A driven solid on solid model

We introduce a variant of the solid on solid interface model which is formed from two distinct particle types. Numerical simulations show that driving one of the particle types leads to an increase in surface fluctuations and in the case of non-conserved dynamics can lead to a change in the steady state height. We theoretically explain these results in terms of stochastic density functional theory.

I. THE MODEL

We consider a model of a surface delimiting a bulk phase which contains two different particle types A and B. The effective hamiltonian for the model is

$$H[\mathbf{n}_A, \mathbf{n}_B] = J\sum_{i=1}^{N} |h_{i+1} - h_i|^k - \mu_A \sum_{i=1}^{N} n_{Ai} - \mu_B \sum_{i=1}^{N} n_{Bi}. \tag{1}$$

Here n_{Ai} and n_{Bi} denote number of particles of type A and B respectively and the site i. The permitted particle configurations are taken to be stacked vertically such that the A particles are at the bottom and the stack of B particles lies on top of that of the A particles (see the figure 1), we are this assuming that the particles in each column are demixed. At each site $h_i = n_{Ai} + n_{Bi}$ and the first term in the Hamiltonian corresponds to the surface tension with a gas phase above the stacks of particles. In the case where $k = 1$ we have the standard non-restricted solid on solid particle Hamiltonian and when $k = 2$ we have the Gaussian version. The model differs from the usual solid on solid model in that a number of particle configurations give rise to the same height configuration (even if there is only one particle type). The grand partition function is given by

$$\Xi = \sum_{\mathbf{n}_A, \mathbf{n}_b} \exp(-\beta H[\mathbf{n}_A, \mathbf{n}_B] - \sum_i \ln(n_{Ai}!) + \sum_i \ln(n_{Bi}!)), \tag{2}$$

the second entropic contribution arises from the fact that there are $N_A!N_B!/\prod_i n_{A_i}!n_{B_i}!$ ways of choosing the configurations specified by n_{A_i} and n_{B_i} among the total number of $N_A = \sum_i n_{A_i}$ and $N_B = \sum_i n_{B_i}$ particles which are indiscernible among particles of the same type. The motivation for a two particle theory is that when one develops a continuous, off lattice theory, based on Brownian dynamics, any single particle theory is insensitive to constant driving due to Galilean invariance, the presence of two different particle types breaks this invariance and yields non-equilibrium effects.

The grand partition function can also be written as

$$\Xi = \Xi = \sum_{\mathbf{n}_A, \mathbf{n}_b} \exp(-\beta H_e[\mathbf{n}_A, \mathbf{n}_B]) \tag{3}$$

where H_e is the effective Hamiltonian

$$H_e[\mathbf{n}_A, \mathbf{n}_B] = H[\mathbf{n}_A, \mathbf{n}_B] - T\sum_i \ln(n_{Ai}!) + T\sum_i \ln(n_{Bi}!) \tag{4}$$

The statics of the above can be reduced to the study of a single particle model by making the change of variable $n_{Bi} = h_i - n_{Ai}$, doing this the sum over the variables n_{Ai} may be trivially carried out and we find

$$\Xi = \sum_{\mathbf{h}} \exp(-\beta J \sum_i |h_{i+1} - h_i|^k - \sum_i \ln(h_i!) + \beta \sum_i \mu_e h_i), \tag{5}$$

where

$$\mu_e = \frac{1}{\beta} \ln(\exp(\beta\mu_A + \beta\mu_B) \tag{6}$$

is the effective chemical potential for the variables h_i. This reduced theory can be numerically solved in equilibrium by transfer matrix methods.

The goal of this paper is to study how this modified solid on solid model is modified when subjected to driving. The driving here is introduced by adding a force acting on the particles of type A which are subjected to local diffusive or Kawasaki dynamics. The particles of type B are also subjected to diffusive dynamics.

Purely diffusive dynamics is implemented using the following algorithm. At each Monte Carlo step a particle of type A or B is chosen from site i with a probability proportional to pn_{Ai} and $(1-p)n_{Bi}$ respectively. This means that, at any given Monte Carlo step, the probability one tries to move a particle of type A at site i to the left or right is given by $p(A_i) = pn_{Ai}/(pN_A + (1-p)N_B)$, while the corresponding probability one tries to move a particle of type B is $pn_{Ai}/(pN_A + (1-p)N_B) = Cpn_{Ai}$. The associated energy change is ΔH is computed and the acceptation of the move is made based on the Metropolis algorithm. For instance, the probability of moving a particle of type A from site i to $i+1$ is given by $q_{1\to 2} = \frac{1}{2}Cpn_{Ai}\min\{1, \exp(-\beta[H_2 - H_1])\}$, where H_1 and H_2 denote the energy of

the initial and attempted final state respectively, here C is a global normalisation constant. The reverse move occurs with probability $q_{2\to1} = \frac{1}{2}Cp(n_{Ai+1}+1)\min\{1, \exp(-\beta[E_1 - E_2])\}$. The ratio of the equilibrium Boltzmann weights of the final and initial states is given by

$$\frac{W_2}{W_1} = \frac{\exp(-\beta E_2)}{(n_{Ai+1}+1)!(n_{Ai}-1)!} \times \frac{n_{Ai}!(n_{Ai+1})!}{\exp(-\beta E_1)} = \frac{n_{Ai}}{(n_{Ai+1}+1)} \exp(-\beta[E_2 - E_1]) = \frac{q_{1\to2}}{q_{2\to1}}, \tag{7}$$

and we see that detailed balance is respected. The value of p sets the relative values of the diffusion constants of the particles of type A and B. It is important to note here that we could have implemented an alternative diffusion dynamics as follows. One chooses a site randomly rather that a particle and attempt to moves a particle to a neighbouring left or right site the move is then accepted with probability $q_{1\to2} = \frac{1}{2}Cpn_{Ai}\min\{1, \exp(-\beta[H_{e2} - H_{e1}])\}$, where H is the effective Hamiltonian, however this does not lead to a dynamics of diffusing particles as the mobility of each site should be proportional to the number of particles at each site.

An added aspect to this model is that we consider the case where the particles of type B are not conserved and can be exchanged with a reservoir. Given a non conserving move has been selected, for to change the particle number at site particle at site i by ±1, we accept the change with probability $\min\{1, \exp(-\beta[H_{e2} - H_{e1}])\}$, this means that the number of particles of type B do not affect the rate at which the moving is attempted, this is physical as it is only the uppermost particle that is involved. The dynamics thus defined again obeys detailed balance.

Therefore combined conserved and diffusive Monte Carlo is implemented via the following discrete time algorithm. With probability p_d we choose to implement a diffusive change and with probability $1-p_d$ we implement a nonconserving move. In the case of a diffusive move a particle of type A is chosen at size i with probability $pn_{Ai}/(pN_A+(1-p)N_B)$ and a particle of type B is chosen with probability $pn_{Ai}/(pN_A + (1-p)N_B)$. The particle chosen attempts to move left or right with probability $1/2$, the change is accepted with probability $\min\{1, \exp(-\beta[H_2 - H_1])\}$. The algorithm is not perfect from a physical point of view as as the density of particles increases the probability of diffusion should increase relative to that of evaporation. That is to say $\frac{p_d}{1-p_d} \sim (pN_A + (1-p)N_B)/L$ where L is the number of sites. However as $N_{A/L} = \overline{n}_{A/B}$ is an extensive quantity the approximation will be good for large $\overline{n}_{A/B}$.

For a nonconserving more a site i is selected randomly and uniformly. With probability $1/2$ one attempts to add a particle and with probability $1/2$ one attempts to takeaway a particle. The resulting change is accepted with probability $\min\{1, \exp(-\beta[H_{e2} - H_{e1}])\}$

To test the algorithm with a view to studying the driven system, we have implemented it in the case of no driving and have compared the results with the equilibrium transfer matrix for the effective parameter h_i which we carried out via numerical diagonalisation of the truncated transfer matrix.

II. CONTINUUM THEORY

In order to understand the statics of the model we write a continuum version of the theory with two field $n_A(x)$ and $n_B(x)$ and we take the a Gaussian form for the surface energy

$$H = \int dx \frac{\sigma}{2}[\frac{d}{dx}(n_A + n_B)]^2 + V(n_A(x), n_B(x)) \tag{8}$$

where σ is where

$$V(n_A(x), n_B(x)) = -\mu_A n_A(x) - \mu_B n_B(x) + T n_A(x)[\ln(n_A(x)) - 1] + T n_A(x)[\ln(n_A(x)) - 1]. \tag{9}$$

We have used Stirlings formula and thus assumed that the typical value of $n_A(x)$ and $n_B(x)$ are large. We now expand $V(n_A(x), n_B(x))$ by writing $n_A(x) = \overline{n}_A + \phi_A(x)$ and $n_A(x) = \overline{n}_A + \phi_A(x)$ where $(\overline{n}_A, \overline{n}_B)$ is the minimum of $V(n_A, n_B)$. Here we find

$$\overline{n}_A = \exp(\beta\mu_A) \text{ and } \overline{n}_B = \exp(\beta\mu_B) \tag{10}$$

This gives an effective Hamiltonian for the fluctuations ϕ_A and ϕ_B

$$H_f = \frac{\sigma}{2} \int dx [\frac{d}{dx}(\phi_A + \phi_B)]^2 + m_A^2 \phi_A^2(x) + m_B^2 \phi_B^2(x) \tag{11}$$

where

$$m_A^2 = \frac{T}{\sigma \overline{n}_A} \text{ and } m_B^2 = \frac{T}{\sigma \overline{n}_B} \tag{12}$$

A straight forward calculation then shows that the Fourier transform of the connected height-height fluctuation correlation function is

$$\tilde{C}_{hh}(k) = \frac{T}{\sigma}\frac{1}{k^2 + m_e^2}, \tag{13}$$

where $m_e^2 = m_A^2 m_B^2/(m_A^2 + m_B^2)$. We this find

$$\langle h^2 \rangle = \frac{T}{2\sigma m_e} = \frac{1}{2}\sqrt{\frac{T\overline{h}}{\sigma}}, \tag{14}$$

where $\overline{h} = \overline{n}_A + \overline{n}_B$. We thus see that the height fluctuations scale as

$$\delta h \sim (\overline{h})^{\frac{1}{4}}, \tag{15}$$

thus for large average height the expansion carried out here is justified.

III. CONSERVED DIFFUSIVE DYNAMICS OF THE CONTINUUM MODEL

Assuming Brownian dynamics for the particles, the stochastic density functional equations for the continuum fields n_A and n_B are given by

$$\frac{\partial n_A(x)}{\partial t} = \frac{\partial}{\partial x}\beta D_A n_A(x)\frac{\partial}{\partial x}\frac{\delta H}{\delta n_A(x)} + \frac{\partial}{\partial x}\sqrt{2D_A n_A(x)}\eta_A(x,t) \tag{16}$$

and

$$\frac{\partial n_B(x)}{\partial t} = \frac{\partial}{\partial x}\beta D_B n_B(x)\frac{\partial}{\partial x}\frac{\delta H}{\delta n_B(x)} + \frac{\partial}{\partial x}\sqrt{2D_B n_B(x)}\eta_B(x,t) \tag{17}$$

where D_A and D_B are the diffusion constants of the particles. The noise terms are independent , zero mean, spatiotemporal Gaussian white noise with

$$\langle \eta_A(x,t)\eta_A(x',t')\rangle = \langle \eta_B(x,t)\eta_B(x',t')\rangle = \delta(x-x')\delta(t-t'). \tag{18}$$

As we are interested in what happens when one of the species is driven, we add a term

$$H_D = -\int dx x f n_A(x) \tag{19}$$

to the Hamiltonian, this corresponds to a force which pushes the particles of type A to the right. We also assume periodic boundary conditions, and thus a current will exist in the resulting steady state. This introduces term in the equation for $n_A(x)$ which becomes

$$\frac{\partial n_A(x)}{\partial t} + \frac{\partial}{\partial x}D_A\beta f n_A(x) = \frac{\partial}{\partial x}\beta D_A n_A(x)\frac{\partial}{\partial x}\frac{\delta H}{\delta n_A(x)} + \frac{\partial}{\partial x}\sqrt{2D_A n_A(x)}\eta_A(x,t). \tag{20}$$

It is important to note that in the absence of the particles of type B, the resulting equation for the field $n_A(x,t)$ can be rendered independent of the force f via the Galilean transformation

$$n(x,t) = n(x - vt, t) \tag{21}$$

where $v = D_A\beta f$ is the induced drift on the particles of type A. Note that the Galilean invariance can also be broken if the force f acts on both particle types but the diffusion coefficients D_A and D_B are different.

We now expand the deterministic part of the two equations to first order in the density fluctuations about its mean value and the noise terms to zeroth order. This approximation respects detailed balance for the effective quadratic Hamiltonian and has been used with accuracy in a wide variety of contexts. The resulting dynamics of of a model B and Fourier transforming in space gives

$$\frac{\partial\tilde{\Phi}(k,t)}{\partial t} = -\beta\tilde{A}(k)\Phi(k,t) + \tilde{\eta}(k,t), \tag{22}$$

where

$$\Phi(k,t) = \begin{pmatrix} \tilde{\phi}_A(k,t) \\ \tilde{\phi}_B(k,t) \end{pmatrix} \tag{23}$$

The noise correlation function is given by

$$\langle \tilde{\eta}^T(k,t)\tilde{\eta}(k',t')\rangle = 4\pi\tilde{R}(k)\delta(t-t')\delta(k+k') \tag{24}$$

where

$$\tilde{R}(k) = 2\begin{pmatrix} D_A\overline{n}_A k^2 & 0 \\ 0 & D_B\overline{n}_B k^2 \end{pmatrix}, \tag{25}$$

and

$$\tilde{A}(k) = \sigma\begin{pmatrix} D_A\overline{n}_A k^2(k^2+m_A^2) - i\frac{D_A k f}{\sigma} & D_A\overline{n}_A k^4 \\ D_B\overline{n}_B k^4 & D_B\overline{n}_B k^2(k^2+m_B^2). \end{pmatrix} \tag{26}$$

The Fourier transform steady state correlation function matrix defined by

$$\langle \tilde{\Phi}^T(k)\tilde{\Phi}(k')\rangle = 2\pi\delta(k+k')\tilde{C}(k) \tag{27}$$

is then given by the solution to the Lyapounov equation

$$\tilde{A}(k)\tilde{C}(k) + \tilde{C}(k)\tilde{A}^T(-k) = 2T\tilde{R}(k). \tag{28}$$

Solving this we find that

$$\tilde{C}_{hh}(k) = \frac{T}{\sigma}\frac{k^2(m_A^2+m_B^2)(D_A\overline{n}_A[k^2+m_A^2]+D_B\overline{n}_B[k^2+m_B^2])^2 + \frac{f^2}{\sigma^2}D_A^2(2k^2+m_A^2+m_B^2)}{k^2(D_A\overline{n}_A[k^2+m_A^2]+D_B\overline{n}_B[k^2+m_B^2])^2(m_A^2m_B^2+k^2(m_A^2+m_B^2)) + \frac{f^2}{\sigma^2}D_A^2(k^2+m_A^2)(k^2+m_B^2)}. \tag{29}$$

In the equilibrium or non-driven system where $f=0$ the above formula yields the static result Eq. (13). Of particular interest is the strong driving limit where we find that as $f\to\infty$ the result

$$\tilde{C}_{hh}(k) = \frac{T}{\sigma}\left[\frac{1}{k^2+m_A^2} + \frac{1}{k^2+m_B^2}\right] \tag{30}$$

The effect of strong driving is to decouple the fluctuations of n_A and n_B and we see that the total height fluctuation is that of the sum two independent interfaces. The height variance is then given by

$$\langle h^2\rangle_s = \frac{T}{2\sigma m_d} \tag{31}$$

where

$$m_d = \frac{m_A m_B}{m_A+m_B} \tag{32}$$

From this we find that

$$\frac{\langle h^2\rangle_s}{\langle h^2\rangle_{eq}} = \frac{m_A+m_B}{\sqrt{m_A^2+m_B^2}}. \tag{33}$$

We also see that, as m_A and m_B are positive, the fluctuations in limit of infinite driving are always larger than in the equilibrium state.

To carry out further analysis we simplify the problem any assuming that the species A and B have the same diffusion constants and chemical potentials and that the only difference is that the applied driving force only acts on particles of type A. We thus write $m_A = m_B = m$, $\overline{n}_A = \overline{n}_B = \overline{n}$ and $D_A = D_B = D$. In this case we find

$$\tilde{C}_{hh} = \frac{T}{\sigma}\left[\frac{1}{k^2+\frac{m^2}{2}} + \frac{2f^2}{f^2+8k^4m^2\overline{n}^2\sigma^2+4k^2m^4\overline{n}^2\sigma^2}\left(\frac{1}{k^2+m^2} - \frac{1}{2k^2+m^2}\right)\right] \tag{34}$$

IV. NON CONSERVED DYNAMICS

We now consider the case where the particles of type B are in contact with a reservoir of the same particles in a vapour phase. To model this we modify the dynamics of the B phase by introducing a component of non-conserved dynamics for these particles

$$\frac{\partial n_B(x)}{\partial t} = \frac{\partial}{\partial x}\beta D_B n_B(x)\frac{\partial}{\partial x}\frac{\delta H}{\delta n_B(x)} + \frac{\partial}{\partial x}\sqrt{2D_B n_B(x)}\eta_B(x,t) - K_B\beta\frac{\delta H}{\delta n_B(x)} + \sqrt{2K_B}\eta'_B(x,t), \tag{35}$$

here if $\eta'_B(x,t)$ is a new spatio-temporal white noise independent of the others, the undriven system obeys detailed balance. Now the average value of the n_B is determined by taking the average in the steady state. As the system is invariant under translation, the average of the first diffusive term on the right-hand-side is zero and so we find

$$\langle\frac{\delta H}{\delta n_B(x)}\rangle = 0, \tag{36}$$

where the averaging is over the system in the steady state. Again invariance by translation in space can be applied to write

$$\langle\frac{\partial V(n_A,n_B)}{\partial n_A}\rangle = 0 \tag{37}$$

Here we have $V(n_A,n_B) = U(n_A) + U(n_B)$ where $U(x) = Tx(\ln(x)-1) - \mu x$ and so expanding about $\overline{n}_A$ we find to second order that

$$\langle U'(\overline{n}_A) + U''(\overline{n}_A)\phi_A + \frac{1}{2}U'''(\overline{n}_A)\phi_A^2\rangle = 0, \tag{38}$$

the equation to first order gives

$$U'(\overline{n}_A) = 0 \tag{39}$$

which gives $\overline{n}_A = n_m$ where n_m is the value for which U attains its minimum. However if we keep the next order term we find

$$U'(\overline{n}_A) + \frac{1}{2}U'''(\overline{n}_A)\langle\phi_A^2\rangle = 0. \tag{40}$$

If the renormalization of the average value of $\overline{n}_A$ is assumed to be small we can write

$$\overline{n}_A = n_m + \delta, \tag{41}$$

which gives

$$\delta = -\frac{1}{2}\frac{U'''(n_m)}{U''(n_m)}\langle\phi_A^2\rangle. \tag{42}$$

For the (entropic) potential in question here we have

$$\delta = \frac{1}{2n_m}\langle\phi_A^2\rangle, \tag{43}$$

we thus see that the average height of the interface is increased due to fluctuations. The non-equilibrium fluctuations are stronger an thus the height increases under driving. Clearly when K is small it causes a small correction to the previous result on out of equilibrium