The Diffusion of Sticky Particles in One Dimension

Driven Stochastic Transport in Low-Dimensional Systems

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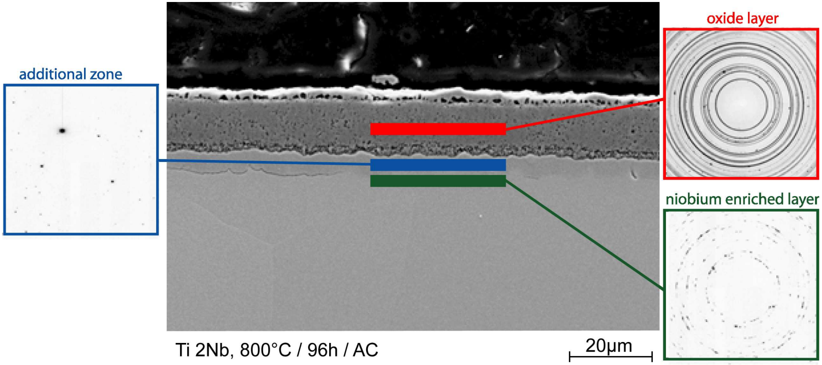
Contents

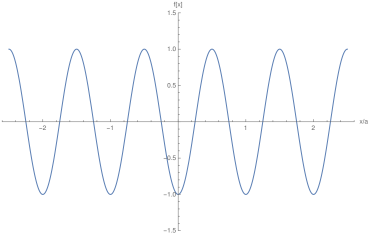
Model Motivation
Formation of an Oxide Layer in Titanium

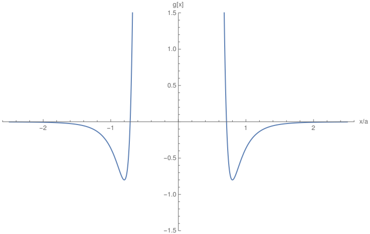


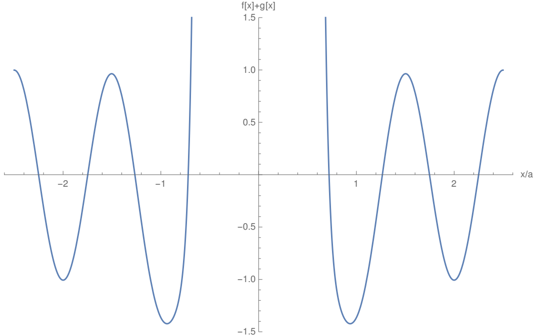
Model Motivation
The Diffusion of Oxygen Atoms in Titanium

Model Motivation

Interactions Between Particles in a Periodic Potential







Model Motivation

My 1D Sticky Lattice Model

$$
\begin{array}{rcll}
\cdots VOV \cdots & \longrightarrow & \cdots VVO \cdots & \text{with rate } 1 \\
\cdots VOV \cdots & \longrightarrow & \cdots OVV \cdots & \text{with rate } 1 \\
\cdots OOV \cdots & \longrightarrow & \cdots OVO \cdots & \text{with rate } \lambda \\
\cdots VOO \cdots & \longrightarrow & \cdots OVO \cdots & \text{with rate } \lambda
\end{array}
$$

- Let $\zeta = 1 - \lambda$, and ρ_i be the ensemble-averaged occupation probability of the i^{th} site in the mean-field approximation.
- Then

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

- Just set the LHS to zero for the steady state.

- Let the lattice spacing be a, and let us take the long-wavelength limit of our MFT, with x as our spatial coordinate, promoting $\rho_i(t)$ to the field $\rho(x,t)$.
- Then we find that

$$\frac{\partial \rho}{\partial t} = \frac{1}{2}a^2\left[(2-2\zeta\rho(4-3\rho))\frac{\partial^2\rho}{\partial x^2} - \zeta\,(2-3\rho)\left(\frac{\partial \rho}{\partial x}\right)^2\right] + \mathcal{O}(a^4).$$

- We can rewrite this as the continuity equation $\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0$, where

$$J = -a^2\left[1-\zeta(4-3\rho)\rho\right]\frac{\partial \rho}{\partial x}$$

Model Phenomenology

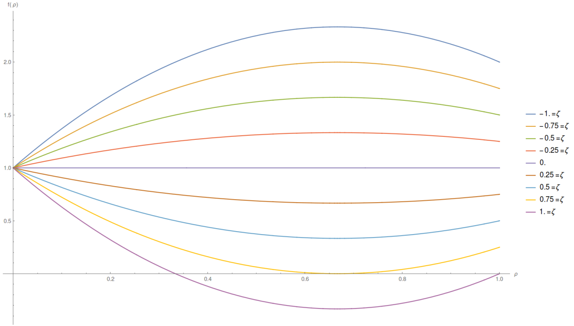
Continuum-Limit MFT Current Flows

- So we can write the current as

$$J = -a^2 f(\rho) \frac{\partial \rho}{\partial x},$$

  where f varies with ζ.

- Varying with respect to ζ yields the following:



Model Phenomenology

Steady State ODE Solutions

- We can actually solve the steady state MFT ODE analytically in the bulk, by recalling that the current flow must be constant and absorbing a:

$$
\begin{aligned}
J_0 &= [1 - \zeta(4 - 3\rho)\rho] \frac{\partial \rho}{\partial x} \\
\int \mathrm{d}x \, J_0 &= \int \mathrm{d}\rho \, [1 - \zeta(4 - 3\rho)\rho] \\
J_0(x - x_0) &= \rho(2\zeta\rho - \zeta\rho^2 - 1),
\end{aligned}
$$

- All we have to do now is solve that cubic for ρ!

- I won't go into the full nature of the solution.
- Our ODE is second order, hence we need to supply two pieces of information to have a well-posed problem.
- We can solve it uniquely on the domain $(0, L)$ where we prescribe the values of ρ on the left and right boundaries to be $\rho_L,\ \rho_R \in (0, 1)$.
- Such a solution is linearly stable so long as $\zeta < \frac{3}{4}$

Numerical Simulation of our Model

Kinetic Monte Carlo

- Recall how we specified our model in the bulk:

$$
\begin{array}{cccl}
\cdots VOV \cdots & \longrightarrow & \cdots VVO \cdots & \text{with rate } 1 \\
\cdots VOV \cdots & \longrightarrow & \cdots OVV \cdots & \text{with rate } 1 \\
\cdots OOV \cdots & \longrightarrow & \cdots OVO \cdots & \text{with rate } \lambda \\
\cdots VOO \cdots & \longrightarrow & \cdots OVO \cdots & \text{with rate } \lambda
\end{array}
$$

- We can simulate it using Kinetic Monte Carlo methods, which are essentially the same as the Gillespie algorithm
- These methods are efficiently implemented in KMCLib (a python-wrapped `C++` code) by Mikael Leetmaa.

Numerical Simulation of our Model

Kinetic Monte Carlo

- We would like to test our MFT predictions about flow rates.
- If we are careful with our boundary conditions, we can setup a situation numerically which should mimic our solution on $(0, L)$ with prescribed boundary values ρ_L and ρ_R.
- The rate of change of the flow through the cell with respect to the concentration gradient across it[1] should be

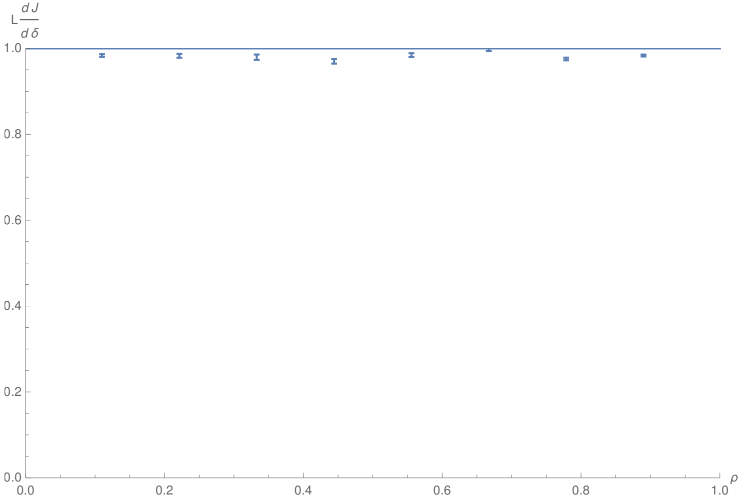
$$L\left(\frac{\partial J}{\partial \delta}\right)_{\delta=0} = 1 - \zeta(4 - 3\rho)\rho,$$

where δ is the concentration difference between the two ends.
- This is something we should be able to directly test using our numerics.

[1] The diffusion coefficient of regular diffusion.

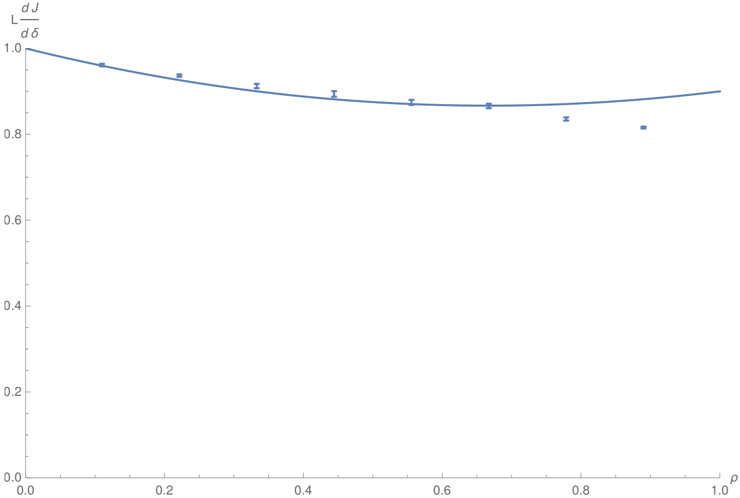
Numerical Results

$\lambda = 1$



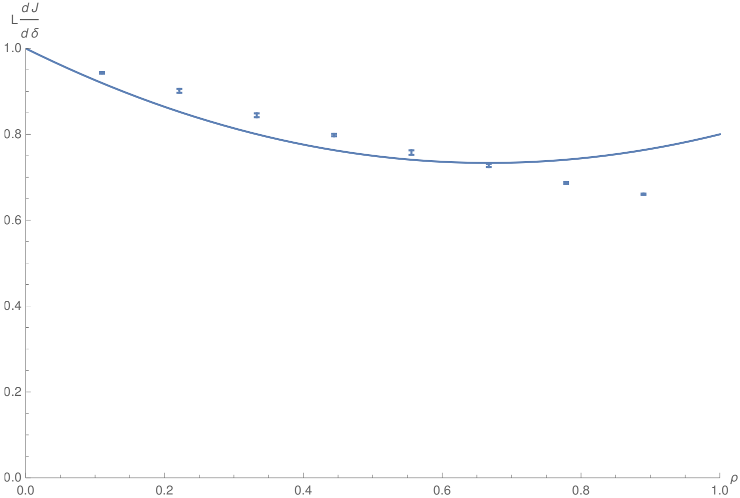
Numerical Results

$\lambda = 0.9$



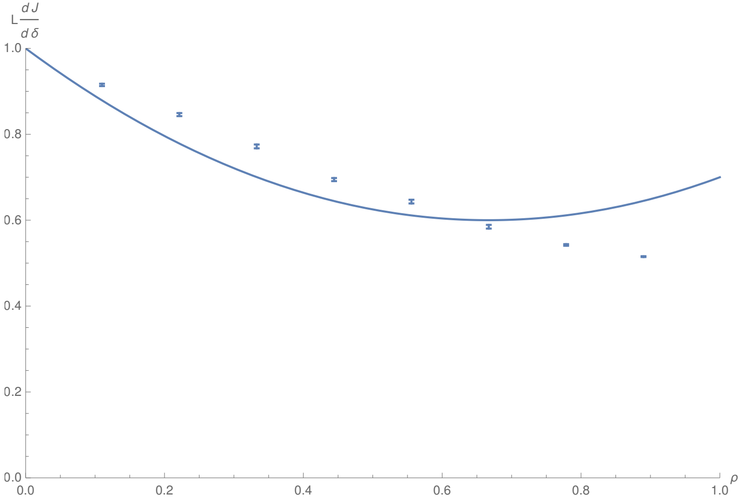
Numerical Results

$\lambda = 0.8$



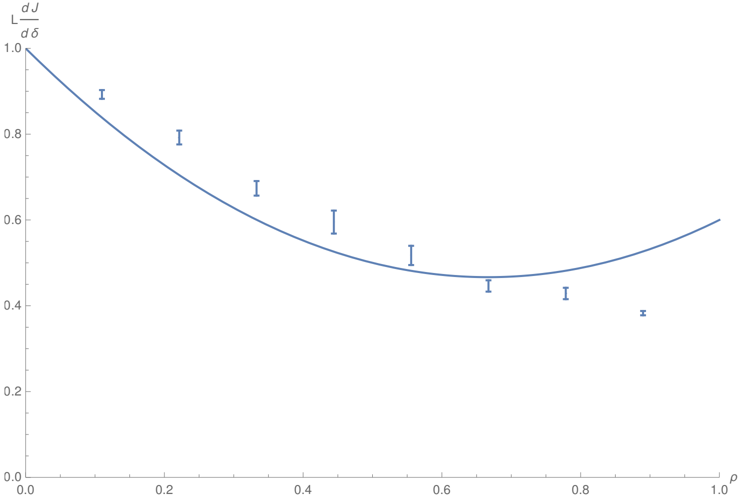
Numerical Results

$\lambda = 0.7$



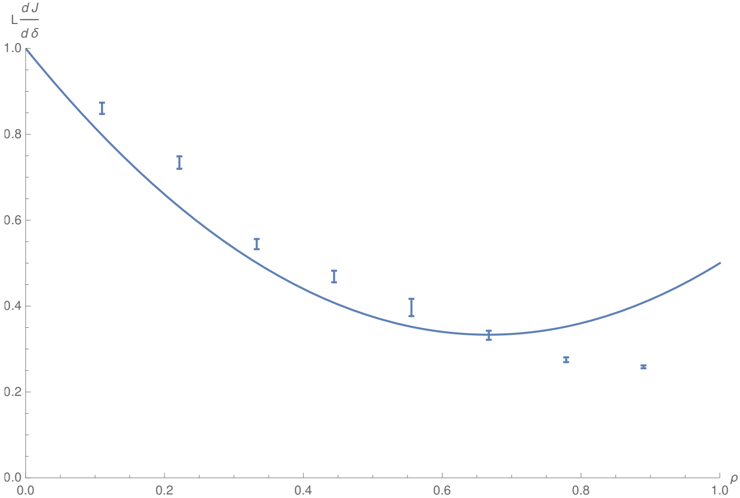
Numerical Results

$\lambda = 0.6$



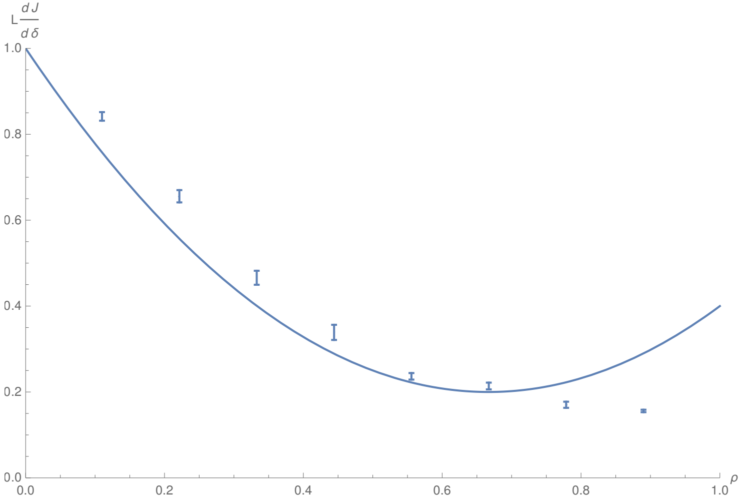
Numerical Results

$\lambda = 0.5$



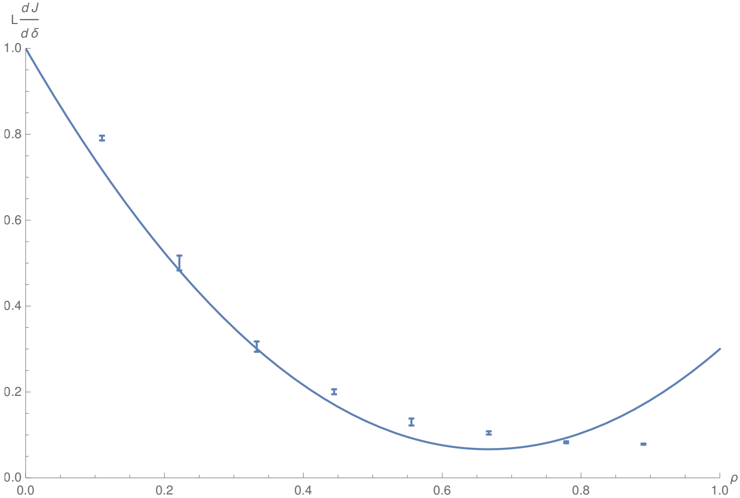
Numerical Results

$\lambda = 0.4$



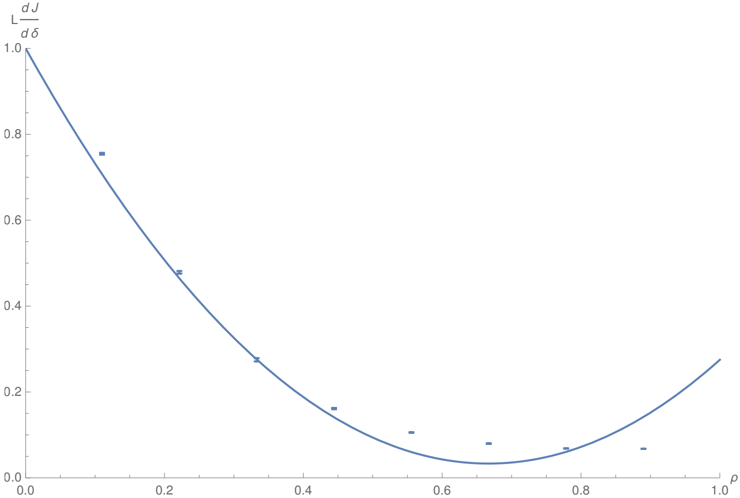
Numerical Results

$\lambda = 0.3$



Numerical Results

$\lambda = 0.275$



Numerical Results

$\lambda = 0.225$