Effects of Short-range Behavior on Interaction Strength Measurements: A Study Using Monte Carlo Simulations

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Steps on a vicinal surface interact via inverse-square elastic and entropic interactions. The step-step interaction strength ($\tilde{A}$) is an important quantity in characterizing a vicinal surface. One of the straightforward ways of measuring it is through the measurement of terrace-width distribution(TWD) of a surface. Steps which cannot touch each other (except at corners) have monatomic height; the associated TWDs are well described by the generalized Wigner surmise. The fit parameter (ϱ) is directly related to the dimensionless energetic interaction strength ($\tilde{A}$). We simulated the TWDs of elastically non-interacting steps with different short-range behavior. Our results indicate that short-range behavior of steps could confound the interaction strength measurements.

Due to their applications in a variety of fields, the study of vicinal surfaces has generated a lot of interested among surface scientists. Step fluctuations, among other surface processes, provide valuable information about the vicinal surface. Since overhangs are energetically forbidden, steps cannot cross each other. This gives rise to an effective entropic repulsion between steps. In addition to this, the strains on a vicinal surface, caused by the sudden extermination of a bulk structure, introduces an elastic interaction between steps. For large step separations, the strengths of both these interactions vary as inverse-square of the distance between steps. As a result, the effective interaction strength can be modeled using a single dimensionless parameter($\tilde{A}$). If steps are prohibited from touching each other, in addition to the no-crossing condition, all the steps are of monatomic height; the minimum separation between steps(d) in this case is 1. The step configurations then correspond to the worldlines of fermions in 1D. The associated TWD can be computed exactly and is given by the generalized Wigner surmise[1]

$$P(s) = a_\varrho s^\varrho e^{-b_\varrho s^2} \tag{1}$$

and the lone fit parameter (ϱ) is related to the dimensionless interaction strength

$$\varrho = 1 + \sqrt{1 + 4\tilde{A}} \tag{2}$$

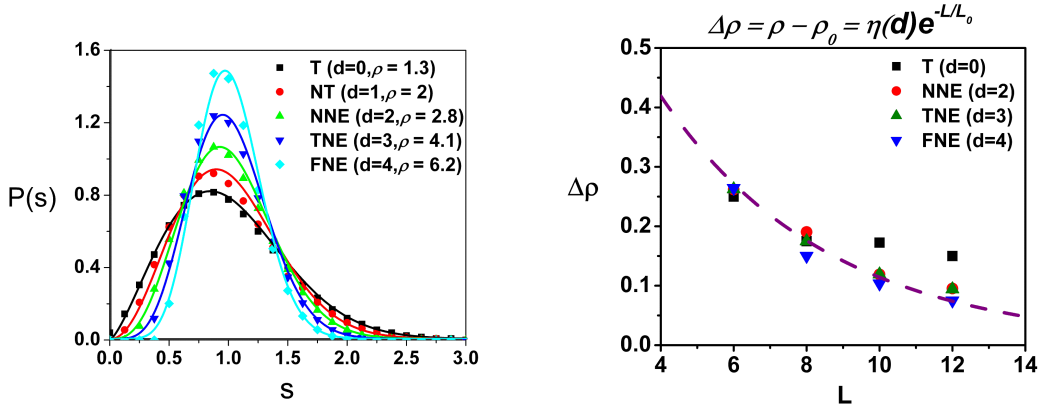
Using Monte Carlo simulations (both metropolis and kinetic), we have simulated the fluctuations of elastically non-interacting steps ($\tilde{A} = 0$) with the following short-range behavior:(i) touching steps (d=0) (ii) steps with hardcore repulsion at small step separations (d>1). From the resultant TWDs, the step-step interaction strength was calculated and compared with the original value of the system ($\tilde{A} = 0$). Our results show that

1. the generalized Wigner distribution describes the TWDs of all of these systems (See Fig.1(a)) and
2. the measured interaction strength is dependent on the type of short-range behavior (given by d) and the mean step spacing (L)

The effects of short-range behavior become smaller as the step separation becomes larger[2] and hence can be modeled as finite-size effects in interaction strength measurements (See Fig.1(b)). The talk discusses this crossover behavior.

References

[1] Hailu Gebremariam, Saul D. Cohen, Howard L. Richards, and T. L. Einstein, *Analysis of terrace-width distributions using the generalized Wigner surmise: Calibration using Monte Carlo and transfer-matrix calculations,* Phys. Rev. B. **69**, 125404 (2004).



(a) (b)

Figure 1: TWDs computed using Monte Carlo simulations: (a) generalized Wigner fits to TWDs of steps with different short-range behavior (b) finite-size effects in interaction strength measurements.

[2] Rajesh Sathiyanarayanan, Ajmi BHadj Hammouda, and T. L. Einstein, *Terrace-width Distributions on Vicinal Surfaces: Effective Attraction Between Noninteracting Touching Steps*, APS March Meeting, New Orleans, 2008