Step Position Distributions and the Generalized Wigner Distribution

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The approximation that justifies the use of the Generalized Wigner Distribution for Terrace Width Distributions also predicts a specific form for the Step Position Distribution (SPD), *i.e.*, the probability density function for the fluctuations of a step about its average position. The predicted form of the SPD is well approximated by a Gaussian, and it agrees well with numerical results obtained from Monte Carlo simulations of the terrace-step-kink model.

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INTRODUCTION

A key factor determining the equilibrium morphology of a vicinal crystal surface is the interaction between the steps on that surface. In many cases, the elastic and electronic contributions to the step-step interaction take the form

$$V(L) = \frac{A}{L^2}\,, \tag{1}$$

where A determines the strength of the step-step interaction and L is the distance between steps. Because this is a typical step-step interaction, and because it has the remarkable property of yielding exact solutions to very plausible approximate theories[1, 2, 3], we confine ourselves in this paper to interactions of the form given in Eq. (1). With this restriction, the quantities discussed in this paper depend only on a single dimensionless parameter,

$$\tilde{A} \equiv \frac{\tilde{\beta} A}{(k_{\rm B}T)^2}\,, \tag{2}$$

where $\tilde{\beta}$ is the step stiffness, $k_{\rm B}$ is Boltzmann's constant, and T is the absolute temperature.

One of the easiest methods[4, 5, 6] for experimentally determining the interaction between steps on a vicinal crystal surface is through the observation of the Terrace Width Distribution (TWD). Typically, this has been done by fitting the TWD to a Gaussian, which is a good approximation and justified by the Gruber-Mullins approximation[7, 8] if the steps strongly repel each other. The step-step interaction is then extracted from the variance of the Gaussian. Unfortunately, however, the Gaussian approximation is only good for strongly interacting steps, and there are conflicting theories[7, 8, 9, 10, 11, 12, 13] regarding the relationship between the step-step interaction and the variance.

Over the past decade[4, 5, 6] it has become apparent that the so-called Generalized Wigner Distribution provides a much better approximation to the TWD. The Generalized Wigner Distribution exhibits the positive skew observed in TWDs from experiments and simulations, and it is a good fit quantitatively to TWDs produced from Monte Carlo simulations of the TSK model. In this article we show that the same theory that predicts the Generalized Wigner Distribution for the TWD also predicts a Gaussian-like distribution for the *position* of steps. For reasons that will be discussed below, the quantitative agreement between the theoretical predictions and measured values of the Step Position Distribution (SPD) are not as good as in the case of the TWD, although the agreement is quite good considering that it is a prediction, not a fit.

PREDICTIONS FROM THE TWO-STEP APPROXIMATION

As was shown in Ref. [3], the Generalized Wigner Distribution can be derived from a phenomenological treatment in which only two steps are treated explicitly, the rest contributing a "confinement potential" related to the two-dimensional pressure and compressibility of the system of steps. We use the usual trick of mapping steps onto the worldlines of one-dimensional spinless fermions, which in this case have the Hamiltonian

$$\mathcal{H} = -\frac{1}{2}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right) + \frac{\tilde{A}}{(x_2 - x_1)^2} + \frac{\omega^2}{2}\left(x_1^2 + x_2^2\right)\,. \tag{3}$$

In this dimensionless formulation, we require that

$$\langle x_2 - x_1 \rangle = 1\,; \tag{4}$$

this fixes the value of ω to

$$\omega = 2b_\varrho\,, \tag{5}$$

where

$$b_\varrho \equiv \left[\frac{\Gamma\left(\frac{\varrho+2}{2}\right)}{\Gamma\left(\frac{\varrho+1}{2}\right)}\right]^2\,, \tag{6}$$

and

$$\varrho = 1 + \sqrt{1 + 4\tilde{A}}\,. \tag{7}$$

After a change of variables to

$$x_{\rm cm} = \frac{x_1 + x_2}{2} \quad (8)$$

$$s = x_2 - x_1 \,, \quad (9)$$

this Hamiltonian becomes separable,

$$\mathcal{H} = -\left(\frac{\partial^2}{\partial s^2} + \frac{1}{4}\frac{\partial^2}{\partial x_{\rm cm}^2}\right) + \frac{\tilde{A}}{s^2} + b_\varrho^2\left(s^2 + 4x_{\rm cm}^2\right) \,, \quad (10)$$

and it has the remarkable property that all of the eigenstates are known. The only eigenstate of interest to us at present, however, is the ground state, which can be written

$$\Psi_{0,0}(s, x_{\rm cm}) = \left[a_\varrho^{1/2} s^{\varrho/2} \exp\left(-\frac{b_\varrho s^2}{2}\right)\right] \times \left[\frac{1}{2\sqrt{\pi b_\varrho}} \exp\left(-4b_\varrho x_{\rm cm}^2\right)\right] \,, \quad (11)$$

where

$$a_\varrho = \frac{2b_\varrho^{(\varrho+1)/2}}{\Gamma[(\varrho+1)/2]} \quad (12)$$

is a constant of normalization. The probability of finding the combination a specific combination of relative separation and "center of mass" is, of course, just $\Psi_{0,0}^2(s, x_{\rm cm})$, which can be rewritten in terms of the original variables x_1 and x_2:

$$P(x_1, x_2) = \Psi_{0,0}^2(s, x_{\rm cm}) = \frac{a_\varrho}{\sqrt{\pi b_\varrho}}(x_2 - x_1)^\varrho \exp[-2b_\varrho(x_1^2 + x_2^2)] \quad (13)$$

subject to the constraint $x_2 \geq x_1$. We can integrate out all possible values of x_2 to find the probability density function for x_1:

$$Q_1(x_1) = \int_{x_1}^\infty P(x_1, x_2)\,{\rm d}x_2 = \frac{a_\varrho}{\sqrt{\pi b_\varrho}} \exp(-2b_\varrho x_1^2) \times \int_{x_1}^\infty (x_2 - x_1)^\varrho \exp(-2b_\varrho x_2^2)\,{\rm d}x_2 \,. \quad (14)$$

As should be expected, the mean value of x_1 is $-1/2$ and the mean value of x_2 is $+1/2$, so we define the analytic SPD to be the calculated probability density function for $x_1 - \langle x_1\rangle$:

$$Q(x) \equiv Q_1\left(x + \frac{1}{2}\right) = \frac{a_\varrho}{\sqrt{\pi b_\varrho}} \exp\left[-2b_\varrho\left(x + \frac{1}{2}\right)^2\right] \times \int_x^\infty \left(x_2 - x + \frac{1}{2}\right)^\varrho \exp(-2b_\varrho x_2^2)\,{\rm d}x_2 \quad (15)$$

Although $Q(x)$ can only be evaluated numerically (it can be rewritten as a complicated expression involving hypergeometric functions, but this does not seem to be genuinely helpful), it is straightforward, though tedious, to calculate its moments. The two most important are the mean, which is zero by definition, and the variance, which is given by

$$\sigma_{\rm SPD}^2 = \frac{1}{4}\left(\frac{\varrho+2}{2b_\varrho} - 1\right) \quad (16)$$

$$\sim \frac{3}{8}\varrho^{-1} \,. \quad (17)$$

These two moments would be enough to entirely specify the SPD if it were a Gaussian distribution, which it should be approximately; the Gruber-Mullins approximation for the TWD, since it concerns the fluctuations in position of only a single step, can be equally well interpreted as an approximation for the SPD. In fact, both the coefficient of skewness[14] and the kurtosis[14] vanish in the limit of strong step-step repulsion. The coefficient of skewness is given asymptotically by

$$\gamma_1 \equiv \frac{\langle(x_1 - \langle x_1\rangle)^3\rangle}{\sigma_{\rm SPD}^3} \sim -\frac{\sqrt{6}}{18}\varrho^{-1/2} \,; \quad (18)$$

note that the coefficient of skewness would have the opposite sign if it had been defined as $\langle(x_2 - \langle x_2\rangle)^3\rangle\sigma_{\rm SPD}^{-3}$. The kurtosis, which is the same regardless of which step is considered, is given asymptotically by

$$\gamma_2 \equiv \frac{\langle(x_1 - \langle x_1\rangle)^4\rangle}{\sigma_{\rm SPD}^4} - 3 \sim \frac{1}{12}\varrho^{-2} \,. \quad (19)$$

The fact that the kurtosis is not exactly zero is not in itself surprising; even within the Gruber-Mullins approximation, the Gaussian distribution is only obtained in the limit of large $\tilde{A}$. The symmetry of our original problem of an infinite number of steps on an infinite vicinal surface, on the other hand, means that the coefficient of skewness, by contrast, *must* be zero for the original problem. Any given step on the surface can be considered "step 1", with its downhill neighbor as "step 2", or it can be considered "step 2", with its uphill neighbor as "step 1"; calling it one or the other breaks the symmetry and permits a nonzero coefficient of skewness.

COMPARISON WITH MONTE CARLO SIMULATIONS

In order to test the usefulness of Eq. (15), we have performed Monte Carlo simulations of the terrace-step-kink (TSK) model and measured the SPD for several values of $\tilde{A}$.

The geometry of the simulated systems was as follows. All simulations were for systems of 30 steps; the length

of each of which was $L_y = 1000a$ (where a is the lattice constant) in the average direction of the steps (the y-direction in "Maryland notation"). The mean step separation was $\langle L \rangle = 10a$, and periodic boundary conditions were applied.

The dynamic used was a local Metropolis update. The temperature was set at $k_{\rm B}T = 0.45\epsilon$, where ϵ is the kink energy; in a previous study, this was approximately the temperature at which TWDs from the restricted TSK model showed the best agreement with the Generalized Wigner Distribution. Each simulation was equilbrated for at least 500 000 Monte Carlo steps per site (MCSS) at the temperature and value of $\tilde{A}$ at which measurements were taken; the initial configurations, however, were not typically straight steps, but steps that had been equilibrated at some other value of $\tilde{A}$. Data was taken from 500 "snapshots," taken at intervals of 1 000 MCSS.

Although the terrace width is always an integer multiple of a in the TSK model, the average step position can be any rational number, depending only on the size of the simulation. Since the step position x is always an integer, the histogram of positions for any given step need not be symmetric.

In order to show concretely what this means, consider a situation in which a Gaussian distribution with mean μ and variance σ^2 is binned into a histogram as follows. The weight assigned to each integer k is given by integrating the Gaussian between $k-1/2$ and $k+1/2$:

$$\begin{aligned} W(k) &= \frac{1}{\sigma\sqrt{2\pi}} \int_{k-1/2}^{k+1/2} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] \mathrm{d}x \\ &= \frac{1}{2}\left\{ \mathrm{erf}\left[\frac{k-(1/2)-\mu}{2\sigma}\right] \right. \\ &\quad \left. - \mathrm{erf}\left[\frac{k+(1/2)-\mu}{2\sigma}\right]\right\}. \end{aligned} \tag{20}$$

For our example, we choose $\sigma = 2.5$ and three "random" values of μ between -0.5 and +0.5. The results are shown in Fig. 1. Clearly none of the histograms is completely symmetric, and the differences between them are noteworthy.

Something similar can and does happen when the SPDs are calculated from Monte Carlo simulations by binning the positions into histograms. As a result, the statistical uncertainties are considerably larger than they are for the corresponding TWDs, and the SPDs are not perfectly symmetric about their peaks, as can be seen in Figs. 2–3. Note the qualitative similarities between the Monte Carlo results (circles) in Figs. 2–3 and the values of $W(k)$ for $\mu = -0.279$ (squares) and $\mu = -0.131$ (diamonds) in Fig. 1. This agreement suggests that during the process of equlibration, the majority of the steps moved slightly to the left (*i.e.*, uphill).

In spite of this, the agreement of the SPDs calculated from simulations and the theoretical $Q(x)$ calcu-

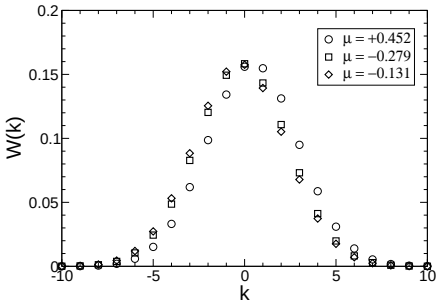

FIG. 1: An illustration of problem that can be caused by the variability of the mean step position when the step position distribution (SPD) is calculted from numerical or experimental results. In this example, Gaussian distributions with identical variances ($\sigma^2 = 2.5^2$) are binned into histograms by means of Eq. (20). The only differences between the three distributions are the values of μ: circles, $\mu = 0.452$; squares, $\mu = -0.279$; diamonds, $\mu = -0.131$.

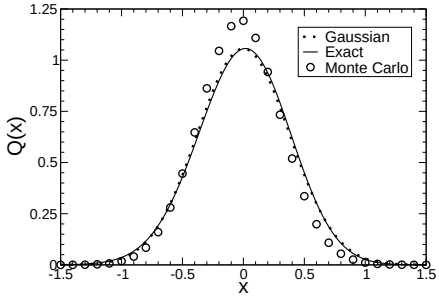

FIG. 2: Comparison of the SPD for $\tilde{A} = 0$ given by Eq. (15) (solid curve) with a histogram SPD from a Monte Carlo simulation (symbols). Also shown is a Gaussian (dotted curve) with a mean of zero and a variance given by Eq. (16).

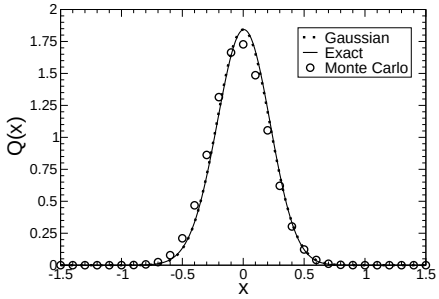

FIG. 3: Comparison of the SPD for $\tilde{A} = 10$ given by Eq. (15) (solid curve) with a histogram SPD from a Monte Carlo simulation (symbols). Also shown is a Gaussian (dotted curve) with a mean of zero and a variance given by Eq. (16).

lated from Eq. (15) is quite good. Even more impressive is the agreement between $Q(x)$ and the Gaussian with zero mean and variance given by Eq. (16). Although Eqs. (18) and (19) imply that the Gaussian approximation will be increasingly good as $\tilde{A}$ becomes large, it is clear from the figures that the Gaussian approximation is good for even for $\tilde{A}=0$.

CONCLUSION

The satisfactory agreement between the SPDs calculated from Monte Carlo simulations and the theoretical SPD given by Eq. (15) are further evidence that the two-step approximation, which also yields the Generlized Wigner Distribution for the TWD, captures the essential physics of a vicinal surface at equilibrium. On the other hand, the nonvanishing coefficient of skewness is clearly an error resulting from the approximation. It is conceivable that the terms in the Hamiltonian given by Eq. (3) representing the net effect of the other steps — *i.e.*, the term $(\omega^2/2)(x_1^2 + x_2^2)$ — could be slightly modified in such a way as to produce a symmetric SPD. However, the asymmetry is already sufficiently small that it seems unlikely that such a modification would be worthwhile, especially since it would almost certainly mar all the main attractions of the current approximation: it is simple, it is separable, and exact expressions are known not only for the ground state but for all of the excited states.

Because the SPD is so well approximated by a Gaussian, it is tempting to compare it directly with Gaussian theories of the TWD. As can be seen in Table 1, in the limit of strongly interacting steps the variance of the SPD is slightly larger than that of the Gruber-Mullins approximation, but less than the variance of the TWD given by either the "Saclay" or "modified Grenoble" approximations. This is reasonable; unlike the Gruber-Mullins Hamiltonian, Eq. (3) does not have fixed walls, so the steps can experience larger fluctuations. In spite of this, since the Gruber-Mullins approximation allows only one step to move, it can be regarded equally as an approximation for the TWD or for the SPD. The fact that the SPD is smaller than the other approximations of the TWD is apparently due to the fact that correlations between fluctuations of adjacent steps are to some degree taken into account in all these approximations, so that they are specifically approximations for the TWD, not the SPD.

In principle, the SPD could be used to determine $\tilde{A}$. However, because the SPD is strongly affected by the random position of the average step position, the TWD is a more practical alternative.

TABLE I: Asymptotic variances in the limit of strong step-step repulsion. The Gaussian-like approximation for the step position distribution (SPD) given by Eq. (15) is compared with selected approximations for the TWD. Except for the Generalized Wigner Distribution, all approximate TWDs are Gaussian approximations. Note also that our approximation for the SPD and the Generalized Wigner Distribution are both independent of the number of interacting steps, whereas the Gaussian approximations are not. (See also Table 1 of Ref. [6].)

Distribution	Reference	Asymptotic Variance
SPD	Eq. (16)	$0.375\varrho^{-1}$
Generalized Wigner	[15, 16, 17]	$0.5\varrho^{-1}$
Gruber Mullins (all steps)	[7]	$0.278\varrho^{-1}$
" (nearest neighbors)	"	$0.289\varrho^{-1}$
Modified Grenoble (all steps)	[9, 10, 15]	$0.495\varrho^{-1}$
" (nearest neighbors)	"	$0.520\varrho^{-1}$
Saclay (all steps)	[11, 12, 13]	$0.405\varrho^{-1}$

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