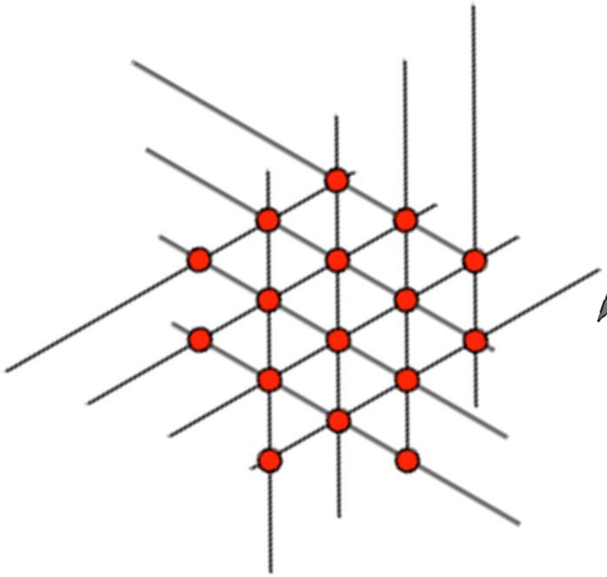
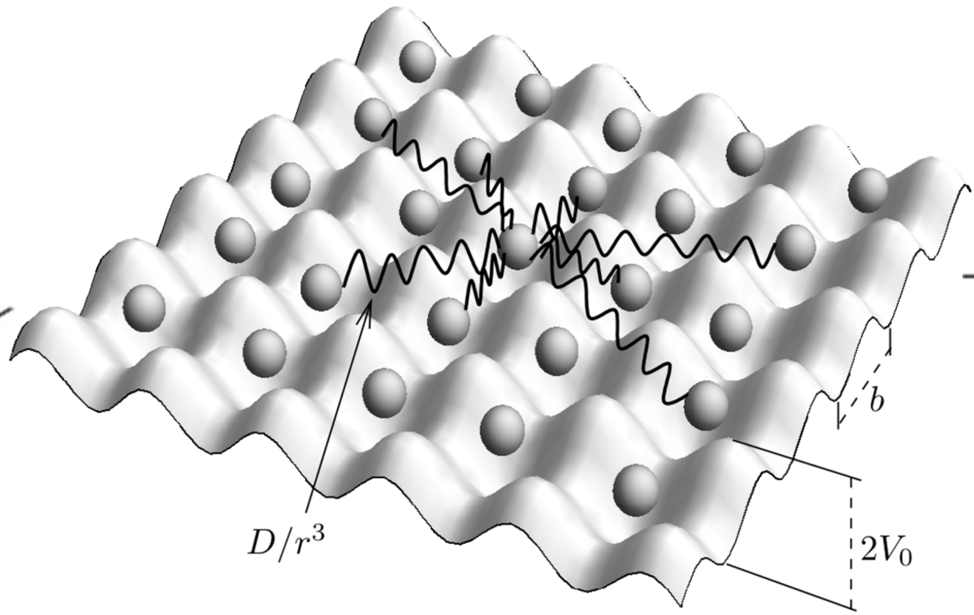
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

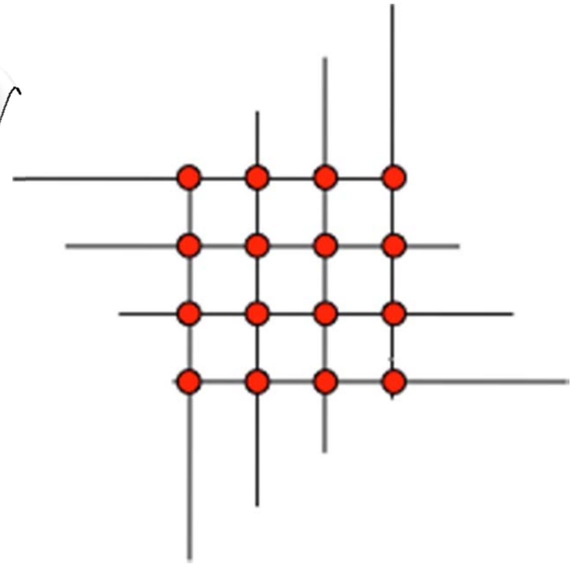
Landau Days 2014

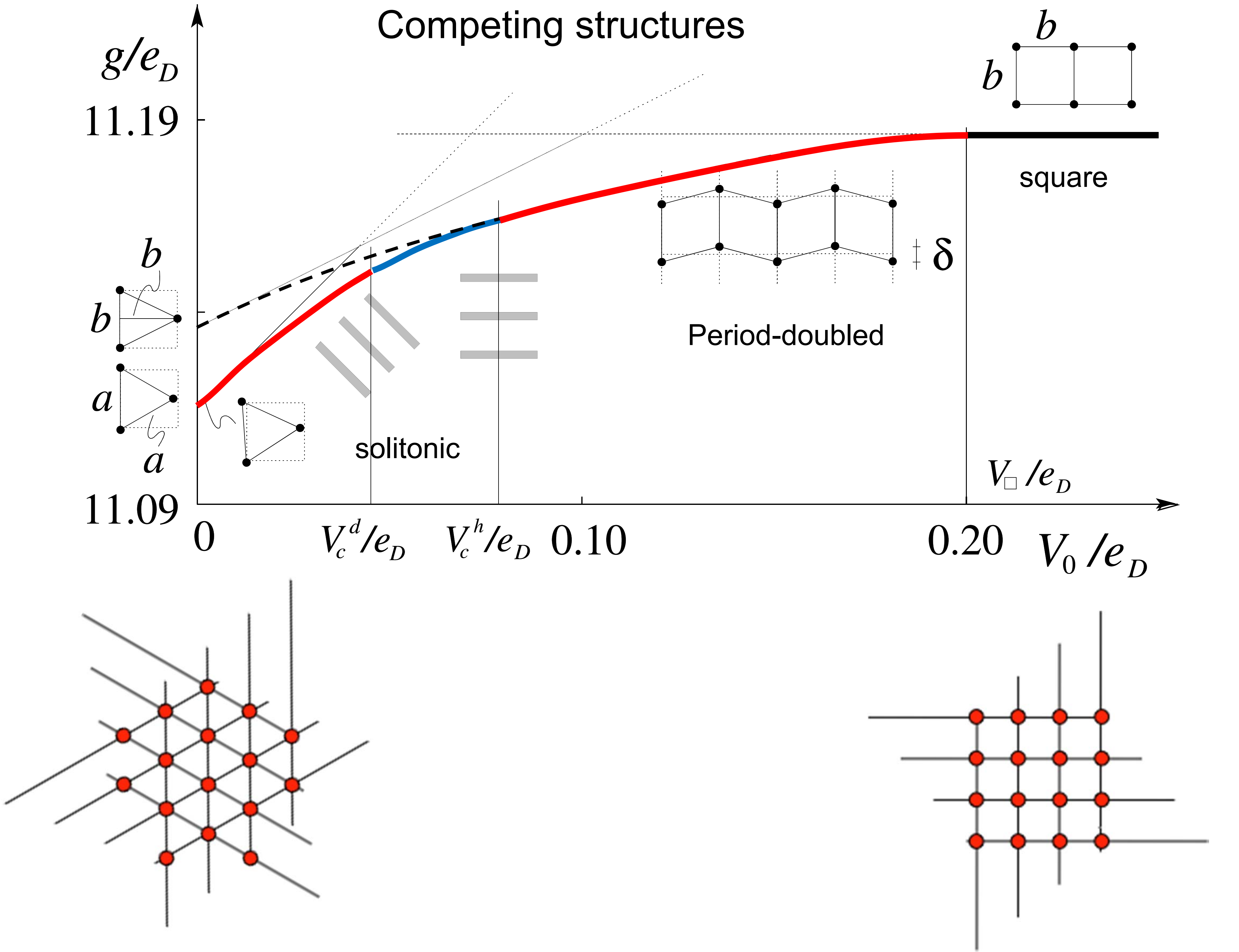
Squaring the triangle – Structural transitions of 2D lattice on a substrate

B. Theiler[1], V. B. Geshkenbein[1], S. E. Korshunov[2], G. Blatter[1]
Institute for Theoretical Physics, ETH Zurich[1]
L.D. Landau Institute for Theoretical Physics[2]









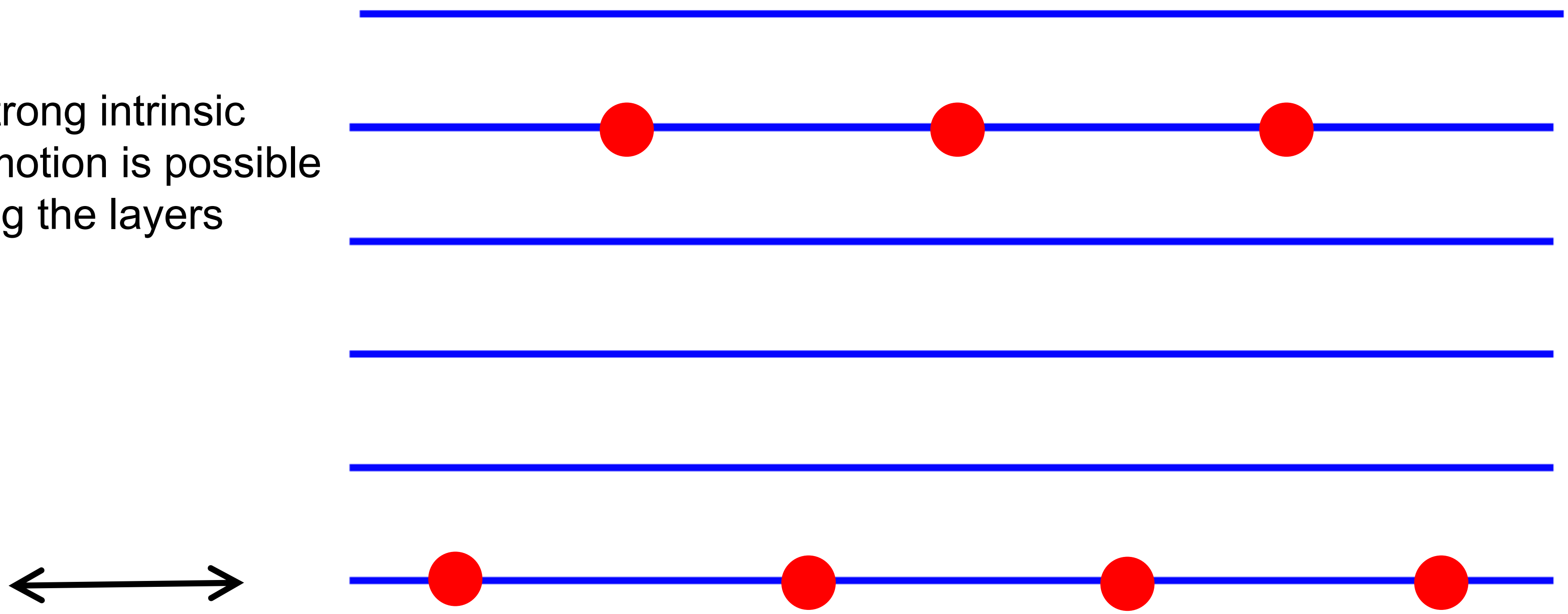
Competing structures
g/e_D
11.19
11.09
b
b
a
a
b
b
solitonic
δ
Period-doubled
square
$V_\square/e_D$
0
V_c^d/e_D
V_c^h/e_D
0.10
0.20
V_0/e_D

Shear Instabilities of a Vortex Lattice in Layered Superconductors

B. I. Ivlev, N. B. Kopnin, and V. L. Pokrovsky

Journal of Low Temperature Physics Vol. 80, 186 (1990)

Due to strong intrinsic pinning motion is possible only along the layers



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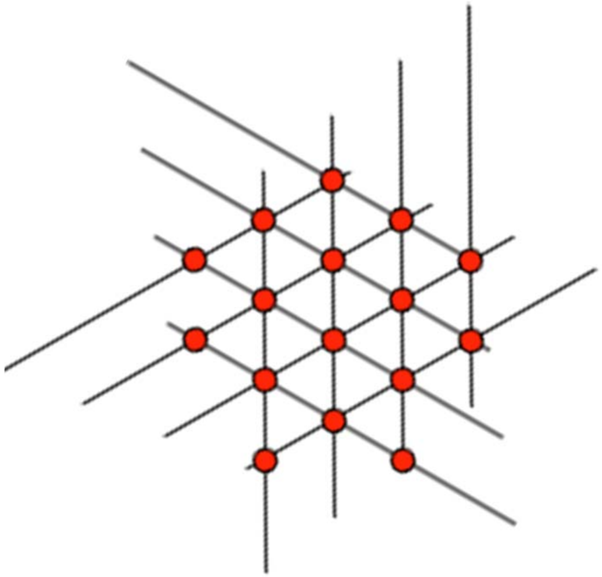
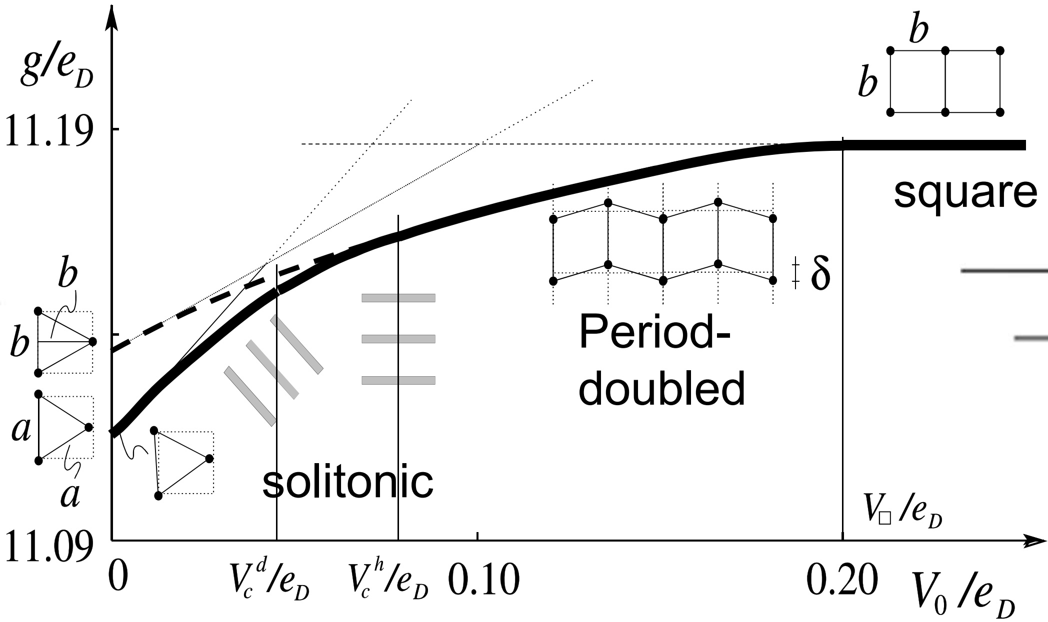
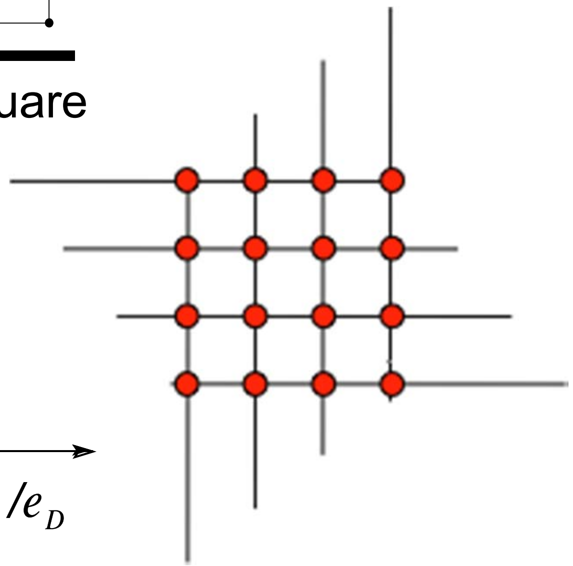


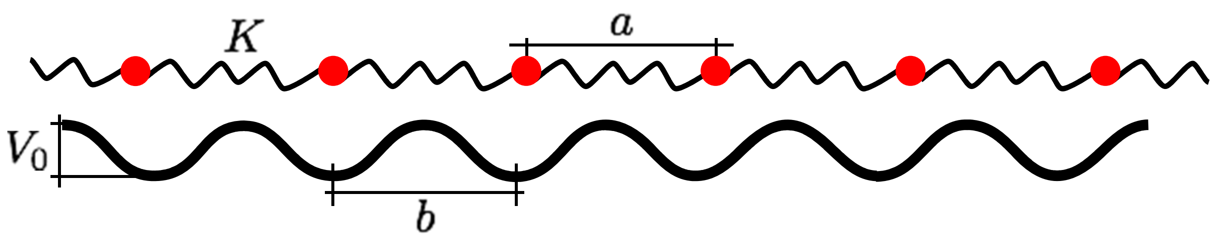




Competing Structures …

… are an old problem in condensed matter physics. The classic problem has been defined in 1D by Frenkel and Kontorova and by Frank and van der Merwe

particle lattice



substrate potential

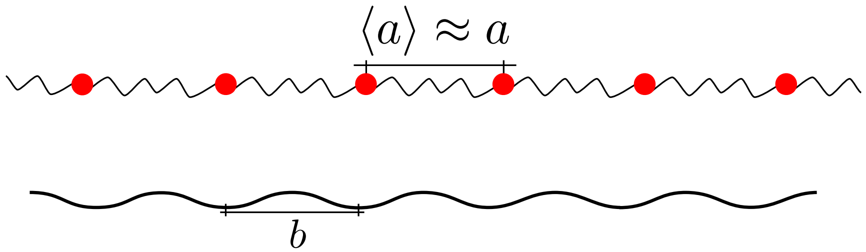
stiff lattice:
misfit parameter

$$s = \frac{a}{b} - 1$$

with lattice deformations:
effective misfit

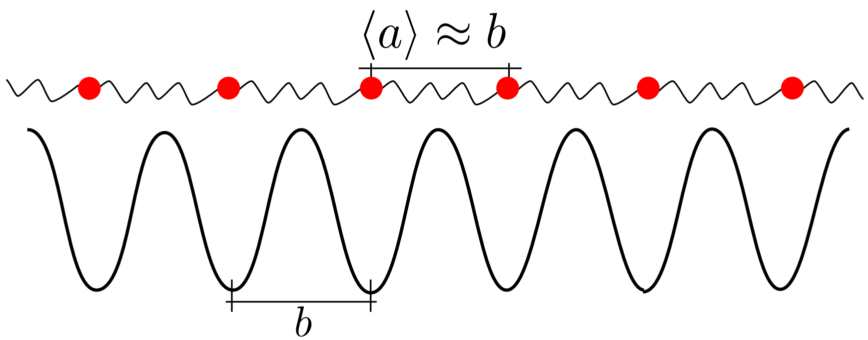
$$s' = \frac{\langle a \rangle}{b} - 1$$

weak substrate



$$s' \approx s$$

strong substrate



$$s' = 0$$

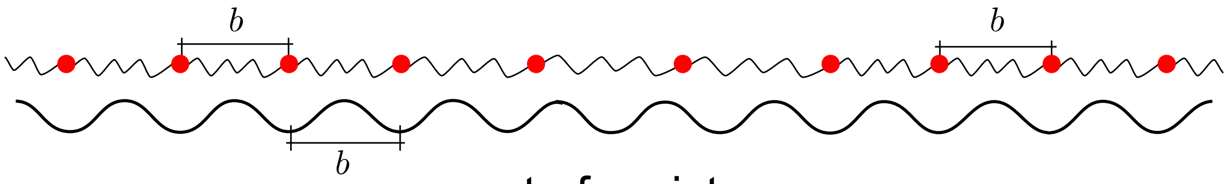
how to go from limit to the other ?

Competing Structures …

… are an old problem in condensed matter physics. The classic problem has been defined in 1D by Frenkel and Kontorova and by Frank and van der Merwe

in registry

in registry



out of registry

with lattice solitons: effective misfit

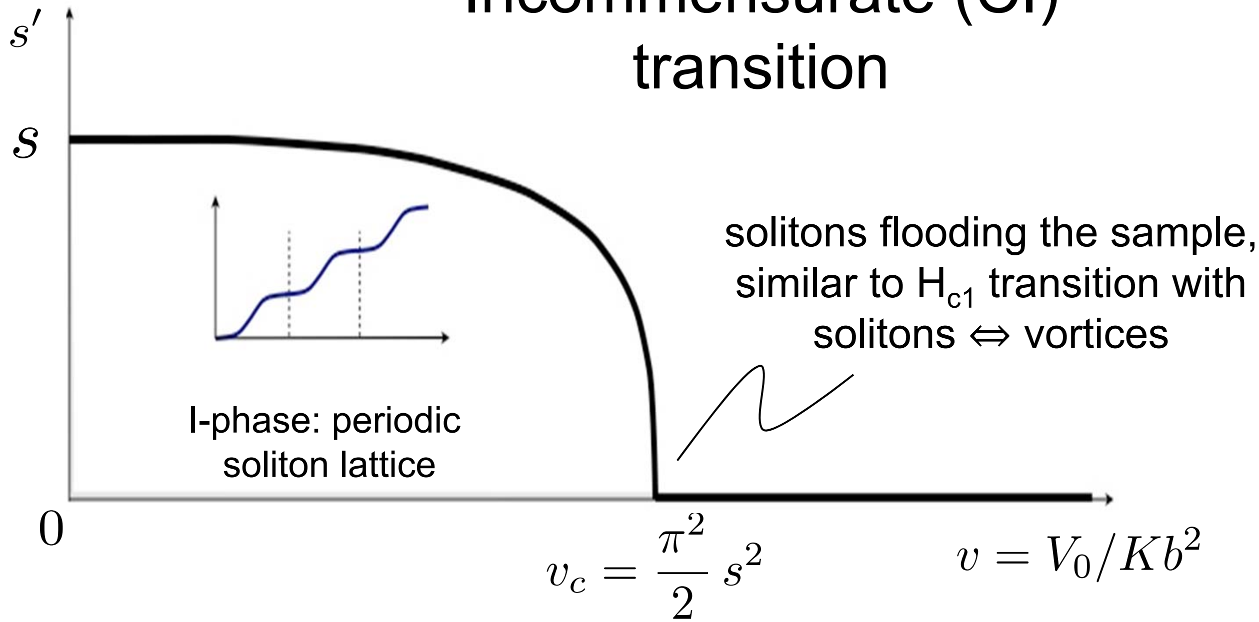
$$0 < s' < s$$

dilution soliton with missing particle

Continuum (elastic) limit:
Sine-Gordon soliton

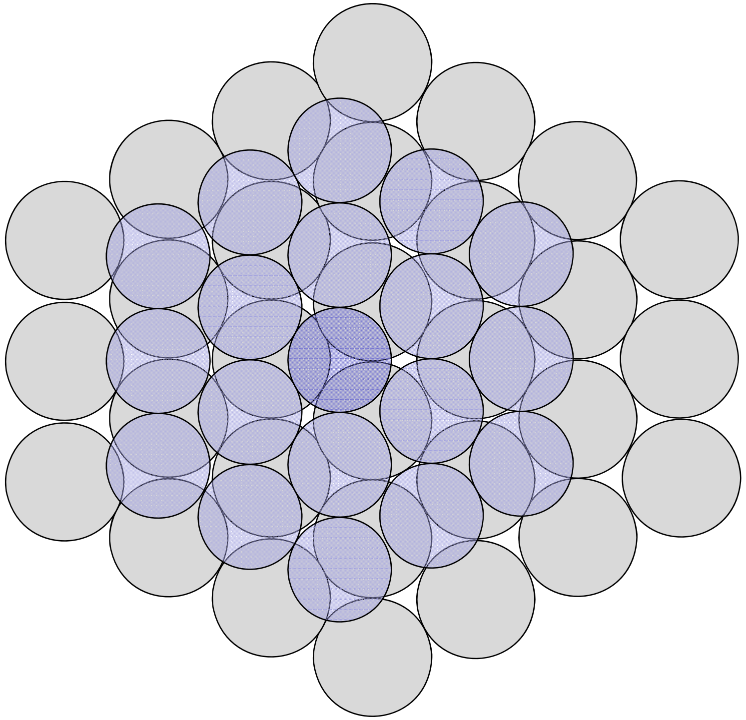
energy	$\varepsilon \sim b\sqrt{V_0 K}$
width	$\ell \sim b\sqrt{K/V_0}$
repulsion	$\propto \exp(-\pi x/\ell)$
density	$L = 1/s'$

Commensurate-Incommensurate (CI) transition



Competing Structures …

… many problems in 2D, the classic one is Krypton on Graphite, Xenon on Platinum, etc.

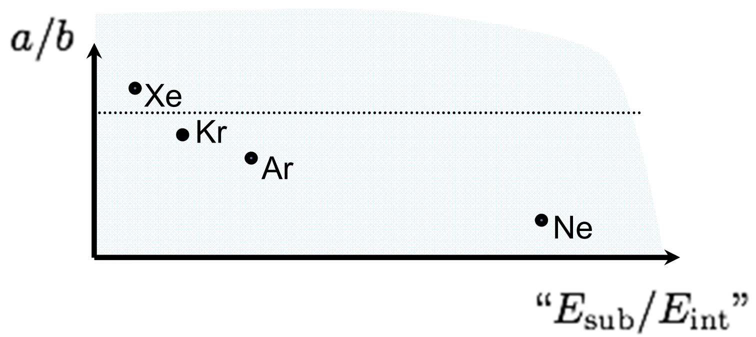


Rare gas monolayers on graphite ($b = 4.26\,\text{Å}$)

Kb^2 $\quad a = 2^{1/6}\sigma$ $\quad V_0$

Adatom	Adatom-adatom ϵ_0 (K)	Adatom-adatom σ (Å)	Adatom-graphite U_{01} (K)	
Ne	35.6	2.78	−3.75	no C-phase
Ar	120.0	3.40	−4.62	no C-phase
Kr	158.0	3.60	−5.00	C-phase
Xe	226.0	4.05	−4.62	C-phase

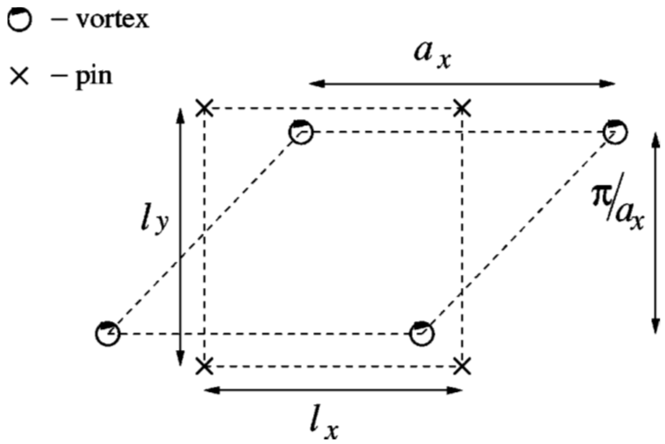
from McTague et al., PRB 19, 5299 (1979)

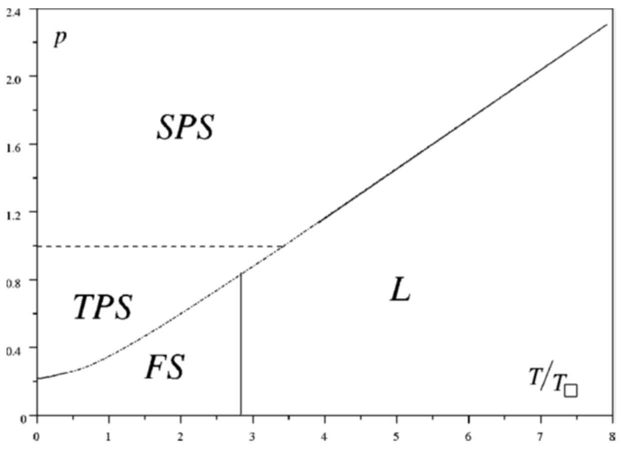


- \`real’ and hence badly tunable system
- triangular lattice on triangular substrate

Competing Structures …

… many problems in 2D, the appropriate one for this conference are **vortices pinned in an artificial defect lattice**





SPS, square pinned solid
TPS, triangular pinned solid
FS, floating solid
L, liquid

Zhuravlev and Maniv, Phys. Rev. B (2003)

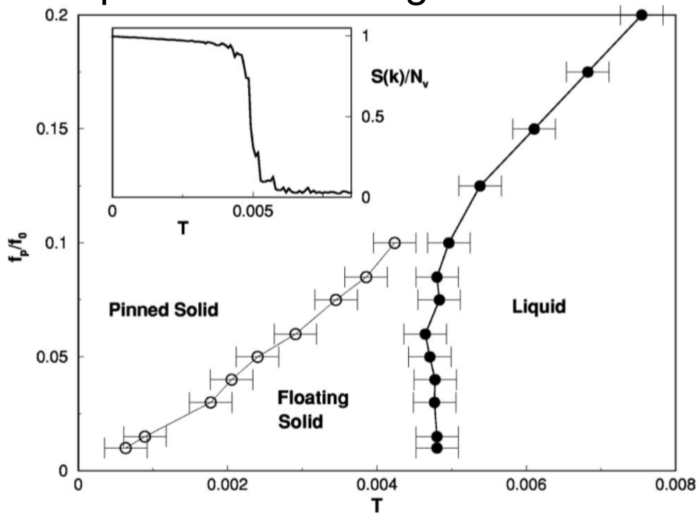
Ginzburg Landau theory
- close to matching field, hence $s \approx 1$
- various low energy phases, isosceles, period doubled
- phase diagram, p = pinning strength, T = temperature

Pogosov, Rakhmanov, and Moshchalkov, Phys. Rev. B (2003)

Continuum elastic theory
- various matching fields
- various low energy phases, deformed triangular, squared, …
- critical currents

Reichhardt et al., Phys. Rev. B (2001)

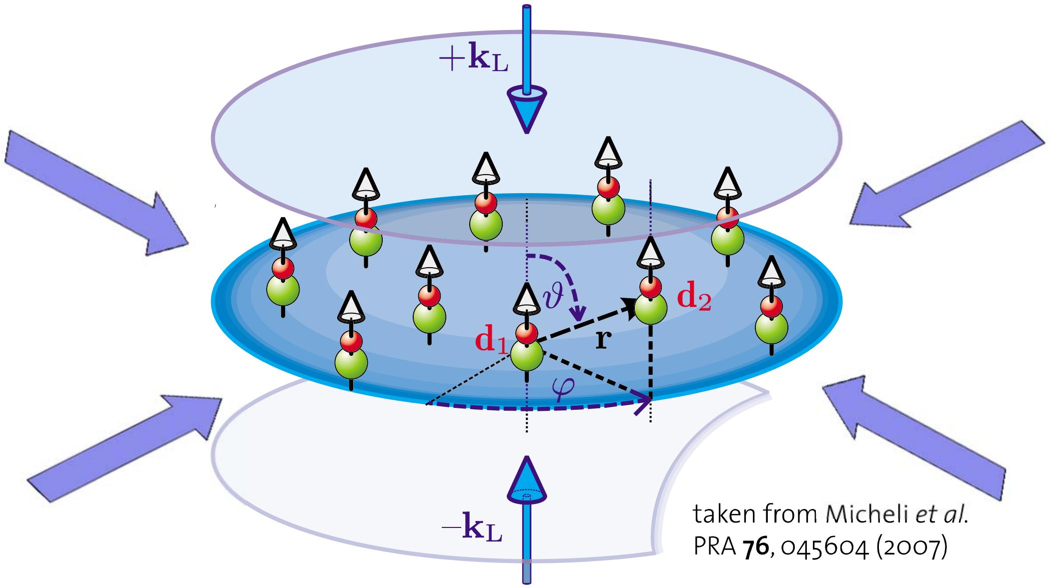
Molecular Dynamics of particles
- close to matching field (and above)
- emphasis on melting



- still a `real', but better tunable system
- triangular lattice on a square substrate

Competing Structures …

… many problems in 2D, the newest one which is fully tunable is implemented with cold gases



- dipolar molecules
- stabilized by vertical electrical field
- subject to (any form of) an optical lattice

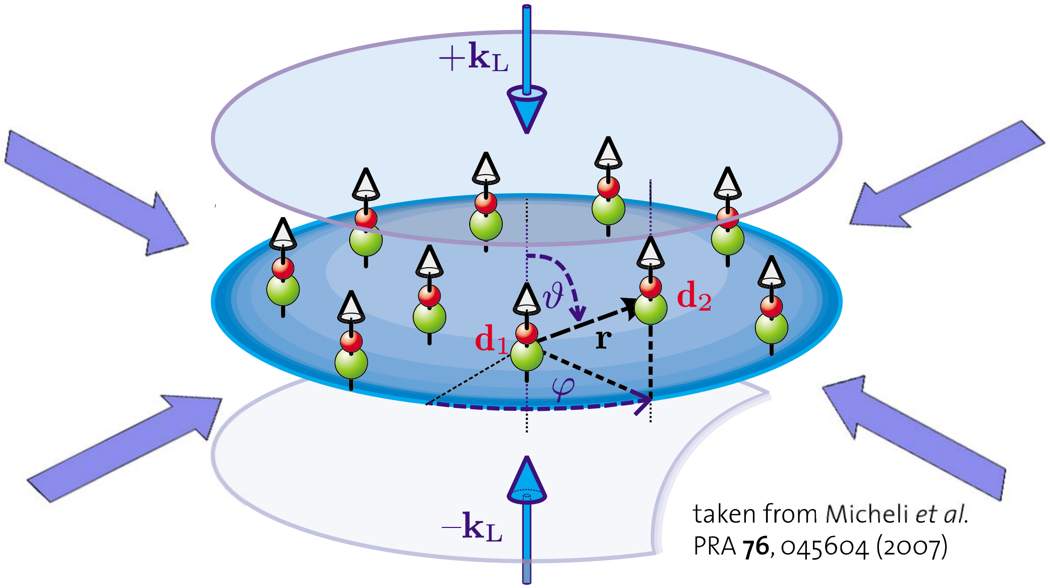
dipolar molecules:
long-range, pure repulsive
interaction D/R^3

square optical lattice
2 modes

$$H = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j}\frac{D}{|\mathbf{R}_i - \mathbf{R}_j|^3} + \frac{V_0}{2}\sum_i \left[2 - \cos(2\pi x_i/b) - \cos(2\pi y_i/b)\right]$$

Competing Structures …

… many problems in 2D, the newest one which is fully tunable is implemented with cold gases



- dipolar molecules
- stabilized by vertical electrical field
- subject to (any form of) an optical lattice

drop fluctuations, both quantum and classical (T=0)

dipolar molecules:
long-range, pure repulsive interaction D/R^3

square optical lattice
2 modes

$$H = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j} \frac{D}{|\mathbf{R}_i - \mathbf{R}_j|^3} + \frac{V_0}{2}\sum_i \left[2 - \cos(2\pi x_i/b) - \cos(2\pi y_i/b)\right]$$

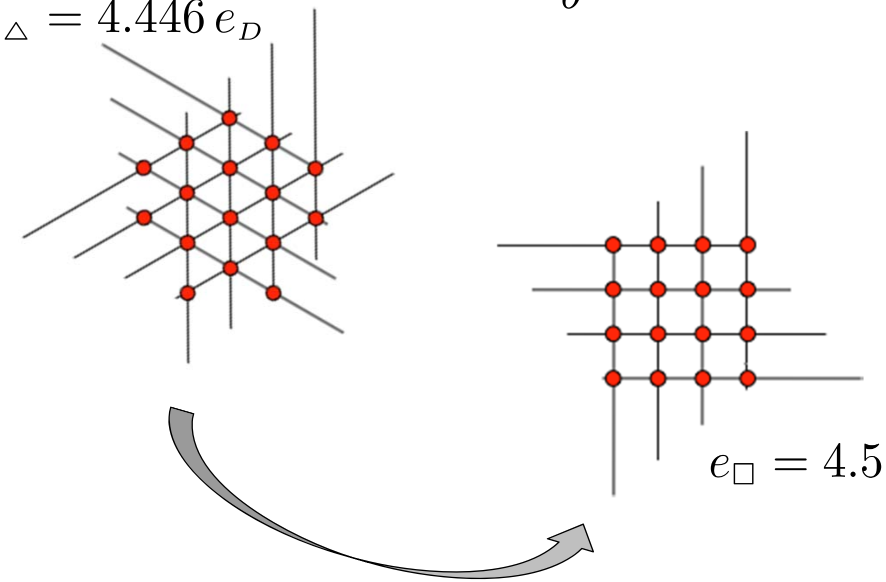
Energy scales

interaction energy

characteristic scale: dipolar energy

$$e_D = \frac{D}{b^3}$$

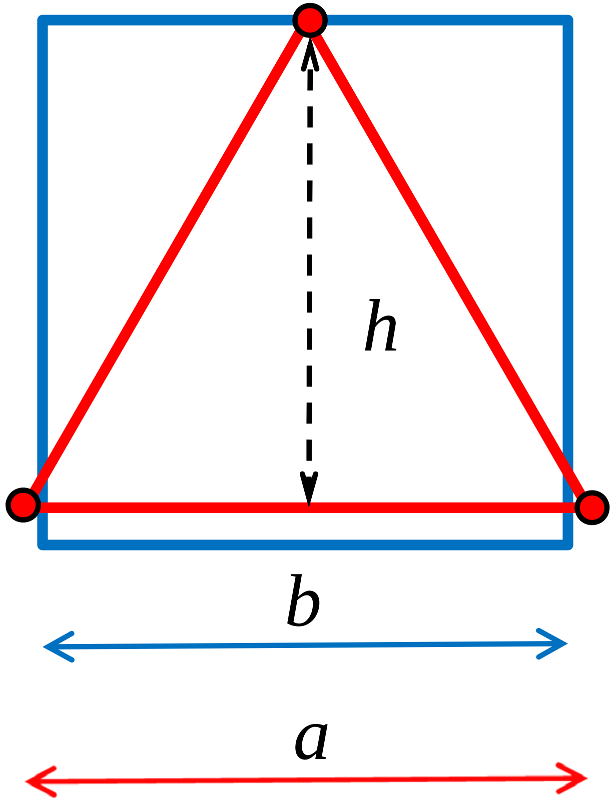
$$e_\triangle = 4.446\, e_D$$



$$e_\square = 4.517\, e_D$$

need characteristic scale for potential

$$V_0 \sim 0.1\ e_D \rightarrow 0.2\ e_D$$



$$a = (4/3)^{1/4}\, b \simeq 1.0746\ b$$

incommensurability parameter

$$s = b\,/\,h - 1 = 0.0746$$

Task

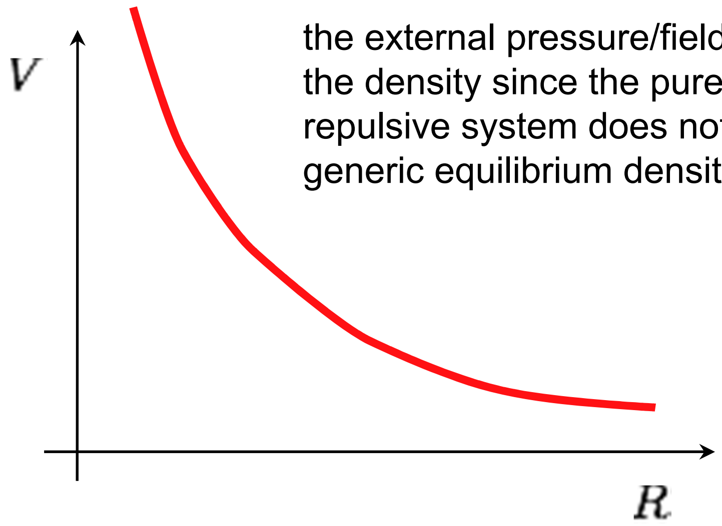
Gibbs free energy

find minimal energy state of

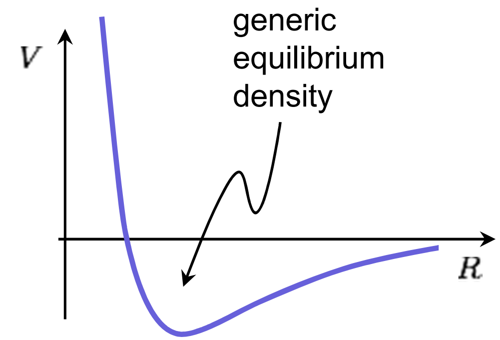
$$G(p,N) = E^{\mathrm{int}}(A,N) + E^{\mathrm{sub}}(N) + pA$$

$$E^{\mathrm{int}}(A,N) = \frac{1}{2}\sum_{i\neq j}^{N} \frac{D}{R_{ij}^3}$$

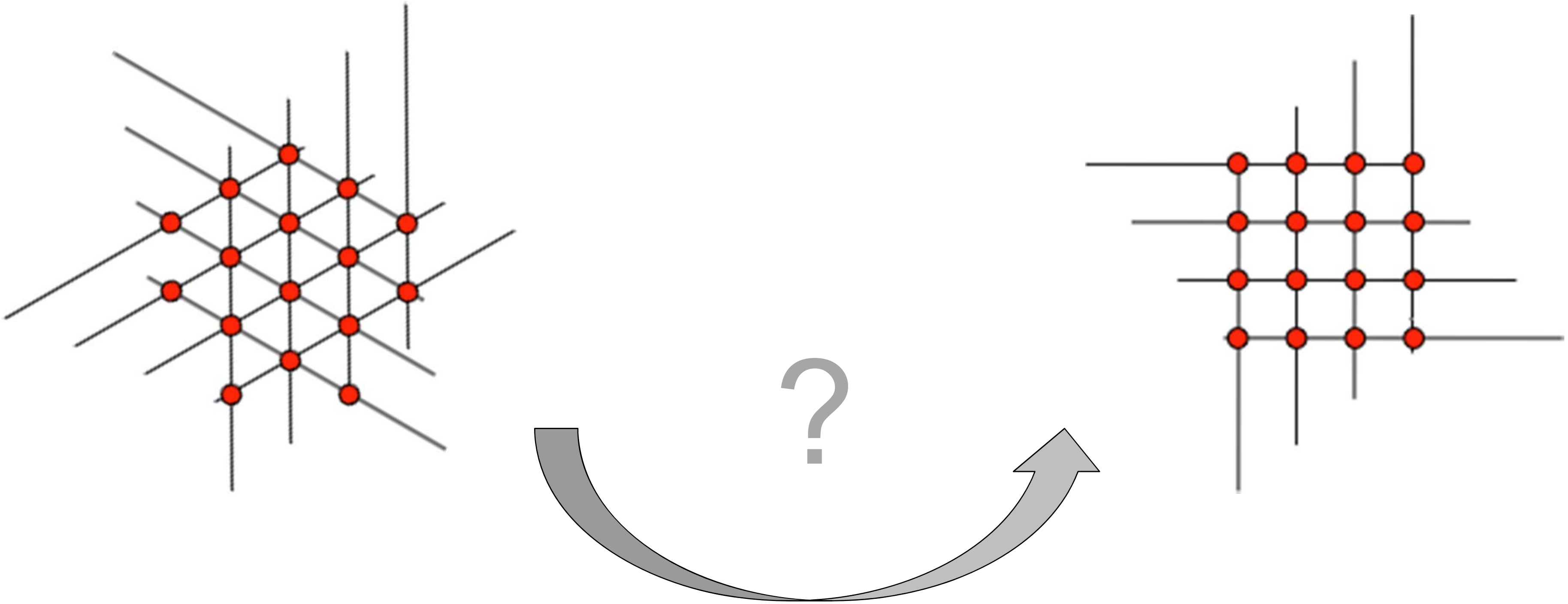
$$E^{\mathrm{sub}}(N) = \sum_i \frac{V_0}{2}\left[2 - \cos(\mathbf{q}_1 \cdot \mathbf{R}_i) - \cos(\mathbf{q}_2 \cdot \mathbf{R}_{)}\right]$$



the external pressure/field defines the density since the purely repulsive system does not have a generic equilibrium density



State diagram



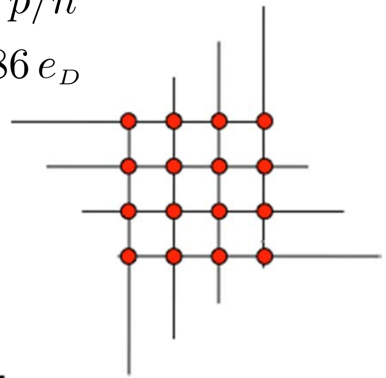
State diagram

simple periodic phases

simplest anticipated phase diagram
at fixed commensurate density

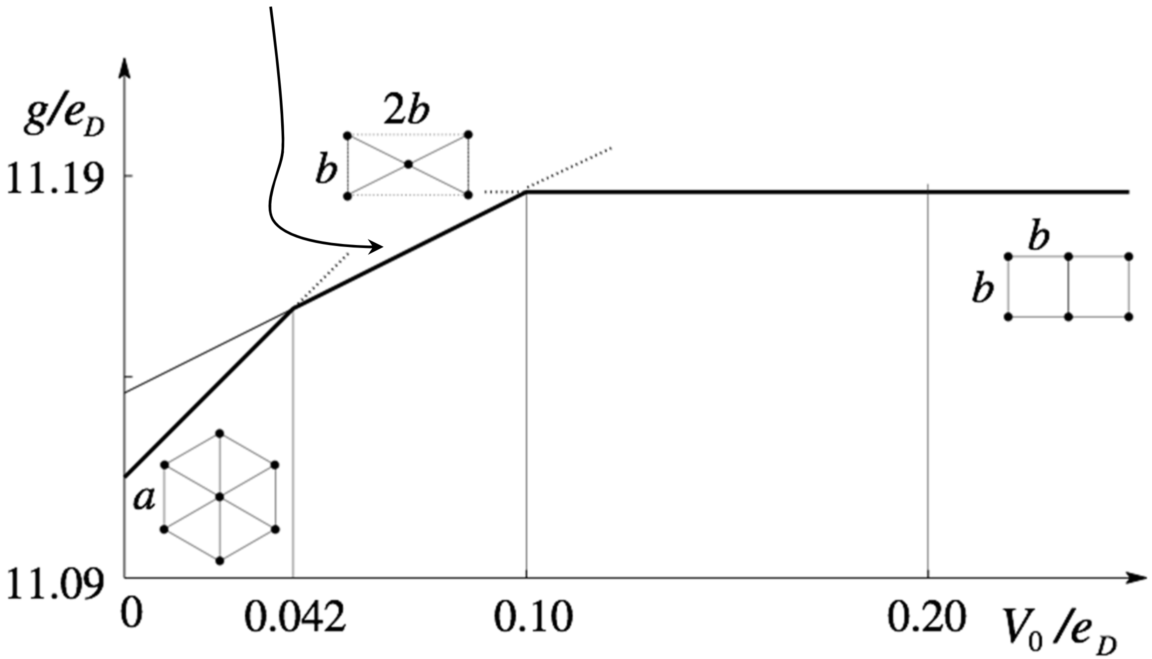
doubly locked phase

$$g_{\square} = e_{\square} + p/n$$
$$= 11.186\, e_D$$



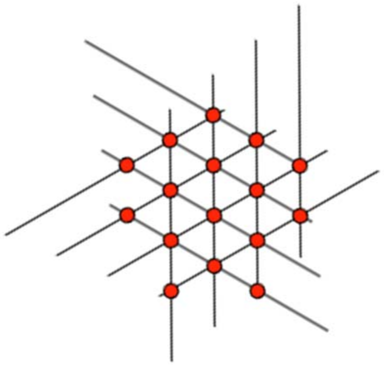
singly locked phase

$$g_{\triangleright} = e_{\triangleright} + p/n + V_0/2$$
$$= 11.136\, e_D + V_0/2$$



floating phase

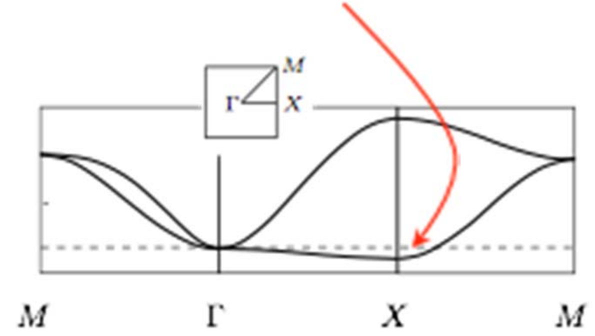
$$g_{\triangle} = e_{\triangle} + p/n + V_0$$
$$= 11.115\, e_D + V_0$$

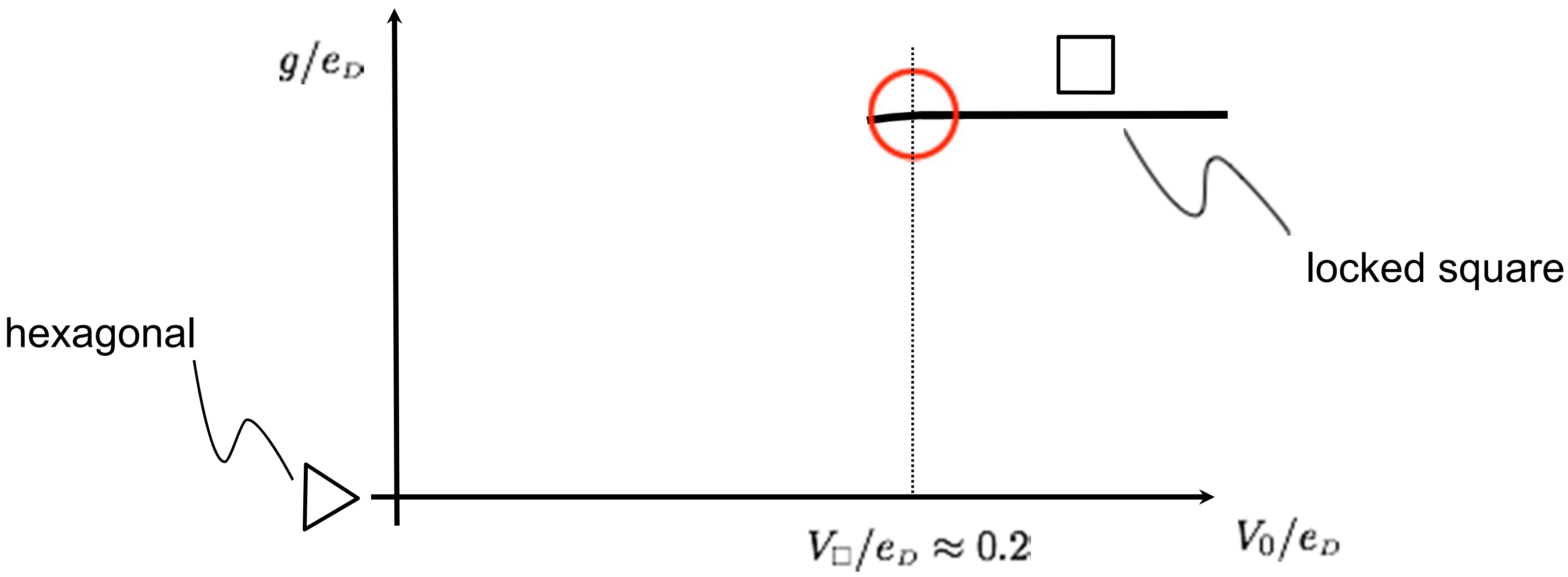


State diagram

A detailed analysis provides the following picture:

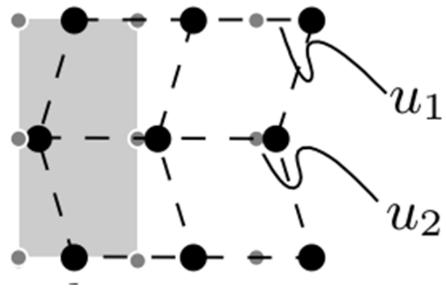
- the square lattice phase undergoes a shear instability (symmetry breaking)





Effective model (pd phase)

Period-doubled phase: Rectangular Bravais lattice
with basis $\{\mathbf{c}_1, \mathbf{c}_2\} = \{(u_1, 0), (u_2, b)\}$



$\delta = u_1 - u_2$: In-cell distortion
$\sigma = (u_1 + u_2)/2$: Center of mass coordinate

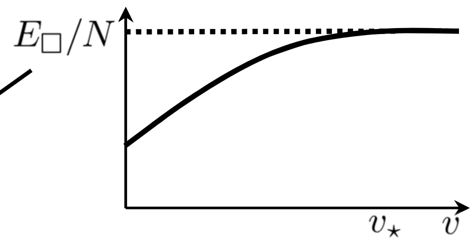
$$E^{\text{sub}}(\delta, \sigma, V_0) = \frac{V_0}{2}\{1 - \cos(q\sigma)\cos(q\delta/2)\}$$

$$E^{\text{int}} = \begin{cases} E_{\square} & \delta = 0 \\ E_{\lozenge} & \delta = b/2 \end{cases}$$

$E^{\text{int}}(\delta) \approx C_1 + C_2[\cos(q\delta) - 1]$ with $C_1 = E_{\square}/N,\ C_2 = (E_{\square} - E_{\lozenge})/2N$

$\partial_\delta E^{\text{tot}} \overset{!}{=} 0 \implies \cos(q\delta/2) = \frac{V_0}{8C_2}\cos(q\sigma)$ (Force balance)

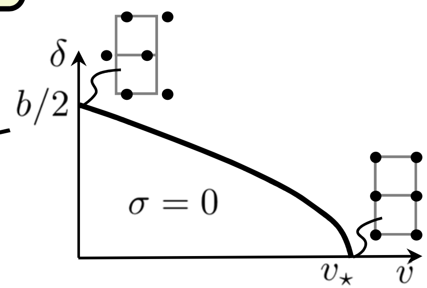
$\partial_\sigma E^{\text{tot}} \overset{!}{=} 0 \implies E_{\text{pd}}(\sigma, V_0) = C_1 + \frac{V_0}{2} - \frac{V_0^2}{32C_2}\cos^2(q\sigma)$



Minima energy	$E_{\text{pd}}(V_0) = C_1 + \frac{V_0}{2} - \frac{V_0^2}{32C_2}$
Translational locking	$\sigma = 0, b/2$
Distortion amplitude	$\delta = \frac{2}{q}\arccos(V_0/8C_2)$

$v_\star = 8C_2 \approx 0.198$

$$\frac{v_\star - v_{c2}}{v_{c2}} \approx -1\%$$

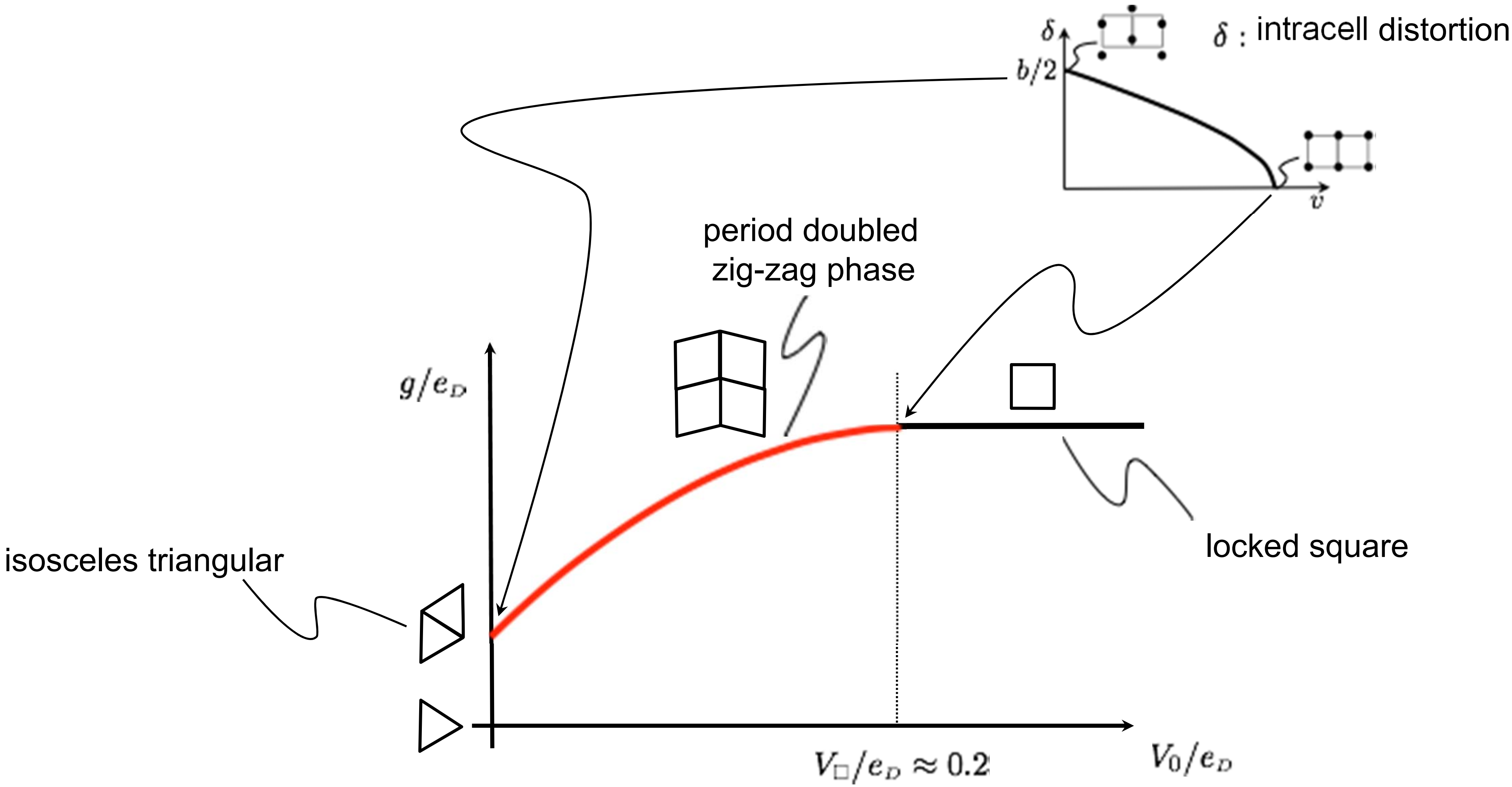


State diagram

simple periodic phases

A detailed analysis provides the following picture:

- the square lattice phase undergoes a shear instability (symmetry breaking)
- the period-doubled phase goes into the isosceles triangular phase (Bravais lattice)

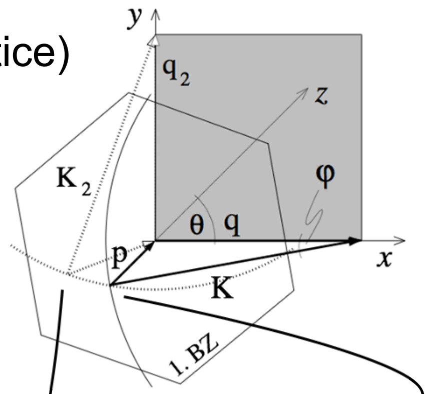


simple periodic phases

State diagram

A detailed analysis provides the following picture:

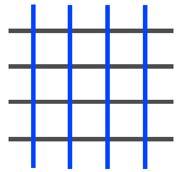
- the square lattice phase undergoes a shear instability (symmetry breaking)
- the period-doubled phase goes into the isosceles triangular phase (Bravais lattice)
- a small substrate potential distorts and rotates the hexagonal phase



substrate potential with

1st harmonic

2nd harmonic



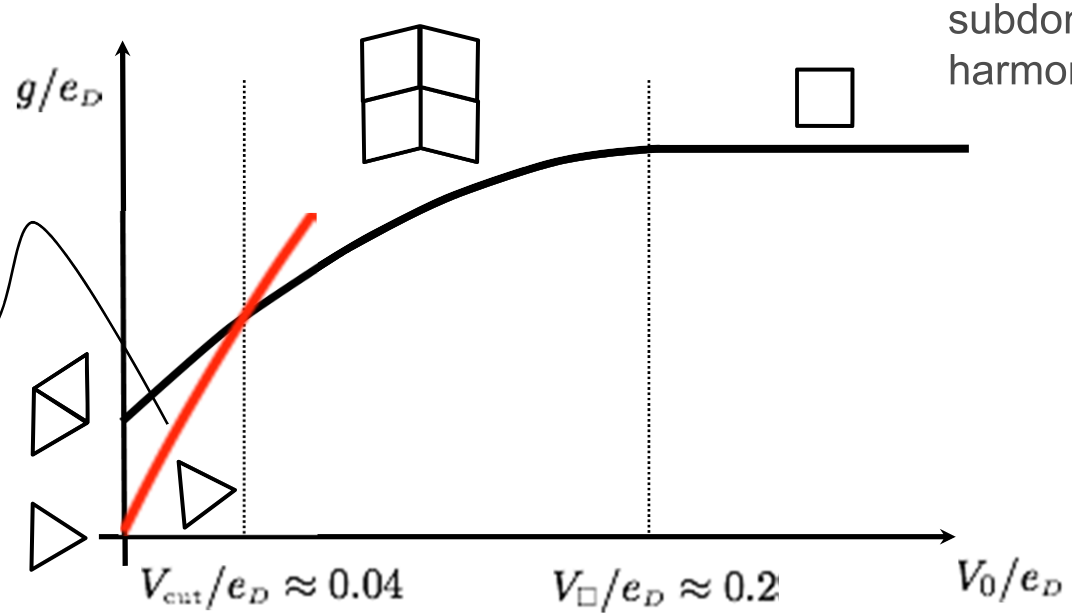
subdominant harmonic at large k

dominant harmonic at small k

rotated & distorted hexagonal

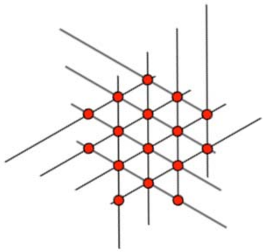
locking angle $\varphi_0 \approx 3.83°$

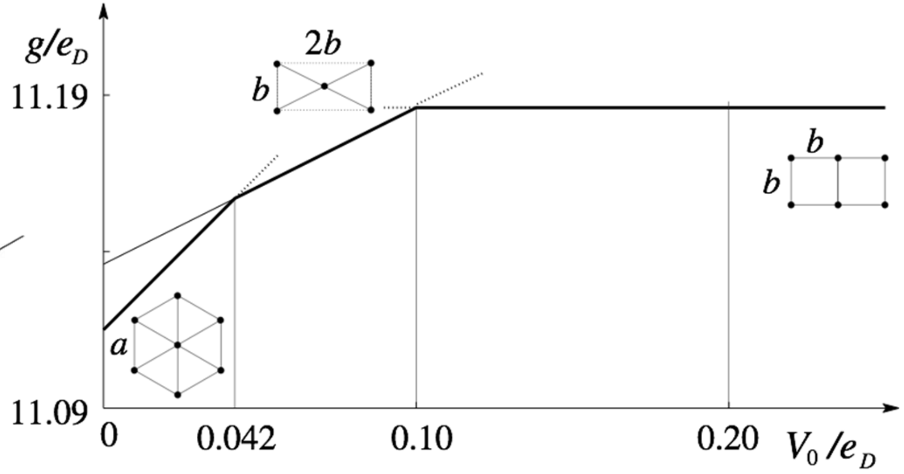
determined by misfit parameter s



Novaco & McTague

State diagram

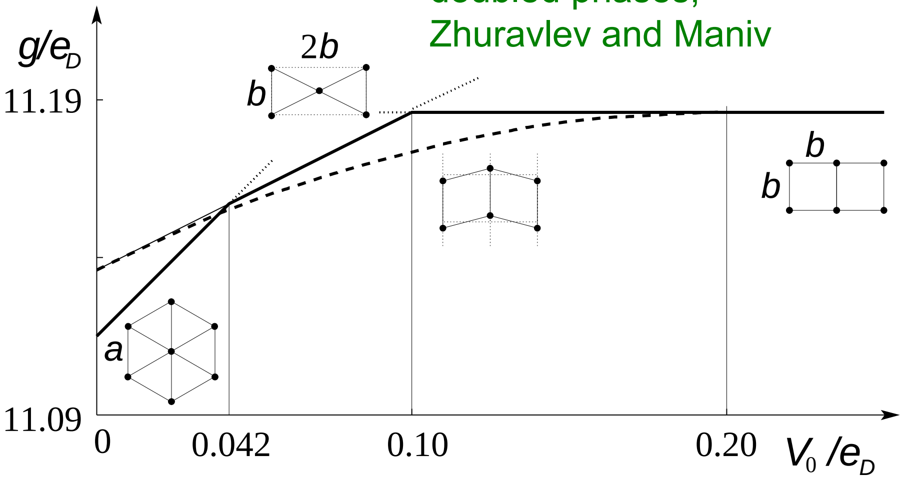




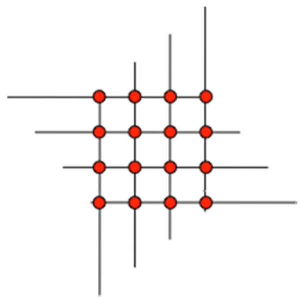
We have gone

from a simple consideration

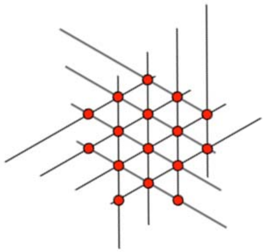
isosceles and period doubled phases, Zhuravlev and Maniv

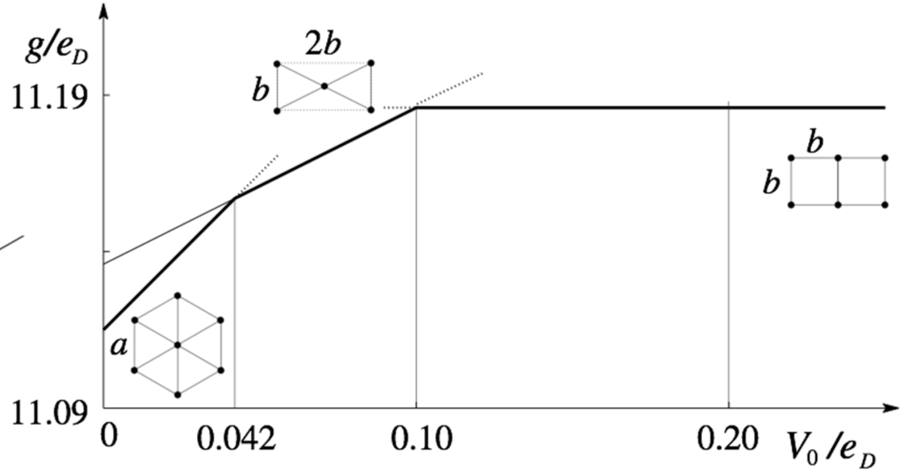


to a more sophisticated result



State diagram

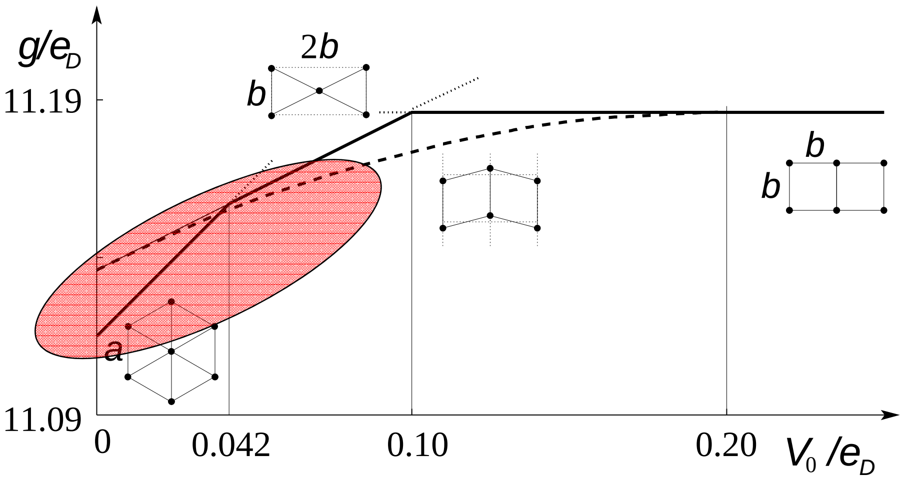


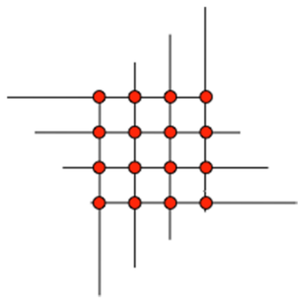


We have gone

from a simple consideration

solitons

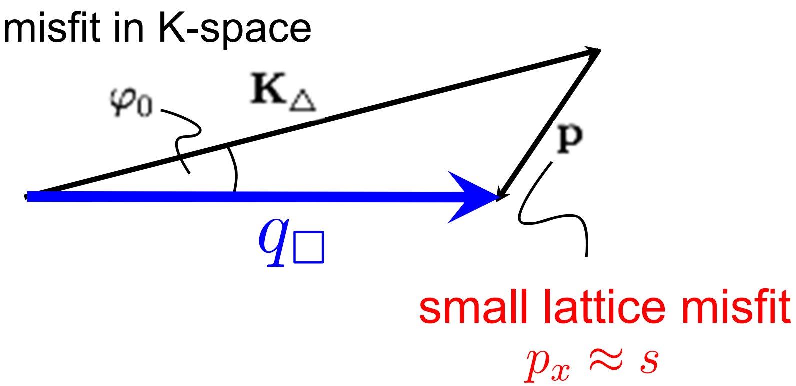




to a more sophisticated result

Resonance approximation (V. L. Pokrovsky and A. L. Talapov 1980)

start from weak potential and small misfit parameter, then the system is well described by a distorted hexagonal phase



$$E \sim C\mathrm{p}^2 u^2/2 + E^{\mathrm{sub}}(\mathrm{p}, u)$$

deformation is biggest for smallest **p**

$$u \propto f^{\mathrm{sub}}(\mathrm{p})/C\mathrm{p}^2$$

Consider only dominant mode of the substrate potential

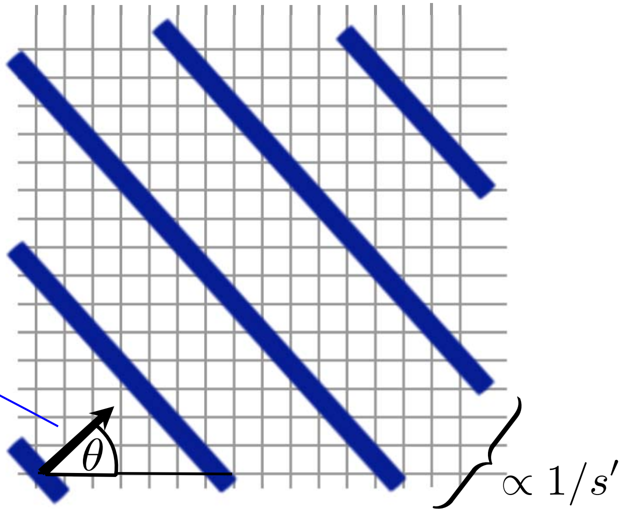
$\longrightarrow$ effective 1D model

Resonance approximation (V. L. Pokrovsky and A. L. Talapov, 1980)

compression

shear

$$\theta = \arctan\left[\sqrt{\frac{\kappa - \mu}{\kappa + \mu}}\right]$$



Near the transition:

single soliton energy

$$\epsilon = \sqrt{\frac{8V_0\gamma}{\Omega_{\mathrm{uc}}\pi^2}}$$

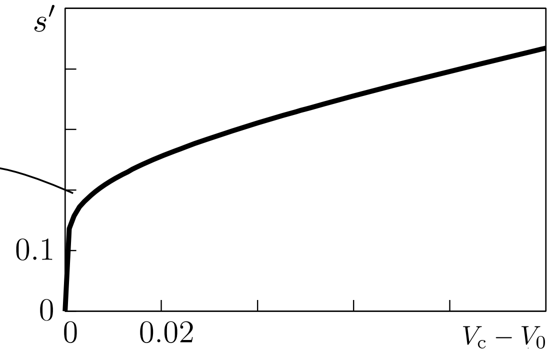
$$\Delta e(s') \approx (\epsilon - \gamma s)s' + 4\epsilon s' e^{-4V_0 n/\epsilon s'}$$

chemical potential

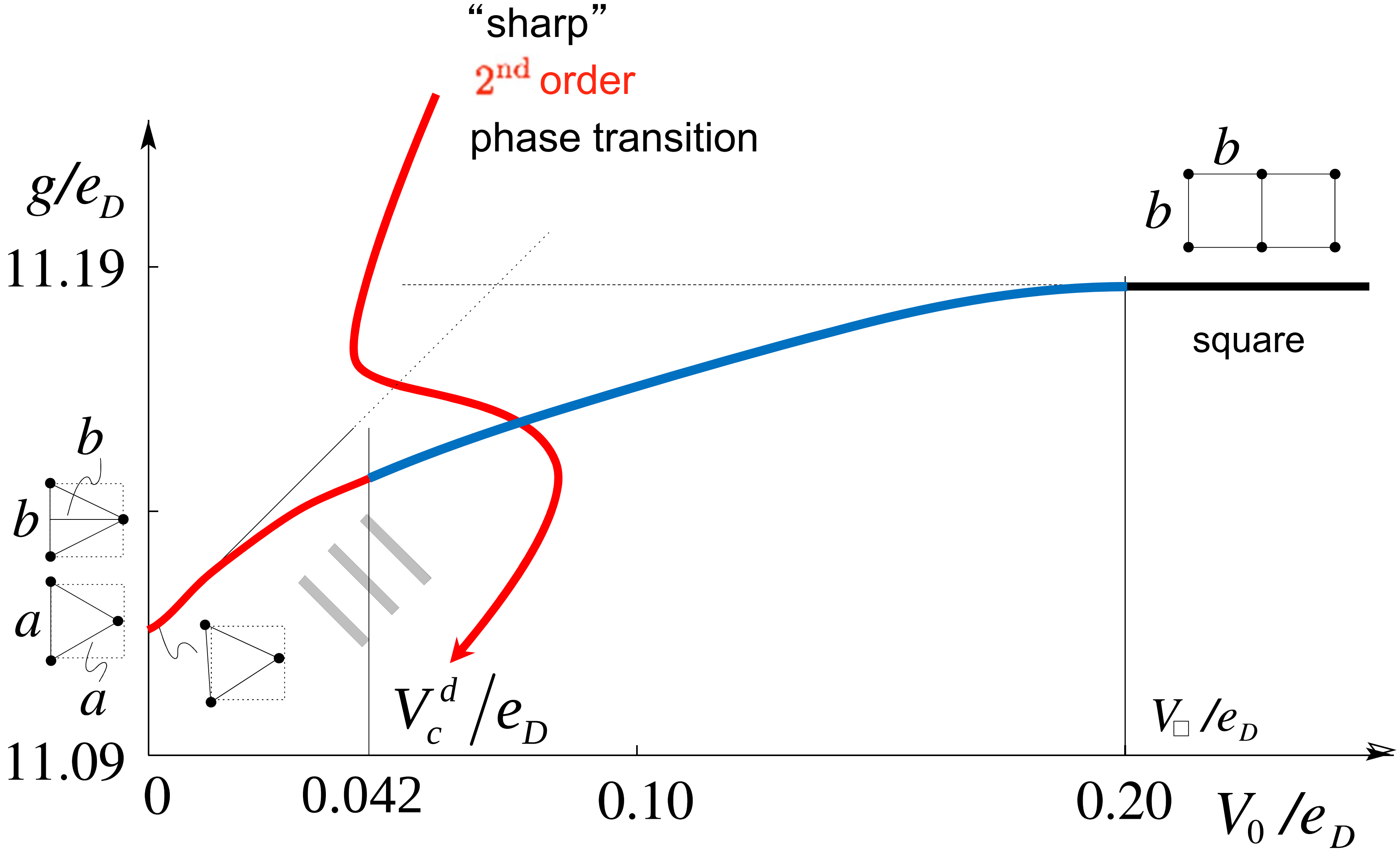
soliton density

soliton-soliton interaction

$$s' \propto -\frac{1}{\ln\left(V_c - V_0\right)}$$

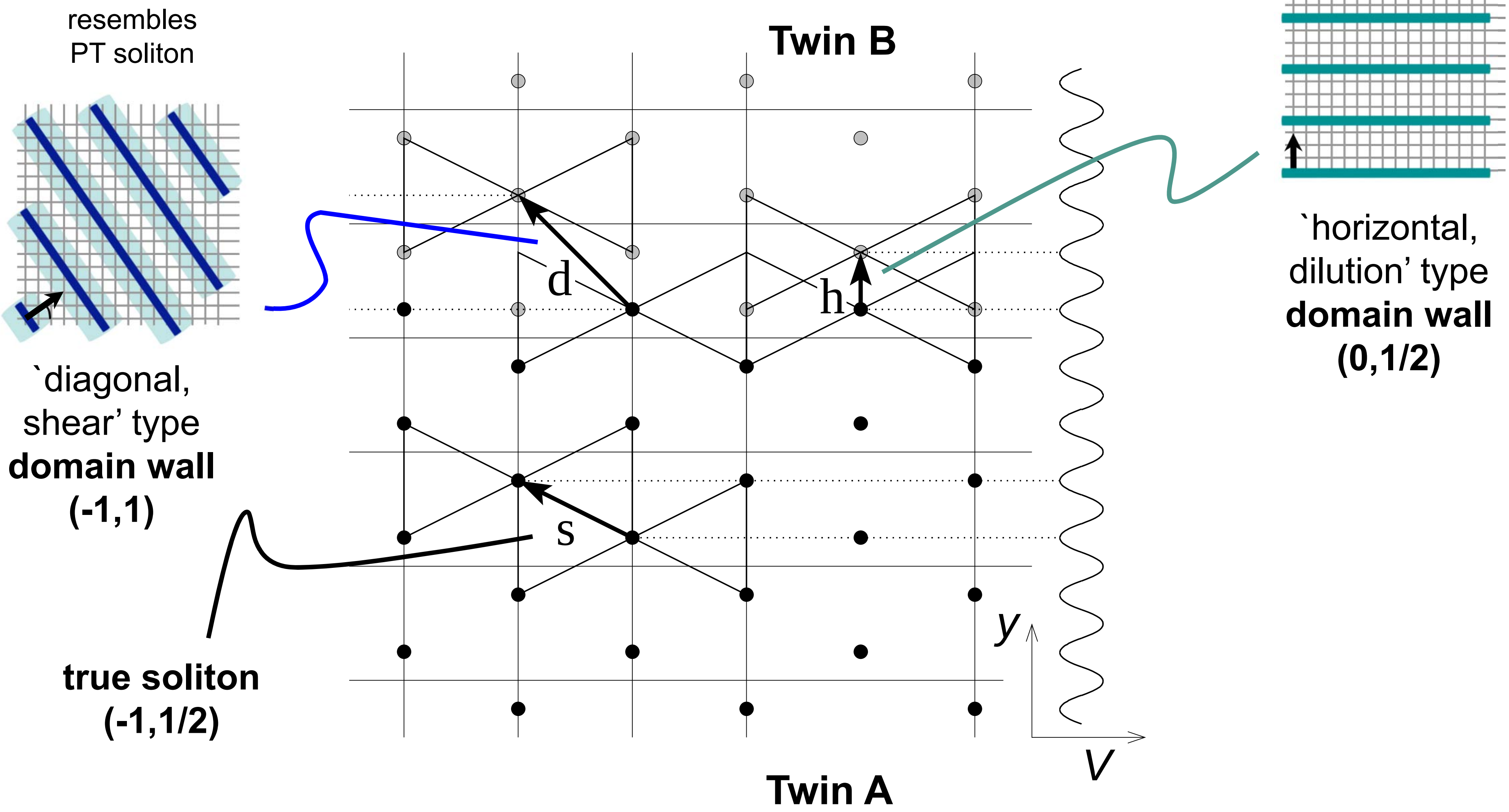


Resonance approximation (Pokrovsky and Talapov)



Two modes in substrate potential

Problem is fully **two-dimensional**, with additional **constraints** on the solitons.
We obtain several candidate solitons:



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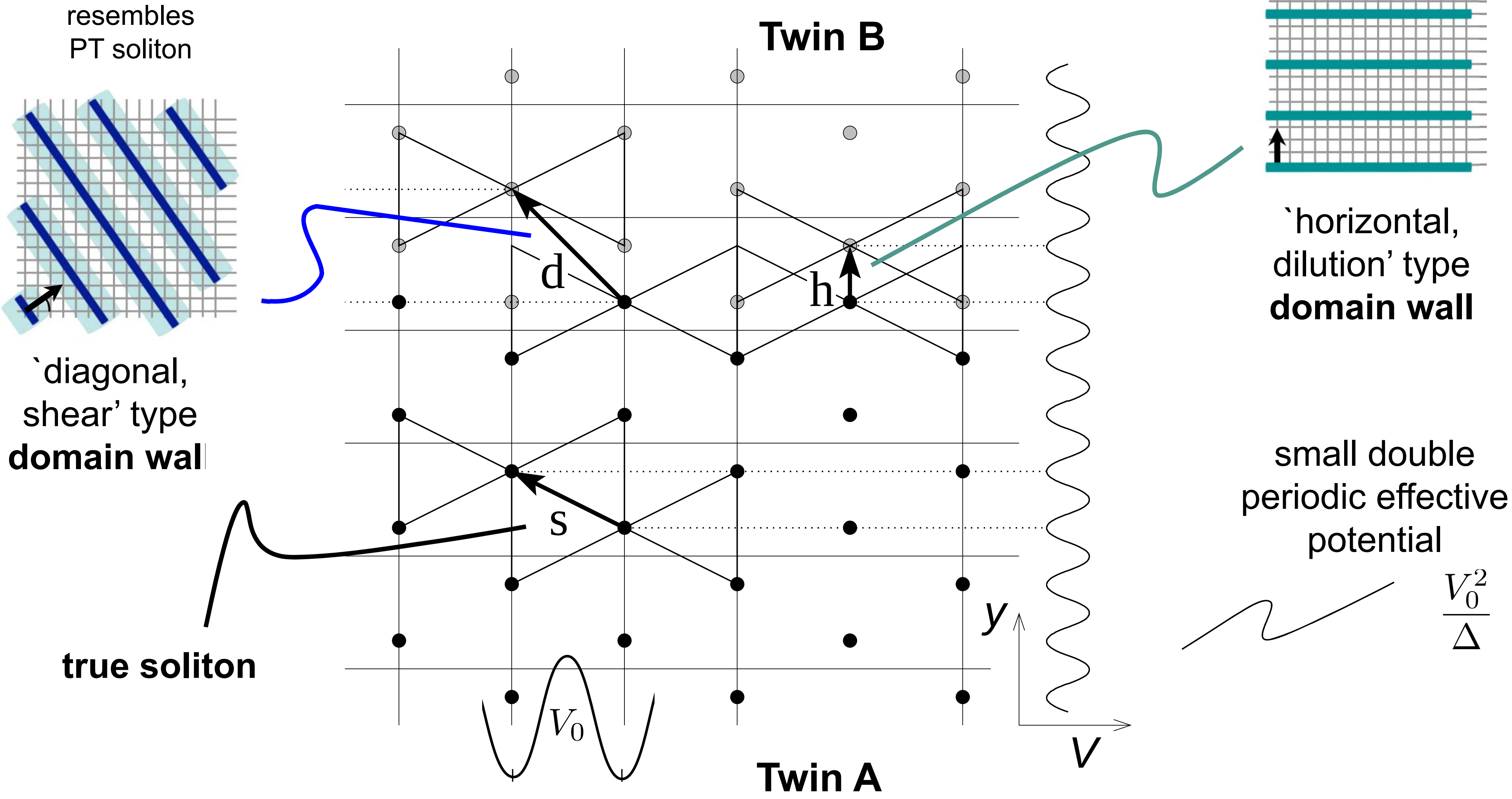
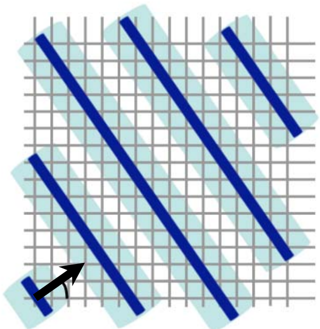


Two modes in substrate potential

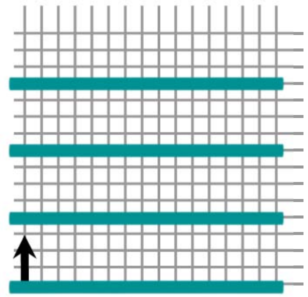
second harmonic — geometric parameters l, m

$$\Delta e = \int_{-\infty}^{\infty} dz \left\{ e_{\rm elast}(\mathbf{v}) - \frac{V_0 n}{2}\cos(qv_x) - \frac{V_0^2 n}{64\Delta}\cos(2qv_y) \right\} - 2\mu s b\left[\left(1+\frac{s}{1-\sigma}\right) l\cos\theta + \left(1-\frac{s}{1-\sigma}\right) m \sin\theta\right]$$

resembles PT soliton



`diagonal, shear' type **domain wall**



`horizontal, dilution' type **domain wall**

soliton width

$$\lambda_{\rm shear} \sim b\sqrt{\frac{\mu/n}{V}} \qquad \lambda_{\rm dil} \sim b\sqrt{\frac{\kappa\Delta}{nV^2}}$$

soliton energy

$$\varepsilon_{\rm s,shear} \sim nb\sqrt{V\mu/n} \qquad \varepsilon_{\rm s,dil} \sim nb\sqrt{\kappa V^2/n\Delta}$$

soliton drive

$$\varepsilon_d \sim -\mu s b$$

soliton entry

$$V_{\rm c,shear} \sim \frac{\mu}{n}s^2 \qquad V_{\rm c,dil} \sim \sqrt{\frac{\Delta n}{\kappa}\frac{\mu}{n}}\, s$$

large κ → shear soliton wins

small misfit s → dilution soliton wins

Task, find the best soliton/domain wall
varying type **(m,n)** and angle θ

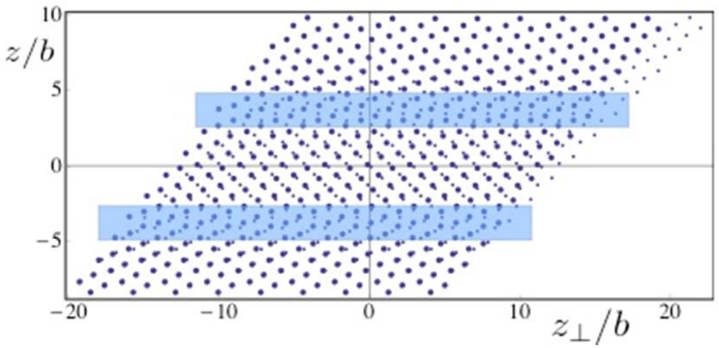
Two modes in substrate potential

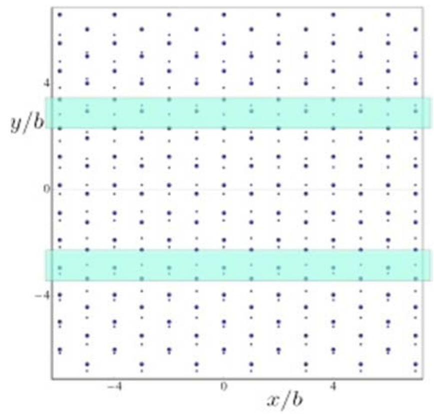
Analytic calculations …

… are not good enough due to large anharmonic effects, specially for shear type solitons

Numerical calculations …

… are doable





etc.

So far, we have found that the first dilution domain-wall **(0,1/2)** wins the game, destroying the period doubled phase at a critical potential

$$V_c^h \approx 0.074 e_D$$

Surprisingly, the optimal domain-wall appears at a finite angle $\sim 45^\circ$ away from horizontal.

Scenario:

When **(0,1/2)** domain-walls flood the sample, they eliminate the second substrate mode. At lower substrate potential, PT solitons enter the system and complete the transition. .

Phase diagram

The final scenario for the conversion of the square to hexagonal lattice seems to be

← period-doubled one-fold locked lattice ← two-fold locked square lattice

← Pokrovski-Talapov shear-soliton lattice ← rotated dilution domain-wall lattice

hexagonal floating ← rotated distorted locked hexagonal