On The Diffusion of Sticky Particles in 1-D

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This is where I would write the abstract. This is probably best left until the end, as then I'll know what I'm actually summarising.

I. INTRODUCTION

There are a great many natural phenomena which involve the diffusion of small particles through solids; the growth of a titanium dioxide layer on the surface of titanium metal exposed to air is a good example [1]. If we wish to answer questions such as why these interfaces grow, or how quickly, we really need to understand how particles diffuse through crystal lattices, especially in the case when they interact with each other. In this paper we will introduce a very simple locally interacting exclusion model of this kind of diffusion, and we will explore the continuum-level implications of such a model.

By way of example, we would intuitively expect that our titanium interface growth problem would involve the diffusion of oxygen through titanium; once the concentration of oxygen is high enough, the medium becomes titanium dioxide. The oxygen atoms do this primarily by hopping between the interstitial sites between the titanium atoms. It is extremely energetically unfavourable for multiple oxygen atoms to occupy such a site, therefore to a good approximation we may regard these oxygen atoms as excluding each other from these sites, just like in ASEP [2, 3].

Next, I am going to assume that the lattice that the oxygen atoms move through is fairly rigid[4], and that the interactions between the oxygen atoms are quite short-ranged[5] Finally, we should note that even though a problem like interface growth happens in three-dimensional space, the problem is rotationally and translationally invariant in a plane perpendicular to the direction of growth; therefore the interesting aspects of the problem are one-dimensional.Indeed, in anisotropic solids it is often the case that diffusion occurs much more rapidly along parallel chains than in other directions.

Putting all these assumptions together, we are motivated to investigate the model described by the rates detailed in Figure I. It is essentially the symmetric exclusion model, only now the presence of an adjacent particle causes the hopping rate to change. I will henceforth refer to the model as the "sticky hopping model", or SHM.

FIG. 1. Filled circles indicate particles, empty circles indicate empty sites (vacancies). Particles randomly move into adjacent vacancies with rate 1 (having rescaled time for notational convenience), unless there is a particle behind the position they're moving from, in which case they move with rate λ; $\lambda < 1$ represents attractive forces between particles, and $\lambda > 1$ repulsive.

II. MODEL PHENOMENOLOGY

It turns out, having run some numerical simulations that we will discuss later, that the sticky hopping model described above exhibits some rather interesting dynamical behaviour; thus, let's try to examine the model using analytic means, then see how these compare with the numerics. About the easiest way to analyse such a model is using mean-field theory (MFT), so let's do that now.

A. Mean-Field Theory Derivation

Let the spacing between lattice sites be a, τ_0 be the non-sticky hopping timescale and the time-averaged[6] occupation probability of the i^{th} lattice site be ρ_i. It is not difficult to show that, in the mean-field approximation regime,

$$\begin{aligned}\tau_0 \frac{\partial \rho_i}{\partial t} = &(1-\rho_i)\left[\left(1-\zeta\rho_{i-2}\right)\rho_{i-1} + \left(1-\zeta\rho_{i+2}\right)\rho_{i+1}\right] \\ &- \rho_i\left[2\zeta\rho_{i-1}\rho_{i+1} - (3-\zeta)\left(\rho_{i-1}+\rho_{i+1}\right) + 2\right],\end{aligned}$$

where $\zeta = 1-\lambda$ is to be regarded as a "stickiness parameter". Switching to the continuum limit by taking $a \to 0$, and neglecting $\mathcal{O}(a^4)$ terms, we may reexpress this as a conserved flow J as follows:

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= -\frac{\partial J}{\partial x}, \\ J &= -\frac{a^2}{\tau_0} A(\rho) \frac{\partial \rho}{\partial x}, \\ A(\rho) &= 1 - \zeta\rho(4-3\rho).\end{aligned}$$

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Thus, the MFT says that the particles should flow at a rate in proportion to their negative concentration gradient multiplied by a prefactor which is quadratic in the local density.

B. Continuum MFT Predictions

C. MFT Solutions

III. NUMERICAL RESULTS

A. Flow in a Block

B. Correlation Functions

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[1] B. Tegner, L. Zhu, C. Siemers, K. Saksl, and G. Ackland, Journal of Alloys and Compounds **643**, 100 (2015).

[2] K. Sugden and M. Evans, Journal of Statistical Mechanics: Theory and Experiment **2007**, P11013 (2007).

[3] T. M. Liggett, *Interacting particle systems* (Springer-Verlag, Berlin, 1985).

[4] I.e. that the titanium atoms are quite tightly bound and don't move that much, which is reasonable as they are metal atoms in a metal.

[5] Any electrostatic forces should be rapidly screened by the metal, thus the main interaction should be via short-range electrostatics and electron sea distortion.

[6] Or ensemble-averaged, assuming ergodicity.