Abstract Submitted for the MAR05 Meeting of The American Physical Society

Collective diffusion in an ordered adsorbate: kinetic lattice gas model approach ZBIGNIEW W. GORTEL, University of Alberta, MAGDALENA A. ZALUSKA–KOTUR, Polish Academy of Sciences — An approach to microscopic kinetics of an interacting lattice gas is proposed to derive an algebraic expression for the coverage dependence of the collective diffusion coefficient in an adsorbate, ordered by strong adatom-adatom repulsive intractions, populating a square lattice of adsorption sites. The starting point are Markovian Master equations for the time dependent probabilities of all accessible microstates of the gas in which jumps of adatoms from occupied to empty adsorption sites are accounted for. The transition rates between the microstates depend on the occupancy state of the adsorption sites around the jumping adatom. The diffusion coefficient is extracted from the lowest eigenvalue of a non-hermitian rate matrix in the long wavelength limit. The eigenvalue is evaluated using an anzatz for the left and the right eigenvectors of the rate matrix with the adsorbate ordering inscribed into the structure of the eigenvectors. Analytic results which have not been obtained yet by any other method are validated by Monte Carlo simulations of the diffusion process.

> Zbigniew W. Gortel University of Alberta

Date submitted: 23 Nov 2004

Electronic form version 1.4