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Stationary States and Scaling Shapes of One-Dimensional Interfaces

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Sub-lattice parallel heat bath dynamics is applied to various one dimensional Solid-On-Solid interface models. The existence of invariant product measures in the gradient variables allows to compute exactly the interface speed as function of the slope. This function can have many convex and concave parts, depending on lattice modulation and unboundedness of the state space. This may be associated with the occurrence of corners in the macroscopic scaling shapes.

KEY WORDS: Heat bath algorithm; sub-lattice parallel dynamics; interfaces; SOS model.

1. INTRODUCTION

The Solid-On-Solid model[(1)] deals with height variables $h_i \in \mathbb{Z}$ or $\mathbb{R}$, indexed by the lattice sites $i \in \mathbb{Z}^d$, here $d = 1$. In $\mathbb{Z}^{d+1}$, the interface is the set of points (i, h_i), and one may think that there is one phase of matter above the interface and another phase below the interface. We are interested in non-equilibrium, at a coarse grained scale where stochastic dynamics is appropriate. The choice of a dynamics is motivated by an energy function, which we take as

$$H = J \sum_i (1 + |h_{i+1} - h_i|^n) - E \sum_i h_i \tag{1.1}$$

For $n = 1$, the first term is proportional to the interface length, and J is the interface energy per unit length. The second term is proportional to the area below the interface. The coefficient E is the difference of free energy per unit area between the two phases.

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We only use H to write a detailed balance condition for our dynamics: suppose h_i is being updated and denote $w_{h_i \to h_i'}$ the probability (or probability density) that h_i goes to h_i', the other h_j's being held fixed. Then we require

$$\frac{w_{h_i \to h_i'}}{w_{h_i' \to h_i}} = e^{-\Delta H} = e^{-J(|h_{i+1}-h_i'|^n + |h'i - h_{i-1}|^n - |h_{i+1}-h_i|^n - |h_i - h_{i-1}|^n) + E(h_i' - h_i)} \tag{1.2}$$

We take $E > 0$, so that the h_i's will go to infinity as time goes to infinity (the phase below the interface grows at the expense of the phase above). We may look at the gradient variables $\eta_i = h_{i+1} - h_i$. A simple case occurs when the gradient variables take values in $\{+1, -1\}$. The model becomes the asymmetric simple exclusion process (ASEP). Under fairly general conditions on the stochastic dynamics, the invariant measures of the ASEP are the product over bonds $(i, i+1)$ of independent identically distributed measures on $\{+1, -1\}$.

This is not the case when the state space of the gradient variables has more than two states. For gradient variables taking values in $\{+1, 0, -1\}$, conditions for invariant product measures were given in ref. 2: the parameters of the dynamics should be restricted to a manifold of co-dimension one, whose equation was given.

In the present paper we start from product measures and find stochastic dynamics which leave them invariant. The *sub-lattice parallel heat bath dynamics* was first used in numerical work. When applied with $E = 0$, it relaxes to the appropriate Gibbs measure. Compared to random sequential updates, it has the advantage of being defined also on the infinite lattice.

Allowing a more general state space and a more general detailed balance condition gives rise to interesting phase diagrams and scaling shapes. As in the cases studied in ref. 2, it is expected that the accidental occurrence of product measures is not responsible for the general features of these diagrams and shapes.

In Section 2 we define sub-lattice parallel heat bath dynamics in $\mathbb{Z}^d$, with invariant product measures. In Section 3 we apply the results to $d = 1$ Solid-On-Solid models. Examples are given in Section 4. In Section 5 we compute the interface speed as function of the interface slope.

2. SUB-LATTICE PARALLEL HEAT BATH DYNAMICS

Denote $e_1, \ldots, e_d$ an orthonormal basis in $\mathbb{Z}^d$. An oriented lattice bond starting from $i \in \mathbb{Z}^d$ in the e_n direction is denoted $i, i + e_n$. We consider random variables $\eta_{i,\,i+e_n} \in \mathbb{Z}$ called bond variables. In $d = 1$ they can be identified with gradient variables.

An equivalence relation $\sim$ is given between sets of $2d$ bond variables incident upon a site i. This equivalence relation is assumed to be such that

$$(\eta_{i-e_1,\,i}, \eta_{i,\,i+e_1},\dots, \eta_{i-e_d,\,i}, \eta_{i,\,i+e_d}) \sim (\eta_{i,\,i+e_1}, \eta_{i-e_1,\,i},\dots, \eta_{i,\,i+e_d}, \eta_{i-e_d,\,i}) \tag{2.1}$$

An arbitrary configuration around i is in equivalence with the configuration obtained by symmetry about the center i. An example of such an equivalence relation is the following: $\eta \sim \eta'$ at i if and only if

$$\eta_{i-e_1,\,i} + \eta_{i,\,i+e_1} + \dots + \eta_{i-e_d,\,i} + \eta_{i,\,i+e_d} = \eta'_{i,\,i+e_1} + \eta'_{i-e_1,\,i} + \cdots + \eta'_{i,\,i+e_d} + \eta'_{i-e_d,\,i} \tag{2.2}$$

which may be interpreted as equal total charge around i.

Another example: $\eta \sim \eta'$ at i if and only if $(\eta_{i-e_1,\,i}, \eta_{i,\,i+e_1},\dots, \eta_{i-e_d,\,i}, \eta_{i,\,i+e_d})$ is a permutation of $(\eta_{i,\,i+e_1}, \eta_{i-e_1,\,i},\dots, \eta_{i,\,i+e_d}, \eta_{i-e_d,\,i})$, which can be interpreted as identical list of particles present around i.

The lattice $\mathbb{Z}^d$ is bipartite: sites are even or odd according to the parity of the sum of their coordinates. This allows to define two equivalence relations $\sim_o$ and $\sim_e$ between configurations:

$$\eta \underset{o}{\sim} \eta' \qquad \text{if and only if} \quad \eta \sim \eta' \text{ at } i \quad \forall i \text{ odd}$$

and

$$\eta \underset{e}{\sim} \eta' \qquad \text{if and only if} \quad \eta \sim \eta' \text{ at } i \quad \forall i \text{ even}$$

Next we introduce $2d$ probability measures on $\mathbb{Z}$ denoted $Q_1, R_1,\dots, Q_d, R_d$, and the two candidates for stationary measures under the dynamics to be defined:

$$\begin{aligned} \mu^e(\eta) &= \prod_{i \text{ even}} \prod_{n=1}^{d} Q_n(\eta_{i-e_n,\,i})\, R_n(\eta_{i,\,i+e_n}), \\ \mu^o(\eta) &= \prod_{i \text{ odd}} \prod_{n=1}^{d} Q_n(\eta_{i-e_n,\,i})\, R_n(\eta_{i,\,i+e_n}) \end{aligned} \tag{2.3}$$

Time is discrete, $t \in \mathbb{Z}^+$. Given a configuration $\eta^{2t} = \eta$ at some even time, the configuration at time $2t+1$ is distributed according to

$$\mathbb{P}(\eta^{2t+1} = \eta' \mid \eta^{2t} = \eta) = \begin{cases} \dfrac{\mu^o(\eta')}{\sum_{\eta'' \sim_o \eta} \mu^o(\eta'')} & \text{if} \quad \eta' \underset{o}{\sim} \eta \\ 0 & \text{otherwise} \end{cases} \tag{2.4}$$

and similarly at the following time

$$\mathbb{P}(\eta^{2t+2} = \eta \mid \eta^{2t+1} = \eta') = \begin{cases} \dfrac{\mu^e(\eta)}{\sum_{\eta'' \sim_e \eta'} \mu^e(\eta'')} & \text{if} \quad \eta \underset{e}{\sim} \eta' \\ 0 & \text{otherwise} \end{cases} \tag{2.5}$$

Let us compute

$$\sum_{\eta} \mathbb{P}(\eta^{2t+1} = \eta' \mid \eta^{2t} = \eta)\, \mu^e(\eta)$$

$$= \sum_{\eta \sim_o \eta'} \frac{\mu^o(\eta')}{\sum_{\eta'' \sim_o \eta} \mu^o(\eta'')}\, \mu^e(\eta)$$

$$= \mu^o(\eta') \frac{\sum_{\eta \sim_o \eta'} \mu^e(\eta)}{\sum_{\eta'' \sim_o \eta'} \mu^o(\eta'')}$$

$$= \mu^o(\eta') \prod_{i \text{ odd}} \frac{\sum^i_{\eta \sim \eta'} \prod_{n=1}^d Q_n(\eta_{i-e_n,\, i})\, R_n(\eta_{i,\, i+e_n})}{\sum^i_{\eta'' \sim \eta'} \prod_{n=1}^d R_n(\eta''_{i-e_n,\, i})\, Q_n(\eta''_{i,\, i+e_n})} \tag{2.6}$$

where $\sum^i$ means a sum over bond variables incident upon i. Now (2.1) allows a change of summation variable in the denominator:

$$\eta''_{i-e_n,\, i} = \eta_{i,\, i+e_n}, \qquad \eta''_{i,\, i+e_n} = \eta_{i-e_n,\, i}$$

so that numerator and denominator cancel out and

$$\sum_{\eta} \mathbb{P}(\eta^{2t+1} = \eta' \mid \eta^{2t} = \eta)\, \mu^e(\eta) = \mu^o(\eta') \tag{2.7}$$

Similarly

$$\sum_{\eta'} \mathbb{P}(\eta^{2t+2} = \eta \mid \eta^{2t+1} = \eta')\, \mu^o(\eta') = \mu^e(\eta) \tag{2.8}$$

Therefore μ^e and μ^o are exchanged under the dynamics, and both are invariant from t to $t+2$.

3. DYNAMICS FOR $d=1$ SOS MODELS

In $d=1$ the notation may be simplified with $\eta_i = \eta_{i,\, i+e_1}$ and $\eta_{i-1} = \eta_{i-e_1,\, i}$. Bond variables may be identified with the gradient of height variables, $\eta_i = h_{i+1} - h_i$. We choose the equivalence relation (2.2): $\eta \sim \eta'$ at i if and only if $\eta_{i-1} + \eta_i = \eta'_{i-1} + \eta'_i$, or $h_{i+1} - h_{i-1} = h'_{i+1} - h'_{i-1}$. The odd and even invariant measures are

$$\mu^e(\eta) = \prod_{i \text{ even}} Q(\eta_{i-1})\, R(\eta_i)\,, \qquad \mu^o(\eta) = \prod_{i \text{ odd}} Q(\eta_{i-1})\, R(\eta_i) \tag{3.1}$$

The rules (2.4)(2.5) for the dynamics take the form

$$\mathbb{P}(\eta^{2t+1} = \eta' \mid \eta^{2t} = \eta) = \prod_{i \text{ odd}} \frac{Q(\eta'_{i-1})\, R(\eta'_i)}{Z(\eta_{i-1} + \eta_i)}\, \delta(\eta'_{i-1} + \eta'_i - \eta_{i-1} - \eta_i) \tag{3.2}$$

where $\delta(\,\cdot\,)$ is a Kronecker delta and

$$Z(\gamma) = \sum_\alpha Q(\alpha)\, R(\gamma - \alpha)$$

Similarly

$$\mathbb{P}(\eta^{2t+2} = \eta \mid \eta^{2t+1} = \eta') = \prod_{i \text{ even}} \frac{Q(\eta_{i-1})\, R(\eta_i)}{Z(\eta'_{i-1} + \eta'_i)}\, \delta(\eta_{i-1} + \eta_i - \eta'_{i-1} - \eta'_i) \tag{3.3}$$

For the height variables, (3.2) translates into

$$\mathbb{P}(h^{2t+1} = h' \mid h^{2t} = h)$$
$$= \prod_{i \text{ odd}} \frac{Q(h'_i - h'_{i-1})\, R(h'_{i+1} - h'_i)}{Z(h_{i+1} - h_{i-1})}\, \delta(h'_{i+1} - h'_{i-1} - h_{i+1} + h_{i-1}) \tag{3.4}$$

We see that all the $h'_{2i} - h_{2i}$ take on the same value. The dynamical rule for the gradient variables does not fixed that value. We fix it to 0:

$$h_{2i}^{2t+1} = h_{2i}^{2t} \quad \forall i \tag{3.5}$$

For the same reason we fix

$$h_{2i+1}^{2t+2} = h_{2i+1}^{2t+1} \quad \forall i \tag{3.6}$$

It is then sufficient to define the dynamics for

$$h^{2t} = \{h_i^{2t} \colon i \text{ even}\}, \qquad h^{2t+1} = \{h_i^{2t+1} \colon i \text{ odd}\}$$

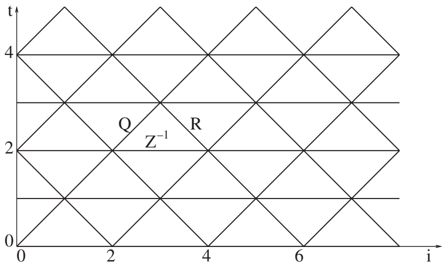

Fig. 1. SOS model in two space-time dimensions.

Given an initial configuration h^0, the probability distribution of heights up to some time T takes on the explicit form

$$\mathbb{P}(h^{0\leqslant t\leqslant T} \mid h^0) = \prod_{\substack{i+t \text{ odd} \\ 0\leqslant t\leqslant T-1}} \frac{Q(h_i^{t+1}-h_{i-1}^t)\, R(h_{i+1}^t-h_i^{t+1})}{Z(h_{i+1}^t-h_{i-1}^t)} \tag{3.7}$$

We now have a two space-time dimensional SOS model, with Boltzmann weights Q, R and Z^{-1} associated to bonds parallel to the first diagonal, second diagonal and horizontal axis respectively (Fig. 1).

The same construction works with real height and bond variables. Now Q and R are densities with respect to the Lebesgue measure,

$$Z(\gamma) = \int Q(\alpha)\, R(\gamma-\alpha)\, d\alpha$$

and (3.1) and (3.7) become

$$\begin{aligned} \mu^e(d\eta) &= \prod_{i \text{ even}} Q(\eta_{i-1})\, R(\eta_i)\, d\eta_{i-1}\, d\eta_i\,, \\ \mu^o(d\eta) &= \prod_{i \text{ odd}} Q(\eta_{i-1})\, R(\eta_i)\, d\eta_{i-1}\, d\eta_i \end{aligned} \tag{3.8}$$

$$\mathbb{P}(dh^{0\leqslant t\leqslant T} \mid h^0) = \prod_{\substack{i+t \text{ odd} \\ 0\leqslant t\leqslant T-1}} \frac{Q(h_i^{t+1}-h_{i-1}^t)\, R(h_{i+1}^t-h_i^{t+1})}{Z(h_{i+1}^t-h_{i-1}^t)}\, dh_i^{t+1} \tag{3.9}$$

4. EXAMPLES

The case $\eta_i \in \{+1, 0, -1\}$ has been thoroughly studied in ref. 2. Here we concentrate on cases where the probability measures Q and R have densities with respect to the Lebesgue measure on $\mathbb{R}$ or the uniform measure on $\mathbb{Z}$ of the form

$$Q_\lambda(\eta) = e^{-J|\eta|^n + (\lambda + \frac{E}{2})\eta}/\text{norm.}, \quad R_\lambda(\eta) = e^{-J|\eta|^n + (\lambda - \frac{E}{2})\eta}/\text{norm.} \tag{4.1}$$

with $n = 1, 2$ or 4, $J > 0$, $E > 0$. The parameter λ is in the range $\lambda \in (-J + E/2, J - E/2)$ for $n = 1$ and $\lambda \in (-\infty, +\infty)$ for $n > 1$.

The transition rates (3.2) take the form

$$\mathbb{P}(\eta^{2t+1} = \eta' \mid \eta^{2t} = \eta) = \prod_{i \text{ odd}} \frac{e^{-J(|\eta'_{i-1}|^n + |\eta'_i|^n) + \frac{E}{2}(\eta'_{i-1} - \eta'_i)}}{\tilde{Z}(\eta_{i-1} + \eta_i)} \delta(\eta'_{i-1} + \eta'_i - \eta_{i-1} - \eta_i) \tag{4.2}$$

with

$$\tilde{Z}(\gamma) = \sum_{\alpha \in \mathbb{Z}} e^{-J(|\alpha|^n + |\gamma - \alpha|^n) + \frac{E}{2}(\gamma - 2\alpha)} \tag{4.3}$$

The dynamics is thus independent of λ, and admits a one-parameter family of invariant measures indexed by λ.

The transition rates for heights (3.4)–(3.6) take the form

$$\mathbb{P}(h^{2t+1} = h' \mid h^{2t} = h) = \prod_{i \text{ odd}} \frac{e^{-J(|h'_i - h_{i-1}|^n + |h_{i+1} - h'_i|^n) + Eh'_i - \frac{E}{2}(h_{i-1} + h_{i+1})}}{\tilde{Z}(h_{i+1} - h_{i-1})} \tag{4.4}$$

where $\tilde{Z}$ is the same as (4.3). If we define $w_{h_i \to h'_i}$ as the factor indexed by i in (4.4), we find that it obeys (1.2).

For the Gaussian case, $n = 2$ with continuous variables, we find that $\tilde{Z}(\gamma)$, now defined with an integral over α, is proportional to $\exp(-J\gamma^2/2)$, hence a more explicit form for (4.4) and for the space-time measure:

$$\mathbb{P}(dh^{0 \leqslant t \leqslant T} \mid h^0) = \prod_{\substack{i+t \text{ odd} \\ 0 \leqslant t \leqslant T-1}} \left(e^{-J(|h_i^{t+1} - h_{i-1}^t|^2 + |h_{i+1}^t - h_i^{t+1}|^2 - \frac{1}{2}|h_{i+1}^t - h_{i-1}^t|^2)} \cdot e^{\frac{E}{2}(h_i^{t+1} - h_{i-1}^t) + \frac{E}{2}(h_i^{t+1} - h_{i+1}^t)} dh_i^{t+1}\right)/\text{norm.} \tag{4.5}$$

5. INTERFACE MEAN SLOPE AND SPEED

Let

$$\langle \eta \rangle_Q = \int \eta \, Q(\eta) \, d\eta, \qquad \langle \eta \rangle_R = \int \eta \, R(\eta) \, d\eta$$

and similarly with sums instead of integrals in the case of discrete variables. In the stationary states (3.1) constructed with Q and R, the interface mean slope, which we denote $\tan\theta$, is given by

$$\tan\theta = \tfrac{1}{2}\left(\langle\eta\rangle_Q + \langle\eta\rangle_R\right) \tag{5.1}$$

The corresponding mean speed $V(\tan\theta)$ is defined as the average variation of any h_i between t and $t+2$, as two time steps are necessary for each h_i to be updated once:

$$\begin{aligned} V(\tan\theta) &= \mathbb{E}(h_i^{t+2} - h_i^t) \\ &= \mathbb{E}((h_i^{t+2} - h_{i-1}^{t+1}) - (h_i^t - h_{i-1}^{t+1})) \\ &= \langle\eta\rangle_Q - \langle\eta\rangle_R \end{aligned} \tag{5.2}$$

We did the computation with $i+t$ even. In the second line of (5.2), $(h_i^{t+2} - h_{i-1}^{t+1})$ is parallel to the first diagonal, hence distributed according to Q, whereas $(h_i^t - h_{i-1}^{t+1})$ is parallel to the second diagonal, hence distributed according to R. For $i+t$ odd, we first use (3.5) and (3.6).

With (4.1), the mean slope $\tan\theta$ is odd and increasing in the parameter λ. The speed $V(\tan\theta)$ is even in λ and therefore even in $\tan\theta$.

For the usual continuous SOS model, $n=1$ in (4.1) and $\eta_i \in \mathbb{R}$, we find

$$\langle\eta\rangle_Q = \frac{2\lambda+E}{J^2 - \left(\lambda + \frac{E}{2}\right)^2}, \quad \langle\eta\rangle_R = \frac{2\lambda-E}{J^2 - \left(\lambda - \frac{E}{2}\right)^2} \tag{5.4}$$

which gives with (5.1) and (5.2) a parametric representation for the function $V(\tan\theta)$. The speed is minimum at $\theta=0$, increases for $\theta>0$, and $V(\tan\theta)/|\tan\theta| \to 2$ for $\tan\theta \to \pm\infty$. The same occurs with the discrete $n=1$ SOS model, $\eta_i \in \mathbb{Z}$, where

$$\begin{aligned} \langle\eta\rangle_Q &= \frac{e^{-J+\lambda+E/2} - e^{-J-\lambda-E/2}}{1 - e^{-J+\lambda+E/2} - e^{-J-\lambda-E/2} + e^{-2J}} \\ \langle\eta\rangle_R &= \frac{e^{-J+\lambda-E/2} - e^{-J-\lambda+E/2}}{1 - e^{-J+\lambda-E/2} - e^{-J-\lambda+E/2} + e^{-2J}} \end{aligned} \tag{5.5}$$

For the Gaussian case, $n=2$ and $\eta_i \in \mathbb{R}$, we find

$$\tan\theta = \frac{\lambda}{2J}, \quad V = \frac{E}{2J}, \tag{5.3}$$

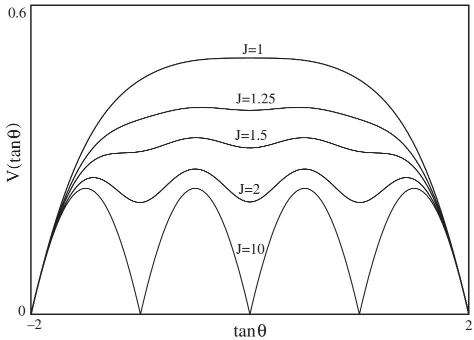

Fig. 2. Quadratic RSOS model, $N = 2$, $E = 1$.

the speed is independent of the slope. For $n = 2$ with discrete variables $\eta_i \in \mathbb{Z}$, the speed is periodic of period 1 in $\tan\theta$.

A Restricted Solid On Solid (RSOS) model is obtained by restricting the state space of the gradient variables to a finite set: $\eta_i \in \{-N, -N+1, \ldots, N-1, N\}$. The case $N = 1$ was studied in ref. 2. For $N = 2$, the computed speed function of the slope is shown on Fig. 2 for various values of J. The graph for $J = 10$ is the same as for $J = \infty$, or zero temperature, and is easily understood in terms of configurations of minimal energy. In the range of allowed slopes, the RSOS model coincides with the corresponding SOS model in that limit.

The macroscopic shape of a growing cluster or a dissolving corner modelled by our interface dynamics stems from the function $V(\tan\theta)$.[3]

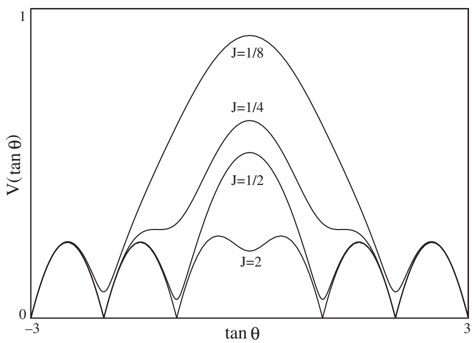

Fig. 3. Quartic RSOS model, $N = 3$, $E = 1$.

Consider an initial corner $h_i^0 = \tan\theta_0\ |i|$. The resulting macroscopic shape is determined by the concave envelope of the function $V(\tan\theta)$ in the interval $[-\tan\theta_0, \tan\theta_0]$. Straight portions in the envelope are unstable: the corresponding slopes are absent from the macroscopic shape which shows corners instead. From Fig. 2 one expects no corner for $J=1$, one corner for $J=1.25$, and three corners for $J=1.5$, with a suitable $\tan\theta_0$.

For $n \neq 1, 2$ the function $V(\tan\theta)$ must be tabulated numerically, which can be done with arbitrary precision as this involves only two integrals over $\mathbb{R}$ or sums over $\mathbb{Z}$. For $n>2$ and $\eta_i \in \mathbb{R}$, the speed is maximum at $\theta=0$ and goes to zero as $\tan\theta \to \pm\infty$. For $n=4$, $V(\tan\theta) \sim E/(J\tan^2\theta)$ as $\tan\theta \to \pm\infty$.

For the Restricted Solid On Solid (RSOS) model with $N=3$ and $n=4$, the computed speed function of the slope is shown on Fig. 3 for various values of J.

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