Step Interactions from Step-Step Correlations: Recent Progress and Remarkable Results for High-Temperature Vicinal Si(111)

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We begin by reviewing theoretical machinery for deducing the strength of repulsions between steps from spatial correlations. There are some noteworthy advantages to studying step-step correlation functions rather than just the terrace width distribution function (i.e. correlations between adjacent steps). Highlights of this work are summarized. These ideas and traditional analyses of spatial and temporal correlations are applied to REM data for vicinal Si(111) above the sublimation temperature, but with a compensating flux, and find striking behavior for the apparent step repulsion strength. To distinguish the atomic-scale mechanisms of evaporation-condensation and diffusion step-to-step, correlations of symmetric combinations of step displacements can be used. This idea is being applied to a chemically heterogeneous Si surface as well as the Si data. Using a Schrödinger equation approach, one can not only present a justification for the generalized continuum Wigner surmise but also contend with complicated step interactions more complicated than inverse square, as might occur due to step interactions mediated by surface states or for small step separations where contributions beyond the leading asymptotic term become important.

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I. INTRODUCTION

At ISSI2k in Nagoya, I spoke of several new directions in the theoretical investigation of the distributions of steps on vicinal surfaces [1]. It was motivated by a decade of quantitative measurements of the widths ℓ of terraces on vicinal surface. A major reason for examining the terrace width distribution (TWD), describing the fluctuations of ℓ from the average value $\langle \ell \rangle$, is that it offers a way to assess the strength of the elastic (and/or dipolar) repulsion between steps. Most notably, we have recognized that since steps on vicinal surfaces should share general features of fluctuating systems, the TWD should exhibit certain universal properties. In this summary paper, we document progress in these and related directions over the last year or so, with some noteworthy experimental illustrations.

To review some basics and set notation, standard analysis procedures of TWD's make a continuum approximation in the direction along the steps, called $\hat{y}$ in "Maryland notation." (The perpendicular direction in the terrace plane, in the "downstairs" direction, then becomes $\hat{x}$.) In the highly successful [2] step continuum approach to vicinal surfaces, equilibrium properties are described in terms of two parameters: the step stiffness $\tilde{\beta}$ and some measure of the strength of the step-step repulsion. The former is essentially the thermal energy divided by the diffusivity, so that

$$\langle [x(y,t) - x(y',t)]^2 \rangle = (k_B T/\tilde{\beta})|y - y'| \tag{1}$$

With ℓ as the difference of the values of x on adjacent steps at the same y and t, the interaction between steps consists of an elastic repulsion per length, to leading order A/ℓ^2, and a temperature-dependent "entropic" repulsion—also $\propto \ell^{-2}$—arising from the physical restriction that steps cannot cross each other. Because step overhangs are physically forbidden and assuming there is insufficient thermal energy to produce islands or pits on the terraces, the set of step configurations in 2D space maps into the world lines describing the evolution of non-crossing particles (spinless fermions or hard bosons) in 1D space. This mapping is what leads to most of the progress in theoretical understanding. In the subsequent description of TWD's, A appears only in form of a *dimensionless interaction strength*

$$\tilde{A} \equiv A\tilde{\beta}(k_B T)^{-2} \ . \tag{2}$$

In experimental systems $\tilde{A}$ is typically between 0 and 15 [2–5] (cf., esp., Table 2 of Ref. [1]).

A. Gaussian Approximations to TWDs

Written in terms of the dimensionless parameter $s \equiv \ell/\langle\ell\rangle$, the TWD, $P(s)$, is not just normalized but has unit mean. The Gaussian approximation to the TWD takes the form:

$$P(s) \approx P_{\mathrm{G}}(s) \equiv \frac{1}{\sigma_G\sqrt{2\pi}} \exp\left[-\frac{(s-1)^2}{2\sigma_G^2}\right] \ . \tag{3}$$

If the repulsion between steps is not too small, the motion of each step is confined near its mean position; a Gruber-Mullins (GM) argument (in which a single step is treated as active and its two neighbors are fixed at twice $\langle\ell\rangle$) shows that, like a fermion in a quadratic potential, the ground-state density is a Gaussian with that [6,7]

$$\sigma^2 = K\tilde{A}^{-1/2}. \tag{4}$$

For the GM case, with interactions only between nearest-neighbor steps, K is $1/\sqrt{48} \approx 0.144$. If all steps interact with A/ℓ^2, then the effective interaction increases by about 8 %, decreasing the variance, and so K (to 0.139).

The Grenoble group [8,9] argued that the GM-derived variance underestimates (for given $\tilde{A}$) the true variance: For very large $\tilde{A}$ the entropy of interaction between steps becomes negligible. Then, assuming *both* steps bounding a terrace fluctuate independently, the σ^2 of the TWD should be the *sum* of the variances of the fluctuations of each step, i.e. *twice* the variance obtained in the GM picture. Due to anticorrelations, σ^2 and so K increase by a factor of 1.801.

Including entropic repulsions in an average way [10] amounts to replacing $\tilde{A}$ in Eq. (4) by an effective interaction strength $\tilde{A}_{\mathrm{eff}} \equiv (1/4)\left(\sqrt{4\tilde{A}+1}+1\right)^2$ obtained from the cubic term of the expansion of the projected free-energy of a vicinal surface as a function of misorientation slope [11]. This modification extends to smaller $\tilde{A}$ the range of viability of this (modified) asymptotic limit. In this approximation, including interactions with all steps decreases σ^2 and so K by nearly 10%. The Saclay group [12], alternatively, makes a continuum approximation in the $\hat{x}$-direction as well as $\hat{y}$ and invokes correlation functions from roughening theory to obtain a result of the form of Eq. (4), again with $\tilde{A}_{\text{eff}}$ replacing $\tilde{A}$, in which σ^2 and K are about 85% of the Grenoble value.

Since the various Gaussian approaches make different fundamental approximations, the detailed relationships between the width of the Gaussian and $\tilde{A}$ differ notably. Even when a TWD can be well fit by a Gaussian, the estimation of $\tilde{A}$ can be ambiguous.

B. Symmetry and Wigner Approximation to TWDs: CGWD

Wigner proposed that fluctuations in the spacings of energy levels of a system (originally nuclei) should exhibit certain universal features depending only on the symmetry—orthogonal, unitary, or symplectic—of the underlying couplings. This insight, developed using random-matrix theory [13,14], has been widely applied to fluctuation phenomena in chaotic systems. The pathway to this valuable information is the description of the equilibrium fluctuations of steps using the (Calogero [15]-)Sutherland [16] model of spinless fermions in 1D, interacting with a repulsion decaying as the inverse square of separation. Remarkably, the TWD becomes equivalent to the distribution of the energy spacings, which can be solved exactly by random-matrix methods for the three symmetries. According to the so-called Wigner surmise, these exact solutions for the three distribution of fluctuations can be approximated by [17]

$$P_\varrho(s) = a_\varrho s^\varrho \exp\left(-b_\varrho s^2\right), \quad \text{with} \quad b_\varrho = \left[\frac{\Gamma\left(\frac{\varrho+2}{2}\right)}{\Gamma\left(\frac{\varrho+1}{2}\right)}\right]^2 \quad \text{and} \quad a_\varrho = \frac{2b_\varrho^{(\varrho+1)/2}}{\Gamma\left(\frac{\varrho+1}{2}\right)}, \tag{5}$$

where b_ϱ is associated with unit mean of $P(s)$ and a_ϱ comes from normalization.

The variance of $P_\varrho(s)$ is

$$\sigma_W^2 = \frac{\varrho+1}{2b_\varrho} - 1 \underset{\varrho\to\infty}{\sim} \frac{1}{2\varrho}. \tag{6}$$

The three symmetries correspond to the values $\varrho = 1$, 2, or 4, respectively. This trio of expressions are outstanding approximations [17]. From the mapping of the step problemonto the Sutherland Hamiltonian [16] comes the relation

$$\tilde{A} = \varrho(\varrho - 2)/4, \tag{7}$$

Inverting Eq. (7) gives $\varrho = 2\sqrt{\tilde{A}_{\text{eff}}}$.

The three special values of ϱ correspond to $\tilde{A} = -1/4$, 0, or 2, respectively. The second case describes steps interacting only via the entropic repulsion, while the first indicates a physically unlikely attraction (which also is not strong enough to produce bunching). The third case, $\tilde{A} = 2$, corresponds to a rather moderate repulsion. As documented in Table 1 of Refs. [1,10], the variance of Wigner's $P_\varrho(s)$ is nearly the same as the exact value. The Saclay and GM estimates are a few percent too low, while the modified Grenoble estimate is much too high.

The crucial question is how to generalize to other values of $\tilde{A}$. We denote use of Eq. (5) for *arbitrary* value of $\varrho \geq 2$, with ϱ related to $\tilde{A}$ by Eq. (7) as the CGWD (continuum generalized Wigner distribution). While no symmetry arguments justify the CGWD form, there are arguments in its favor: $P_\varrho(s)$ should give a decent approximation of the TWD for values of $2 \leq \varrho \leq 4$ since the range in parameter space is small; the Gaussian approximations are manifestly invalid in this regime. For very large $\tilde{A}$, the Grenoble viewpoint becomes compelling: the leading term in the expansion of σ_W^2 in Eq. (6) implies that $K_W = 1/4$ in Eq. (4), with $\tilde{A}_{\text{eff}}$ replacing $\tilde{A}$. (Thus, the CGWD variance approaches the [modified] Grenoble estimate nicely, while the Saclay estimate is notably too small.) Since the CGWD does well for both $\varrho \to \infty$ and ϱ=4, it is a promising candidate for intermediate values. The CGWD not only has the Gaussian behavior expected (from random-walker analogies) at large s but also reproduces the exact power of s for $s \ll 1$: In this limit, the many-step correlation function becomes identical to the pair correlation function, which $\propto s^\varrho$, with a prefactor similar to a_ϱ [18,19]. Finally, we can derive the CGWD from a Schrödinger-equation approach [20].

To test numerically the accuracy of Eq. (5) we have applied standard Monte Carlo methods to the simplest adequate model, the terrace-step-kink (TSK) model for a vicinal simple cubic lattice with unit lattice constant,with kinks of energy ϵ. (Cf. Natori's discussion of the TASK model in this volume.) The stiffness $\tilde{\beta}_{TSK}$ of an isolated step—needed to extract A from $\tilde{A}$—is then simply $2k_BT\sinh^2(\epsilon/2k_BT)$ [21]. This model is obviously *discrete* in the $\hat{y}$ as well as the $\hat{x}$ directions [7,12,21].

C. Monte Carlo Tests

In Fig. 2 of Ref. [1] (cf. note added in proof) we provided some preliminary results for the case $\langle\ell\rangle = 6$ at $k_BT/\epsilon = 0.5$, with $L_y = 200$ and 10 steps. In addition to the standard Metropolis algorithm [22], we use the "refusal-free" n-fold way [23,24], especially for large $\tilde{A}$ (or at low T), where it is believed to be much more efficient than the Metropolis algorithm. The elastic repulsion is here considered only between neighboring steps, a common simplification in Monte Carlo [7,12]. The key result was that the CGWD provides globally the best accounting of the variance as a function of $\tilde{A}$.

Since then we have performed more thorough Monte Carlo simulations to check on the discrepancy between the Metropolis and the n-fold way results in the figure just cited. Our straightforward Metropolis routine could be improved so that it was adequately efficient, even at high $\tilde{A}$. Our n-fold way routine, in contrast, was quite inefficient, especially given the large number of energy classes. Accordingly, we focus our attention on the Metropolis runs. We used larger lattices with 40 steps and $\langle\ell\rangle = 12$, with at least 5 runs at each $\tilde{A}$. To highlight the difference between the various approximations, we plot in Ref. [25] the variance times ϱ, which would be 0.49 in the modified Grenoble and 0.41 in the Saclay Gaussian approximations. The Monte Carlo data rises from the Gruber-Mullins value at small $\tilde{A}$ to the modified Grenoble value at large $\tilde{A}$, tracking closely the prediction of the GCWD. This excellent agreement is curious since the GCWD includes interactions between all steps while our Monte Carlo simulations only allowed nearest steps to interact. Monte

Carlo simulations with essentially all steps interacting (at the same given value of $\tilde{A}$) should have a greater effective repulsion and so a smaller value of the variance, reasoning confirmed by test Monte Carlo simulations. The resulting disagreement, relatively minor on the scale of the experimental errors involved in this subject, should not cause fundamental alarm, since there is no reason to believe that the CGWD would provide an exact solution for the variance at arbitrary $\tilde{A}$.

II. STEP-STEP CORRELATION FUNCTIONS

As advocated as ISSI2k [1] we have analyzed the step correlation function, i.e. the probability of finding another step a specified distance away, regardless of how many steps might lie between them. (For the TWD, no other step can lie between them: it is a many-particle correlation function.) Writing S for this separation divided by $\langle \ell \rangle$, we seek the function $h_\varrho(S)$. Qualitatively, $h_\varrho(S)$ initially increases as S^ϱ, peaks near unity, dips and repeaks at integer values of S, with a monotonically decreasing envelope of these oscillations, so that $h_\varrho(S)$ eventually approaches unity. An advantage of considering $h_\varrho(S)$ is that Forrester [18] produced an exact (but complicated) solution for it at even-integer values of ϱ. While the often-used "harmonic," lattice approximation [26,27] for $h_\varrho(S)$—essentially embodying the Grenoble perspective—proved inadequate for deducing ϱ from data. Fortunately, a recently constructed asymptotic expression [28] provides a good description for $S > 1/2$ (for arbitrary ϱ) and can be joined to $a_\varrho S^\varrho$ for smaller S (cf. discussion near the end of section 2.2 of Ref. [1]).

We applied these ideas in studying REM data for slightly vicinal Si(111) at high temperature, $T = 1100$°C, at which there is sizable sublimation, about 0.015 BL/s. To compensate, a second Si wafer is placed close by, $\sim 100\mu$m away. This "source" wafer is heated independently to a T slightly above the "sample" wafer to ensure that there is no systematic motion—advancement or retraction—of the steps on the sample. (The unique sample holder has been described in detail in Ref. [29].) The experiment and analysis are described in greater detail in Ref. [30]. While the experiment is clearly a steady state situation, it is not obvious that true equilbrium exists since the global system does not have a well-defined T and since there is DC current in the sample (for heating) that can produce an electromigration force. The atomistic motion appears to be EC, but includes a *three-dimensional* component. Of particular interest is comparison with previous investigations of the fluctuations of vicinal Si(111) system by several groups at lower temperatures, primarily in the narrow thermal range above the phase transition (at ~ 860°C) from 7×7 to "1×1" — where steps are already very mobile — but below the onset of significant sublimation.

We first determined the stiffness $\tilde{\beta}$ in three different ways. The most reliable method, making use of Eq. (1), finds slightly above half the $\tilde{\beta}$ of 30 meV/Å obtained at 900°C [31], deemed a calibration standard [32]. From the detailed study by Akutsu and Akutsu [32], which takes into account the geometry of Si(111), we estimate that the stiffness should be reduced by a similar factor of about 1/2.

From the TWD using CGWD, we deduced $\varrho \approx 5$, i.e. $\tilde{A} \approx 4$. However, we feared (without justification, evidently) that this estimate might be biased toward too broad a distribution, i.e. too weak an interaction, due to the occasional but pervasive disappearance (and reappearance) of step images in the digitized frames. Hence, we also — as previously advocated [1]—extracted the step-step correlation function from the data. Since there are only about half a dozen steps in the typical frames, the experimental $h_\varrho(S)$ will vanish for large S. Assuming a simple form for the envelope of $h_\varrho(S)$, we could describe the experimental pair correlations for $\tilde{A}$ around 6 ± 1.

For comparison, at 900°C $\tilde{A}$ is 1.7 [33]. Since $\tilde{A}$ is expected to *decrease* with increasing temperature (cf. Eq. (2); A is normally insensitive to T), our $\tilde{A}$ is strikingly large. We find behavior more like step-flow in growth [34] or etching, even though the coverage is essentially constant. In other words, this steady state situation is not simply equilibrium behavior for 3-dimensional evaporation-condensation, in spite of many similarities. In particular, given the small rate of 3D events, one must question whether some other dramatic change in the surface—but not the steps—has occurred between 900°C and 1100°C. Such changes are known to occur in electromigration on Si(111): behavior between 1000°C and 1180°C is distinctly different from behavior in lower (and in higher) temperature regimes [35].

Alternatively, associated with a deposition rate F is a meandering width which can be *narrower* than that associated with thermal fluctuations restrainted by energetic and entropic repulsions [36], given in Eqs. (4,6). For the *uncompensated* desorption flux at 1100°C, this criterion becomes [30] $d > 400$nm, which is consistent with results in an electromigration experiment on Si(111) [37]. Narrowing during growth has been observed in Monte Carlo simulations [34].

A third possibility, brought out during workshop discussion, was that the electromigration associated with the heating of the sample by DC current might be involved. (Note that this is not equivalent to step bunching, since we are concerned with the fluctuations about the mean positions of the steps, not what this mean is.)

III. CORRELATIONS OF IN-PHASE FLUCTUATIONS

We first summarize some the key results [38] for correlation functions for a vicinal surface, then note some recent applications. Writing the fluctuations of the $n^{\underline{th}}$ step around its mean position as $x_n(y,t)$ implies $\langle x_n(y,t)\rangle_{y,t} = 0$. Definitions of the reduced stiffness $\mathcal{S}$ (which has dimensions of length) and of dimensionless measures of the terrace diffusion ($a_q^{\pm}$) and the step-edge diffusion ($b_q^{\pm}$) are [in terms of the kinetic coefficients $\nu_{\pm}$ and the terrace (D_t) and step (D_s) diffusion constants]

$$\mathcal{S} \equiv \Omega\tilde{\beta}/k_BT, \quad a_q^{\pm} \equiv D_t|q|/\nu_{\pm}, \quad b_q^{\pm} \equiv D_s a_{\perp} q^2/\nu_{\pm} \tag{8}$$

the motion of a step can be shown to be related to the position of it and its neighbors by

$$\dot{x}_n(y,t) = -\sum_q \tau_q^{-1} x_{nq}(t) e^{iqy} = -\sum_q \left\{ A_q x_{nq}(t) - B_q \left[x_{n-1,q}(t) + x_{n+1,q}(t) \right] \right\} q^2 e^{iqy}, \tag{9}$$

$$\text{with} \quad A_q \equiv \mathcal{S}(\nu_+ I_q^- + \nu_- I_q^+) \quad \text{and} \quad B_q \equiv \mathcal{S}(\nu_+ a_q^+ + \nu_- a_q^-)/(2E_q \cosh(|q|\ell)). \tag{10}$$

$$\text{Here}\quad E_q \equiv \left[a_q^+(1+b_q^-)+a_q^-(1+b_q^+)\right]+\left[a_q^+a_q^-+\left(1+b_q^+\right)\left(1+b_q^-\right)\right]\tanh(|q|\ell); \tag{11}$$
$$I_q^\pm \equiv \frac{1}{E_q}\left\{a_q^\mp\left(1+2b_q^\pm\right)+\left[a_q^+a_q^-+b_q^\mp\left(1+b_q^\pm\right)\right]\tanh(|q|\ell)\right\}.$$

However, the in-phase/acoustic fluctuations $x_\Sigma(y,t) \equiv \sum_n x_n(y,t)$ satisfy the simpler relation

$$\dot{x}_\Sigma(y,t) = -\sum_q (A_q \mp 2B_q)x_{\Sigma q}(t)q^2 e^{iqy}. \tag{12}$$

Ref. [38] describes the important limiting casesof Eq. (9), and the crossover between them. Two limiting cases are particularly important to aid in distinguishing evaporation-condensation (EC) from diffusion step-to-step (DSS). In the limit $|q|\ell \longrightarrow \infty$, each step behaves as if isolated [39]. Correspondingly $B_q \longrightarrow 0$, so the set in Eq. (9) decouples and reduces to a similar result for the isolated step, with $\mathcal{S}\nu_\mp q^2 I_q^\pm \longrightarrow 1/\tau_q^\mp$.

For isolated-step evaporation-condensation (EC), case B of Ref. [40], the rate-limiting step for mass transport around an isolated step is the random attachment/detachment of adatoms (or vacancies) at the step. This happens in three distinct limits: (i) $a_q^\pm \gg 1$ and $b_q^\pm = 0$, with no motion along the step edge and a uniform reservoir of atoms on the surface. (ii) $b_q^\pm \gg 1$ and $a_q^\pm = 0$, so no terrace diffusion and a reservoir of adatoms at kink sites. Remarkably, this limit also gives q^2 kinetics even though there is no diffusion on the terraces! (iii) $a_q^\pm \gg 1$ and $b_q^\pm \gg 1$, with detachment limited motion on both terraces and steps. Then terms of unity may be ignored, with the eventual usual result $1/\tau_q = 2\mathcal{S}(\nu_+ + \nu_-)q^2$ [31].

For diffusion from step to step (DSS), case D of Ref. [40], the steps are close to each other (i.e. $|q|\ell \ll 1$, implying $\tanh(|q|\ell) \approx \sinh(|q|\ell) \approx |q|\ell$ and $\cosh(|q|\ell) \approx 1$). No step-edge diffusion is allowed ($D_s = 0$). There are three distinct limits: The mass transport is terrace diffusion limited ($a_q^\pm \ll 1$) such that (i) $a_q^\pm \ll |q|\ell \ll 1$, or such that (ii) $|q|\ell \ll a_q^\pm \ll 1$. Alternatively, mass transport is rate-limited by detachment kinetics so that (iii) $|q|\ell \ll 1 \ll a_q^\pm$ in such a way that $a_q^\pm|q|\ell \gg 1$. For the first two cases

$$\dot{x}_\Sigma(y,t) = -\mathcal{S}D_t^2\left(\frac{\nu_+ + \nu_-}{\nu_+\nu_-}\right)x_\Sigma''''(y,t)\ \text{(i)} \qquad \text{or} \qquad \dot{x}_\Sigma(y,t) = -\mathcal{S}D_t\ell x_\Sigma''''(y,t)\ \text{(ii)}. \tag{13}$$

The result for $x_\Sigma(y,t)$ arises because mass is conserved for the step array as a whole in the terrace-diffusion limited kinetics. In the third case $\dot{x}_\Sigma(t) = \mathcal{S}(\nu_+ + \nu_-)x''_\Sigma(t)$.

Lyubinetsky et al. [41] recently applied this idea to Al/Si(111) ($\sqrt{3}\times\sqrt{3}$) using variable-temperature STM. This is the first study of fluctuations on a chemically heterogeneous surface. Measurements were made over a wide range of temperatures, 770 – 1020 K; at the lower limit, the step mobility became too slow, while at the upper limit Al diffusion into the bulk as well as sublimation occurred. From repeated scans over the same y, $G(y,t) \equiv \langle |x_n(y,t_0+t) - x_n(y,t_0)|^2\rangle_{n,t_0}$ is computed. At all temperatures, the traces showed behavior consistent with $t^{1/2}$—characteristic of evaporation-condensation—rather than $t^{1/3}$ or $t^{1/4}$ evolution. To check whether this temporal scaling might be due to DSS, $G_\Sigma(y,t)$ was studied at 870 and 970K. At 870K, the exponent is 0.45, so consistent with evaporation-condensation dominated dynamics. At 970K, the exponent fell to 0.37, suggesting that diffusion plays an increased role.

In studying the high-temperature behavior of Si(111) mentioned earlier [30], $G_\Sigma(q,t)$ showed behavior consistent with evaporation-condensation behavior. Thus, this approach is both feasible and provides a useful complement of information.

IV. INTERACTIONS MEDIATED BY SURFACE BANDS

The oscillatory nature of the indirect interaction between chemisorbed atoms on metal surfaces [42] has attracted theorical attention for over three decades [43]. Usually the mediation is by bulk electronic states, thereby producing interactions which are anisotropic and which exhibits a rapid decay, $1/d_{ij}^5$ with the adatom separation d_{ij} [44]. Although qualitative understanding of the features of the indirect interaction are long known [44], quantitative agreement between theory and experiment proved elusive due to the complicated nature of the substrate electronic states and the interplay of all occupied energy levels at small d_{ij}. While only states near the Fermi level ϵ_F are important at asymptotically large d_{ij} [45], the rapid decay renders these interactions unmeasurable. The recognition [46] that the decay is much slower, going like d_{ij}^{-2} when there are surface states near ϵ_F, provided a means to progress. However, only very recently did theorists [47,48] apply these ideas to the surface states on (111) noble metals, which consist of a single, circularly symmetric, free-electron like band, with in-surface Fermi wavevector $q_{\rm F}$ and Fermi level $\epsilon_{\rm F} = (\hbar q_{\rm F})^2/2m_{\rm eff}$. For two adatoms, '$i$' and '$j$', at asymptotic separation, $d_{ij} \gg \lambda_{\rm F}/2$, the long-range adatom-pair interaction energy is [47,48]

$$\Delta E_{\rm pair}(d_{ij};\delta_F) \simeq -\epsilon_{\rm F} \left(\frac{2\sin(\delta_F)}{\pi}\right)^2 \frac{\sin(2q_{\rm F}d_{\rm ij}+2\delta_F)}{(q_{\rm F}d_{\rm ij})^2} \tag{14}$$

Here the single-adsorbate scattering can be characterized by the Fermi-level phase shift δ_F, which STM measurements of standing-wave patterns [49] show to be large: $\delta_F \approx \pi/2$.

Recent STM investigations of Cu and Co on Cu(111) and Ag(111) [50,51] have not only revealed a direct correlation between inter-adsorbate distances and the period $\lambda_F/2 = \pi/q_F$ of the surface-wave oscillations around the adsorbates, but have also experimentally determined both the asymptotic decay and strength of this electronic adsorbate pair interaction. Similar effects might well arise in step-step interactions [1,42].

V. BEYOND THE WIGNER DISTRIBUTION: SCHROEDINGER APPROACH

As also noted in the ISSI2k proceedings [1], the generalized Wigner distribution can be derived from a plausible, phenomenological model in which two steps interact with each other directly and with other steps through a position-dependent pressure. The arguments have been improved in a manuscript revised since ISSI2k (but cited in the proceedings paper) [20]. Generalizations to more general step-step interactions lead to predictions that are in good agreement with TWDs derived from numerical transfer-matrix calculations and Monte Carlo simulations. This phenomenological approach allows the step-step interaction to be extracted from experimental TWDs. Applications are being made to a large collection of data for vicinal Cu surfaces taken by both Giesen at FZ–Jülich and van Gastel at Leiden at various misorientations and temperatures. The analysis is still in progress.

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