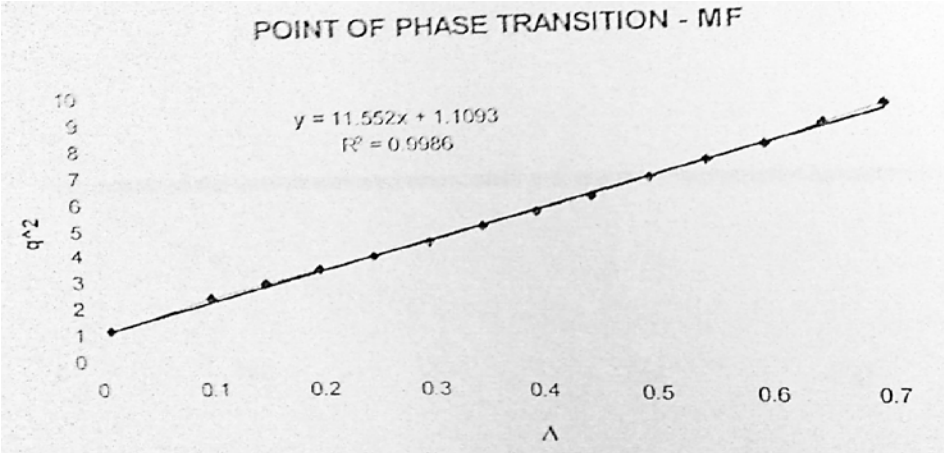
We can discuss model phase transitions using draw of plot of function zeroes in the imaginary q sheet. The low density and high density phases and phase transition for a 100 site chain in below figures are seen respectively:



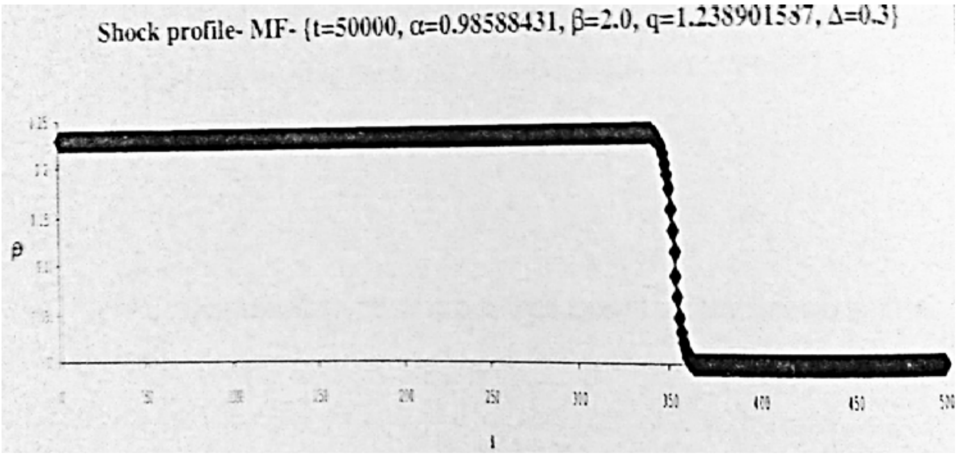




This problem can be solved and discussed using mean field approximation too. Giving different values to α , β and Δ in a computer program code which has written for mean field approximation, a linear function of q^2 versus Δ is obtained: $q^2 = 1.093 + 11.552\,\Delta$ while in exact matrix solution, transition point has $q^2 = 1 + \Delta$ form. This difference is because of the mean field approximation ignores correlations between particles.



But giving different values to models parameters which contemporary confirm two constraints $\alpha = (q^{-1} - q + \beta)\Delta$, (21) and $q^2 = 1.093 + 11.552\,\Delta$ a shock form function is obtained instead of a linear function for density distribution. It is seen in the figure that shock moves toward the left side of chain before the system attached to steady state but in steady states, it would be localized in a point.



This studied model here, can be used for different cases of stochastic systems. For example, a path in which observers with their cars go toward ceremony place or sport race that its one end is closed, a path contains many vehicles that is ended to a checkpoint, a long array of people to take food or water and … or to confirm their identification to permit entering a specific place, a current of flux into a vessel with a one closed end, a sound vessel or tube with a one closed end and so on. The results show that these models have two different phases and a shock profile.

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