Interactions Between Steps: Entropic, Elastic, and Electronic

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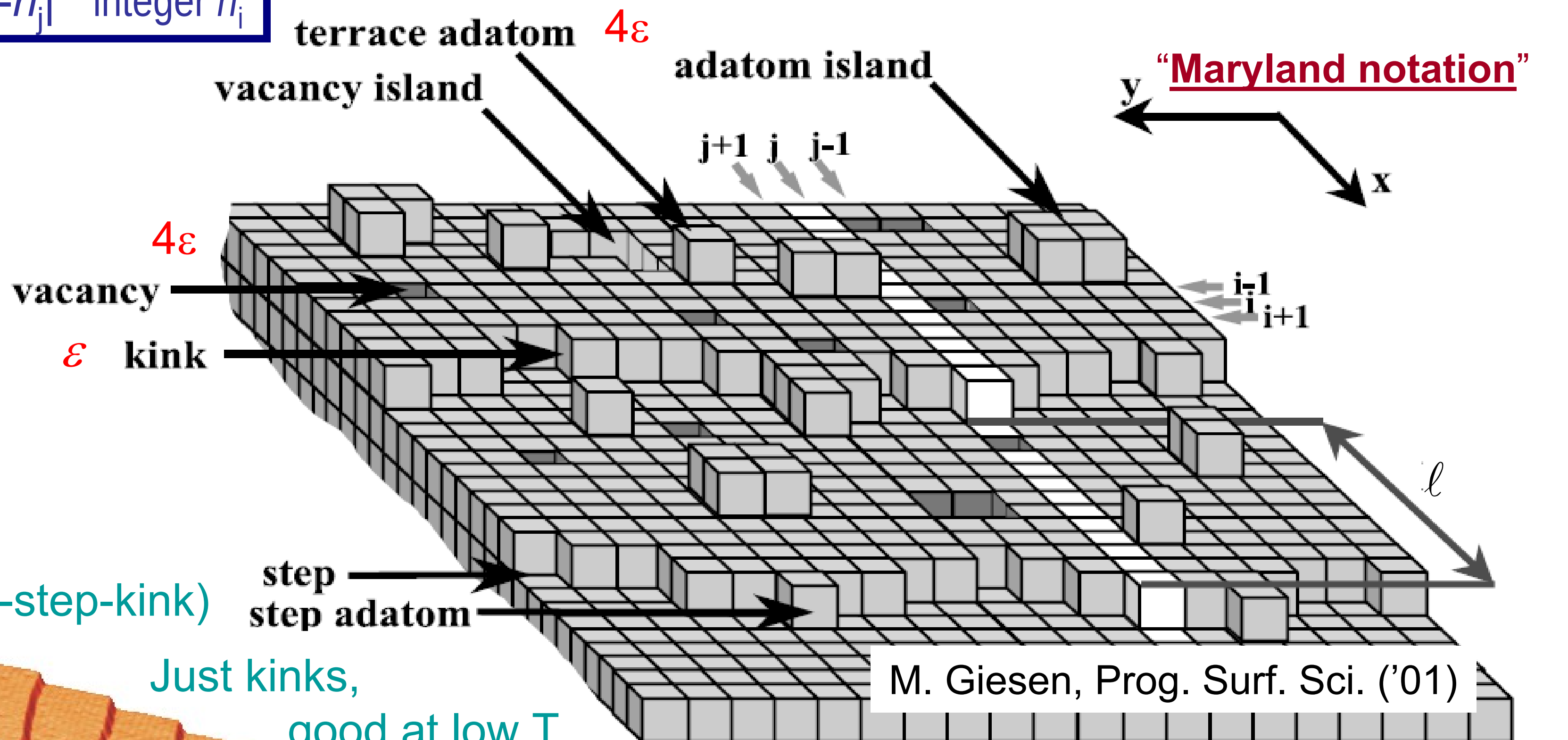
- Stiffness, characteristic energies, etc.
- Terrace width distributions, entropic interactions
- Steps on vicinal surfaces as meandering fermions in (1+1)D...¿interactions?
- Elastic interactions, consequences of simplest isotropic LR form
- Corrections at short range, finite-size effects
- Scaling forms, generalized Wigner distribution for TWD; meaning of ϱ
- Interactions mediated by surface states; new length scale, breakdown of scaling
- Fluctuations of a facet edge (shoreline), understanding Spohn's results

SOS (solid-on-solid) model of vicinals

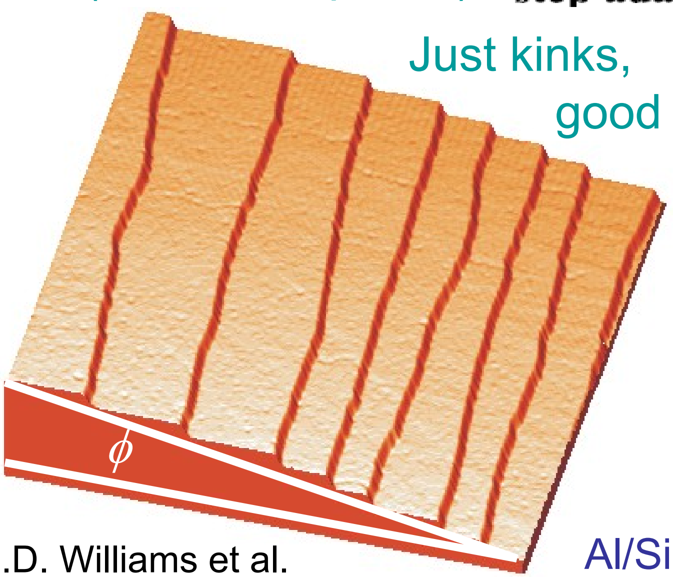
$H = \varepsilon \sum_{\langle ij \rangle} |h_i - h_j|$ integer h_i



M. Giesen, Prog. Surf. Sci. ('01)

TSK (terrace-step-kink)

Just kinks,
good at low T



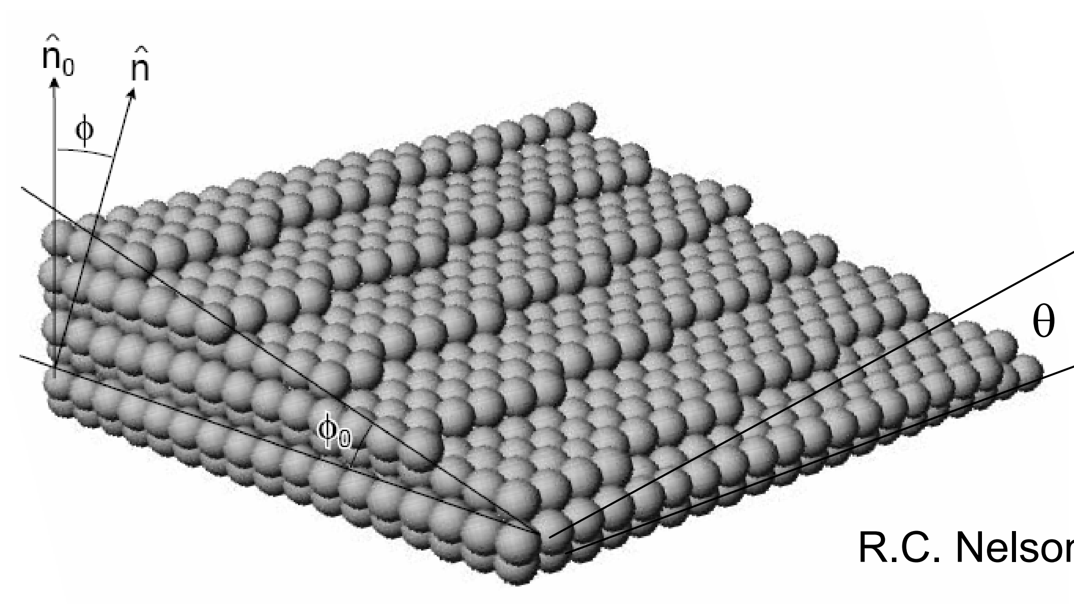
E.D. Williams et al.

Al/Si(111) - (√3×√3)R30°, STM

ϕ is the *misorientation angle*, fixed

Mean step spacing $\langle \ell \rangle \propto 1/\tan(\phi)$

Slope $m = \tan(\phi)$ is a thermodynamic density



R.C. Nelson, TLE, et al., Surf. Sci. 295 ('93) 462

f : *projected* free energy per area = surface free energy per area/cos(ϕ)

Vicinal expansion: $f = f_0 + (\beta/h) \tan \phi + g \tan^3 \phi = f_0 + [\,(\beta/h) + g \tan^2 \phi] \tan \phi$

$\tan \phi = h / \langle \ell \rangle$ = step density $\qquad$ β since 1 dimension lower than γ ?!?

Rough: $f - f_0 \propto \tan^2 \phi$

Kink energy ε: $f(\phi_0,\theta) = f_0 + (\tan(\phi_0)/h)[\beta(0) + (\varepsilon/b) \tan \theta]$

Extracting key energies from slab calculations

- To estimate energy of flat (singular) surface from slab calculation:

$$\mathscr{E}_{\text{fl}} - \mathscr{N}_{\text{fl}} E_{\text{bulk}} = 2 A_{\text{fl}} f_0$$

- To estimate step energy per length, use **awning** ("auvent") approximation:

Step [free] energy per length β = *f* of riser × length along riser – *f* of terrace plane × shaded length [*f* has units of energy/length^2]

{001} $$\beta_{100-\text{str}} \approx \left(\frac{\sqrt{3}}{2} f_{111} - \tfrac{1}{2} f_{100} \right) a_1$$

{111} $$\beta_{\text{A}} \approx \left(f_{100} - \frac{\sqrt{3}}{3} f_{111} \right) a_1 \qquad \beta_{\text{B}} \approx \left(f_{111} - \tfrac{1}{3} f_{111} \right) a_1 \frac{\sqrt{3}}{2} = f_{111} a_1 / \sqrt{3}$$

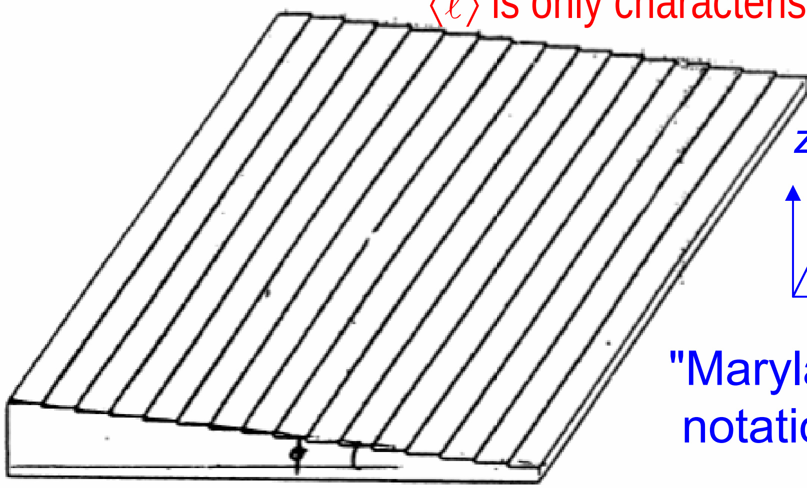
- Similarly, kink energy ε_k can be obtained using a lower-D awning approximation.

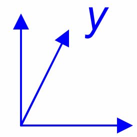
R.C. Nelson, TLE, et al., Surf. Sci. 295 ('93) 462

Terrace-Width Distribution $P(s)$ for Special Cases

"Perfect Staircase" $\ell = \langle \ell \rangle \equiv 1/\tan \phi$ $s \equiv \ell / \langle \ell \rangle$

$\langle \ell \rangle$ is only characteristic length in x

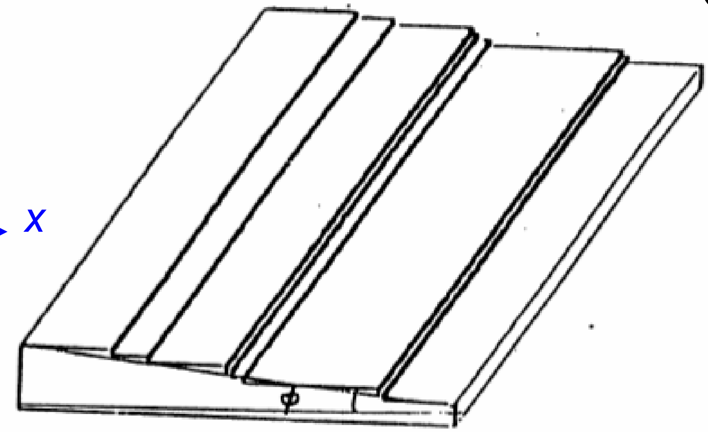




"Maryland notation"

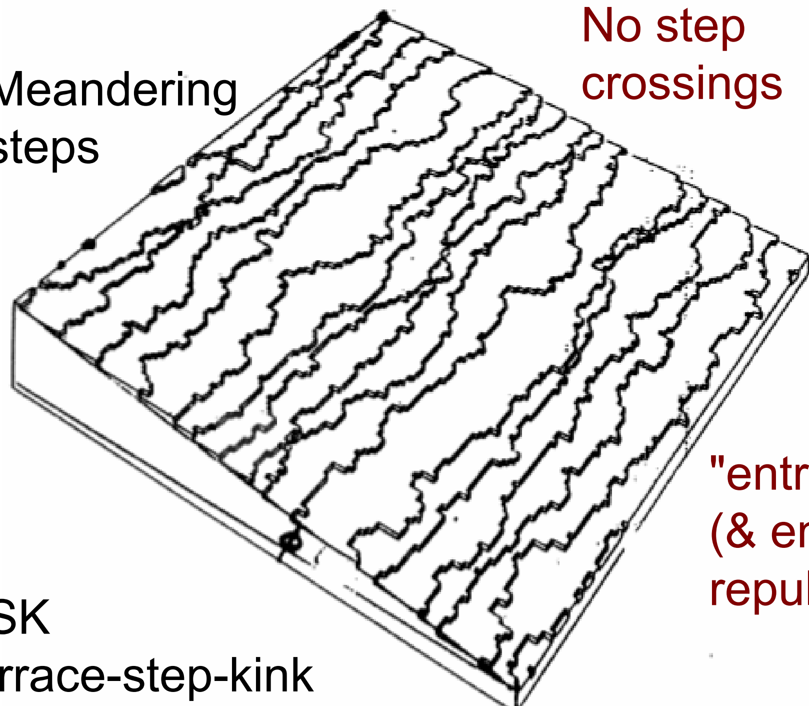
Straight steps, randomly placed

Geometric distribution: $P(s) = e^{-s}$



Meandering steps

No step crossings

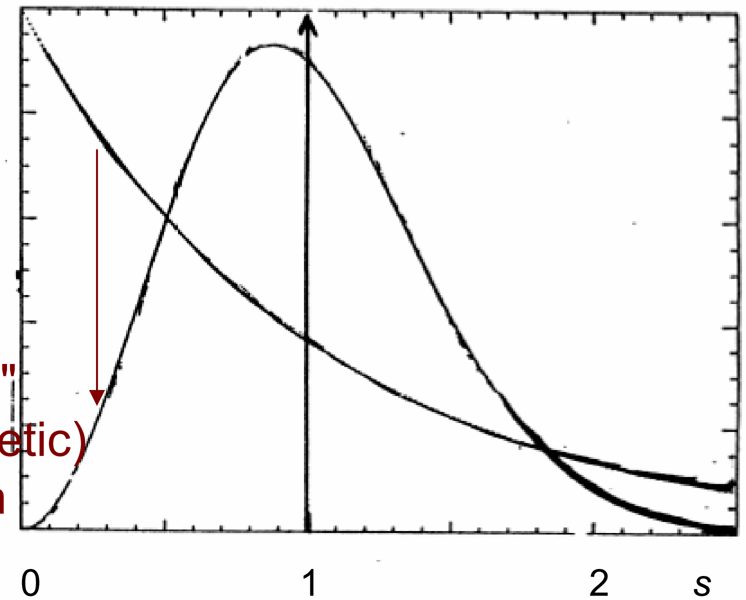


TSK

terrace-step-kink

kink energy ε

Scaled TWD: $P(s)$ indep. of $\langle \ell \rangle$

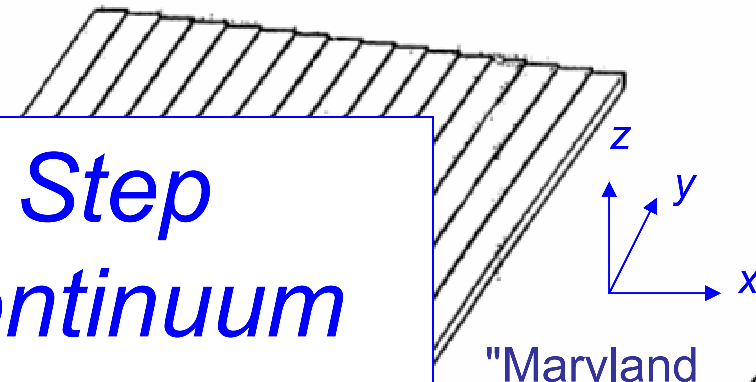


"entropic" (& energetic) repulsion

"static correlation" $\langle x_n(y) - x_{n-1}(y) - \langle \ell \rangle \rangle_{y,n}$

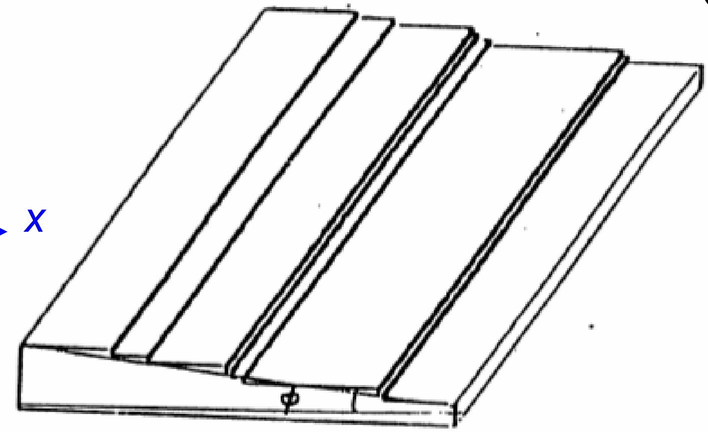
Terrace-Width Distribution $P(s)$ for Special Cases

"Perfect Staircase" $\ell = \langle \ell \rangle \equiv 1/\tan \phi$ $s \equiv \ell / \langle \ell \rangle$



"Maryland notation"

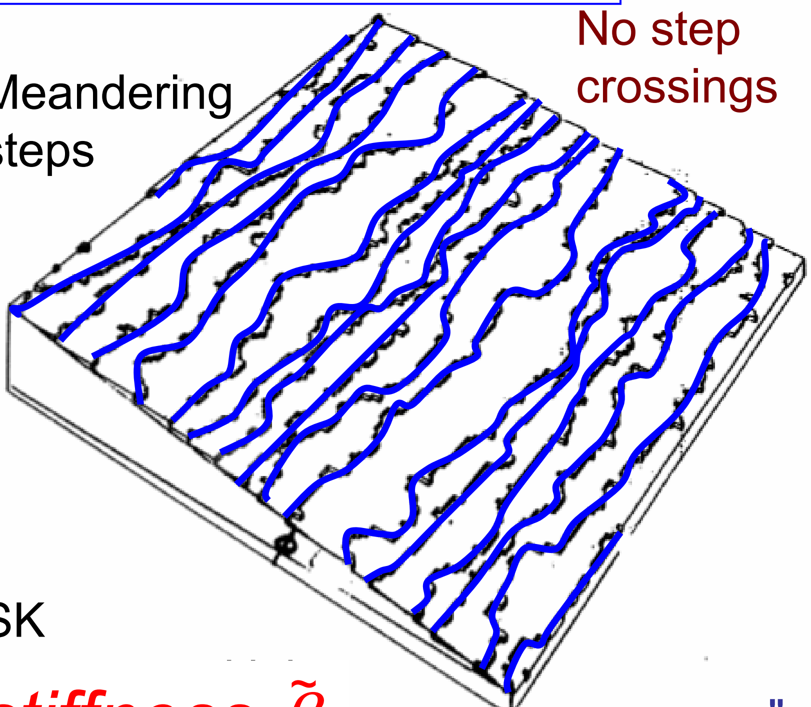
Straight steps, randomly placed
Geometric distribution: $P(s) = e^{-s}$



Step Continuum Model

Meandering steps

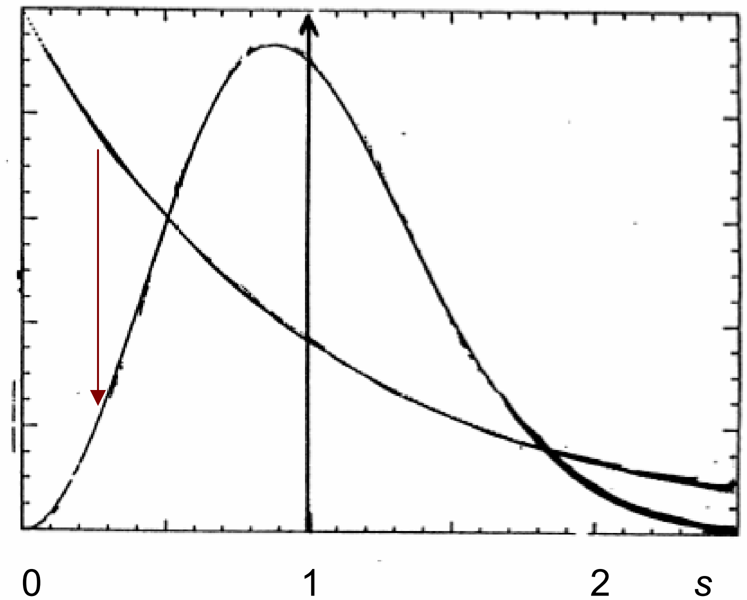
No step crossings



TSK

stiffness $\tilde{\beta}$

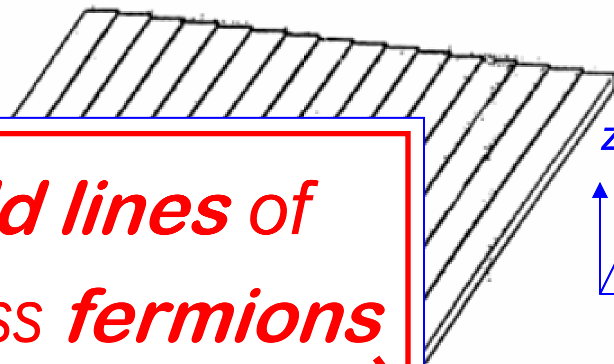
Scaled TWD: $P(s)$ indep. of $\langle \ell \rangle$



"static correlation" $\langle x_n(y) - x_{n-1}(y) - \langle \ell \rangle \rangle_{y,n}$

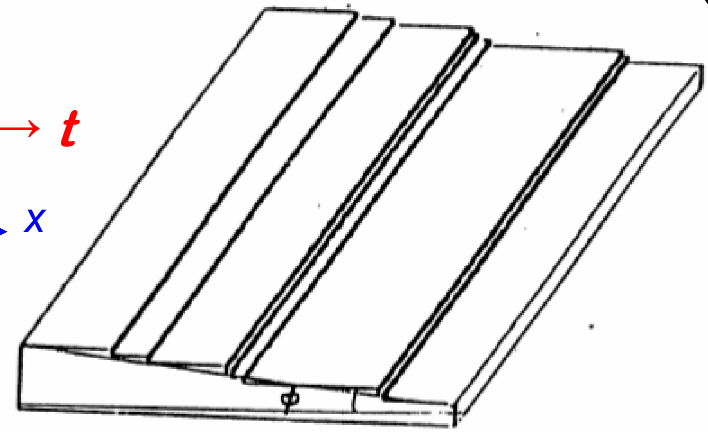
Terrace-Width Distribution $P(s)$ for Special Cases

"Perfect Staircase" $\ell = \langle \ell \rangle \equiv h/\tan\phi$ $s \equiv \ell / \langle \ell \rangle$



Straight steps, randomly placed

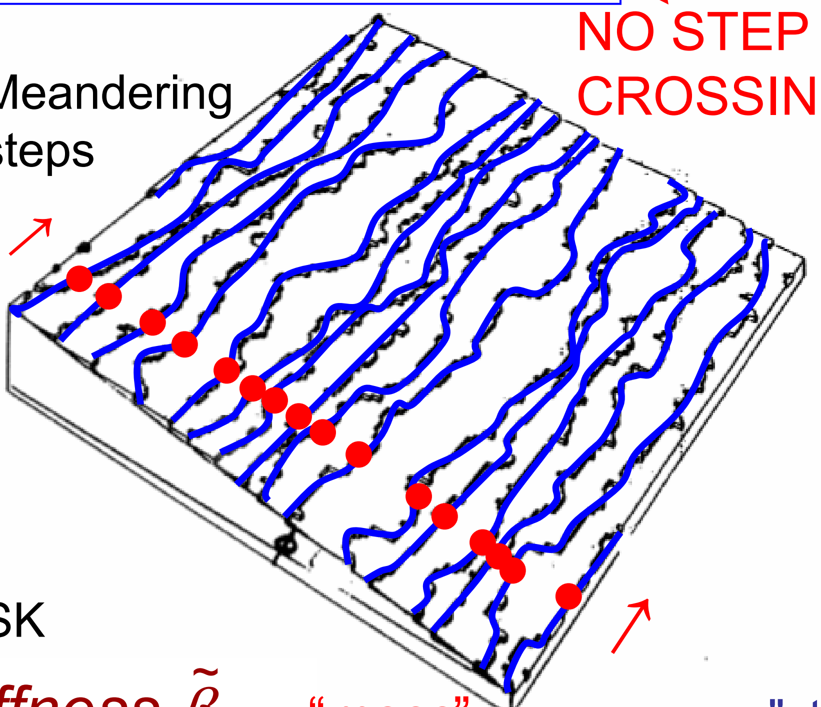
Geometric distribution: $P(s) = e^{-s}$



World lines *of spinless* ***fermions*** *evolving in* ***1D***

NO STEP CROSSINGS

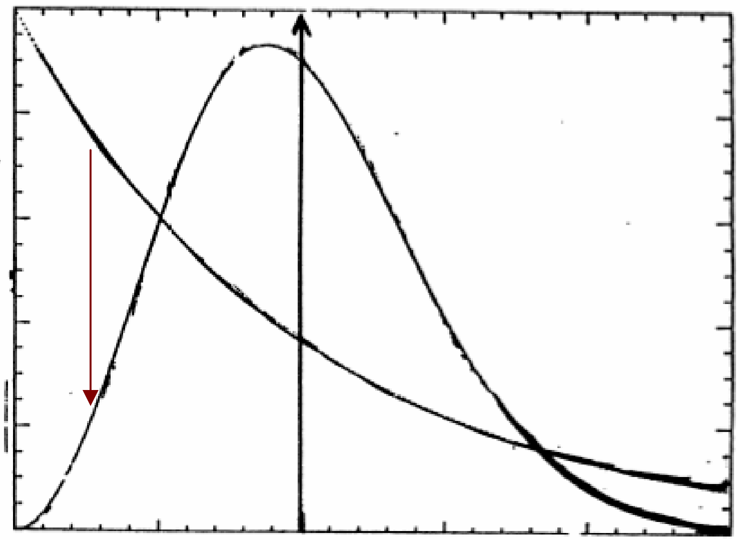
Meandering steps



TSK

stiffness $\tilde{\beta}$ → "*mass*"

Scaled TWD: $P(s)$ indep. of $\langle \ell \rangle$



"static correlation" $\langle x_n(y) - x_{n-1}(y) - \langle \ell \rangle \rangle_{y,n}$

Steps as polymers in 2D ⇒ non-crossing

THE JOURNAL OF CHEMICAL PHYSICS VOLUME 48, NUMBER 5 1 MARCH 1968

Soluble Model for Fibrous Structures with Steric Constraints

P.-G. de Gennes

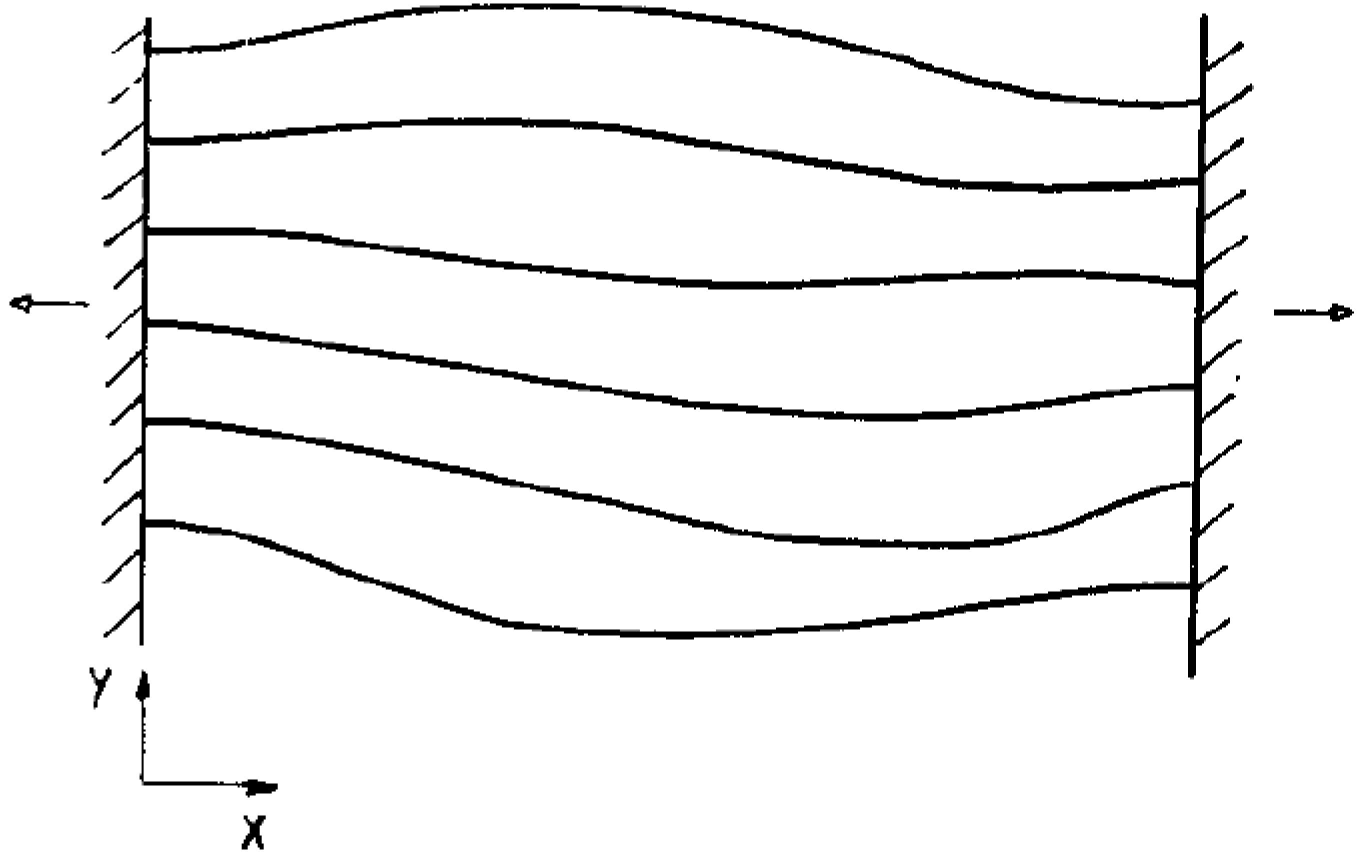
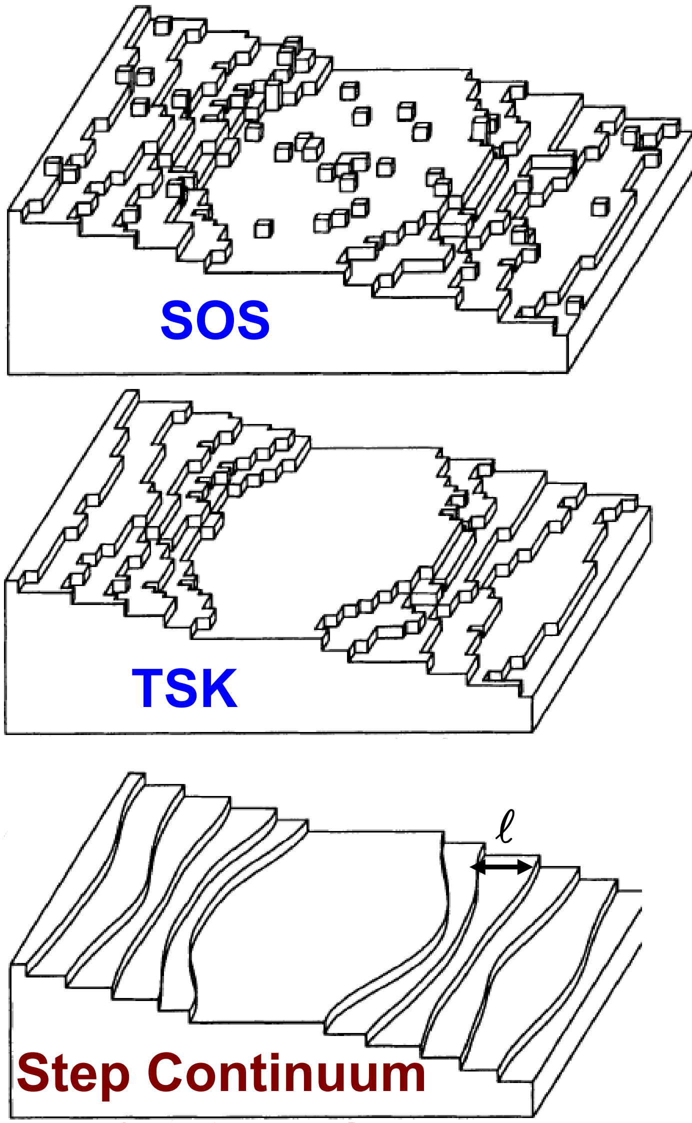


Fig. 1. Model for a two-dimensional fiber structure.

Models & Key Energies

Discrete/atomistic → Step Continuum



ε *energy of unit height difference between NN sites*
+ hopping barriers, attach/detach rates

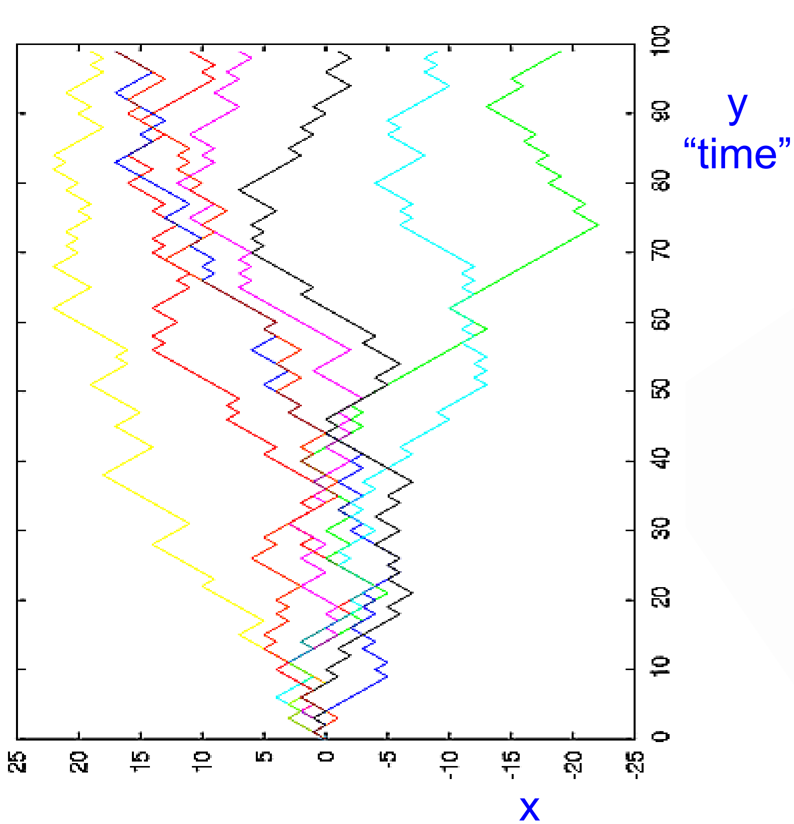
kink energy

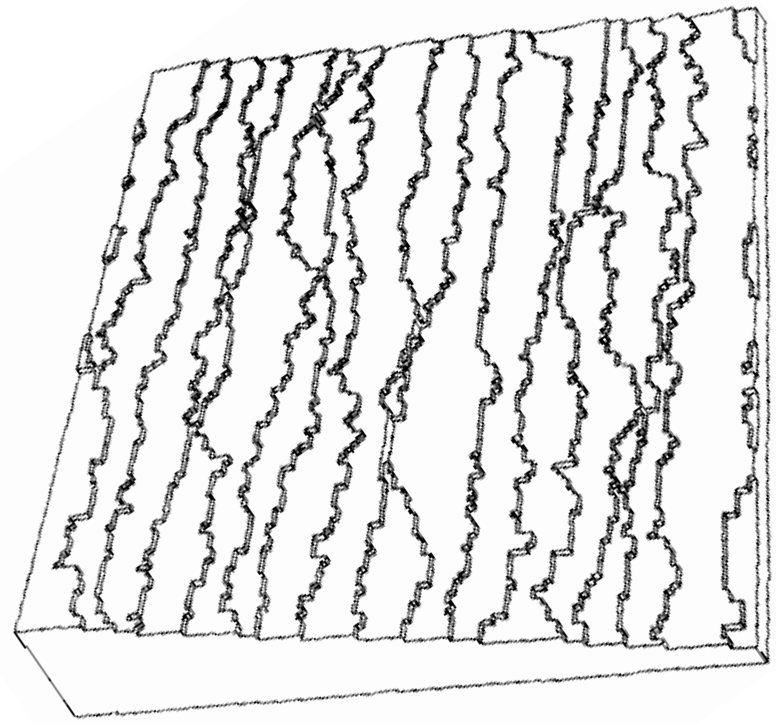
$\tilde{\beta}$ *step stiffness* $\beta(\theta) + \beta''(\theta)$: inertial "mass" of step

A *strength of step-step repulsion A/ℓ^2*

Γ *rate parameter, dependent on microscopic transport mechanism*

Main test: Self-consistency of these 3 parameters to explain many phenomena
Coarse-grain: Relation of 3 nano/mesoscale parameters to atomistic energies??





(b)

$$\langle [x(y+y_0) - x(y_0)]^2 \rangle_{y_0} = b^2\, |y|/a_{\parallel} = (k_B T/\tilde{\beta})\, |y| \quad \rightarrow (\ell/\pi)^2 \ln(|y|/a_{\parallel})$$

Handwaving argument:

"time" (or y) until hit $\propto \ell^2 \Rightarrow$ # hits/"time" $\propto 1/\ell^2 \Rightarrow$ entropic int'n [per length] $\propto 1/\ell^2$

Lose entropy $k_B \ln(2)$ at each hit $\Rightarrow$ free energy rises by $k_B T \ln(2)$

Formal proof: M.E. & D.S. Fisher, Phys. Rev. B 25 ('82) 3192

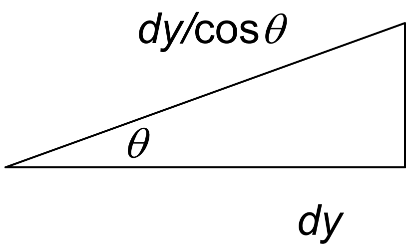
Why Stiffness ? $\tilde{\beta}$

$$\mathcal{E} = \int \beta(\theta)\sqrt{1+\left(\frac{dx}{dy}\right)^2}\,dy \sim \text{const.} + \frac{\tilde{\beta}(0)}{2}\int \left(\frac{dx}{dy}\right)^2 dy \rightarrow \frac{\text{“}m\text{”}}{2}\int \left(\frac{dx}{dt}\right)^2 dt$$

$$\mathcal{E} = \int \beta(\theta)\sqrt{1+\tan^2\theta}\,dy = \int dy\left[\beta(0) + \frac{1}{2}\beta''(0)\theta^2\right] / \cos(\theta)$$

$$\approx \int dy\left[\beta(0) + \frac{1}{2}\beta''(0)\theta^2\right]\left(1 + \frac{1}{2}\theta^2 + \dots\right)$$

$$\approx \int dy\left[\beta(0) + \frac{1}{2}\{\beta(0) + \beta''(0)\})\theta^2\right]$$



$\beta(0)$ due to greater path length

$\beta''(0)$ due to different orientation

M.P.A. Fisher, D.S. Fisher, & J.D. Weeks, PRL 48 ('82) 368

What if we expand around θ_0, where $\beta'(\theta_0) \neq 0$?

$$\beta(\theta) = \beta(\theta_0) + \beta'(\theta_0)(\theta-\theta_0) + \frac{1}{2}\beta''(\theta_0)(\theta-\theta_0)^2 + \dots,$$

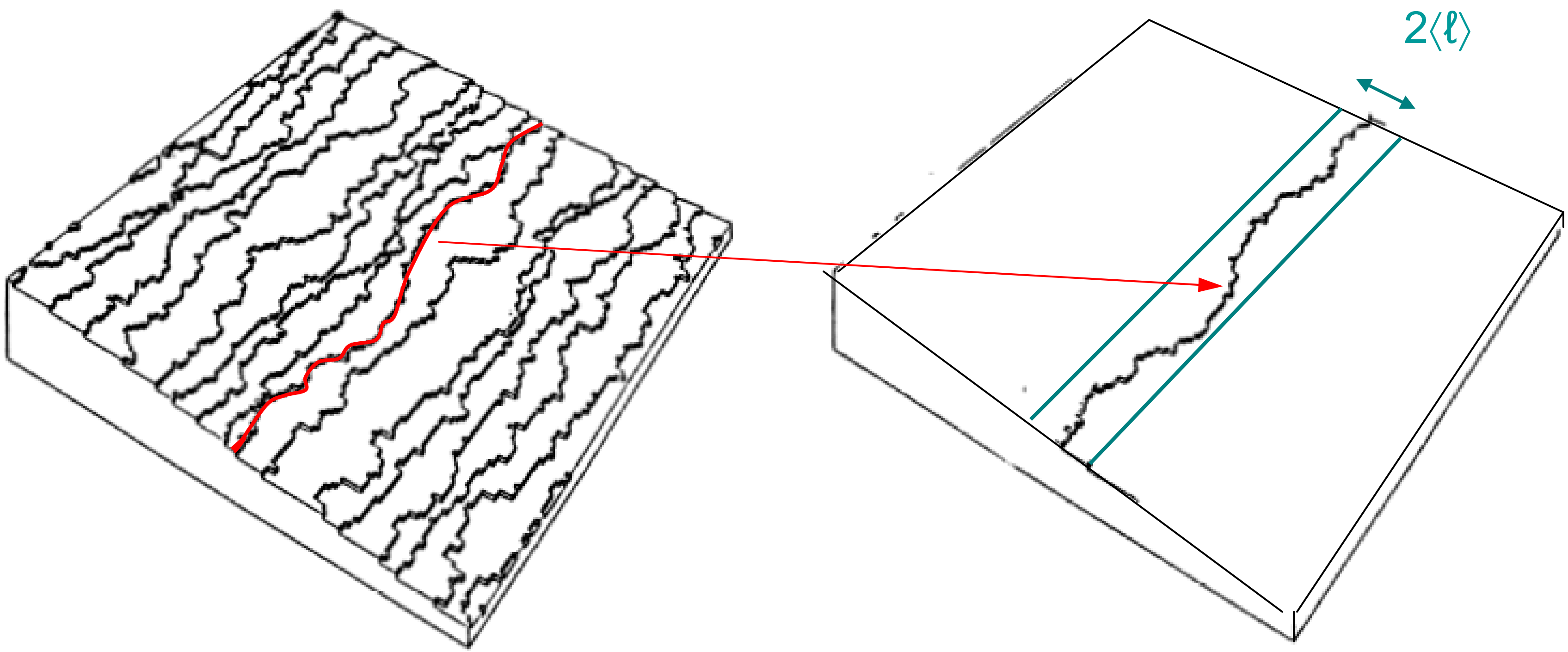
To create this unfavorable orientation, one must apply a torque $-\beta'(\theta_0)$ $(\theta - \theta_0)$ which cancels linear term

H.J. Leamy, G.H. Gilmer, K.A. Jackson, in: *Surface Physics of Crystalline Materials*, ed. by J.M. Blakely (Academic, New York, 1976)

$$\tilde{\beta}(\theta_0) \equiv \beta(\theta_0) + \beta''(\theta_0)$$

Formal proof in T.J. Stasevich dissertation

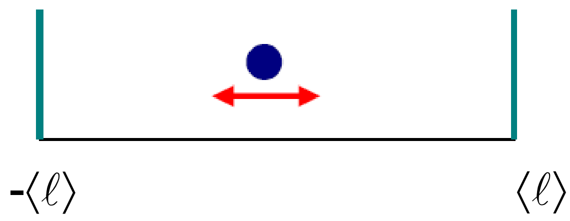
Essence of Gruber-Mullins (MF)



Single active step meanders between 2 steps separated by twice mean spacing.

Fermion evolves in 1D between 2 fixed infinite barriers 2⟨ℓ⟩ apart.

1D Schrödinger equation



$$\frac{\hbar^2}{2m} \rightarrow \frac{(k_B T)^2}{2\tilde{\beta}}$$

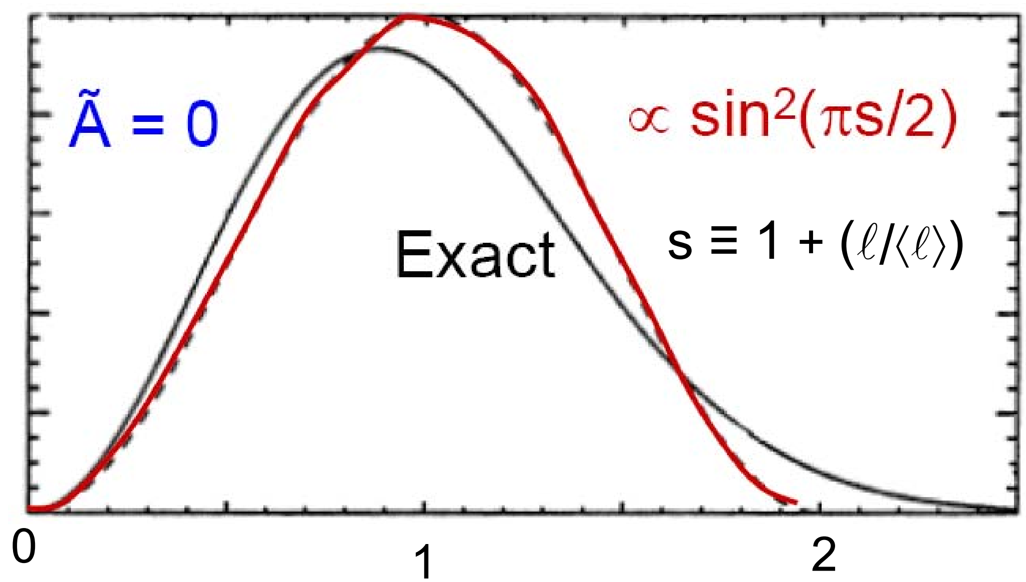
$$-\frac{(k_B T)^2}{2\tilde{\beta}} \frac{\partial^2}{\partial \ell^2} \psi(x) = E\, \psi(x)$$

Ground State

$$\psi_0(x) = \frac{1}{\langle \ell \rangle} \cos\left(\frac{\pi \ell}{2\langle \ell \rangle}\right)$$

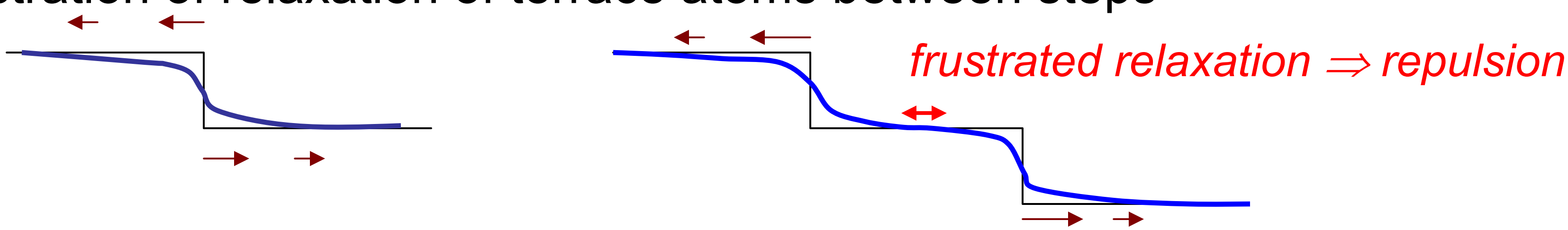
$$E_0 = \frac{(k_B T)^2 \pi^2}{8\tilde{\beta}\langle \ell \rangle^2}$$

Remarkably, E_0 is exactly the entropic repulsion!



Origin of elastic (dipolar) step repulsions

- Frustration of relaxation of terrace atoms between steps



- Energy/length: $U(\ell) = A/\ell^2$ (Same y for points on two interacting steps separated by ℓ along $x \Rightarrow$ "instantaneous")

Importance of step repulsions

- 1 of 3 parameters of continuum step model of vicinals
- Determine 2D pressure
- Determine morphology: e.g. bunch or pair
- Drives kinetic evolution in decay
- Elastic and entropic repulsions $\propto \ell^{-2}$ (entropic from $-\partial^2/\partial\ell^2$)

  $\Rightarrow$ universality of $\langle\ell\rangle^{-1}P(\ell)$ vs. $s \equiv \ell/\langle\ell\rangle$ so $P(s;\langle\ell\rangle) \rightarrow P(s)$ *scaling*

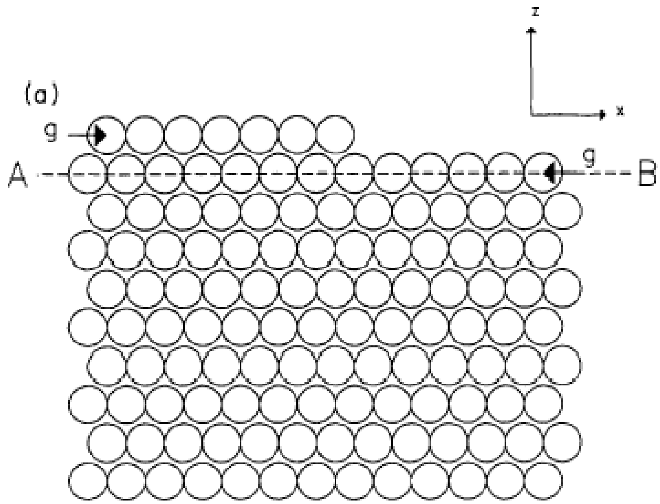
Metallic surface states ⇒ additional oscillatory term in *U*

$U(\ell) \propto \ell^{-3/2} \cos(4\pi\ell/\lambda_F + \phi)$ **new length scale λ_F**

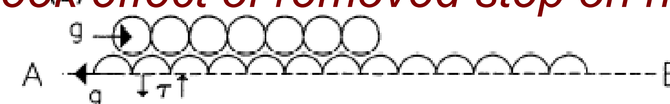
Per Hyldgaard & TLE, J. Crystal Growth **275**, e1637 (2005) [cond-mat/0408645].

How the stress dipole at step edges arises

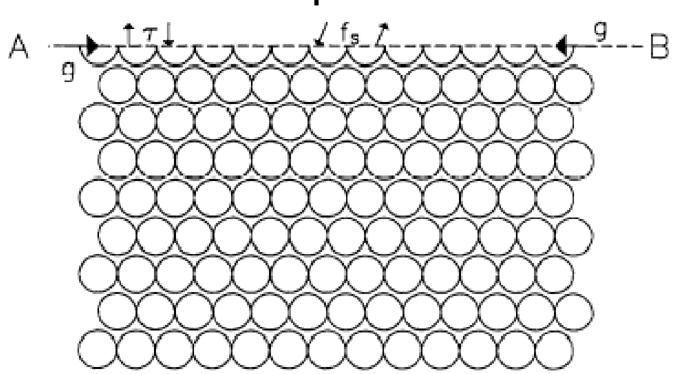
Marchenko argument:stress dipole



Need to get to flat surface for simple calc; seek effect of removed step on next layer



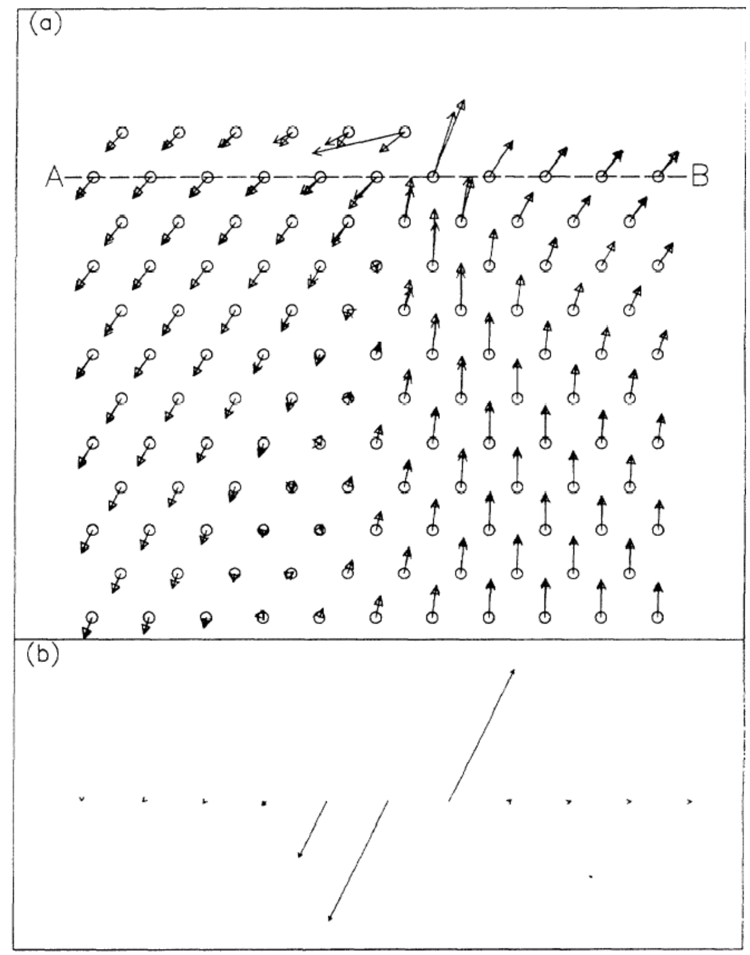
Torque due to surf. stress τ



V.I. Marchenko & Y.A. Parshin, Sov. Phys. JETP 52 ('80) 129

Stewart et al., PRB **49** ('94) 13848

2D classical: springs (beyond NN) for Si



$$E(\ell) = 2\frac{1-\nu^2}{\pi Y}\frac{(\tau h)^2+\xi^2}{\ell^2} = A/\ell^2$$

Some useful reviews re elastic interactions…

P. Nozières, in C. Godrèche (ed.), Solids Far from Equilibrium [Lectures at Beg-Rohu Summer School], Cambridge University Press ('93) p. 1.

P. Müller & A. Saúl, Elastic effects on surface physics, Surf. Sci. Rept. 54 ('04) 157.

H. Ibach, The role of surface stress in reconstruction, epitaxial growth and stabilization of mesoscopic structures, Surf. Sci. Rept. 29 ('97) 193

and articles by Nanosteps attendees

P. Müller & A. Saúl, Elastic effects on surface physics, Surf. Sci. Rept. 54 ('04) 157.

B. Houchmandzadeh & C. Misbah, Elastic Interaction Between Modulated Steps on Vicinal Surfaces, J. Phys. (France) I 5 ('95) 685; P. Peyla, A. Vallat, & C. Misbah, Elastic interaction between defects on a surface, J. Crystal Growth 201/202 ('99) 97

V.B. Shenoy & C.V. Ciobanu, Orientation dependence of the stiffness of surface steps: an analysis based on anisotropic elasticity, Surf. Sci. 554 ('04) 222; C.V. Ciobanu, D.T. Tambe, & V.B. Shenoy, Elastic interactions bet'n [100] steps and bet'n [111] steps on TiN(001), Surf. Sci. 582 ('05) 145

F. Leroy, P. Müller, J.-J. Métois & O. Pierre-Louis, Vicinal silicon surfaces: From step density wave to faceting,Phys. Rev. B 76 ('07) 045402

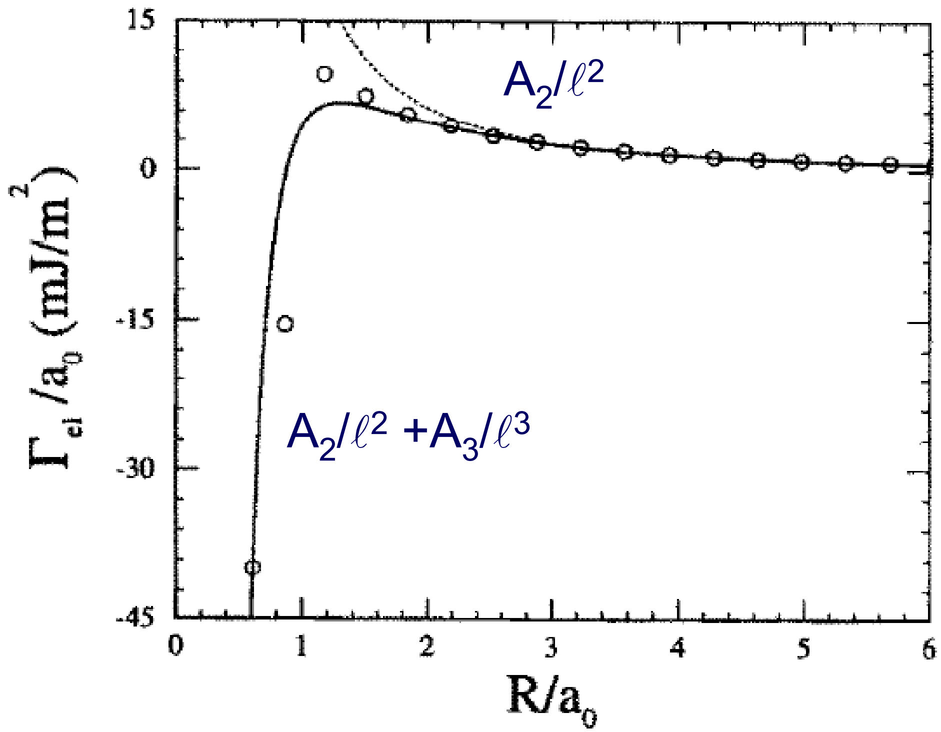


Fig. 8. The elastic component of the step energy $\Gamma = R\gamma_{01n} - (na_0\gamma_{001})/2 = \gamma_{step}^{[100]} + \gamma_{int}(R)$ for [110] steps on the (001) Cu surface as a function of step spacing, R. The circles represent the energies determined based on our atomistic simulation results while the dashed and solid lines are calculated using the parameters found in fitting the $(\bar{1}1m)$ surface energies to Eq. (7) with $k_{max} = 2$ and 3, respectively.

Najafabadi & Srolovitz, use EAM & study EAM metals: Ni, Pd, Pt, Cu, Ag, Au

$$E_{tot} = \sum_{i=1}^{N} \sum_{j \neq i} \phi(r_{ij}) + \sum_{i=1}^{N} F\left(\sum_{j \neq i} \rho(r_{ij}) \right)$$

- A_2/ℓ^2 OK for $\ell > 3a_0$
- Need A_3/ℓ^3 also, for $\ell < 3a_0$
- Including A_4/ℓ^4, too, does not improve much

R. Najafabadi, D.J. Srolovitz / Surface Science 317 (1994) 221

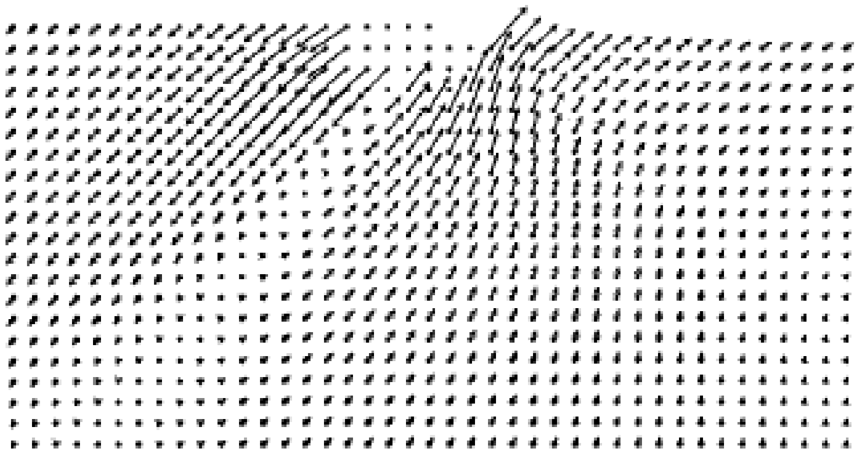
Table 1
The material dependent coefficients ζ_k of the R^{-k} terms in the expansion of the interaction energy between [100] steps (Eq. (7)) extracted from fitting the simulated $(01n)$ surface energies; The ζ_k are reported for fits to the expansion with $k_{max} = 2$, 3 and 4 for each of the six fcc metals examined; The goodness of fit parameter χ^2 would be zero for a perfect fit

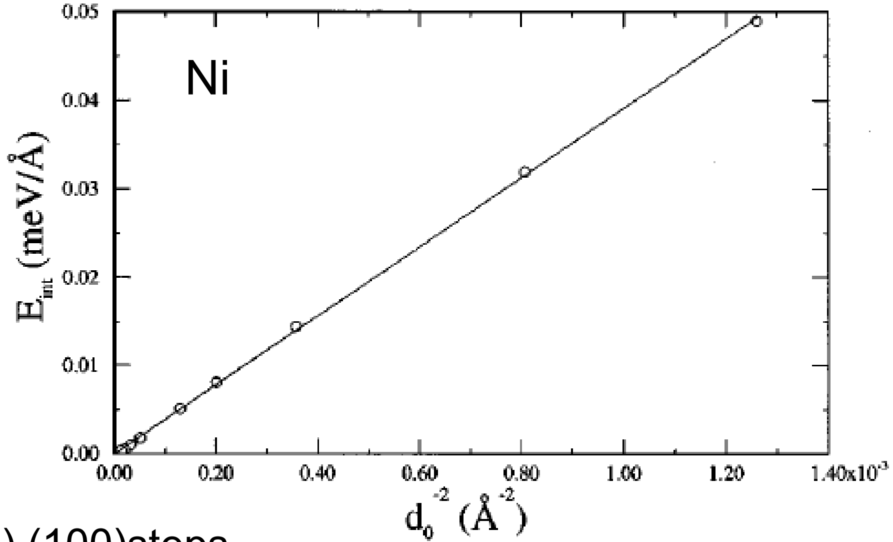
	$10^{13}\zeta_2$ (J/m)	$10^{13}\zeta_3$ (J/m)	$10^{13}\zeta_4$ (J/m)	χ^2
Ag	19			0.0013
	20	−7		0.0003
	20	−3	−7	0.0003
Au	73			0.0271
	88	−60		0.0022
	85	−34	−49	0.0021
Cu	41			0.0014
	47	−23		0.0007
	46	−14	−18	0.0006
Ni	26			0.0027
	28	−10		0.0003
	28	−5	−11	0.0003
Pd	87			0.0278
	101	−55		0.0032
	97	−22	−62	0.0030
Pt	146			0.0565
	165	−74		0.0081
	161	−40	−65	0.0078

Table 2
The material dependent coefficients ζ_k of the R^{-k} terms in the expansion of the interaction energy between [110] steps (Eq. (7)) extracted from fitting the simulated $(\bar{1}1m)$ surface energies

	$10^{13}\zeta_2$ (J/m)	$10^{13}\zeta_3$ (J/m)	$10^{13}\zeta_4$ (J/m)	χ^2
Ag	26			0.0003
	36	−34		0.0002
	34	−16	−35	0.0002
Au	108			0.0077
	142	−141		0.0004
	135	−78	−122	0.0003
Cu	56			0.0031
	78	−92		0.0017
	72	−48	−85	0.0017
Ni	36			0.0007
	48	−60		0.0004
	44	−29	−60	0.0004
Pd	126			0.0073
	165	−166		0.0004
	156	−97	−134	0.0004
Pt	206			0.0138
	263	−255		0.0015
	247	−123	−254	0.0016

How far apart must steps be just inverse-square repulsion?





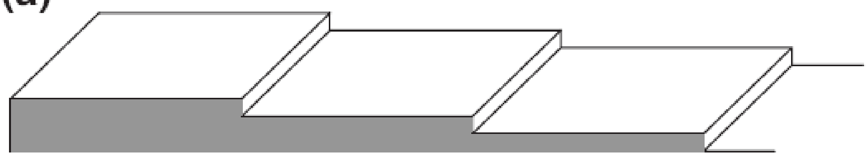
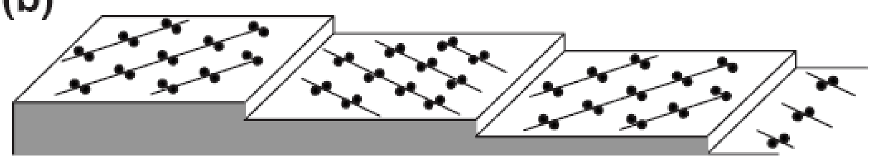
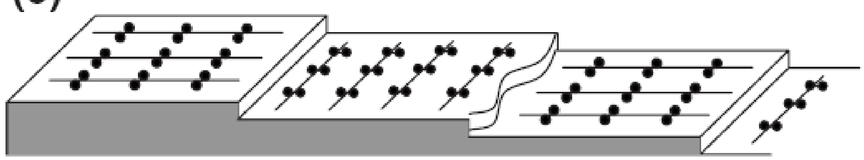
Displacements (200x magnification near Ni(001) (100)steps (zig-zag), separated by 300a_0 [Shilkrot&Srolovitz, PRB 53 ('96) 11120]

$$E_{int} = \frac{A_1}{\ell} + \frac{A_2}{\ell^2} + \frac{A_3}{\ell^3}$$

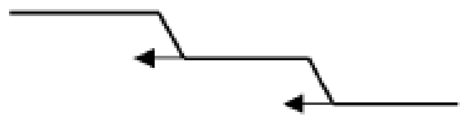
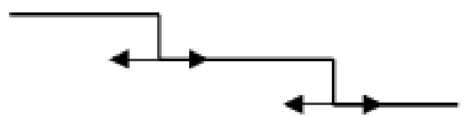
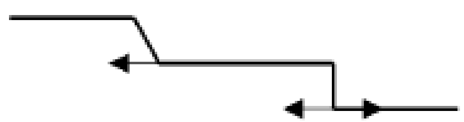
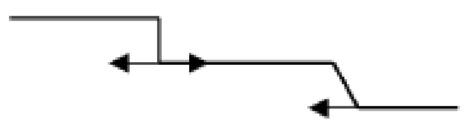
	A_1 (eV)	A_2 (eV Å)	A_3 (eV Å^2)
Au	-0.0003 ± 0.0002	0.17 ± 0.02	-0.62 ± 0.34
Ni	$-0.000\,03\pm0.000\,02$	0.045 ± 0.001	-0.14 ± 0.02

Including anisotropy (Stroh formalism) improves fit with dipole

Elastic Interactions on Principal Faces of Si

(a) 	**Vicinal (111)** Identical terraces Identical steps Dipôles
(b) 	**Vicinal (001) in the [100] direction** Different terraces Different steps Monopoles
(c) 	**Vicinal (001) in the [110] direction** Different terraces Identical steps Monopoles + dipoles

Leroy, Müller, Métois, Pierre-Louis, PRB 76 (’07) 045402

mo-mo		$\alpha_1 \ln(L/2\pi a)$	$\alpha_1 = \dfrac{Ea^2 m_o^2}{\pi(1-\nu^2)}$
di-di		$\alpha_2 (a/L)^2$	$\alpha_2 = \dfrac{2A^2(1-\nu)^2}{\pi E a^4}$
mo-di		$\alpha_3 (a/L)$	$\alpha_3 = -\dfrac{Am_o}{\pi a}(1+\nu)$
di-mo		$-\alpha_3 (a/L)$	

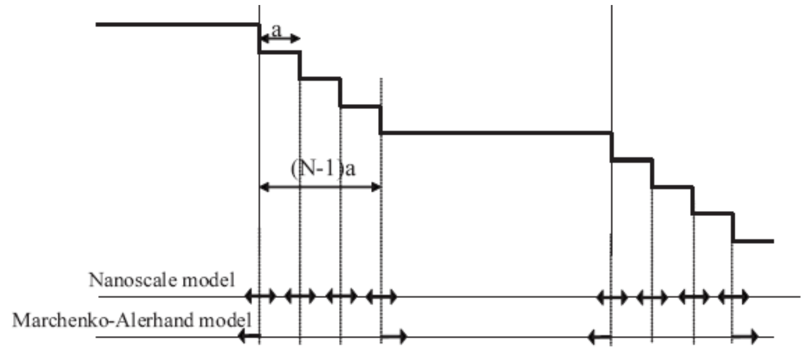


TABLE III. (a) Elastic energy W/L for dipoles. Moreover the expressions are given per unit step-length, thus the unity is an energy over surface area. (b) Elastic energy W/L for alternated monopoles. Notice that $A_{dip}=+\frac{1-\nu^2}{\pi E}A^2$ but $A_{monop}=\frac{(1+\nu)(1-2\nu)}{\pi E}F_y^2$ (see the Appendix). The + and − signs arise, respectively, for N even and N odd. Moreover, the expressions are given per unit step length; thus, the unity is an energy over surface area.

(a)	Intrabunch	Interaction between two bunches (interbunch)	Interaction energy for an infinite periodic surface
Exact expression	$\frac{A_{dip}}{a^2}\sum_{i<j,j}\frac{1}{(i-j)^2}$	$\frac{A_{dip}}{a^2}\sum_{i,j=1}^{N}\frac{1}{[M+(i-j)]^2}$	$\frac{A_{dip}}{a^2}\sum_{k}\sum_{i,j=1}^{N}\frac{1}{[kM+(i-j)]^2}$
Approximated expression	$\frac{A_{dip}}{a^2}\left[N\frac{\pi^2}{6}-1-\ln N\right]$	$-\frac{A_{dip}}{a^2}\ln\left[1-\left(\frac{N}{M}\right)^2\right]$	$-\frac{A_{dip}}{a^2}\ln\left[\frac{\sin\left(\frac{\pi N}{M}\right)}{\left(\frac{\pi N}{M}\right)}\right]$

(b)	Intrabunch	Between two bunches (interbunch)	For an infinite pattern of bunches
Exact expression	$\frac{A_{mon}}{a_0^2}\sum_{i<j,j=1}^{N}(-1)^{j-i}\ln\left((j-i)\frac{a}{a_0}\right)$	$\frac{A_{mon}}{a_0^2}\sum_{i,j=1}^{N}(-1)^{j-i}\ln\left((M+j-i)\frac{a}{a_0}\right)$	$\frac{A_{mon}}{4a_0^2}\sum_{k}\sum_{i,j=1}^{N}(-1)^{j-i}\ln\left[\left((kM+j-i)\frac{a}{a_0}\right)\right]$
Approximated expression	$\frac{A_{mon}}{4a_0^2}\left[2N\ln\left(\frac{\pi a_0}{2a}\right)-1\pm\ln N\right]$	$\pm\frac{A_{mon}}{4a_0^2}\ln\left[1-\left(\frac{N}{M}\right)^2\right]$	$\pm\frac{A_{mon}}{4a_0^2}\ln\left(\frac{\sin\left(\frac{\pi N}{M}\right)}{\left(\frac{\pi N}{M}\right)}\right)$

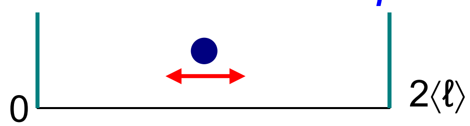
Particle in 1D Box vs. Exact

$$E = \int \beta\sqrt{1+x'^2}\,dy \sim \text{const.} + \int \frac{\tilde{\beta}x'^2}{2}$$

$x'^2 \to \dot{x}^2$

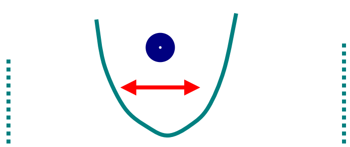
1-D Schrödinger eqn $\quad \frac{\hbar^2}{2m} \to \frac{(k_B T)^2}{2\tilde{\beta}}$

- *Free fermions: repulsion just entropic*



$$\psi_0 = \frac{1}{\langle \ell \rangle} \sin\left(\frac{\pi x}{2\langle \ell \rangle}\right) \qquad E_0 = \frac{(k_B T)^2 \pi^2}{8\tilde{\beta}\langle \ell \rangle^2}$$

- $U(\ell) = A/\ell^2$, large A

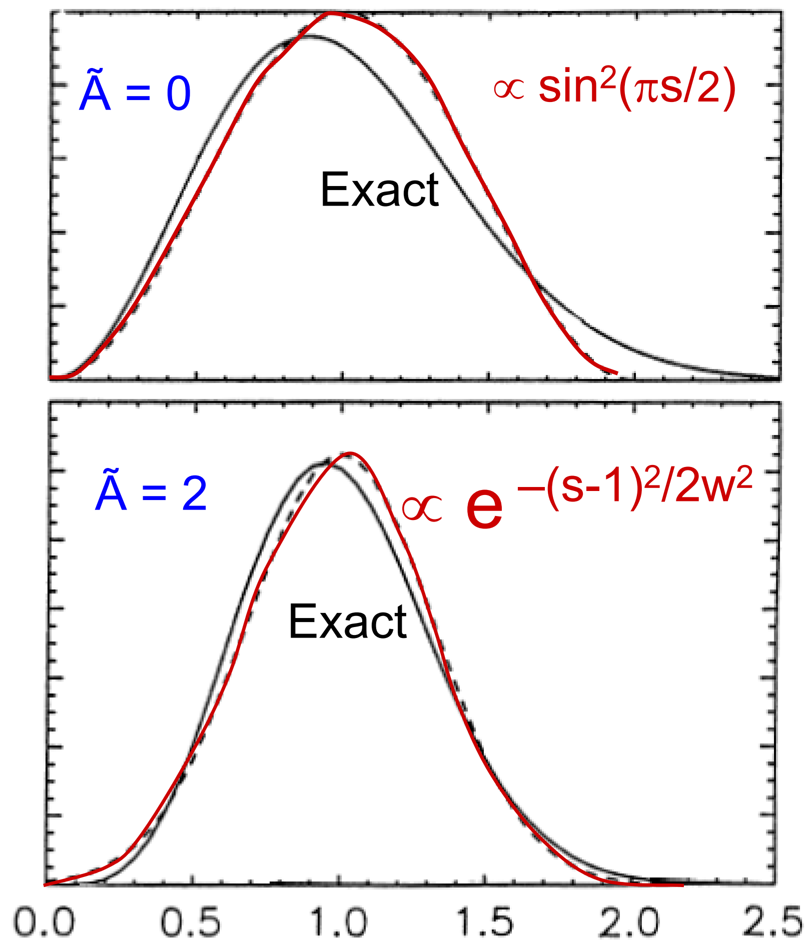


$$\psi_0 \propto e^{-x^2/4w^2} \qquad w^4 = \frac{(k_B T)^2}{8\tilde{\beta}U''(\langle \ell \rangle)}$$

$$w = \text{const.}\ \tilde{A}^{-1/4}\langle \ell \rangle$$

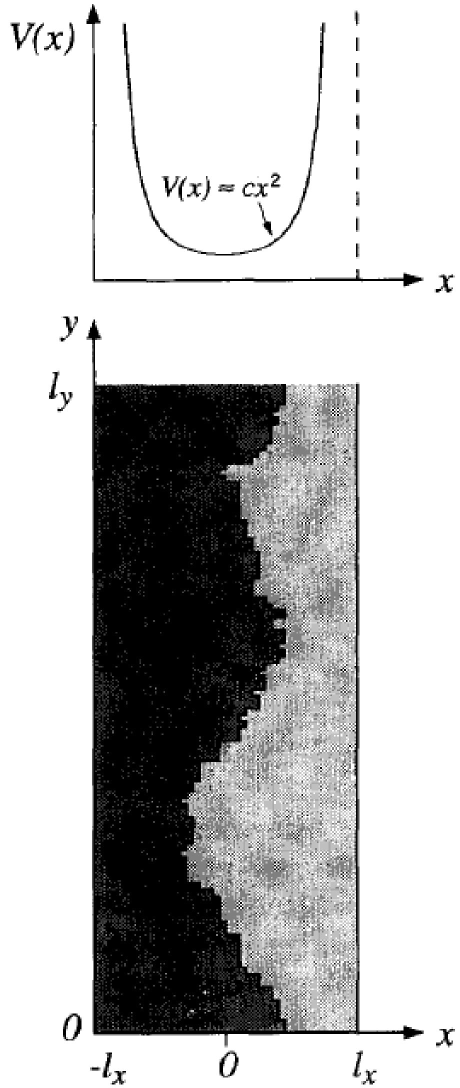
A enters only as Ã: $\quad \tilde{A} \equiv \frac{\tilde{\beta}A}{(k_B T)^2}$

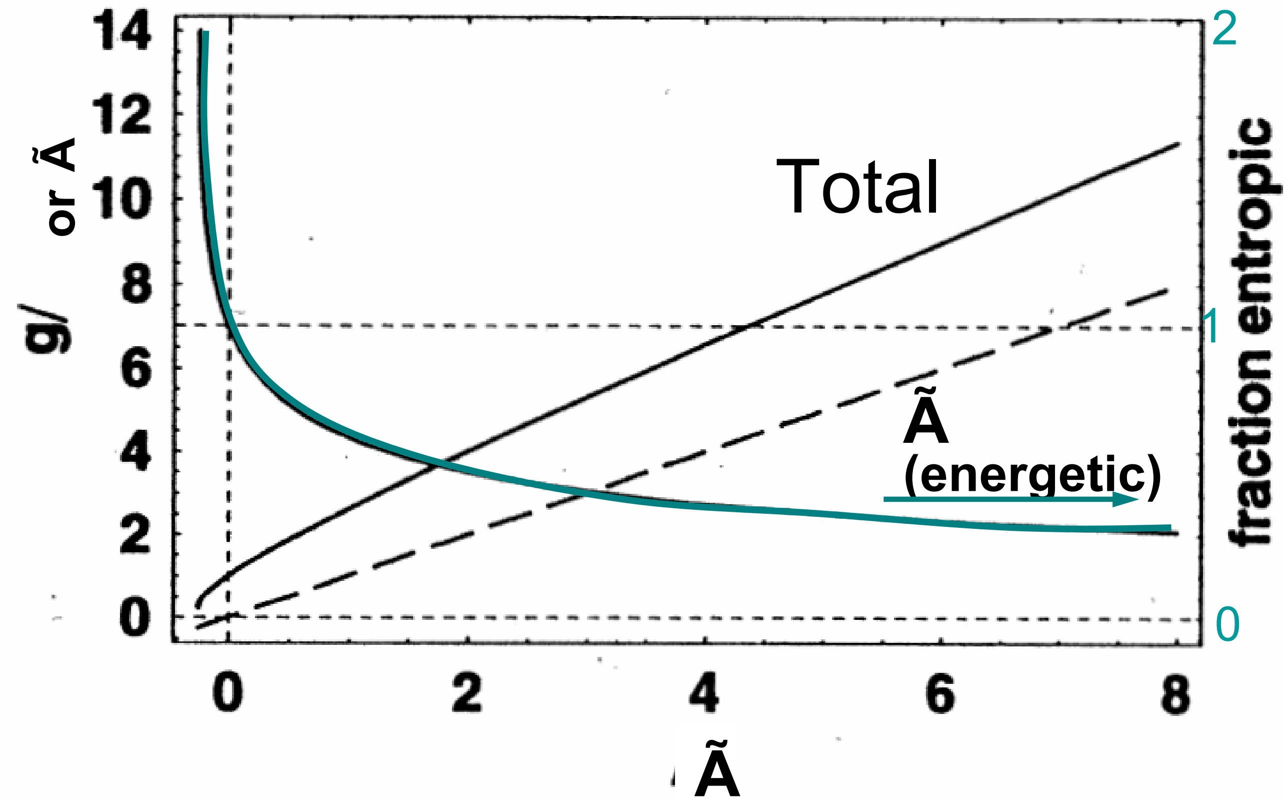
const. *changes with approximation*



Entropic & Elastic Not Simply Additive!

Large Ã keeps steps apart, decreasing contribution of entropic relative to energetic



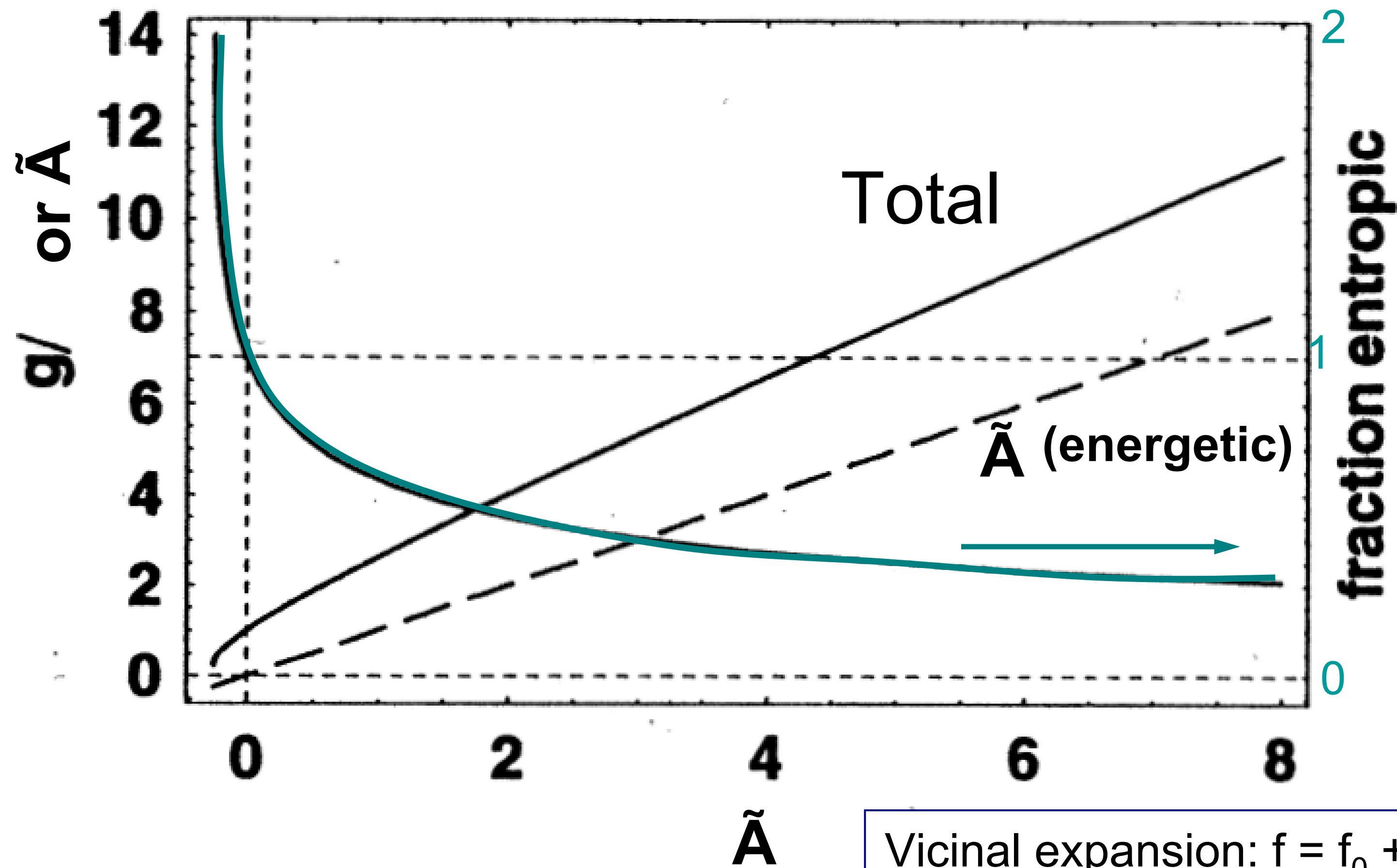


Vicinal expansion: $f = f_0 + (\beta/h)\tan\phi + g\tan^3\phi$

$g = (\pi^2/6)(kT)^2/\tilde{\beta}$ x Total

Entropic & Elastic Not Simply Additive!

Large Ã keeps steps apart, decreasing contribution of entropic relative to energetic



Total is

$\frac{1}{4}[\sqrt{(4\tilde{A}+1)} + 1]^2$

$=(\varrho/2)^2$

Vicinal expansion: $f = f_0 + (\beta/h) \tan\phi + g \tan^3\phi$

$g = (\pi^2/6)(kT)^2/\tilde{\beta} \times$ Total

Jayaprakash, Rottman, & Saam, PRB 30 ('84) 6549 & factor 2 error

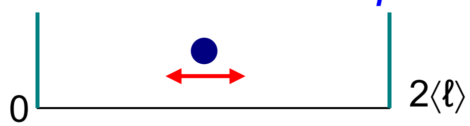
Particle in 1D Box vs. Exact

$$E = \int \beta\sqrt{1+x'^2}\,dy \sim \text{const.} + \int \frac{\tilde{\beta}x'^2}{2}$$

$x'^2 \to \dot{x}^2$

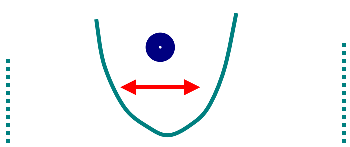
1-D Schrödinger eqn $\quad \dfrac{\hbar^2}{2m} \to \dfrac{(k_B T)^2}{2\tilde{\beta}}$

- *Free fermions: repulsion just entropic*



$$\psi_0 = \frac{1}{\langle \ell \rangle}\sin\left(\frac{\pi x}{2\langle \ell \rangle}\right) \qquad E_0 = \frac{(k_B T)^2 \pi^2}{8\tilde{\beta}\langle \ell \rangle^2}$$

- $U(\ell) = A/\ell^2$, large A

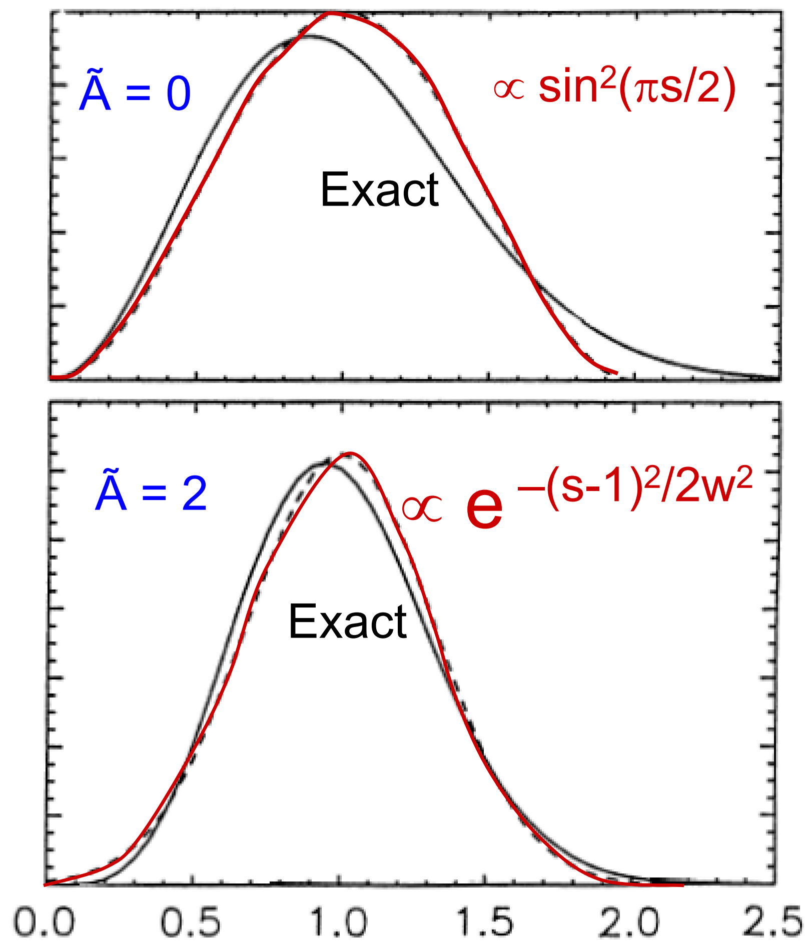


$$\psi_0 \propto e^{-x^2/4w^2} \qquad w^4 = \frac{(k_B T)^2}{8\tilde{\beta}U''(\langle \ell \rangle)}$$

$$w = \text{const.}\ \tilde{A}^{-1/4}\langle \ell \rangle$$

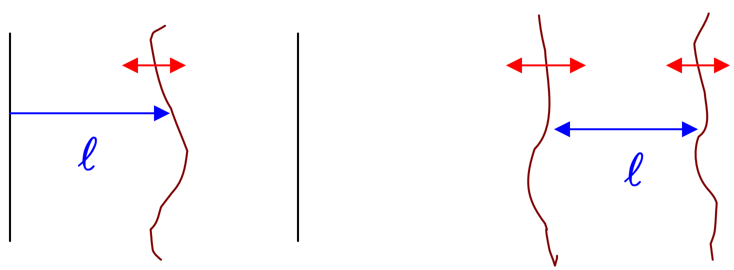
A enters only as Ã: $\quad \tilde{A} \equiv \dfrac{\tilde{\beta}A}{(k_B T)^2}$

const. *changes with approximation*



Steps in 2D → fermion worldlines in 1D

- Step non-crossing ⇒fermions or hard bosons
- Energy ∝ path-length × free energy/length β, expand ⇒ 1D Schrödinger eqn., $m \to$ stiffness $\tilde{\beta}$
- Analogous to polymers in 2D (deGennes, JCP '68)
- Only dependence on A via $\tilde{A} \equiv \tilde{\beta} A/(k_B T)^2$ $\qquad \ell/\langle \ell \rangle$
- Mean-field (Gruber-Mullins): 1 active step, $0 \le s \le 2$
  - $\tilde{A}$ =0: particle in box, $P(s) = \psi_0^2 \propto \sin^2(\pi s/2)$, $\varepsilon_0 \propto T^2/\tilde{\beta}\langle \ell \rangle^2 \to$ *entropic repulsion*
  - $\tilde{A} \ge 1½$: parabolic well, $P(s) \propto \exp[-(s-1)^2/2w_M^2]$, $w_M \propto \tilde{A}^{-1/4}\langle \ell \rangle$
- $\tilde{A} \to \infty$: "phonons", variance of $P(s)$ is $2w_M^2$, not w_M^2

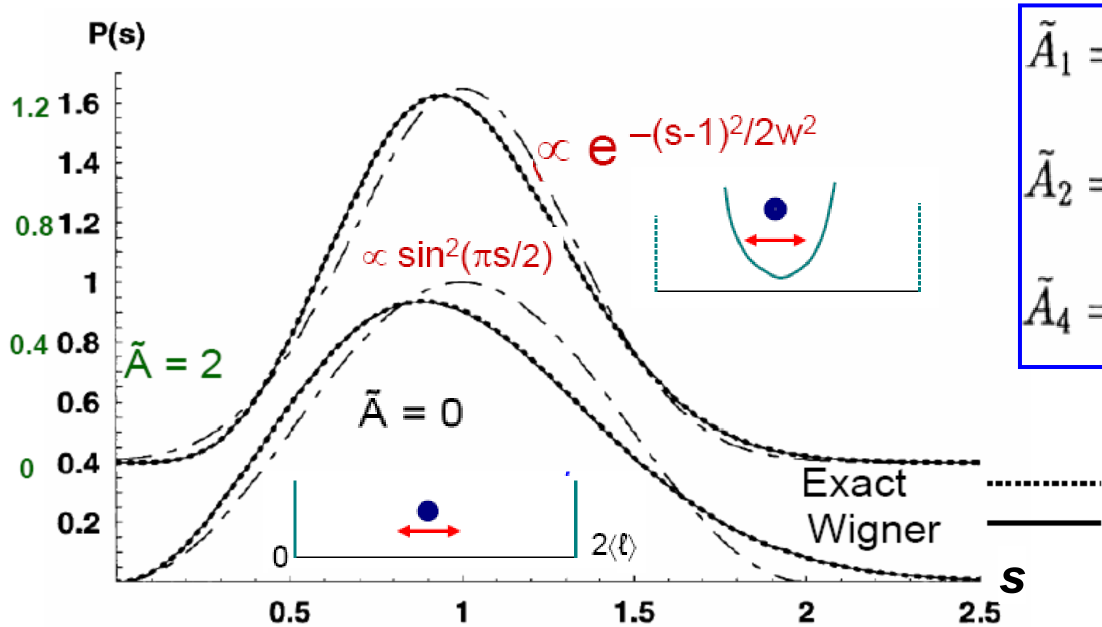


Comparison of prefactors for Gaussian approximations

Measure variance σ^2 of TWD $\qquad \sigma^2 = \kappa_X / \varrho$

Model	*Approximation*	*NN/all*	κ_X
Gruber-Mullins	*Single active step*	NN	(0.289)
		all	(0.277)
Grenoble	*Entropy completely neglected, Independent steps*	NN	(0.520)
		all	(0.475)
Grenoble, modified	*Entropy included only in average way*	NN	0.520
		all	0.475
Saclay	*Continuum roughening theory*	all	$4\pi^{-2} \cong 0.405$
Wigner	*Wigner surmise*	all	(1/2)

Wigner Surmise (WS) for TWD (terrace-width distribution)



$\tilde{A}_1 = -1/4: \quad P_1(s) = \frac{\pi}{2} s \exp\left(-\frac{\pi}{4} s^2\right)$

$\tilde{A}_2 = 0: \quad P_2(s) = \frac{32}{\pi^2} s^2 \exp\left(-\frac{4}{\pi} s^2\right)$

$\tilde{A}_4 = 2: \quad P_4(s) = \left(\frac{64}{9\pi}\right)^3 s^4 \exp\left(-\frac{64}{9\pi} s^2\right)$

$U(\ell) = A/\ell^2$

$$\tilde{A} \equiv \frac{\tilde{\beta} A}{(k_B T)^2}$$

Generalizing from the special cases: **WS → GWS**

- The three special cases correspond to $\varrho = 1$, 2, and 4.
- $\tilde{A}$ and ϱ are related by: $\tilde{A} = (\varrho - 2)\varrho/4$; $\varrho = 1 + \sqrt{1 + 4\tilde{A}}$
- Simplest interpolation expression: $P_\varrho(s) = a_\varrho s^\varrho \exp(-b_\varrho s^2)$
- Two conditions on $P_\varrho(s)$: normalization & unit mean
  $\Rightarrow$ values of a_ϱ, b_ϱ (in terms of Γ functions).

Calogero-Sutherland Model's Ground State & Random Matrices

Calogero-like Hamiltonian:

$$\mathcal{H} = -\sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} + 2\frac{\beta}{2}\left(\frac{\beta}{2} - 1\right) \sum_{1\leq i<j\leq N} (x_j - x_i)^{-2} + \omega^2 \sum_{j=1}^{N} x_j^2$$

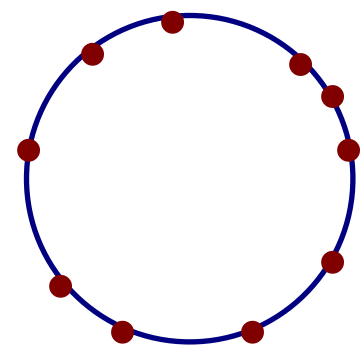
[In the limit $N \to \infty$, $\omega \to 0$; in Calogero $\mathcal{H}$, $x_j^2 \to (x_j - x_i)^2$.]

$$\Psi_0 = \prod_{1\leq i<j\leq N} |x_j - x_i|^{\beta/2} \exp\left(-\frac{1}{2}\omega \sum_{k=1}^{N} x_k^2\right)$$

The ground-state density Ψ_0^2 is recognized as a joint probability distribution function from the theory of random matrices for Dyson's Gaussian ensembles.

Sutherland Hamiltonian:

$$\mathcal{H} = -\sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} + 2\frac{\beta}{2}\left(\frac{\beta}{2} - 1\right) \frac{\pi^2}{L^2} \sum_{i<j} \left[\sin\frac{\pi(x_j - x_i)}{L}\right]^{-2}$$



$$\Psi_0 = \prod_{i<j} \left|\sin\frac{\pi(x_j - x_i)}{L}\right|^{\beta/2}, \quad x_j > x_i$$

$$\theta_i \equiv 2\pi x_i/L \quad \Rightarrow \quad \Psi_0^2 = \prod_{i<j} \left|e^{i\theta_j} - e^{i\theta_i}\right|^{\beta}$$

The ground-state density Ψ_0^2 is also a joint probability distribution function from the theory of random matrices, now for Dyson's circular ensembles.

Note that the pair correlation functions and other properties of the ensembles can be evaluated exactly only for the cases $\beta = 1$, 2, or 4, corresponding to orthogonal, unitary, or symplectic symmetry of the ensemble.

Generalized Wigner Surmise (GWS) for TWD

$U(\ell) = A/\ell^2$

$\tilde{A} \equiv \frac{\tilde{\beta} A}{(k_B T)^2}$

Generalizing from the special cases:

- The three special cases correspond to $\varrho = 1$, 2, and 4.
- $\tilde{A}$ and ϱ are related by: $\boxed{\tilde{A} = (\varrho - 2)\varrho/4}$; $\boxed{\varrho = 1 + \sqrt{1 + 4\tilde{A}}}$
- Simplest interpolation expression: $\boxed{P_\varrho(s) = a_\varrho s^\varrho \exp(-b_\varrho s^2)}$
- Two conditions on $P_\varrho(s)$: normalization & unit mean
  $\Rightarrow$ values of a_ϱ, b_ϱ (in terms of Γ functions).

Why is the Wigner surmise is so interesting and universal?

"Stay tuned" until next week!

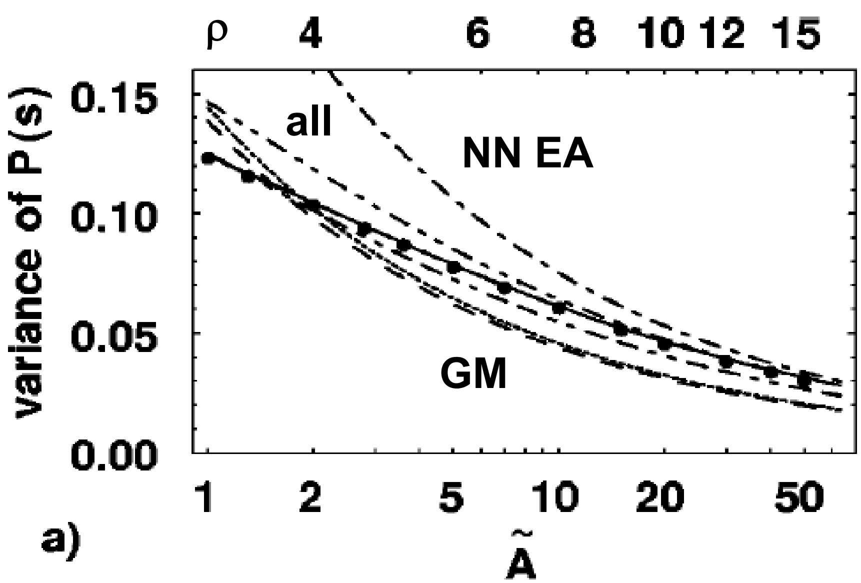
Can still use Gaussian for large Ã, if generalize from $\tilde{A} \propto \sigma^{-4}$ to:

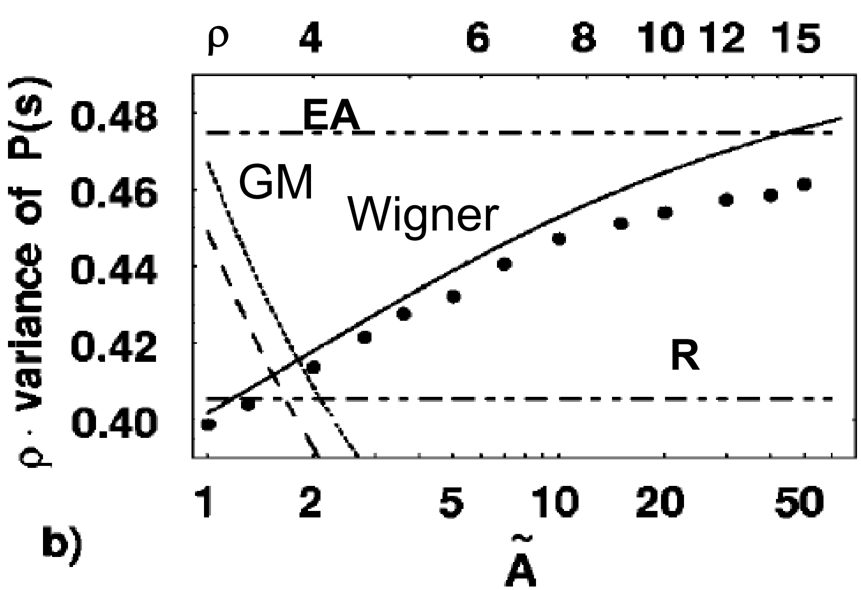
$$\tilde{A} \approx \frac{1}{16}\left[(\sigma^2)^{-2} - 7(\sigma^2)^{-1} + \frac{27}{4} + \frac{35}{6}\sigma^2\right]$$

Discreteness of steps not important for $\langle \ell \rangle \geq 4$

System collapses for $\tilde{A} < -1/4$

Monte Carlo data confronts approximations





Dots: MC data
Line: Wigner
Dashes: Gruber-Mullins (mean field)
Long-short [-short]: Grenoble
(no entropic int'n, EA)
Long-long-short-short: Saclay
(continuum roughening, R)

Lower plot highlights differences:
remove ρ^{-1} asymptotic decay
Wigner is best, quantitatively
and conceptually

Hailu Gebremariam et al.,
Phys. Rev. B 69 ('04)125404

Comparison of variance of $P(s)$ vs. Ã computed with Monte Carlo:

GWS does better, quantitatively & conceptually, than any other approximation

Hailu Gebremariam et al., Phys. Rev. B 69 ('04)125404

Experiments measuring variances of TWDs

Vicinal	T (K)	σ^2	ϱ	$\tilde{A}$	A_W/A_G	A_W (eV Å)	Experimenters
Pt(1 1 0)-(1 × 2)	298		2.2	0.13	–	$\tilde{\beta} = ?$	Swamy, Bertel [36]
Cu(19, 17, 17)	353	0.122	4.1	2.2	0.77	0.005	Geisen [5,54]
Si(1 1 1)	1173	0.11	3.8	1.7	0.96	0.4	Bermond, Métois [55]
Cu(1,1,13)	348	0.091	4.8	3.0	1.27	0.007	Giesen [5,56]
Cu(1 1,7,7)	306	0.085	5.1	4	1.37	0.004	Geisen [5,54]
Cu(1 1 1)	313	0.084	5.0	3.6	1.39	0.004	Geisen [5,54]
Cu(1 1 1)	301	0.073	6.0	6.0	1.58	0.006	Geisen [5,54]
Ag(1 0 0)	300	0.073	6.4	6.9	1.58	$\tilde{\beta} = ?$	P. Wang...Williams
Cu(1, 1, 19)	320	0.070	6.7	7.9	1.64	0.012	Geisen [5,56]
Si(1 1 1)-(7 × 7)	1100	0.068	6.4	7.0	1.67	0.7	Williams [57]
Si(1 1 1)-(1 × 1)Br	853	0.068	6.4	7.0	1.67	0.1	X.-S. Wang, Williams [58]
Si(1 1 1)-Ga	823	0.068	6.6	7.6	1.67	1.8	Fujita...Ichikawa [59]
Si(1 1 1)-Al $\sqrt{3}$	1040	0.058	7.6	10.5	1.85	2.2	Schwennicke...Williams [60]
Cu(1, 1, 11)	300	0.053	8.7	15	1.95	0.02	Barbier et al. [21]
Cu(1, 1, 13)	285	0.044	10	20	2.12	0.02	Geisen [5,56]
Pt(1 1 1)	900	0.020	24	135	2.59	6	Hahn...Kern [61]
Si(1 1 3) rotated	1200	0.004	124	3.8×10^3	2.92	$(27 \pm 5) \times 10^2$	van Dijken, Zandvliet, Poelsema [9]

Experimental Test of Thermal Dependence of Ã

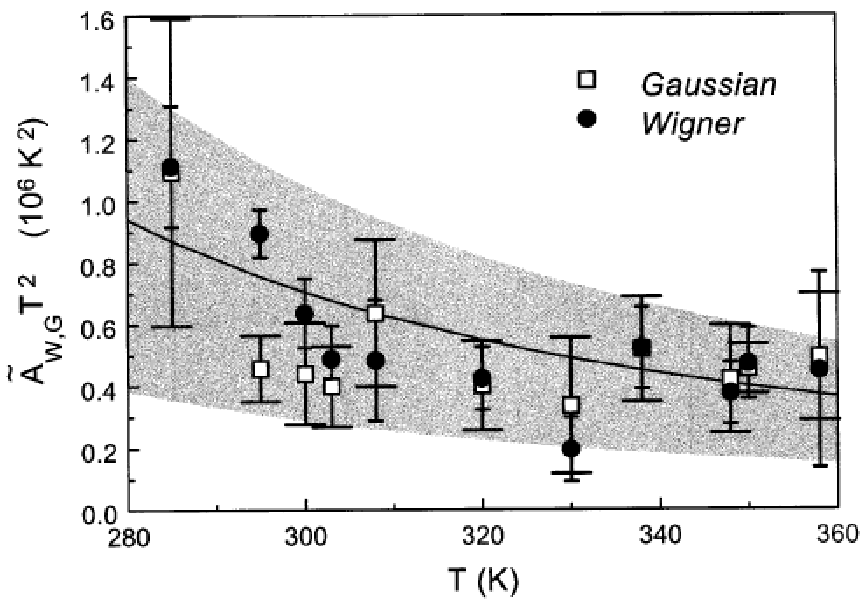
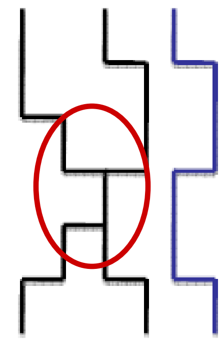


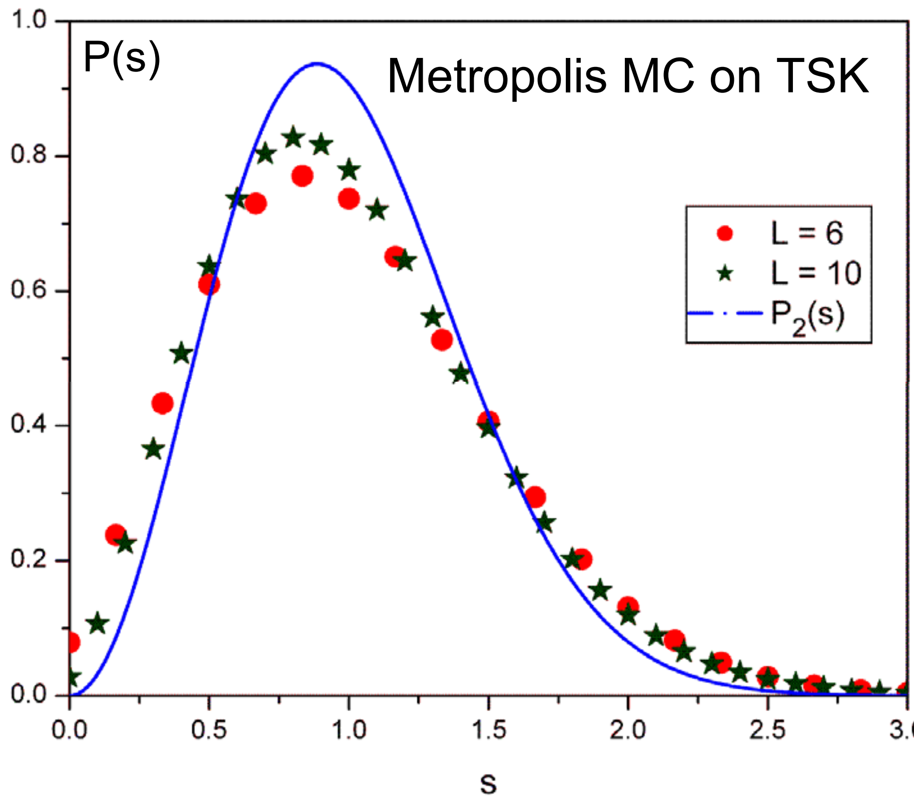
Fig. 6. Temperature dependence of $T^2\tilde{A}_W$ (solid circles) and $T^2\tilde{A}_G$ (open squares) for Cu (1 1 13), with error bars distinguished by narrow and wide feet respectively. The solid curve is calculated from Eq. (1), with $\tilde{\beta}$ obtained from Footnote 4 and A set to 7.1 meV Å, the value determined in Ref. [9]. The gray band blanketing the data corresponds to a range of about ±50% of A.

M. Giesen & TLE, Surface Sci. 449 (00') 191

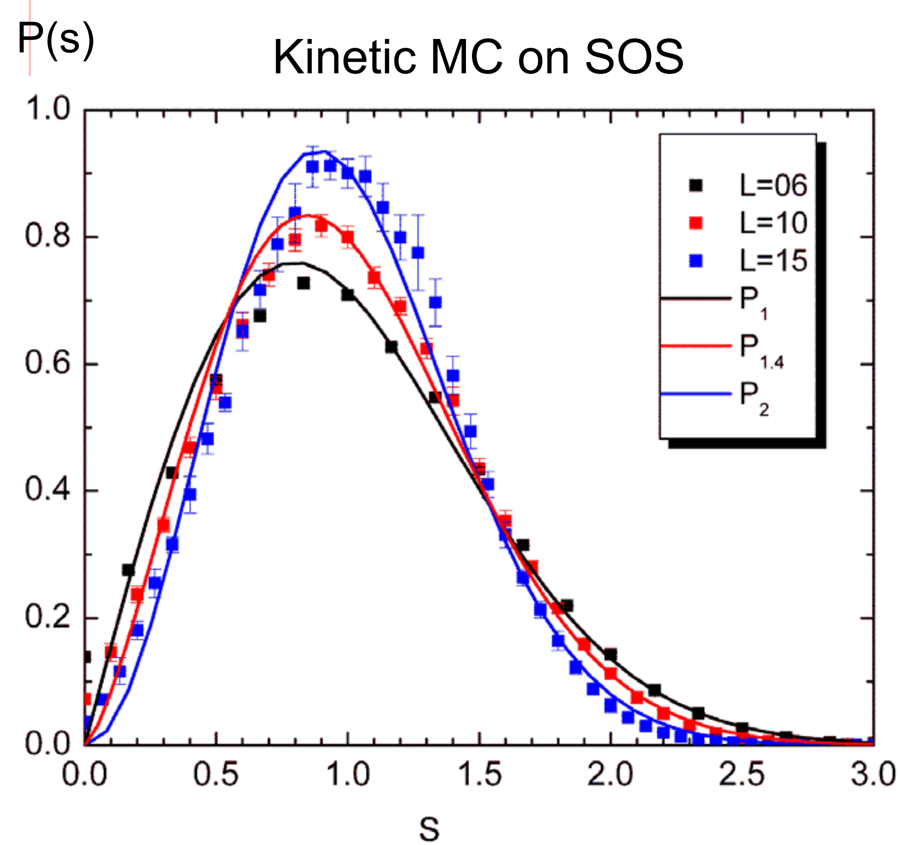
What happens when steps are allowed to touch?

Effective attraction: $\varrho = 2 \rightarrow \varrho < 2$, finite-size dep.





L	6	8	10	12	16
$\varrho(L)$	1	1.3	1.3	1.4	1.45
$\tilde{A}$	-0.25	-0.23	-0.23	-0.21	-0.20



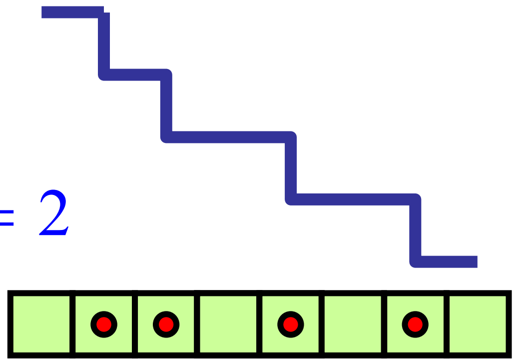
$T = 580$ K $\quad E_d = 1$ eV $\quad E_a = 0.35$ eV

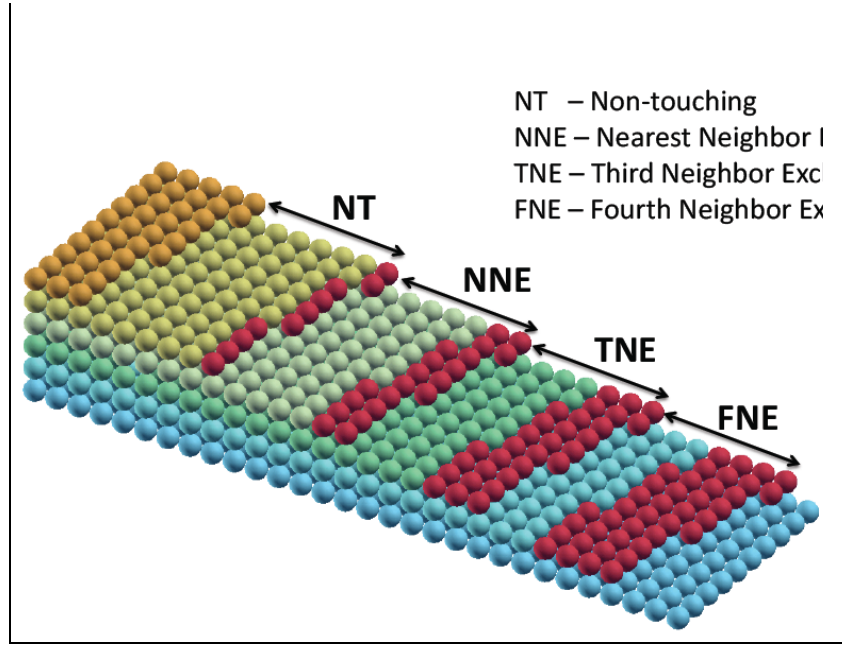
NNI (NT) and NN2 Chains

Kwangmoo Kim

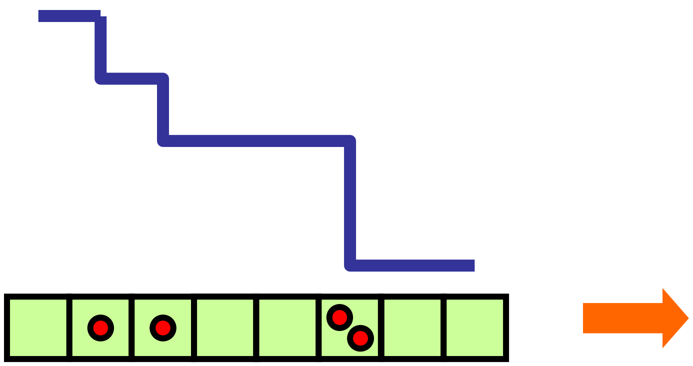
- Map steps onto 1D free-fermions

$\langle L \rangle = 2$

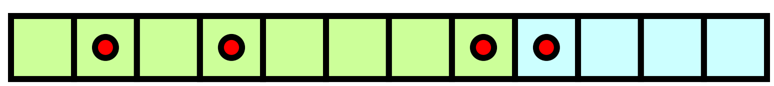




- Overlapping steps (NN2) can be mapped onto Nearest-Neighbor Included (NNI) chain, then *shifted* and *rescaled*



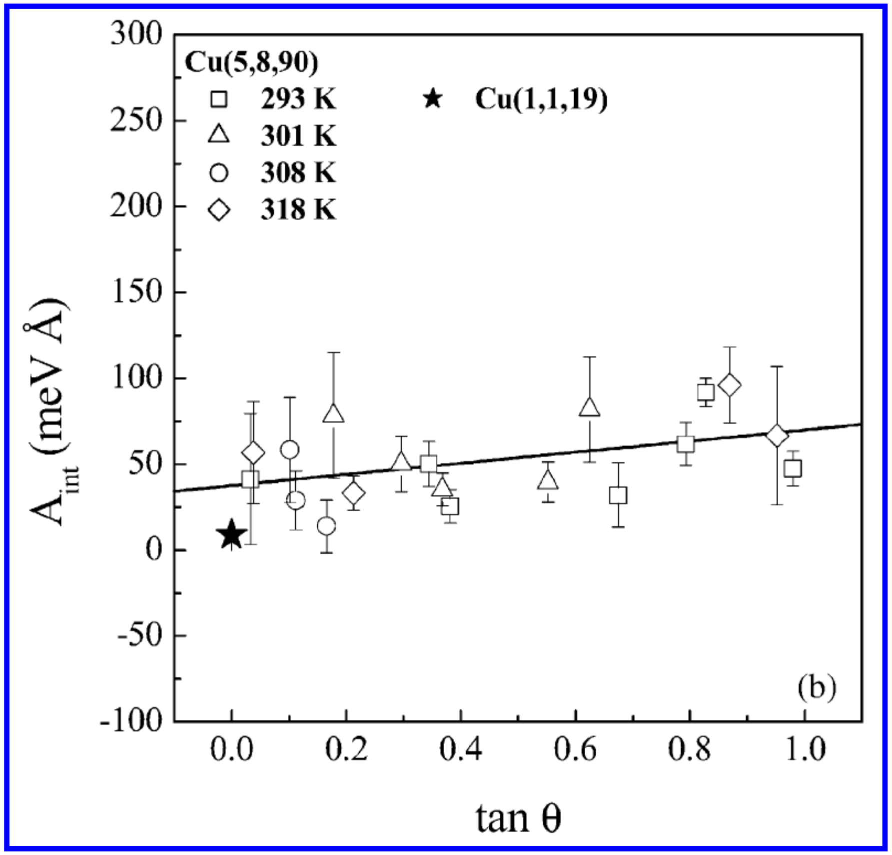
$\langle L \rangle = 3$

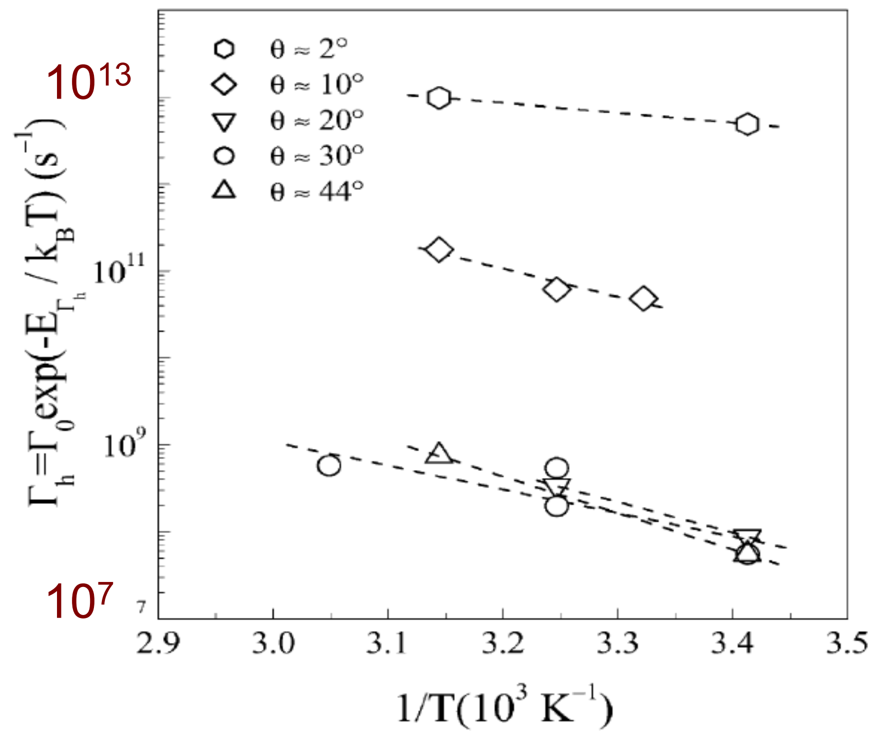


NNE : S.-A. Cheong & C. L. Henley (unpublished); S.-A. Cheong, dissertation

Anisotropy of Repulsion Strength
(is much weaker than edge-diffusion anisotropy)

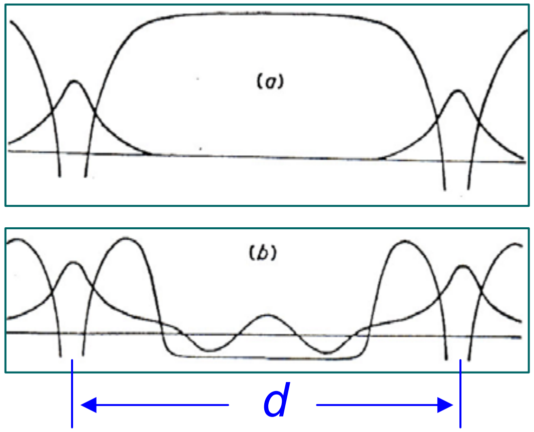
M. Giesen, S. Dieluweit / Journal of Molecular Catalysis A: Chemical 216 (2004) 263





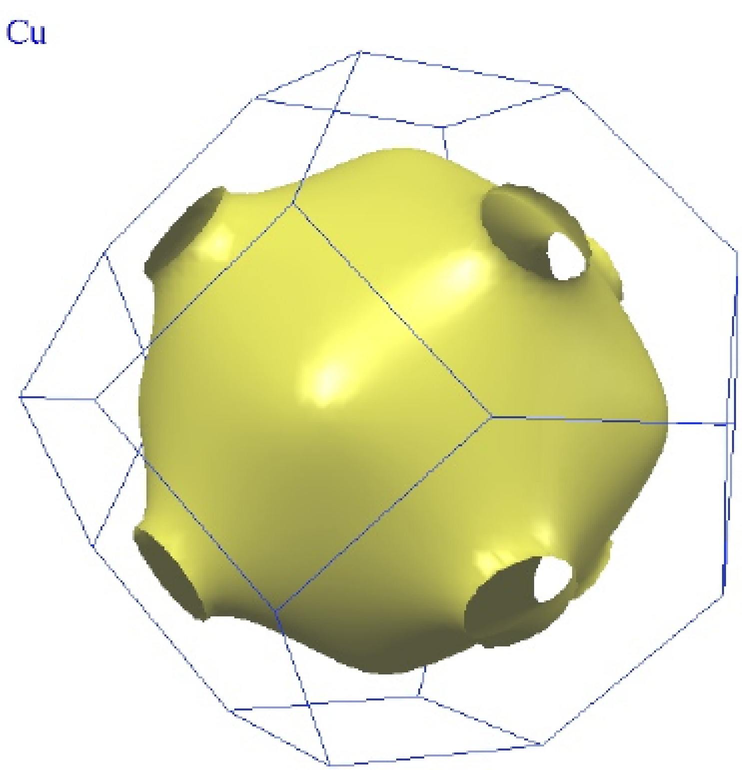
Needs more study, especially from theory perspective

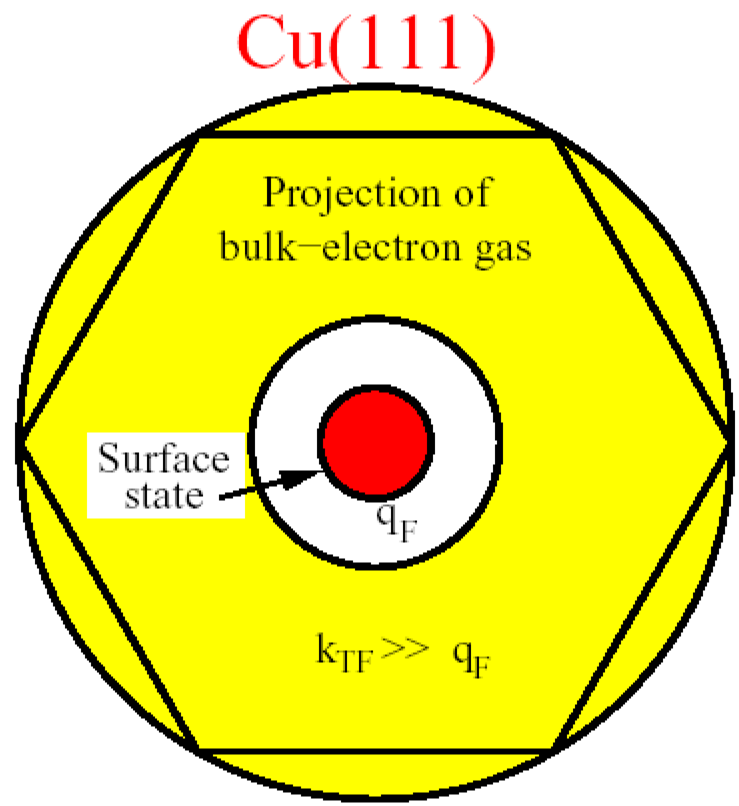
Essence of *Indirect* Interactions



- Symmetry determined by mediating state[s] & by adatom-metal coupling
- Local, screened perturbation of robust substrate ψ
- *Oscillatory* in sign; power-law decay at long range; simple form only when asymptotic & negligibly small
- Overwhelmed by any *direct* interaction at short-range
- Weaker than binding energy & diffusion barrier
- Produces correlations measurable by FIM, STM, …
- Produces ordered 2D superlattices measurable by LEED, RHEED, grazing x-ray...

Metallic Surface State on Noble Metal (111)





	$m_{\text{eff}}/m_{\text{e}}$	ϵ_{F} (eV)	q_{F} (Å^{-1})	$\lambda_{\text{F}}/2$ (Å)	k_{TF}^{-1} (Å)
Cu	$0.44^a/0.46^b$	$0.38^a/0.39^b$	$0.21^a/0.217^b$	$15.0^a/14.5^b$	0.552^d
Ag	$0.40^a/0.53^b$	$0.065^a/0.12^b$	$0.083^a/0.129^b$	$37.9^a/24.4^b$	0.588^d
Au	0.28^b	0.41^b	0.173^b	18.2^b	0.588^d
Si-Ag $\sqrt{3}$	$0.15(7)^c$	$0.25(5)^c$	$0.010(3)^c$	$31(9)^c$	$[k_{\text{DH}}^{-1} \gg \lambda_{\text{F}} \text{ at } 6\text{ K}]^e$

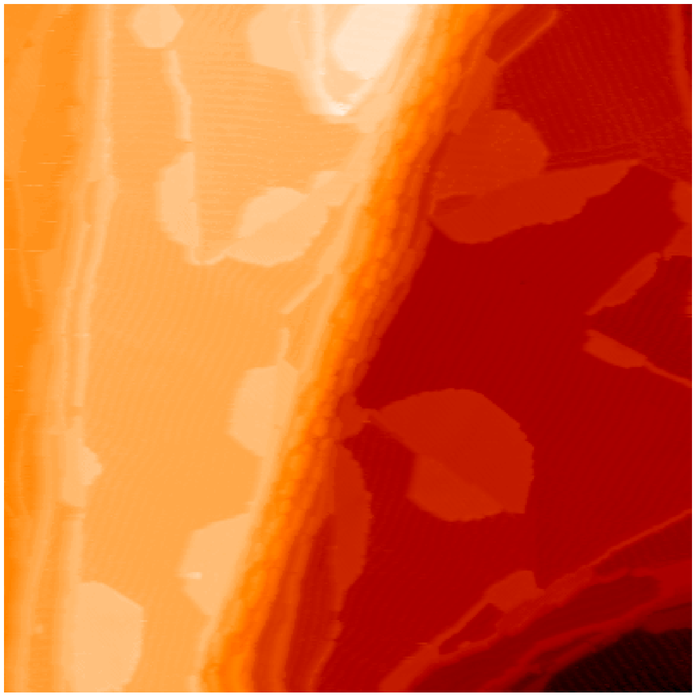
Indirect interaction via bulk vs. surface states

Asymptotically $E_{pair}(d) \propto d^{-n} \sin(2q_F d + 2\delta)$

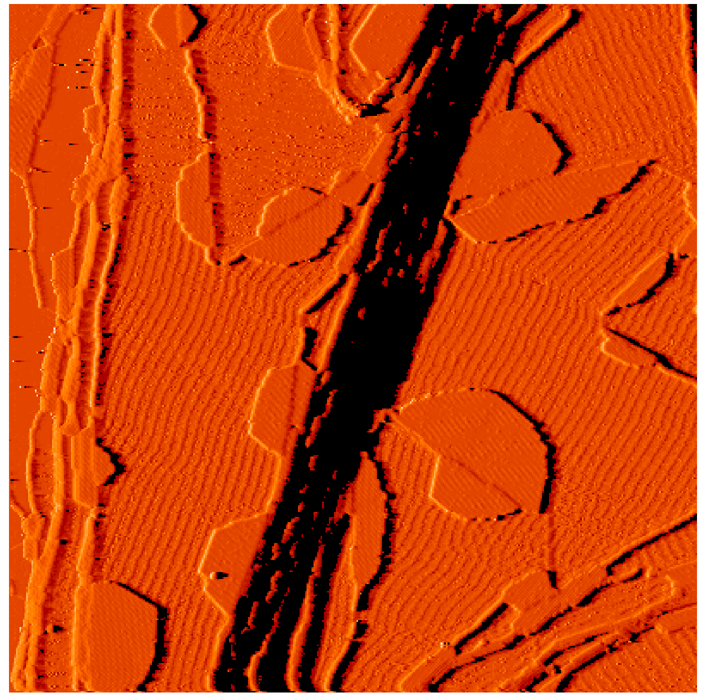
- $\lambda_F /2 \approx 2.3$Å [Cu]
- Anisotropic $\varepsilon_n(\mathbf{k}_\|)$
- Messy computation: multiple 3D bands
- Asymptotic decay envelope $\propto d^{-5} \Rightarrow$ insignificant
- Trio asymptotic $\propto d^{-7}$

- $\lambda_F /2 \approx 15$Å [Cu(111)]
- Circular isotropy $\varepsilon=(\hbar k_\|)^2/2m^*$
- Analytically simple: single parabolic 2D band
- Asym. decay env. $\propto d^{-2}$ $\Rightarrow$ *observable*
- Trio asymptotic $\propto d^{-5/2}$

Ripple Structures in Ag(111) Regions Confined by C_{60} : Evidence of Surface State



Topography image of ripple structures

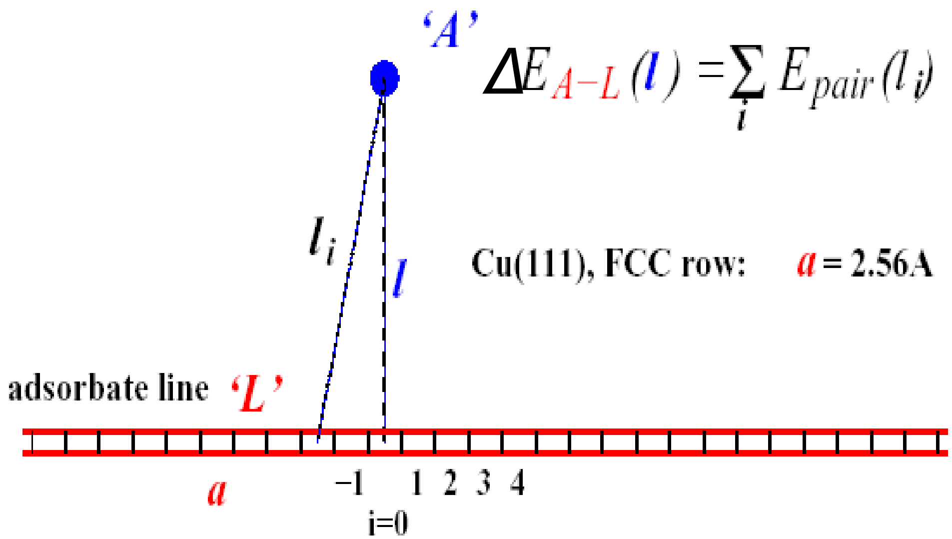


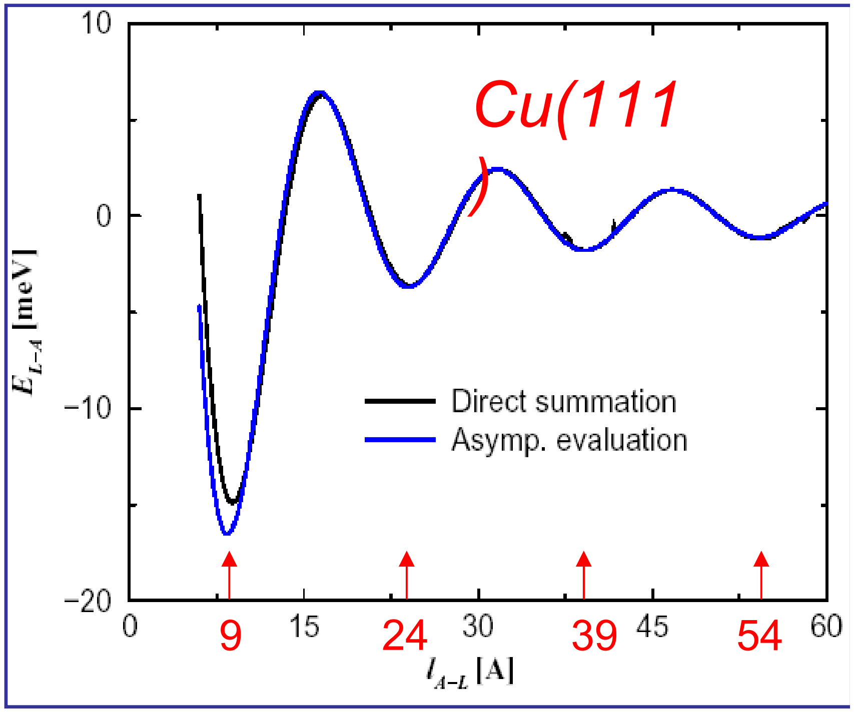
Current image of ripple structures

204.18nm x 204.18nm, V = -1.396V, I = 0.101nA, room temp.

C. Tao & E.D. Williams

Strong, Slowly-Decaying Atom-Adchain Interaction





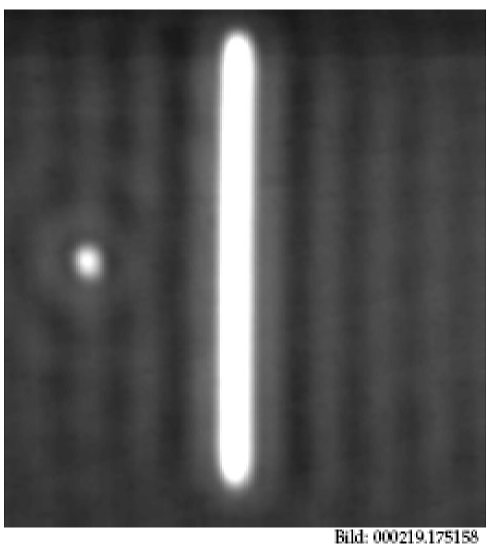
Asymptotic Evaluation:

$$\Delta E_{L-A}(l) \approx - \frac{\varepsilon_F}{\sqrt{\pi}} \left(\frac{2\sin(\delta_F)}{\pi} \right)^2 A(\delta_F) \left(\frac{\lambda_F/2}{a} \right) \frac{\sin(2q_F l + 2\delta_F + \pi/4)}{(q_F l)^{3/2}}$$

Redfield & Zangwill, PRB '92
TLE review '96

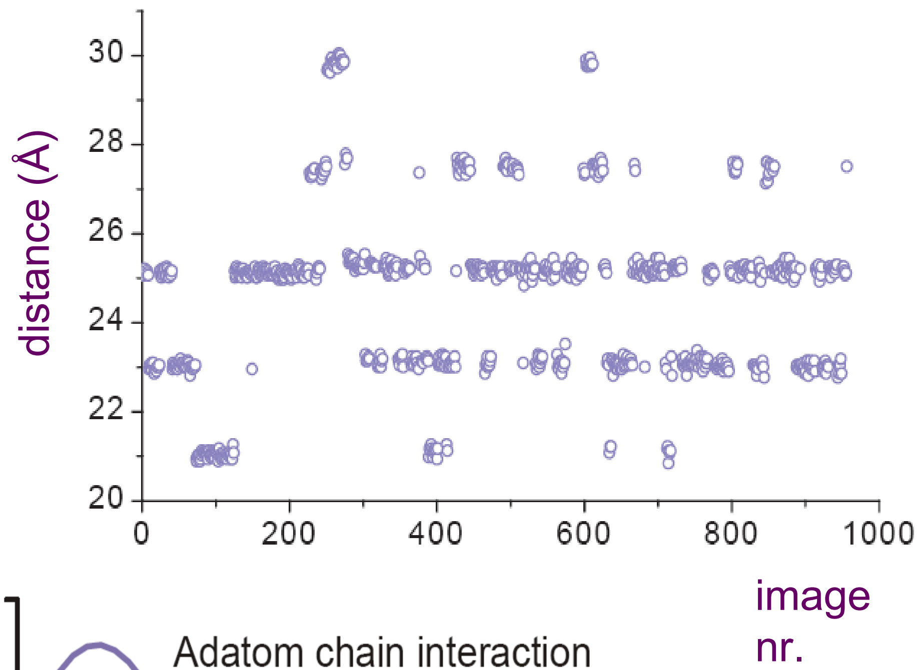
Deducing Chain-Atom Potential from 950^{+} STM images

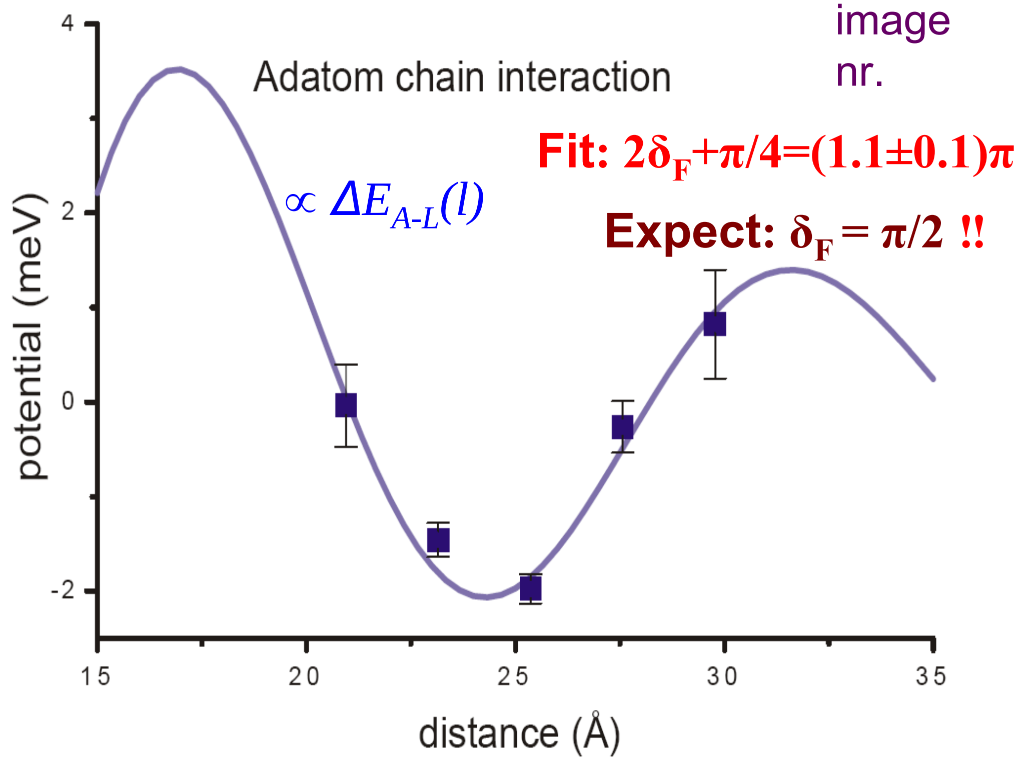
J. Repp, dissertation '02



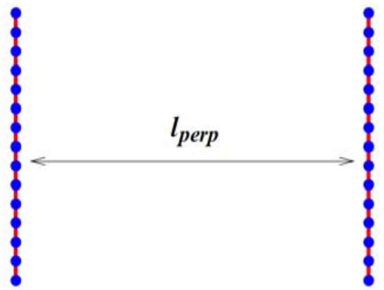
130Å × 130Å; 0.5nA; +100mV

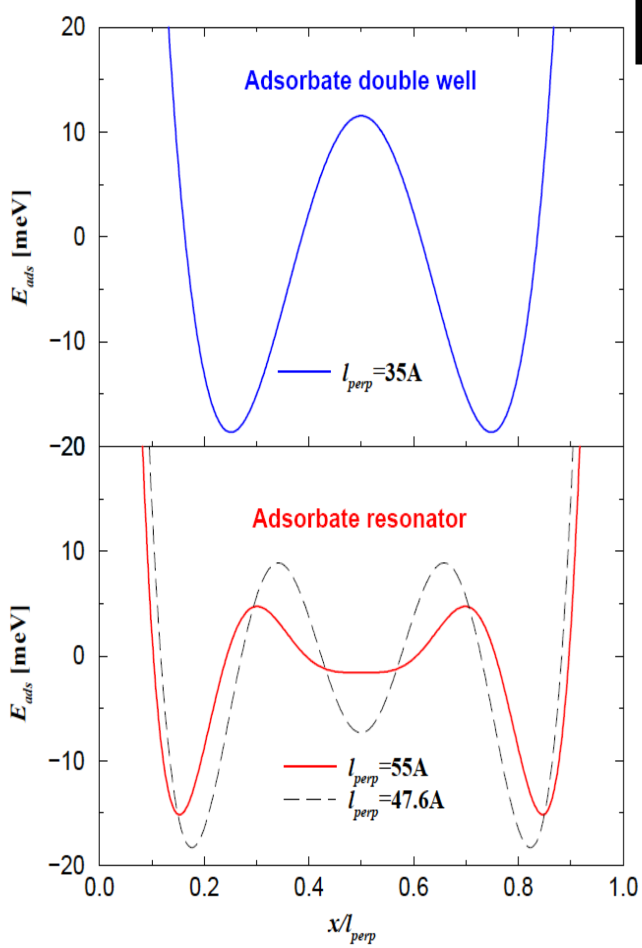
32 hours, T = 12.5K

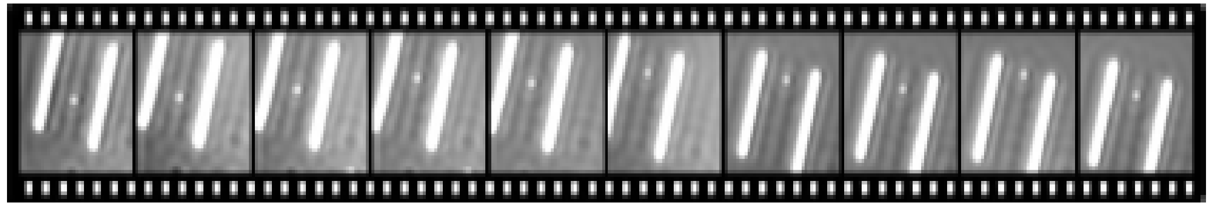




Chain Pairs ⇒ Potential Trough[s]



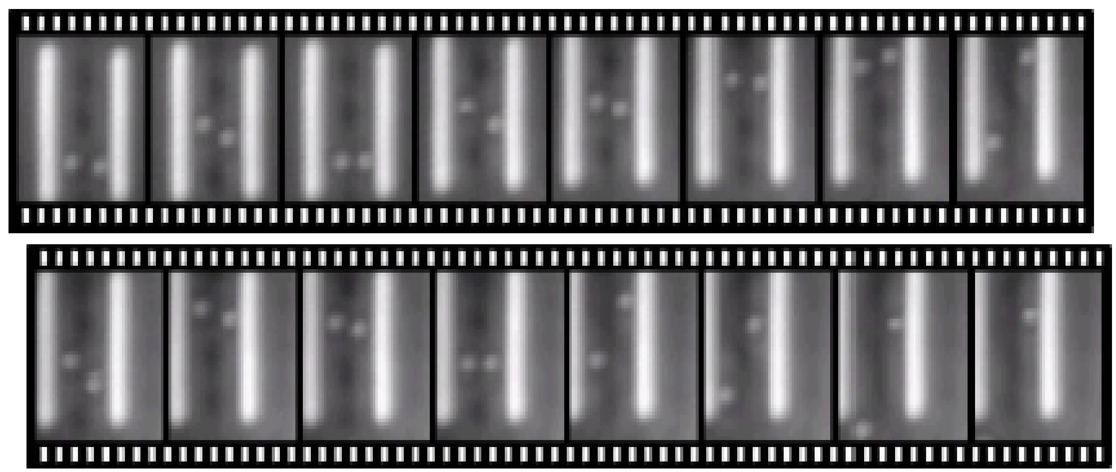




je 100Å × 100Å; 70pA; +105mV

l_{perp} = 55Å, 19 hours, T = 12K

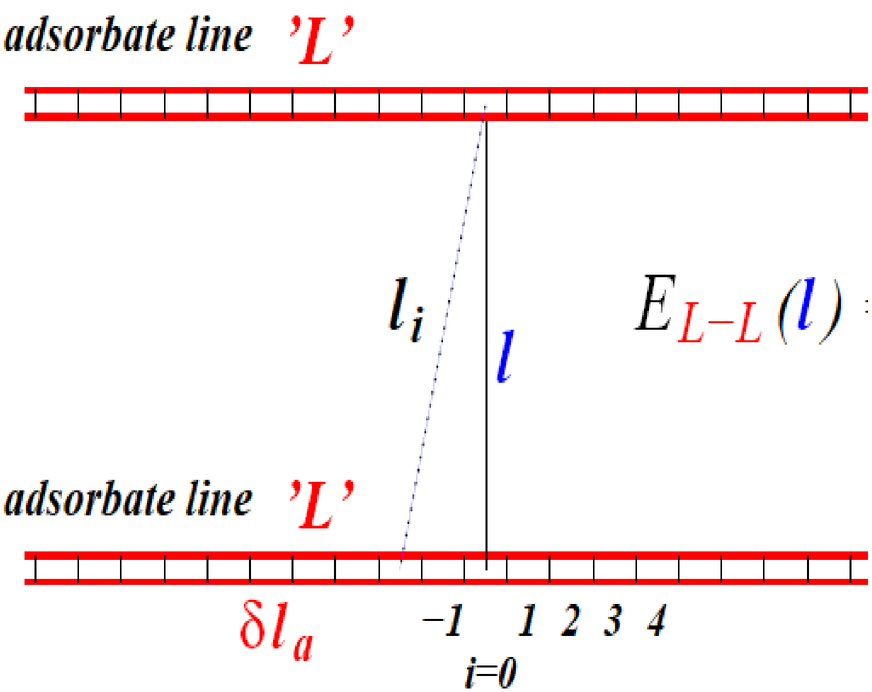
1 or 2 Cu atoms 1-D diffusing in parallel troughs *J. Repp*



ie 65Å × 65Å; 200pA; +105mV

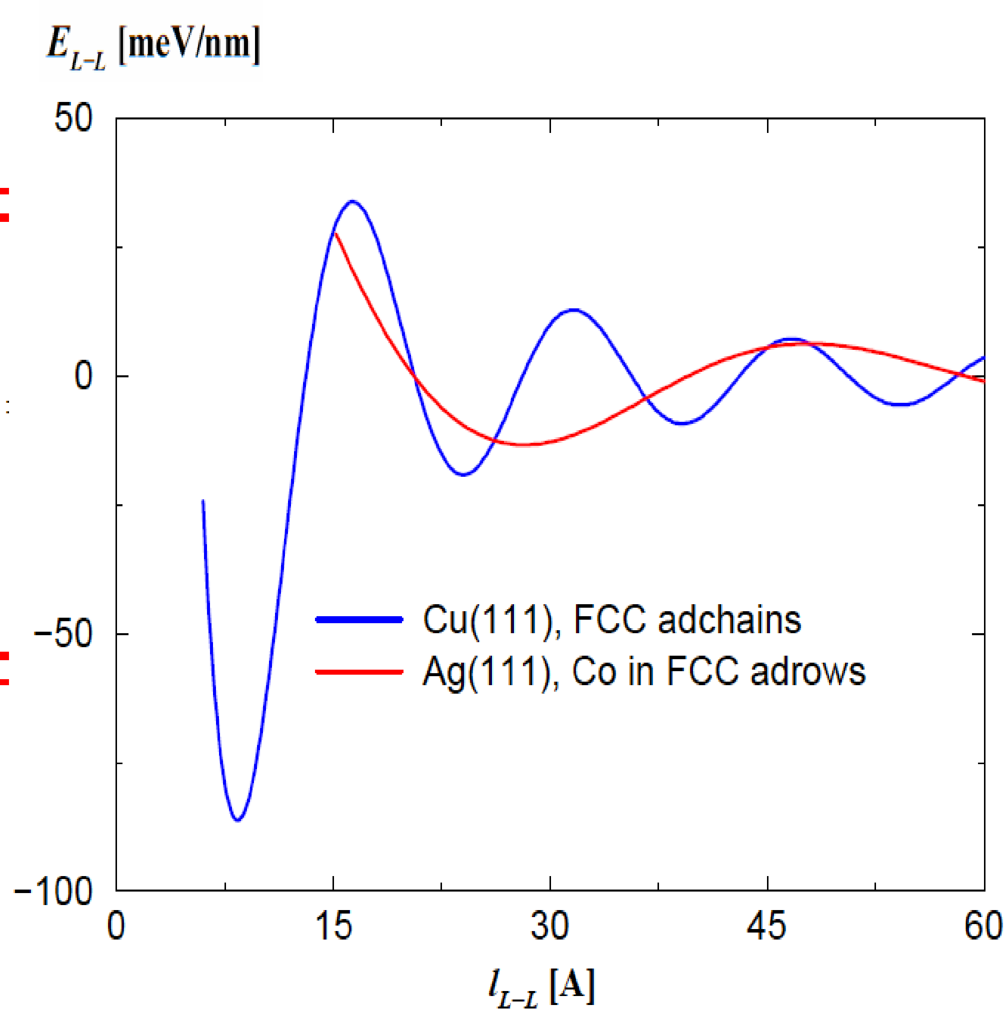
l_{perp} = 35Å, 30 hours, T =

Adchain-Adchain Interaction: Prelude to Steps?



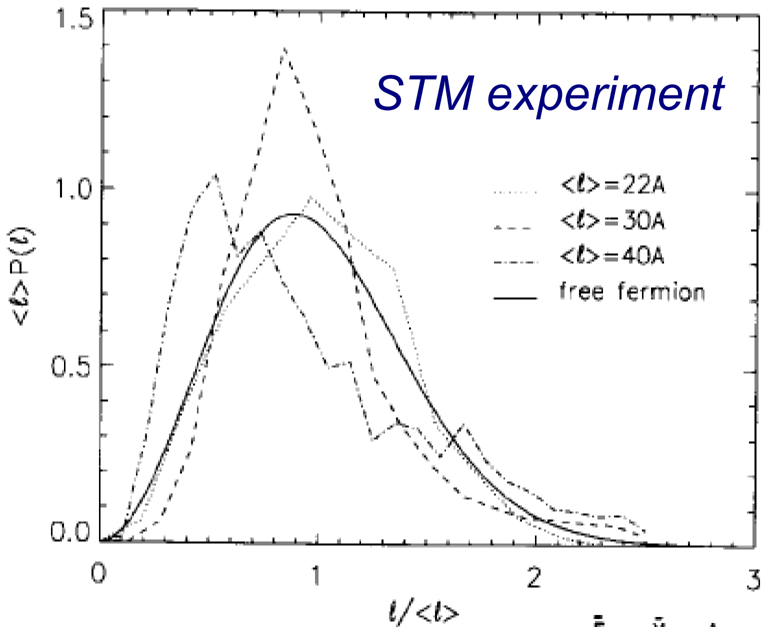
$$E_{L-L}(l) = \sum_i E_{pair}(l_i)$$

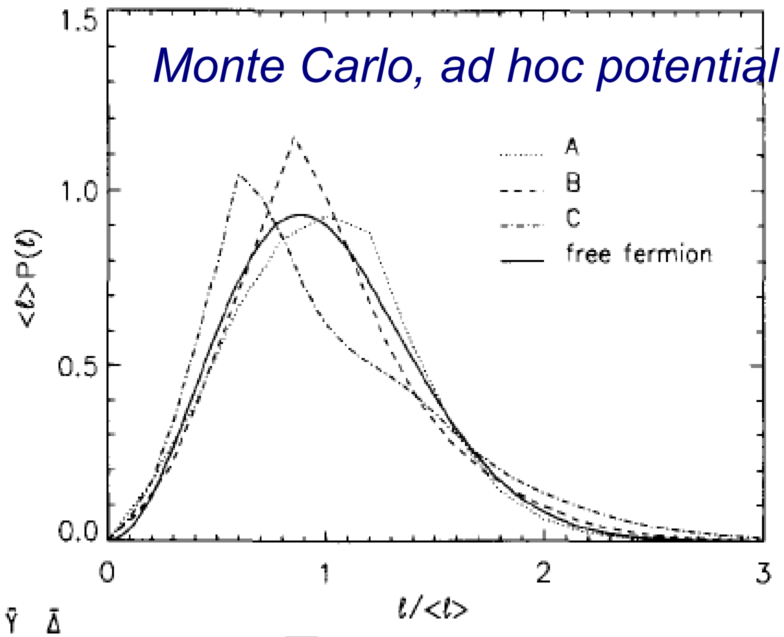
$$E_{L-L}(l) = N\, E_{A-L}(l)$$

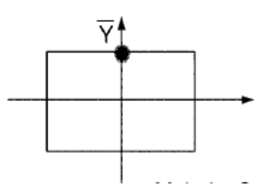


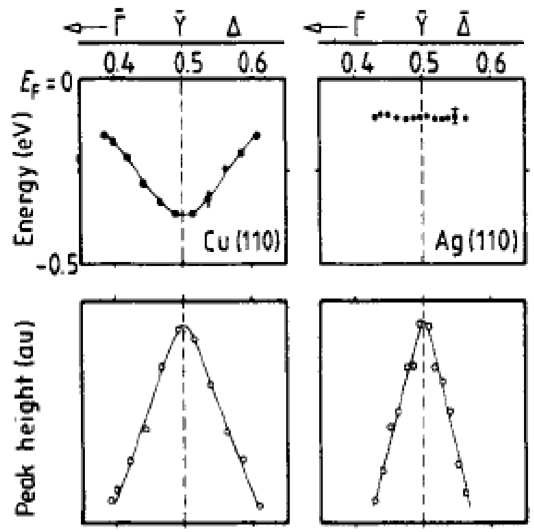
	ε_F [eV]	$(\lambda_F/2)$ [Å]	δ_F
Cu/Cu(111)[a]	0.39	15	$\pm\pi/2^a$
Co/Ag(111)[b]	0.06	38	$\pi/3^b$

Surface-state mediated step interaction wrecks of TWD scaling *W.W. Pai, TLE, J.E. Reutt-Robey, Surf. Sci. 307-9 ('94) 747*

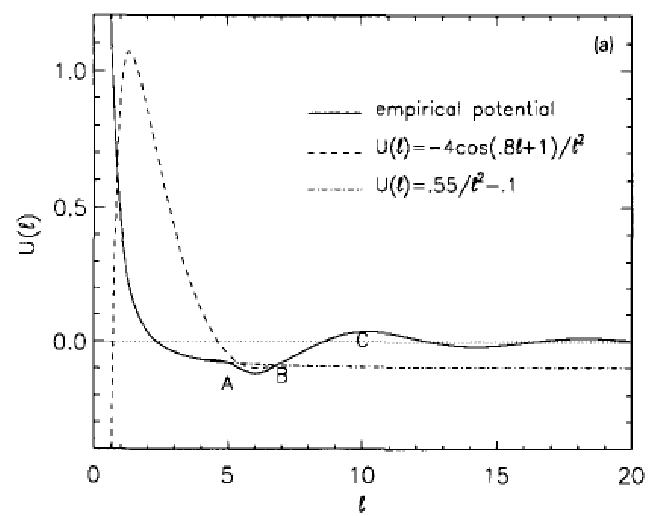








R. Courths…S. Hüfner,
J. Phys. F 14 (1984) 1559



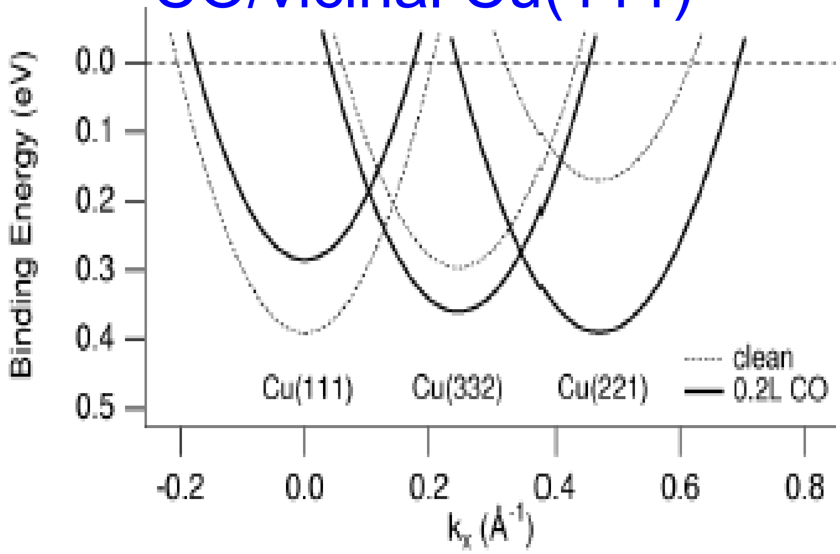
From Chains to Steps: Complications

T. Greber: steps as actors or spectators?

q_F *tunable* by step width & decoration

Baumberger, Greber,..., PRL **88** ('02) 237601

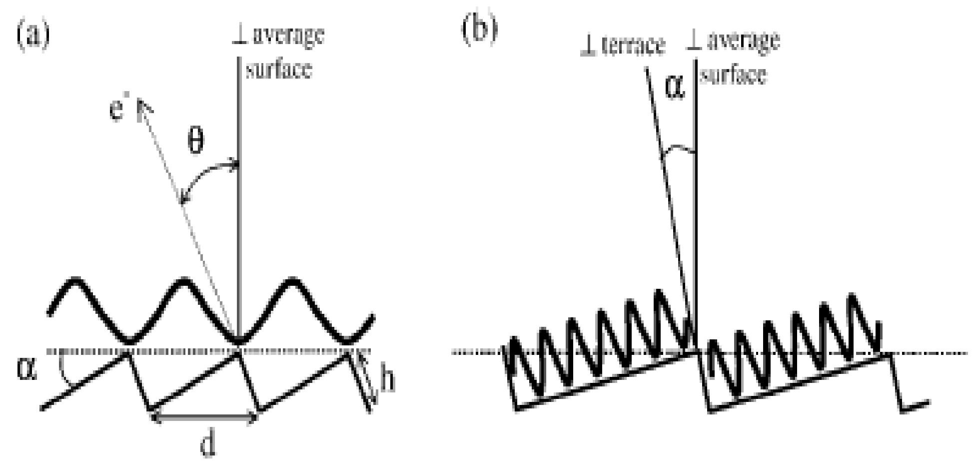
CO/vicinal Cu(111)



Switch from terrace to step modulation

Ortega,…,Himpsel, PRL **84** ('00) 6110

ψ on vicinal Cu(111)



vicinal-dominated

terrace-dominated

switch at α = 7°

Broad Implications of Surface-State Mediated Int'ns

- Distribution $P(\ell/\langle\ell\rangle)$ of terrace widths ℓ becomes dependent on mean step spacing $\langle\ell\rangle$ (rather than universal form depending only on strength of ℓ^{-2} step-step repulsion). [Pai…, Surf Sci '94]
- Equilibrium crystal shape no longer scales arbitrarily with crystal size since introduction of *new length scale* λ_F. *Pokrovsky-Talapov* "critical behavior" of curved region near facet edges should be altered.

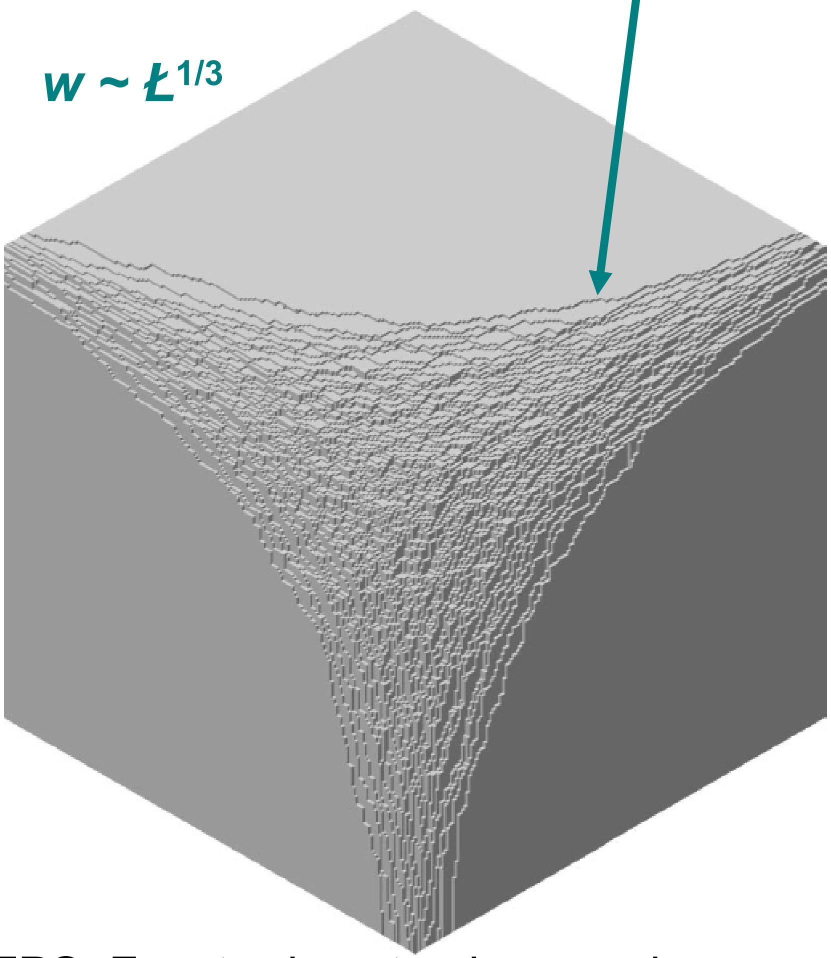
- Pair and trio interactions can affect the pathways of atoms approaching islands/clusters, enhancing or impeding growth.
- Magnetic interactions should have same periodicity as atomic interactions, but there is no obvious *a priori* reason for the phase factor δ_F to be the same, so rich behavior is possible.
- Intriguing possibilities for nanoengineering!

Facet edge vs. isolated step (or single-layer island) & vicinal surface

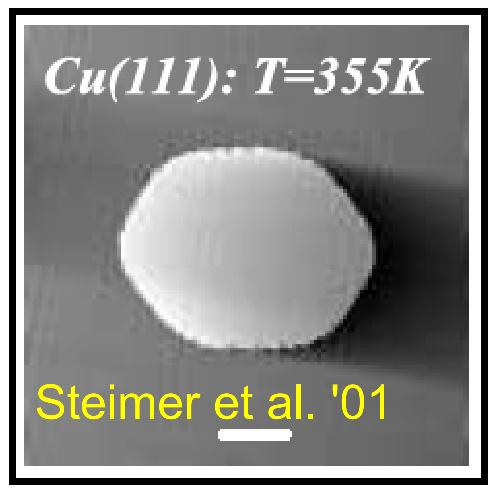
"On the Beach": facet *"shoreline"*
…by a rough sea!

Ł is along *y* direction.

***w ~ Ł*$^{1/3}$**

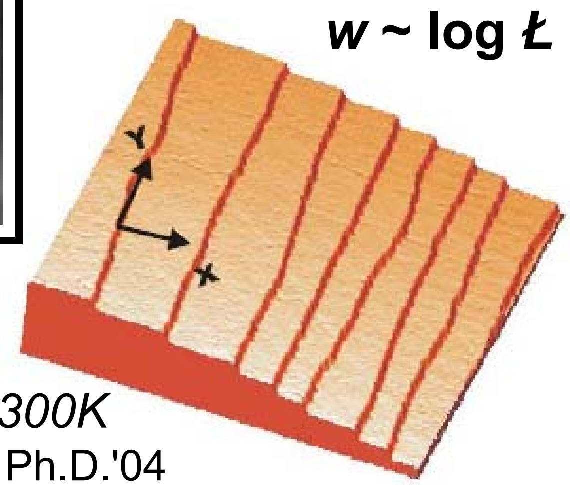


FPS: Facet-edge step has much more space in which to meander than steps in rounded [rough] region.



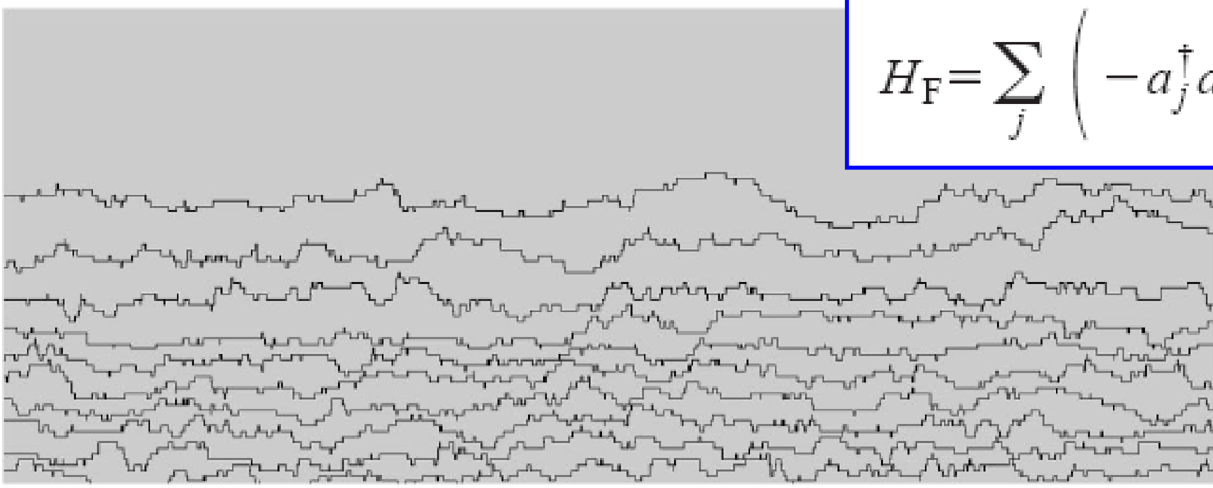
***w ~ Ł*$^{1/2}$**

w ~* log *Ł



Al/Si(111): T=300K
D.B. Dougherty Ph.D.'04

FPS Analysis: steps as [free] fermion world lines



$$H_F = \sum_j \left(-a_j^\dagger a_{j+1} - a_{j+1}^\dagger a_j + 2a_j^\dagger a_j + \frac{j}{\lambda} a_j^\dagger a_j \right)$$

λ^{-1} is Lagrange multiplier
re ***conserved volume,***
→ 0 in macro limit

Exact result for step density $\bar{\rho}_\lambda(j) = \langle \bar{a}_j^\dagger a_j \rangle_\lambda$ in terms of Bessel function J_j & deriv's

Near shoreline, $\lim_{\lambda\to\infty} \lambda^{1/3} \rho_\lambda(\lambda^{1/3} x) = -x \mathrm{Ai}(x)^2 + \mathrm{Ai}'(x)^2$

Shoreline wandering: $\mathrm{Var}[b_\lambda(t) - b_\lambda(0)] \cong \lambda^{2/3} g(\lambda^{-2/3} t)$ $\quad$ *g(s)*: $2|s| \to 1.6264 - 2/s^2$

$$\mathrm{Var}[b_\ell(\ell\tau + x) - b_\ell(\ell\tau)] \cong (\tfrac{1}{2} A \ell)^{2/3} g\left(\frac{A^{1/3}}{2^{1/3}\ell^{2/3}} x\right)$$

$\ell \sim N^{1/3}$ $\quad$ cf. 3-d Ising corner

In scaling regime shoreline fluctuations are *non-Gaussian* & related to GUE multimatrix models.

$\kappa = \frac{1}{2}(\pi\gamma_{PT} k_B T/\tilde{\beta})^2$ $\quad$ where $h = -\frac{2}{3}\gamma_{PT}(r - \rho_0)^{3/2}$ (up to lattice consts)

Heuristic extraction of dynamic/growth exponent β

Isolated steps: $G(t) \equiv \langle [x(t_0+t) - x(t_0)]^2 \rangle_{t_0[,y_0]} \propto t^{2\beta} = \begin{cases} t^{1/2} & \text{A} \\ t^{1/4} & \text{B} \end{cases}$

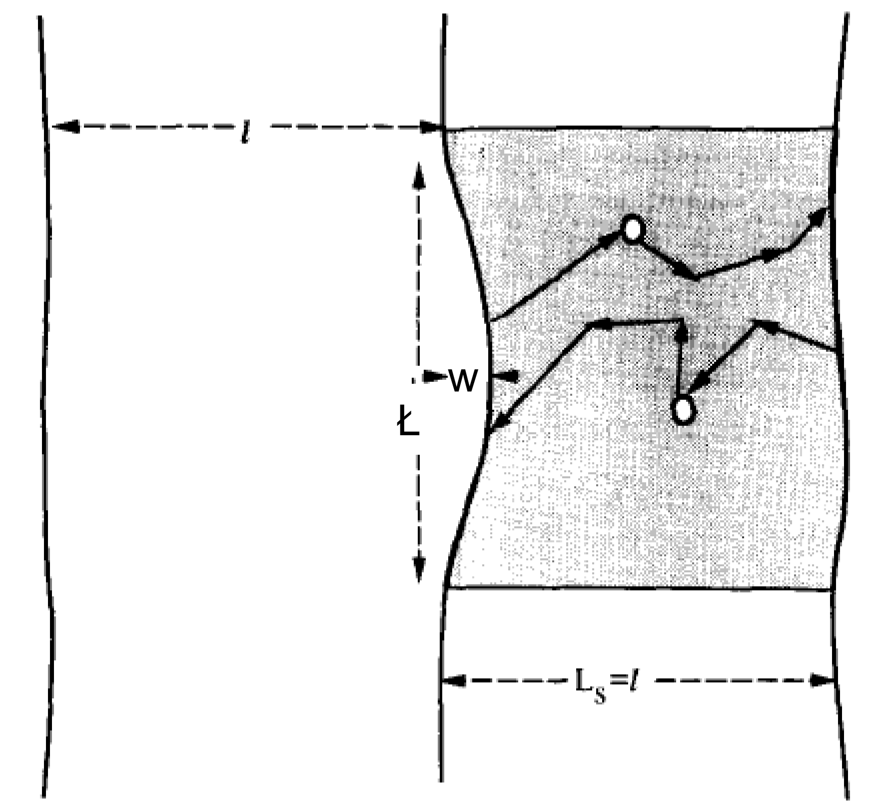


Fig. 1. A stepped surface seen from above. A typical configu-

- # atoms entering/leaving in t: $N(t) \approx c_{eq} Ł L_s t/\tau^*$
- fluctuating area²: $W^2 Ł^2 \approx (\delta N)^2 \approx N(t)$
- Ferrari *et al.* scaling: $W \sim Ł^{\alpha} \rightarrow Ł^{1/3}$
- $L_s \approx a$

A) Attachment-detachment limited

$1/\tau^* \approx$ kinetic coef.

$w \approx t^{1/5}$ or $G(t) \approx t^{2/5}$

B) Step-edge diffusion limited

$1/\tau^* \approx D_{se}/Ł^2$

$w \approx t^{1/11}$ or $G(t) \approx t^{2/11}$

A. Pimpinelli, J. Villain, et al.,
Surf. Sci. **295**, 143 ('93)

A. Pimpinelli, M. Degawa, TLE, EDW, Surface Sci. **598**, L355 (2005).

Scaling approach

$$x(y,t) \rightarrow \tilde{r}(\theta,t) = [r(\theta,t) - \rho_0]/\rho_0$$

$$\delta\mu = a^2\tilde{\beta}\left(\kappa - \frac{1}{\rho_0}\right) \approx \frac{a^2\tilde{\beta}}{\rho_0}\left(-\tilde{r}_{\theta\theta} + \frac{1}{2}\tilde{r}_\theta^2\right)$$

Nonlinear KPZ term in Langevin eqns due to curvature

(or from asymmetric potential due to step neighbor on just 1 side)

$$\frac{\partial \tilde{r}(\theta,t)}{\partial t} = \left(\Gamma_{\mathrm{AD}} \cdots\right)\left[\frac{\partial^2 \tilde{r}}{\partial \theta^2} - \frac{1}{2}\left(\frac{\partial \tilde{r}}{\partial \theta}\right)^2\right] + \eta(\theta,t)$$

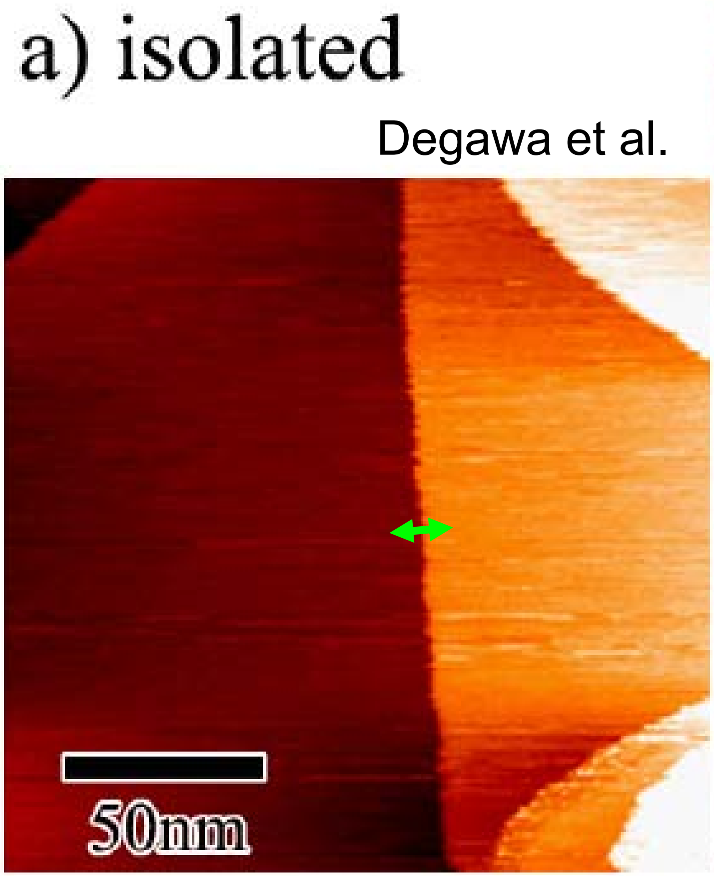
$$\frac{\partial \tilde{r}(\theta,t)}{\partial t} = \left(\Gamma_{\mathrm{SED}} \cdots\right)\left[-\frac{\partial^4 \tilde{r}}{\partial \theta^4} + \frac{1}{2}\frac{\partial^2}{\partial \theta^2}\left(\frac{\partial \tilde{r}}{\partial \theta}\right)^2\right] + \eta_C(\theta,t)$$

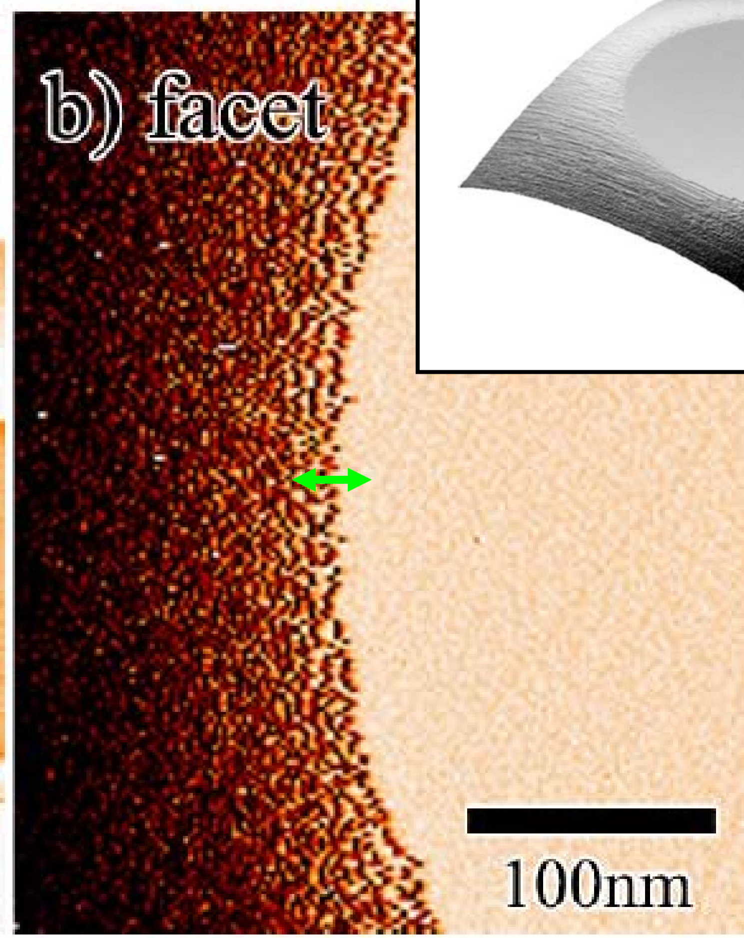
Dilate by *b*, so *Ł'* = *b Ł*, *w'* = *b*$^{\alpha}$ *w*, *t'* = *b*^{z} *t*; equate exponents of *b*

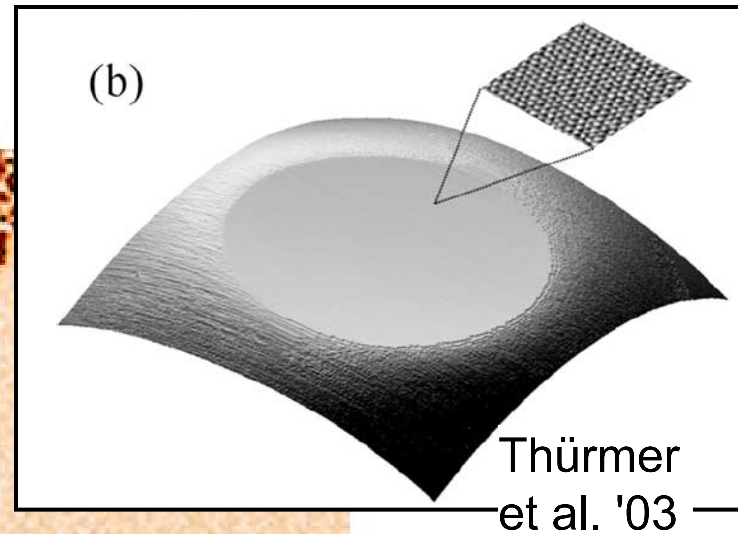
Class	$\partial/\partial t$	Lin. $\nabla^{2,4}$	NL KPZ	Noise	α	z	$\beta = \alpha/z$
Isolated AD	$\alpha - z$	$\alpha - 2$	-	$-(1+z)/2$	$1/2$	2	$1/4$
Isolated SED	$\alpha - z$	$\alpha - 4$	-	$-(3+z)/2$	$1/2$	4	$1/8$
Train AD	$\alpha - z$	$\alpha - 2$	-	$-(2+z)/2$	0 (ln)	2	0
Asymmtr. AD	$\alpha - z$	$\alpha - 2$	$2\alpha - 2$	$-(1+z)/2$	$1/3$	$5/3$	$1/5$
Asymmtr. SED	$\alpha - z$	$\alpha - 4$	$2\alpha - 4$	$-(3+z)/2$	$1/3$	$11/3$	$1/11$

STM images (scanned, not snapshot): step & facet edge

(111) facet [close-packed] on supported Pb crystallite

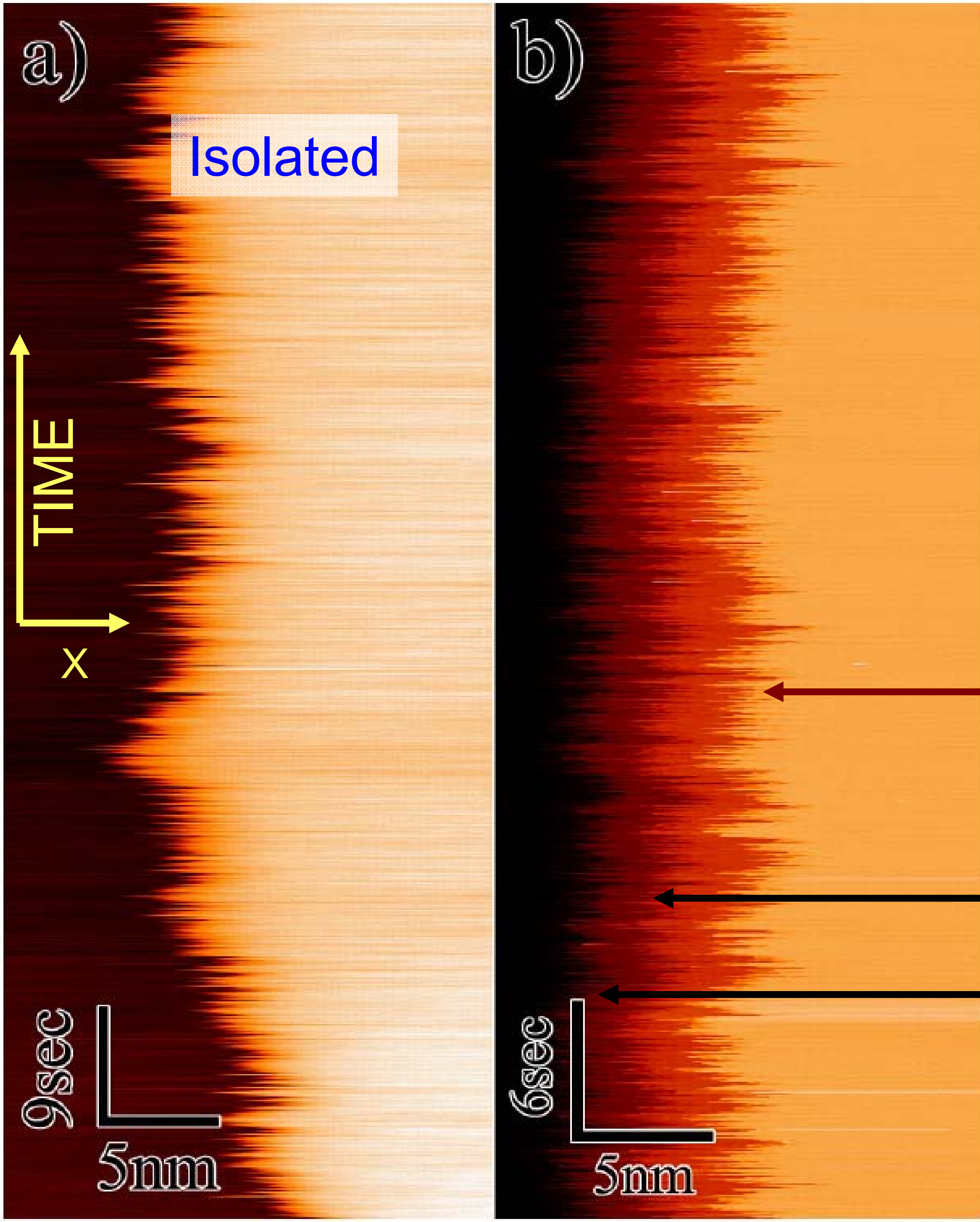






from screw dislocation

Equilibrium fluctuations studied by F. Szalma et al. '06



STM line-scans (pseudoimages)

$$\langle [x(t_0+t)-x(t_0)]^2 \rangle_{t_0}$$

$$\equiv G(t) \propto t^{2\beta}$$

$$w^2 = ½\, G(t\rightarrow\infty)$$

Facet edge (shoreline)

Analyzed on next slide

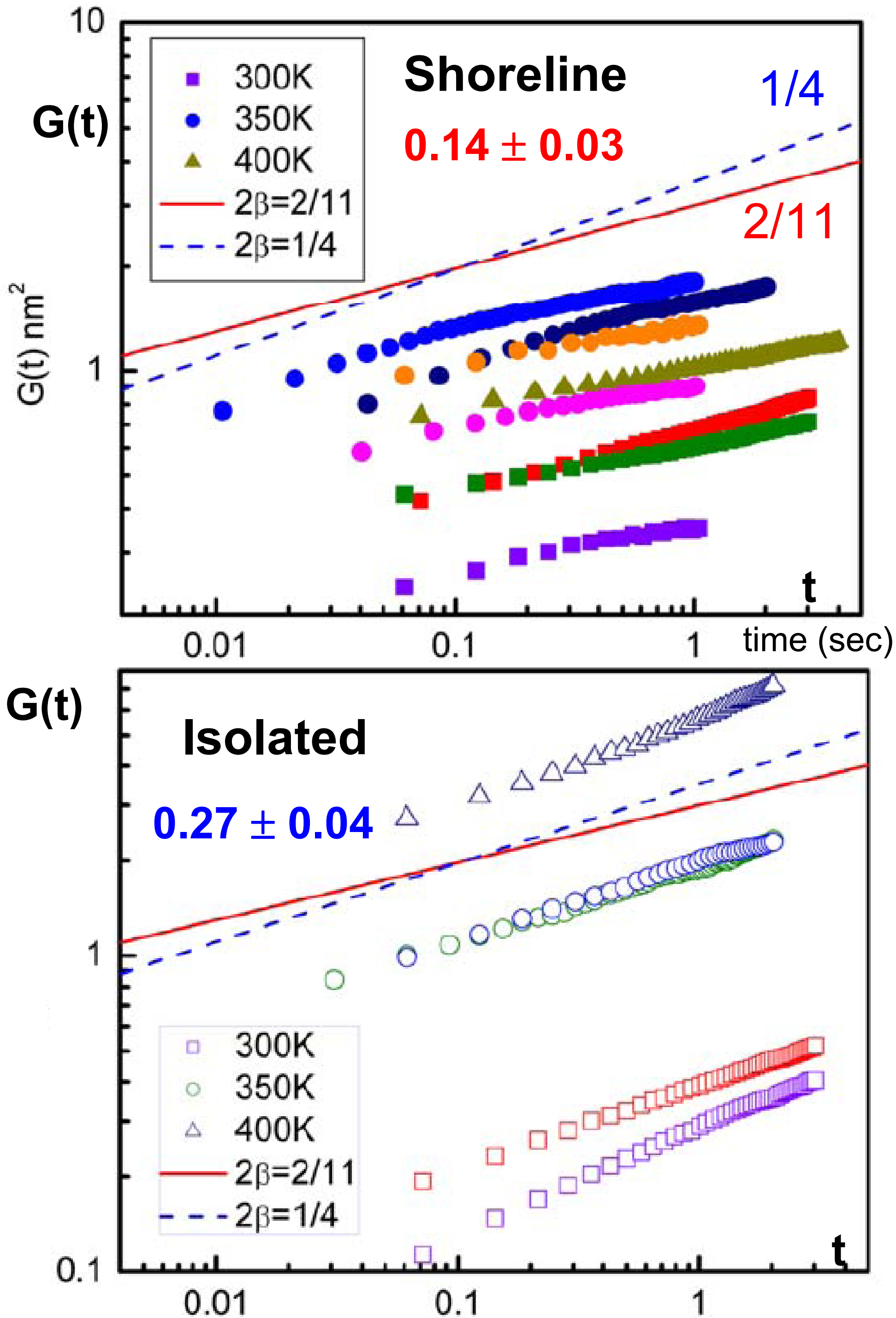
Next step edge

3rd step edge

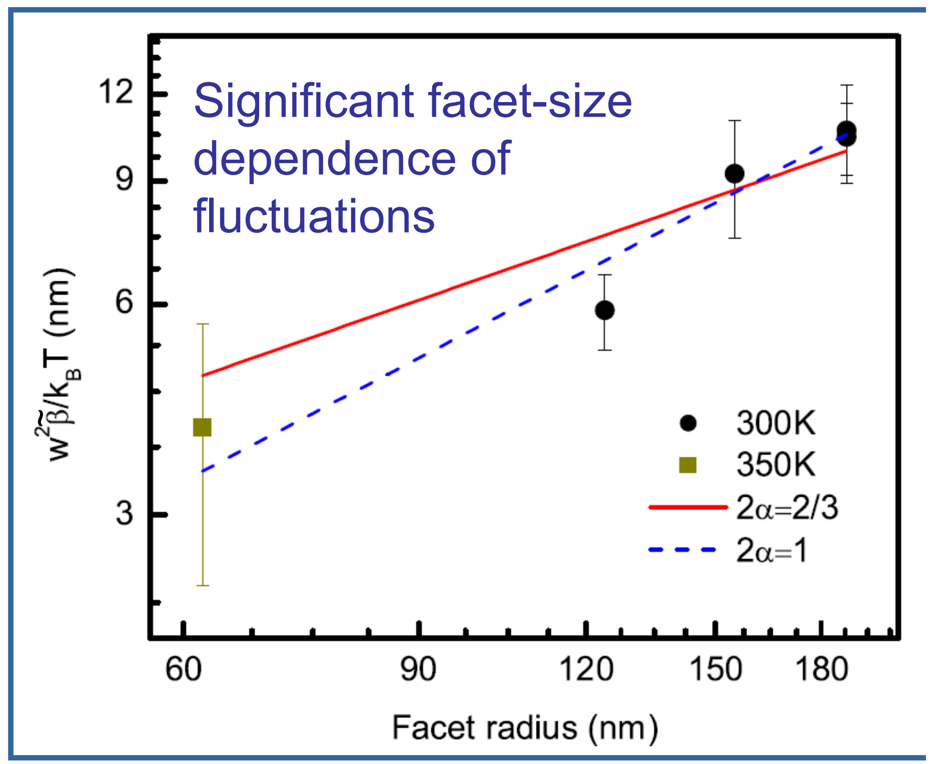
fcc metals (late trans., noble,…):

mass transport by SED (B)

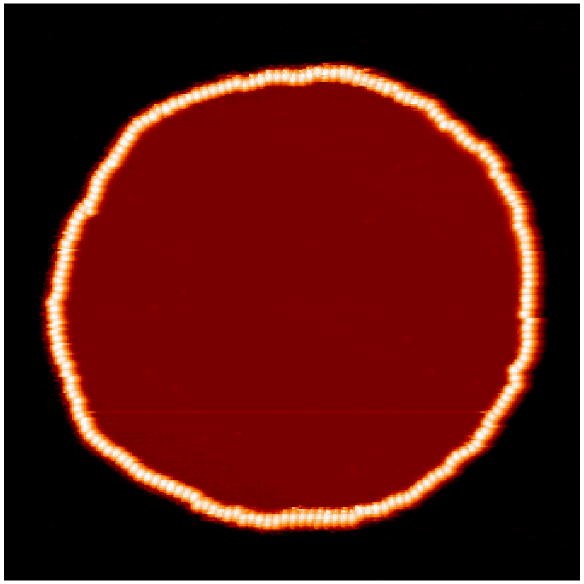
Extract 2β from log-log plot of experimental *G(t)*

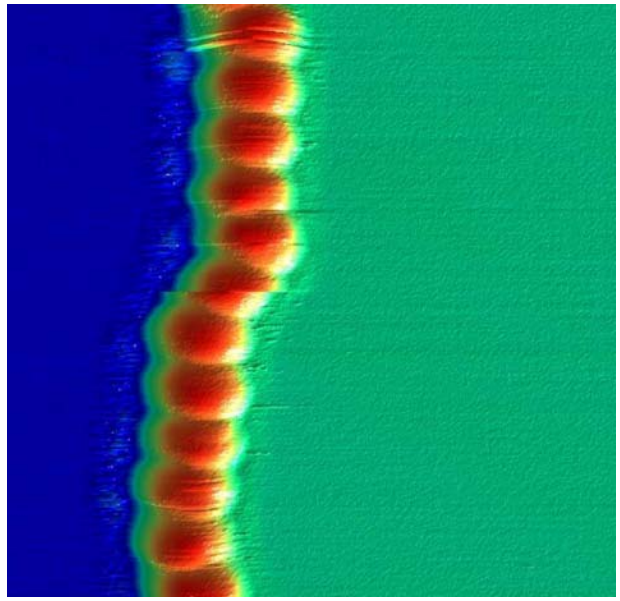


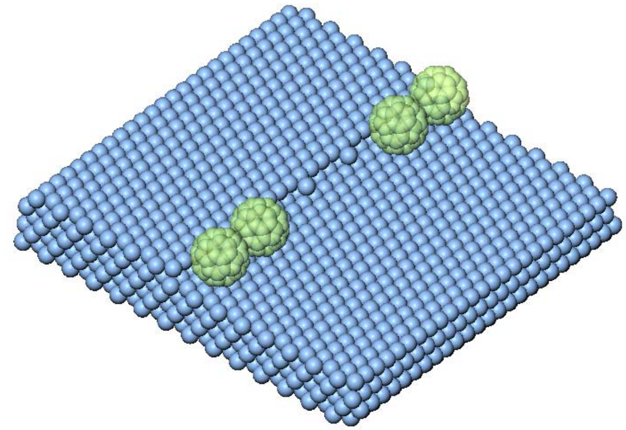
Exponent for facet edge is significantly smaller than for isolated step, with value consistent with expectation for asymmetric SED

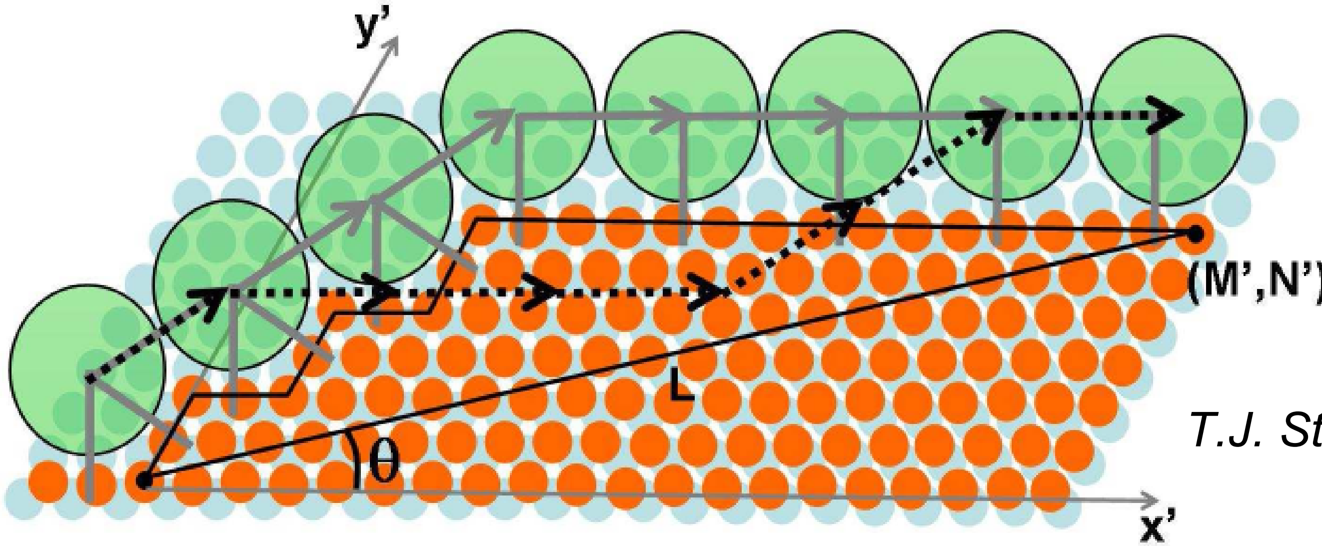


C_{60} on Ag(111)









T.J. Stasevich, C.G. Tao, et al.

Some Take-Away Messages

- Fermion picture is fruitful, and perhaps also seductive
- When energetic repulsions $\propto A/\ell^2$, TWD is independent of $\langle \ell \rangle$
- Entropic and elastic interactions do not simply add
- Generalized Wigner surmise is useful to analyze TWD
- Short-range corrections to elastic interactions may lead to finite-size corrections $\Rightarrow$ may need to do several $\langle \ell \rangle$'s (i.e., ϕ's)
- Interactions mediated by metallic surface states introduce new length scale that leads to dependence of TWD on $\langle \ell \rangle$, no scaling