TIFR/TH/94-15
12 April, 1994

NUMERICAL DIAGONALIZATION STUDY OF THE TRIMER DEPOSITION-EVAPORATION MODEL IN ONE DIMENSION

Peter B. Thomas*, M. K. Hari Menon† and Deepak Dhar‡

Theoretical Physics Group,
Tata Institute of Fundamental Research,
Homi Bhabha Road, Bombay 400 005, India.

ABSTRACT

We study the model of deposition-evaporation of trimers on a line recently introduced by Barma, Grynberg and Stinchcombe. The stochastic matrix of the model can be written in the form of the Hamiltonian of a quantum spin-$\frac{1}{2}$ chain with three-spin couplings given by $H = \sum_i \, [\, (1 - \sigma_i^- \sigma_{i+1}^- \sigma_{i+2}^-)\, \sigma_i^+ \sigma_{i+1}^+ \sigma_{i+2}^+ + h.c\,]$. We study by exact numerical diagonalization of H the variation of the gap in the eigenvalue spectrum with the system size for rings of size up to 30. For the sector corresponding to the initial condition in which all sites are empty, we find that the gap vanishes as L^{-z} where the gap exponent z is approximately 2.55 ± 0.15. This model is equivalent to an interfacial roughening model where the dynamical variables at each site are matrices. From our estimate for the gap exponent we conclude that the model belongs to a new universality class, distinct from that studied by Kardar, Parisi and Zhang.

DAE

PACS numbers: 02.50+s, 75.10.J, 82.20.M, 05.50+q

---

* Present address: Department of Physics, Brookhaven National Laboratory, Upton, NY 11973; Internet: thomas@cmth.phy.bnl.gov

† Internet address: hari@theory.tifr.res.in

‡ Internet address: ddhar@theory.tifr.res.in

Many physical processes such as heterogeneous catalysis, chemical reactions on polymer chains, adsorption on solid surfaces, *etc.* involve evaporation and deposition of reactants on a substrate. Recently Barma *et al.* have introduced a simple model which shows that the excluded volume effect together with dissociation and re-combination of the reactants on the surface can give rise to very interesting dynamical behaviour. In their model they have studied a random deposition-evaporation process of k identical atoms (called k-mers, $k = 1, 2, 3...$) on a surface [1,2]. It has been shown that in one-dimension when $k \geq 3$ the phase space breaks up into an exponentially large number of dynamically disconnected sectors and the model has infinite number of conserved quantities. It is found that in this case the auto-correlation function in the steady state decays with time t as $t^{-1/4}$, $t^{-1/2}$, $t^{-0.59}$ or as $e^{-\sqrt{t}}$, depending on the initial condition. The behaviour of the auto-correlation function for different initial conditions is understood in terms of the random walk of the substrings which constitutes what is called an irreducible string [4]. However for the steady state corresponding to the empty configuration as the initial condition, this analysis does not apply. In this case, for trimer model, Monte Carlo simulations show power law decay of autocorrelation function with an approximate value for the exponent 0.59 [5]. A theoretical understanding of this exponent is still lacking. Thus our main motivation is to understand the dynamics of trimer model in this sector. We have done a study of the trimer model on a one dimensional lattice, by exact diagonalisation of the stochastic matrix in this sector.

In this letter we restrict ourselves to the study of trimers (k=3) on a line (d=1). We consider a ring of L sites. At each site i is a dynamical variable n_i which takes values 0 or 1, depending on whether the site is occupied or not. In time a configuration $\{n_i\}$ evolves stochastically by Markovian dynamics as follows: Any three adjacent empty sites can become occupied with a rate ϵ and any three adjacent occupied site can become empty with a rate ϵ'.

If $P(C, t)$ is the probability that the ring has configuration C at time t, then

$P(C, t)$ satisfies the master equation

$$\frac{\partial}{\partial t} P(C, t) = \sum_{C'} W_{CC'} P(C', t) \tag{1}$$

Where the transition rate matrix $\hat{W}$ for the case $\epsilon = \epsilon'$ can be written as

$$\hat{W} = \epsilon \sum_{i=1}^{L} \left[\left(1 - \sigma_i^- \sigma_{i+1}^- \sigma_{i+2}^-\right) \sigma_i^+ \sigma_{i+1}^+ \sigma_{i+2}^+ + \text{h.c.} \right] \tag{2}$$

where σ_i^- and σ_i^+ are the Pauli annihilation and creation operators at site i.

Since $\hat{W}$ is a stochastic matrix where the transition rates satisfy detailed balance, all its eigenvalues are real and non- positive. The infinite number of conservation laws of this Hamiltonian can be encoded into a single conservation law of the irreducible string [3]. For any configuration the irreducible string is defined as follows: From the L-bit string of 0's and 1's representing the configuration, we recursively delete any consecutive occurrence of three 0's or 1's until no further deletions are possible. The irreducible string is conserved under dynamics and can be used to label uniquely each of the dynamically disconnected sectors. There is a large degeneracy for the eigenvalue 0, reflecting the large number of conservation laws in the model. An example of an eigenvector with zero eigenvalue is any a configuration which has no 3 adjacent 0's or 1's. Such a state cannot evolve in time. The number of such configurations has been shown to vary as μ^L for large L, where μ is the golden mean $(\sqrt{5} + 1)/2$ [3].

We can exactly diagonalise $\hat{W}$ in some almost totally jammed sectors. For example, if the sector corresponds to an irreducible string of length $L - 3$, then it is easy to see that the corresponding stochastic matrix in general has size of $O(L^2)$. Under dynamics the position of the reducible block on the ring changes and its motion can be described as a random walk. In this case it can be shown that the mean square displacement increases linearly with time. This corresponds to a dynamical exponent of $z = 2$. Sectors with irreducible string length $L - 6$

correspond to diffusion of 2 interacting random walkers. In this case the size of the stochastic matrix will be of $O(L^3)$. When the two walkers are next to each other, they stay there longer, which corresponds to an attractive interaction. The dynamical exponent will be 2 in this case also.

The most interesting sector corresponds to the case when the length of the irreducible string (l) is very small compared to L. In this case Monte Carlo simulations [5] have shown that the attractive interaction between these "random walkers" gives rise to a sub-diffusive behavior, with the dynamical exponent $z > 2$. In this paper, we estimate this exponent by numerically diagonalising the stochastic matrix for small systems and assuming finite size scaling.

For numerical diagonalisation it is desirable to reduce the size of the matrix as much as possible by making use of the known symmetries and conservation laws of the model. For periodic boundary conditions, and for the special case of deposition and evaporation rates equal ($\epsilon = \epsilon'$), in addition to the conservation law of the irreducible string, one can make use of the three symmetries of the system namely translation, reflection and flip, to reduce the size of the matrix by about a factor of $2L$. Let $\hat{T}$, $\hat{P}$ and $\hat{F}$ be the operators corresponding to these symmetries. They are defined by

$$\begin{aligned}
\hat{T}\,|n_1, n_2, .., n_i, .., n_L\rangle &= |n_2, n_3, .., n_{i+1}, .., n_L, n_1\rangle \\
\hat{P}\,|n_1, n_2, .., n_i, .., n_L\rangle &= |n_L, n_{L-1}, .., n_i, .., n_1\rangle \\
\hat{F}\,|n_1, n_2, .., n_i, .., n_L\rangle &= |\bar{n}_1, \bar{n}_2, .., \bar{n}_i, .., \bar{n}_L\rangle\,; \qquad \text{where } \bar{n}_i = 1 - n_i
\end{aligned} \tag{3}$$

Here $|n_1, n_2, .., n_i, .., n_L\rangle$ is a vector in the Hilbert space representing the configuration $\{n_i\}$. These operators satisfy the following algebra

$$\begin{aligned}
&[\hat{T}, \hat{F}] = [\hat{P}, \hat{F}] = 0 \\
&\hat{T}^L = \hat{P}^2 = \hat{F}^2 = 1 \\
&\hat{T}\hat{P} = \hat{P}\hat{T}^{-1}
\end{aligned} \tag{4}$$

Note that $\hat{T}$ and $\hat{P}$ do not commute. The three operators which simultaneously commute with $\hat{W}$ and with each other are $\hat{F}$, $\hat{P}$ and $\left(\hat{T}+\hat{T}^{-1}\right)$. Let their corresponding eigenvalues be f, p and $2\cos(k)$ respectively, where $f=\pm 1$, $p=\pm 1$ and $k=2n\pi/L$; $n=0,1,...,L-1$. The simultaneous eigenvectors of these three operators are of the form

$$\begin{aligned}|k,f,p,+\rangle &= (1+f\hat{F})(1+p\hat{P})\sum_{r=1}^{L} T^r \cos(kr)\,|C\rangle \\ |k,f,p,-\rangle &= (1+f\hat{F})(1+p\hat{P})\sum_{r=1}^{L} T^r \sin(kr)\,|C\rangle\end{aligned} \tag{5}$$

where $|C\rangle$ is any of the vectors $|\{n_i\}\rangle$.

We have used the states (5) as the basis for the stochastic matrix. For the null sector, the matrix splits into $2L$ blocks, corresponding to combinations of the 2 eigenvalues of $\hat{F}$ and the L eigenvalues of $\hat{T}$. Of these, due to a Kramers type degeneracy in the eigenvalues for the momentum values k and $2\pi-k$, we can fix p to always be equal to unity, and sweep over only half of the allowed momentum values. For lattice lengths which are not multiples of three, there is an additional degeneracy in the eigenvalues for $f=1$ and $f=-1$, since these states and their flipped counterparts are not connected by the dynamics. Since the size of the null sector $\sim (27/4)^{L/3}L^{-3/2}$ [3], the size of each block $\sim (27/4)^{L/3}L^{-5/2}$. For any lattice length, each block of the matrix is real and sparse, since all rows or columns have at most L non-zero entries.

The difference between the largest and the second largest eigenvalue of the complete matrix is proportional to the inverse relaxation time. The largest eigenvalue is zero and it lies in the block $k=0$, $f=1$. To find the second largest eigenvalue of the full matrix, we have numerically computed the largest eigenvalue in all the other blocks, and the second-largest eigenvalue in the $k=0$, $f=1$ block. Simple iteration of the eigenvector after suitably shifting all the eigenvalues, converged sufficiently fast for these blocks. This method preserves the sparseness of the blocks, which is necessary to keep the memory requirement of the program as low as possible. For the $k = 0$, $f = 1$ block, we computed the second largest eigenvalue, by ensuring orthogonality of the iterated vector to the eigenvector corresponding to the zero eigenvalue.

We have computed these eigenvalues for lattice sizes ranging from $L = 3$ to $L = 30$. When L is a multiple of 3, the irreducible string in the null sector has length zero and in this case we have diagonalized the stochastic matrix for both the $f = 1$ and $f = -1$ case. For the case $f = -1$ the smallest eigenvalue occurs for $k = 2\pi(1 - 1/L)/3$, and for the case $f = 1$ it occurs for $k = 2\pi/3$. When $L = 3n + 1$ and $L = 3n + 2$, where n is an integer, the irreducible string in the sector where the initial state is all empty has length 1 and 2 respectively. In this case, as explained earlier, the eigenvalues for $f = 1$ and $f = -1$ are degenerate. We have estimated the gap exponent z for each of these 4 sets of data, by assuming the scaling relation $\lambda \sim L^{-z}$. We define the effective exponent

$$z_L = \frac{\log[\lambda_{\mathrm{L-3}}/\lambda_{\mathrm{L}}]}{\log[L/(L-3)]}. \tag{6}$$

The sizes of the matrices, eigenvalues and estimate of the dynamical exponent z_L are shown in tables below. The z_L values are also plotted as a function of $1/L$ in figure 1.

Length of the lattice	$f = -1$		
	Matrix Size	λ_{min}	z_L
3	1	-6.00000	
6	1	-2.00000	1.58492
9	2	-0.87113	2.04977
12	10	-0.43876	2.38400
15	35	-0.26065	2.33375
18	170	-0.16932	2.36607
21	815	-0.11744	2.37373
24	4176	-0.08545	2.37929
27	21872	-0.06455	2.38333
30	118175	-0.05020	2.38672

pt

Length of the lattice	$f=1$		
	Matrix Size	$\lambda_{\min}$	z_L
6	1	-2.00000	
9	2	-1.25553	1.14828
12	10	-0.67412	2.16180
15	35	-0.44217	1.88375
18	173	-0.29577	2.21307
21	811	-0.20803	2.28276
24	4186	-0.15213	2.34360
27	21874	-0.11485	2.38637
30	118175	-0.08903	2.41725

Length of the lattice	Matrix Size	$\lambda_{\min}$	z_L
4	1	-1.00000	
7	4	-0.23008	2.62557
10	17	-0.09277	2.54655
13	84	-0.04754	2.54625
16	428	-0.02802	2.54829
19	2305	-0.01806	2.55571
22	12744	-0.01240	2.56472
25	72311	-0.00892	2.57433

Length of the lattice	Matrix Size	$\lambda_{\min}$	z_L
5	1	-1.00000	
8	4	-0.28476	2.67255
11	21	-0.11943	2.72855
14	103	-0.06215	2.70857
17	553	-0.03678	2.70122
20	3014	-0.02372	2.69857
23	16985	-0.01627	2.69933
26	97419	-0.01168	2.70193

It is clear from an inspection of these tables that while the convergence in each sector is reasonably good, there is a large difference between them if we compare them between different sectors. To see if this can be due to the presence of correction to the asymptotic scaling form, we have tried to incorporate various forms for the correction to the scaling. But none of these fit the data well, and at the same time decrease the discrepancy in z between different sectors. This can be seen from the fact that the effective values of z_L do not show a significant tendency to converge to a single value as L increases, for the largest sizes reached in our study.

One of the possible explanations for this is that different sectors have different gap exponents. Though this is quite intriguing, it is somewhat unlikely. The possible reason behind this could be the existence of an infinite number of conserved quantities in the model. It is hoped that further studies will clarify this point.

However, from our data it can be concluded that the gap exponent for all these sectors fall with in the range $z = 2.55 \pm 0.15$. To get a more precise estimate for z one needs further study either of larger size lattices, or by Monte Carlo simulations, or analytical methods.

In figure 2 we have shown a plot of λ versus k (dispersion curve) for three different lattice sizes. This is related to the spectrum of the excitations of the quantum Hamiltonian $\hat{W}$. It is seen that the spectrum for different sizes is qualitatively similar, but shows a complicated, yet un-understood structure as a function of k. We have also studied the same model for the case of unequal deposition-evaporation rates (in this case there is no flip symmetry). The range of estimated value of z is the same as that for equal deposition-evaporation rates.

The stochastic evolution of the trimer model can be mapped to the stochastic dynamics of a string, both ends fixed to the same point, by defining a matrix variable U_i at each site [3]. This matrix U_i has information about the length of the irreducible string corresponding to the substring from site 1 of the lattice upto site i. Under the dynamics the length of this irreducible string changes, and is related to the change in the matrix variables U_i. Thus this model corresponds to a generalisation of the KPZ model where the scalar height variables are replaced by matrix variables. It is well known that $z = 1.5$ for the KPZ model [6]. Our results show that this model falls under a new universality class. It is also different from the model studied recently by Doherty *et al.* which is also a generalisation of the KPZ equation to n component variables. In their model, the dynamical exponent $z = 3/2$ in one dimension, independent of n, though in higher dimensions it depends on n [7].

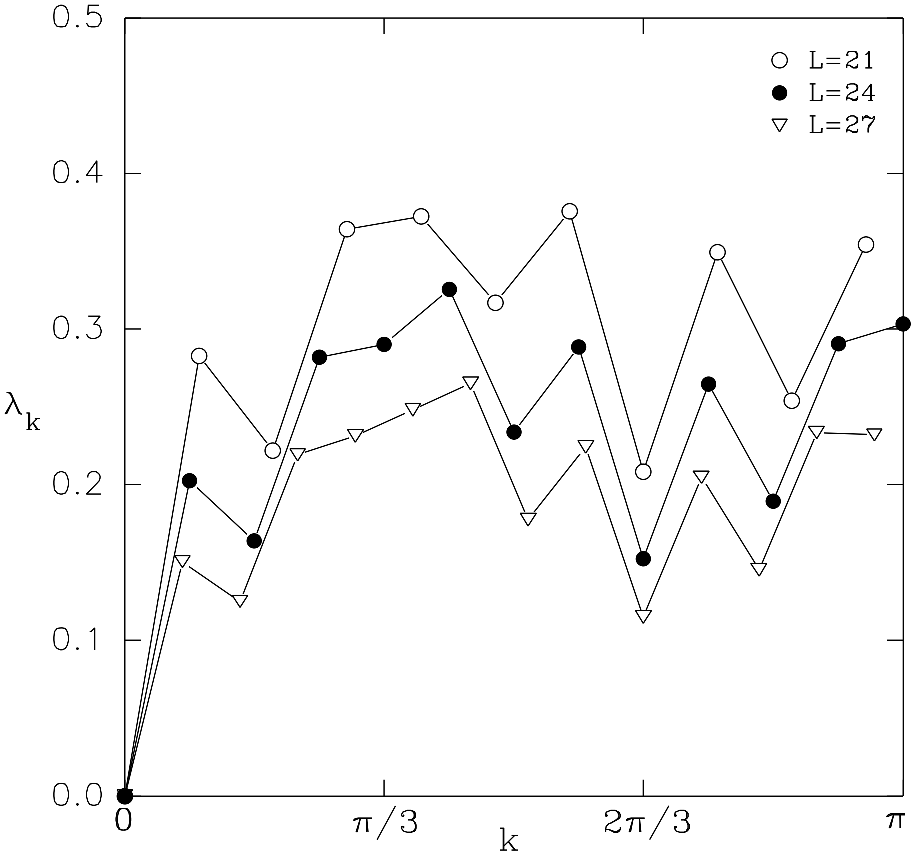
REFERENCES

1. M. Barma, M. D. Grynberg and R. B. Stinchcombe, *Phys. Rev. Lett.* **70**, 1033 (1993).
2. R. B. Stinchcombe, M. D. Grynberg and M. Barma, *Phys. Rev. E*, **47** 4018 (1993)
3. D. Dhar and M. Barma *Pramana* **41** L193 (1993).
4. M. Barma and D. Dhar *Proceedings of the Solid State Physics Symposium* **36C** 489 (1993).
5. M. Barma and D. Dhar , *In preparation*
6. M. Kardar, G. Parisi and Y. C. Zhang *Phys. Rev. Lett.* **56** 889 (1986).
7. J. P. Doherty, M. A. Moore, J. M. Kim and A. J. Bray *Manchester Preprint* (1993).

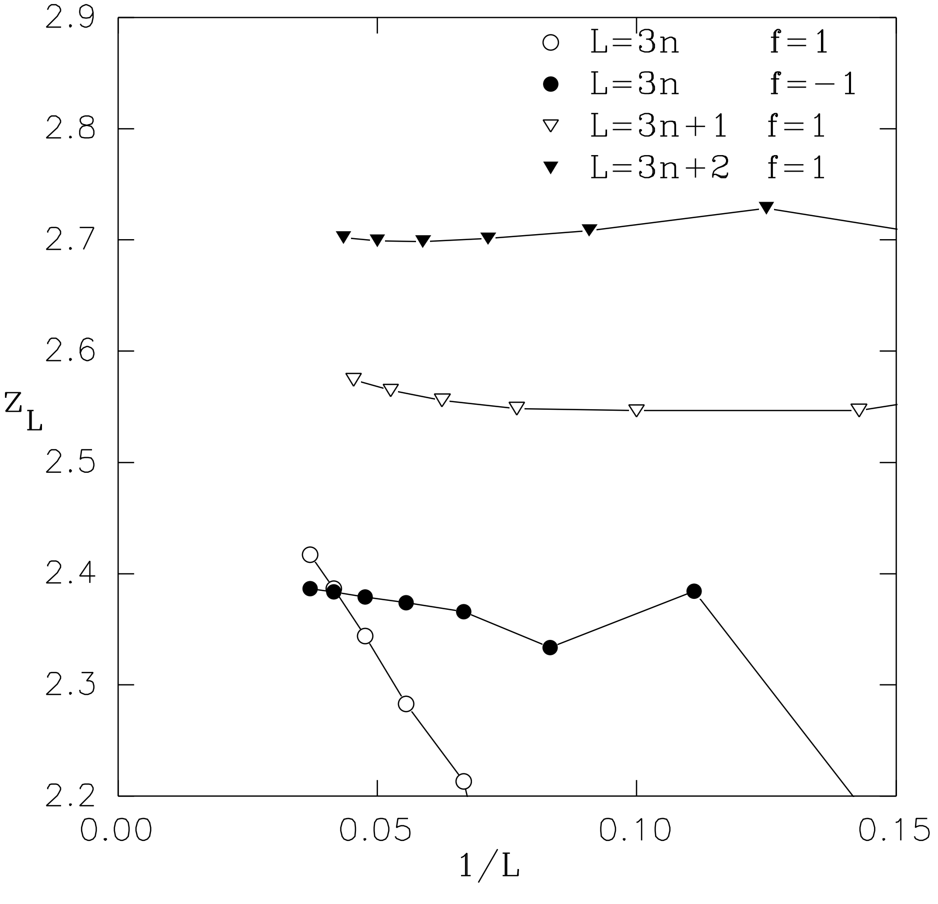
FIGURE CAPTIONS

1. A plot of the effective exponent z_L versus $1/L$, where L is the length of the lattice.

2. Dispersion curve of the quantum Hamiltonian corresponding to the trimer model [Equation (2)].



0.5
0.4
0.3
0.2
0.1
0.0
λ_k
0
$\pi/3$
$2\pi/3$
π
k
L=21
L=24
L=27



2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
z_L
0.00
0.05
0.10
0.15
1/L
○ L=3n f=1
● L=3n f=−1
▽ L=3n+1 f=1
▼ L=3n+2 f=1