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# "Long range logarithmic interaction between steps at vicinal surfaces of quantum crystals"

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**These are preliminary lecture notes, intended only for distribution to participants.**

# Long-Range Logarithmic Interaction between Steps at Vicinal Surfaces of Quantum Crystals

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# OUTLINE

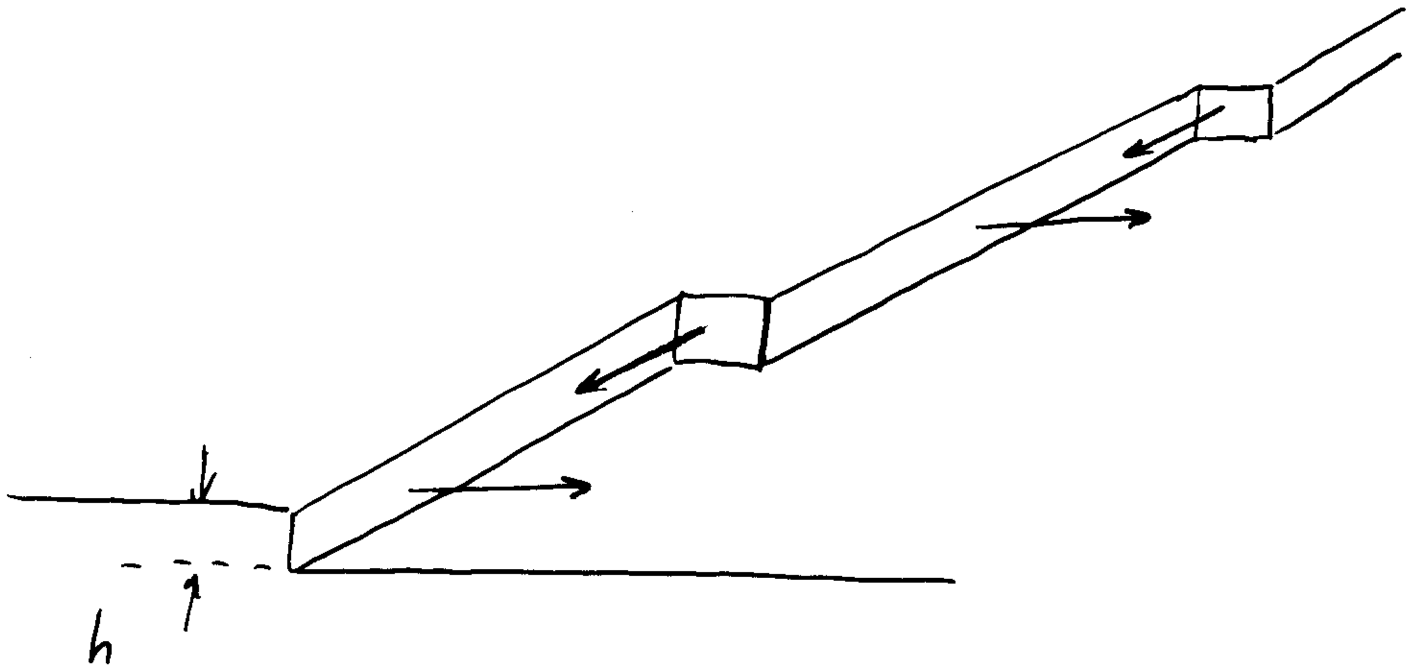
1. Long-wavelength dynamical properties of single-layer steps at vicinal surfaces.

2. Intrinsic surface stress and step-step interaction.

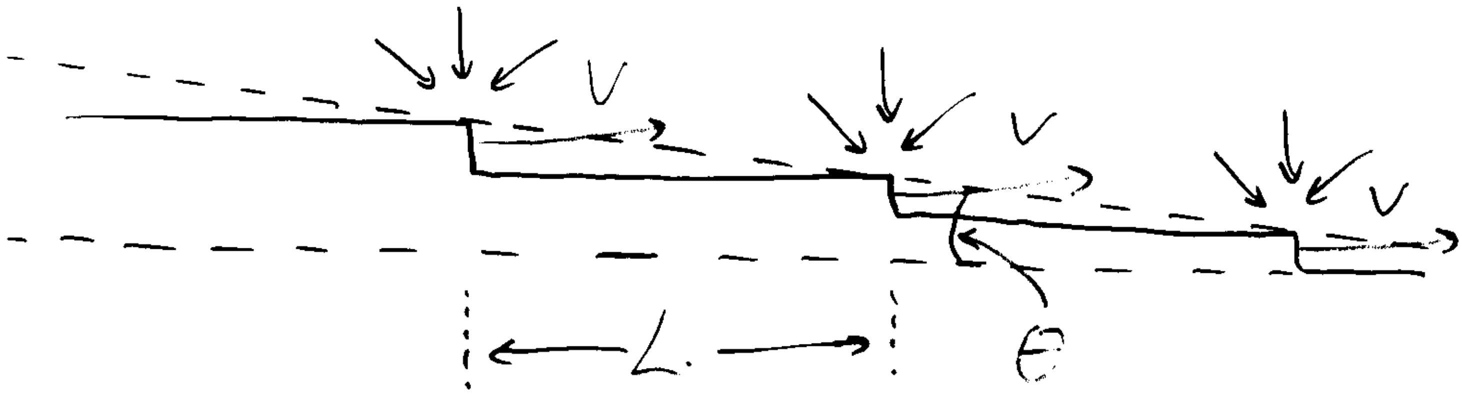
3. Model for thermal-fluctuation induced ISS and logarithmic step-step interaction in QS.

4. $T/\theta$ surface stiffness $\tilde{\alpha}$ of c-facets in $^4He$ crystals.

5. Application to anisotropic surfaces (with dimer rows).




• $\theta = \frac{h}{L} \ll 1$ - small inclination




• $m_{eff.} \sim \rho \cdot \left(\frac{\Delta\rho}{\rho}\right)^2 \cdot \underbrace{h^2} \ln(L/h)$ -

effective mass (per unit line)

( A. Kosevich, Yu. K. '81 - prediction;
'90; '95; '96 - experiments)

- New Branches of surface sound waves with $q_{\parallel} h \ll 1$, trapped by parallel steps at vicinal surface

( Ni(977) surface,

Niu et al. '95 - exp.

Mele, Pykhtin '95 - theory,

boundary conditions with only

- the "geometrical" constrains at the vicinal surface ).

Conclusion from these observations:

Macroscopic (hydrodynamic) boundary conditions work up to $h \sim a$.

In particular, for static elastic strain single-layer step edge should be stress-free.

At c-facet of He crystal,

surface stiffness $\tilde{\alpha}$:

- $\tilde{\alpha} \equiv \alpha + \frac{\partial^2 \alpha}{\partial \theta^2} = \underline{\frac{K}{\theta}}$ for $\theta \ll 1$,

$K = (11 \pm 3) \times 10^{-4}\, T$ (erg/cm$^2$·K),

for $0.05\,K \leq T \leq 0.7\,K$

(Babkin, Alles, Hakonen, Parshin, Ruutu, Saramäki '95)

$\tilde{\alpha} \propto \frac{K}{\,}$ results from

- logarithmic interaction between steps with $\underline{L \gg h}$:

if $\underline{\alpha = \frac{A}{L} - \frac{B}{L} \ln(L/h)}$, $L = \frac{h}{\theta}$.

- $\tilde{\alpha} = B/(h\theta)$ for $\theta \ll 1$.

# C-facet of $^4He$ crystal:

- 1. Isotropic ;
- 2. No surface reconstructions;
- 3. No impurities (adatoms),
- 4. No electronic surface states

- Only lattice (phonon) excitations can contribute to surface states at low enough temperatures.

Intrinsic surface stress (ISS):

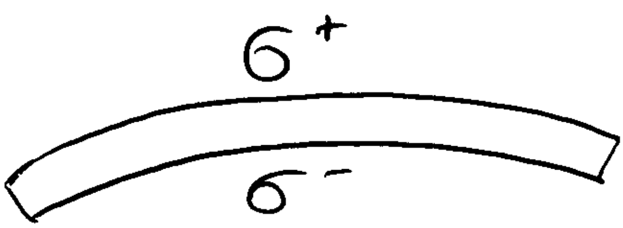
if $\underline{f_\alpha^s(\vec{x}) = \Omega_{\alpha\beta}\nabla_\beta'\delta(\vec{x}-\vec{x}')}$,

where $\Omega_{\alpha\beta} = \Omega_{\beta\alpha}$ – "strength" of surface elastic dipoles,

then $\underline{\sigma_{\alpha\beta}^s = \Omega_{\alpha\beta} n_s}$ – ISS,

where $n_s$ – surface density of elastic dipoles.

- $\underline{\mathcal{E}_{int.} = \int \sigma_{\alpha\beta}^s u_{\alpha\beta}^{ext.} dS}$ – energy of interaction with external elastic strain.




Experiments on bending of thin slabs with $\underline{\sigma^+ \neq \sigma^-}$ (Adatom-induced ISS)

Interaction between two isotropic elastic dipoles:

- $$U_{12}(R) = \Omega_0^{(1)} \Omega_0^{(2)} \frac{1-\sigma^2}{\pi E R^3},$$

  where $\Omega_{\alpha\beta}^{(1,2)} = \Omega_0^{(1,2)} \delta_{\alpha\beta}$

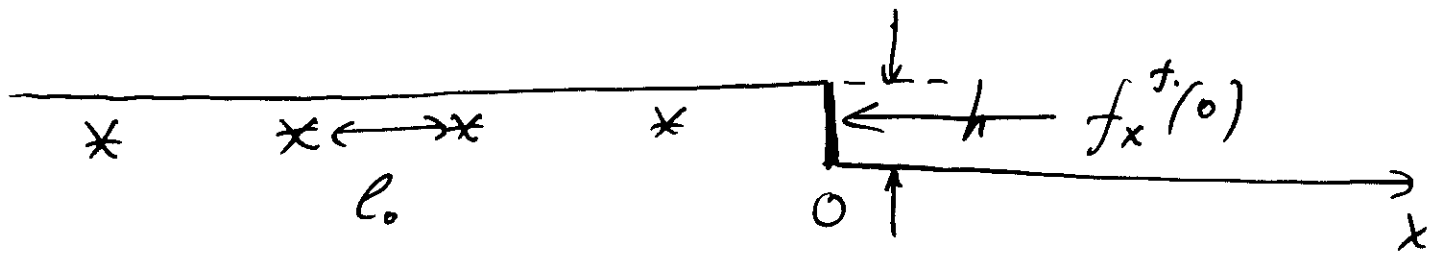
(Andreev, Y. K. '81)

- Interaction between a dipole and its "image" is attractive:

  $U_{12}(R) < 0$, since $\Omega_0^{(1)} \Omega_0^{(2)} < 0$.

- Energy of interaction of two half-planes of elastic dipoles (per unit length of the border line scales as $\Omega_0^{(1)} n_s^{(1)} \Omega_0^{(2)} n_s^{(2)} \ln(L/a)$.

Interaction of 2D array of surface elastic dipoles with <u>stress-free</u> step edge:




$$u_{xx}(0) = \frac{2(1-\sigma^2)}{\pi E}\,\frac{\Omega_0}{l_0^2}\sum_{n=1}^{\infty}\frac{1}{n^2}\,;$$

$$f_x^{f.}(0) = u_{xx}(0)\,\frac{E}{1-\sigma^2}\cdot h \quad (\text{for } h \ll l_0)$$

or $$f_x^{f.}(0) = \frac{\Omega_0}{l_0^2}\,h\,\frac{\pi}{3} \equiv \sigma_0^s\,\frac{h}{l_0}\,,$$

where $$\underline{\sigma_0^s} = \frac{\Omega_0}{l_0}\,\frac{\pi}{3} \simeq \underline{\frac{\Omega_0}{l_0}}\,.$$

- $f_x^{f.}$ – <u>"fictitious"</u> step-edge force, which maintains <u>stress-free</u> boundary conditions.

## In general:

- $f_x^{t.}(0) = \sigma_0^s \, \varphi(h/\ell_0)$,

where

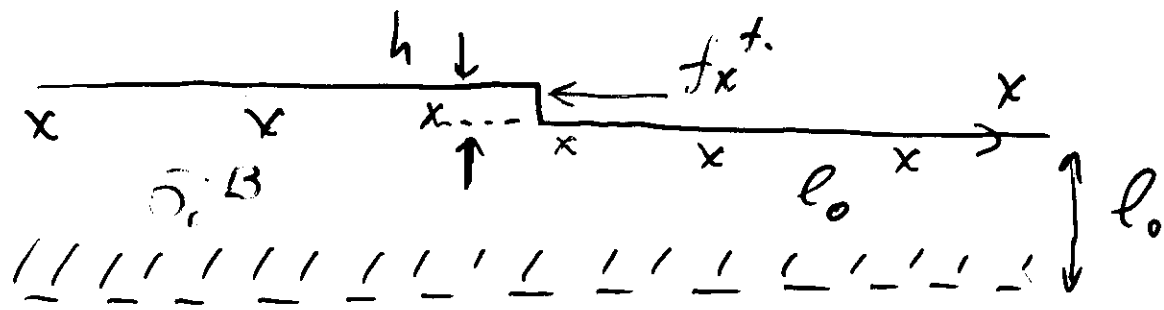
- $\varphi(x) \to x$, for $x \ll 1$;
- $\varphi(x) \to 1$, for $x \gg 1$.

$\Big\}$ form-factor.

(e.g. $\varphi(x) = \frac{2}{\pi}\arctan(x) + \left(1 - \frac{2}{\pi}\right)\frac{x}{1+x^2}$)

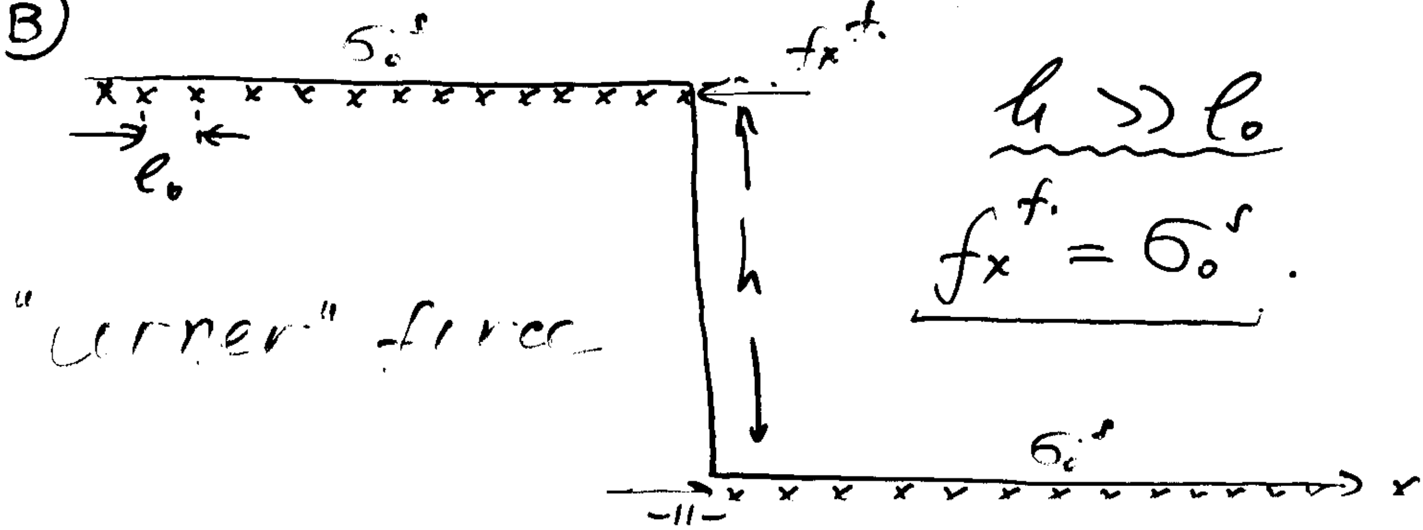
## It means:

(A)




$h \ll \ell_0$, $\quad f_x^{t.} = \sigma_0^s \frac{h}{\ell_0} = \sigma_0^B h$, $\quad \sigma_0^B = \frac{\sigma_0^s}{\ell_0}$

(B)




$h \gg \ell_0$

$f_x^{t.} = \sigma_0^s$.

## Energy of interaction:

- $$\mathcal{E}_1^{int.} = -\frac{2(1-\sigma^2)}{\pi E}(\sigma_0^s)^2\varphi\left(\frac{h}{l_0}\right)\int_{-L}^{-l_0}\int_{l_0}^{L}\frac{dx\,dx'}{(x-x')^2} =$$

$$= -2\,\frac{(1-\sigma^2)}{\pi E}(\sigma_0^s)^2\varphi\left(\frac{h}{l_0}\right)\underline{\ln\left(L/4l_0\right)},$$

if $(h, l_0) \ll L$.

## Contribution to surface energy:

$$\Delta\alpha_s = \frac{2}{L}\,\mathcal{E}_1^{int.} = 4\,\frac{1-\sigma^2}{\pi E}(\sigma_0^s)^2\,\frac{\varphi\left(\frac{h}{l_0}\right)}{h}\,\theta\ln\left(\frac{4\theta l_0}{h}\right),$$

$\theta = h/L \ll 1$ - inclination angle.

- $$+\ \frac{A}{L} = \frac{A\theta}{h},$$

$\underline{A}$ - step formation energy (per unit length of the step)

# Model for ISS $\sigma_0^s$ in QS:

- $\sigma_0^s = \dfrac{E}{1-\sigma^2} \cdot \underline{u_{xx}^0} \cdot a_\perp = \dfrac{E}{1-\sigma^2} \cdot \underline{\dfrac{\Delta u_x^0}{a_\parallel}} a_\perp$ ;

- $(\sigma_0^s)^2 = \left(\dfrac{E}{1-\sigma^2}\right)^2 \cdot \left(\dfrac{a_\perp}{a_\parallel}\right)^2 \cdot \underline{(\Delta u_x^0)^2}$.

<u>We assume</u>, that

- $(\Delta u_x^0)^2 = (\Delta u_y^0)^2 \simeq \langle u_\parallel^2 \rangle_T^S - \langle u_\parallel^2 \rangle_T^B$,

and

- $\langle u_\parallel^2 \rangle_T^S - \langle u_\parallel^2 \rangle_T^B = \underline{\gamma \langle u_\parallel^2 \rangle_T^B}$,

where

- $\gamma \ll 1$ – adjusting parameter.

We estimate:

$$\cdot \left\langle U_{\parallel}^2 \right\rangle_T^B = \frac{K_B T}{M \omega_{0\parallel}^2} \simeq \frac{K_B T}{M C_t^2} \cdot \frac{a_{\parallel}^2}{\pi^2};$$

$$\omega_{0\parallel}^2 \simeq C_t^2 \cdot \left(\frac{\pi}{a_{\parallel}}\right)^2;$$

and

$$\cdot \ h \simeq l_0; \quad \varphi(h/l_0) \simeq 1; \quad h \simeq a_{\perp}.$$

## Contribution to surface energy

$$\Delta \alpha_s = 4 \frac{E}{1-\sigma^2} \cdot \frac{K_B T}{M C_t^2} \cdot \frac{a_{\perp}}{\pi^3} \theta \ln\left(\frac{4\theta a_{\parallel}}{a_{\perp}}\right) \gamma;$$

since $\underbrace{\frac{E}{1-\sigma^2} \cdot \frac{a_{\perp}}{M C_t^2}}$ $\simeq \frac{\rho a_{\perp}}{M} = \frac{M a_{\perp}}{M a_{\parallel}^2 a_{\perp}} = \underline{\frac{1}{a_{\parallel}^2}}$

finally we obtain

$$\cdot \ \underline{\frac{\partial^2 \alpha}{\partial \theta^2} = \frac{T}{\theta} \cdot \frac{4 K_B}{\pi^3 a_{\parallel}^2} \cdot \gamma.}$$

For $a_{\parallel} = 3.3$ Å we obtain

- $$\frac{\partial^2 \alpha}{\partial \theta^2} = K\left(\frac{I}{\theta}\right) \text{ with } \underline{K \simeq 16 \cdot 10^{-3} \gamma} \left(\frac{erg}{cm^2 \cdot K}\right)$$

Experiment gives

- $$K = 1.1 \times 10^{-3} \left(\frac{erg}{cm^2 \cdot K}\right).$$

Thus we have to assume

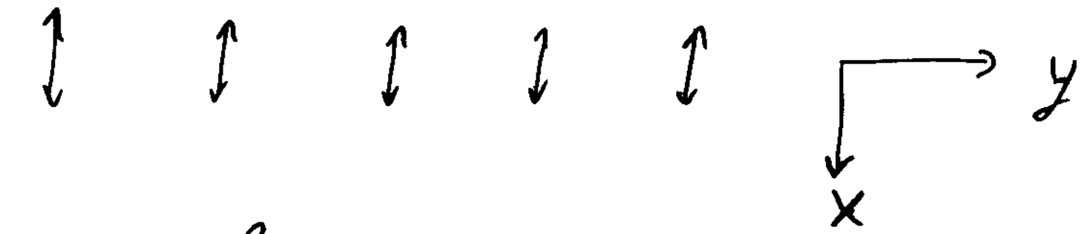
- $$\gamma \simeq \frac{1}{14} \simeq 7\,\%.$$

One can compare $\gamma$ with

- $$\frac{c_t^2 - c_R^2}{c_t^2} \simeq 10\% \quad (\text{for } \sigma = 1/3).$$

At <u>anisotropic surface</u>, one has to consider 2D array of <u>anisotropic elastic dipoles</u> (due to <u>reconstruction</u> e.g., dimers at Si(001) surface).

For dimer row along OY,

- 


one has

- $\Omega_{xx} \gg \Omega_{yy}$.
- The method is useful also for describing the interaction between <u>vacancies (voids)</u> in dimer rows

# Conclusions

1. 2D array of elastic surface dipoles mediate long-range logarithmic interaction between steps at vicinal surfaces.
2. In quantum solid elastic surface dipoles can be induced by the difference thermal mean-square displacements.
3. At anisotropic surfaces, anisotropic elastic surface dipoles can be induced by surface dimers.