Phason Elastic Energy

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Phasons and Phonons

Phasons are slowly varying, long wave length distortions of the perp space coordinates ("phason coordinates") of a quasicrystal.

Analogous to phonons (sound waves), which are slowly varying, long wave length distortions of the physical space coordinates of a solid.

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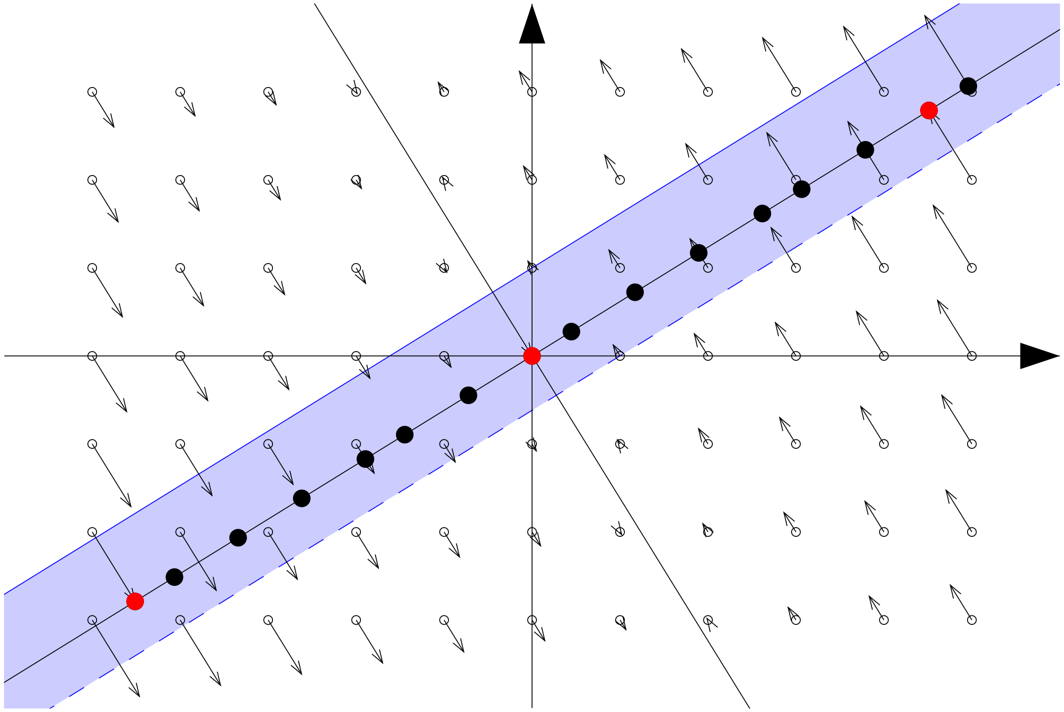
Quasicrystal should be stable against phasons and phonons. Phasons and phonons should be excitations of the quasicrystal.

Energy spectrum of such excitations is relevant for thermal stability and other physical properties.

Linear Phason Strain



A linear phason strain can be applied by shearing the higher-dimensional crystal: $x^\perp \rightarrow x^\perp + A x^\parallel$.

Periodic approximants are constructed this way.

Perfect Quasicrystal vs. Random Tiling

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The density of matching rule violations varies linearly with the norm of the phason strain.

If the energetics is governed by matching rules, there should be a phase transition between the perfect quasicrystal at low temperature, and the random tiling at high temperature.

Energetics of a Toy Model

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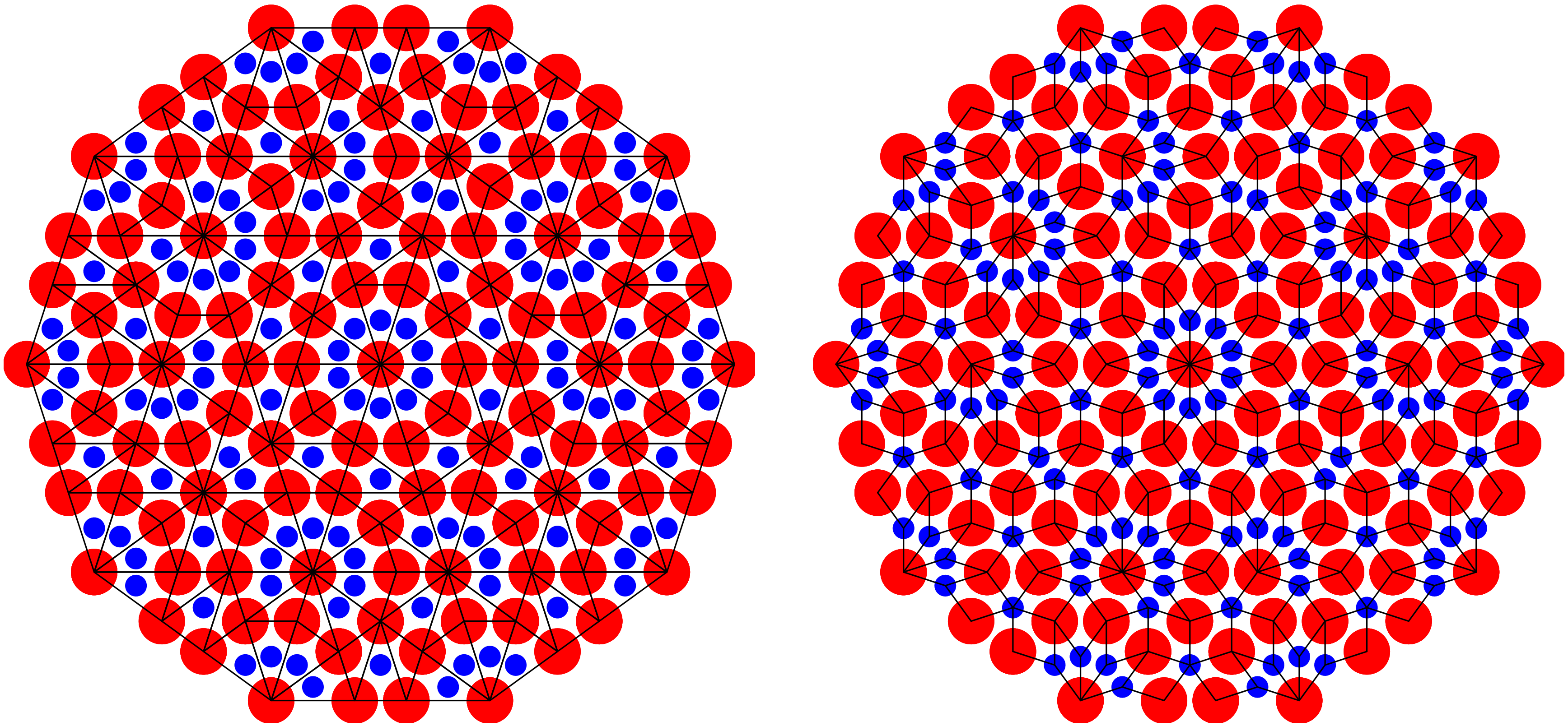
We study here in detail the low temperature energetics of a simple toy model with simple pair interactions.

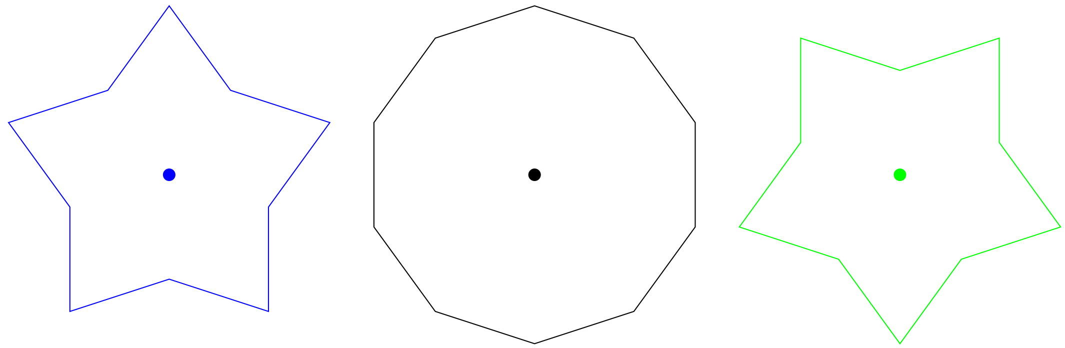
This is mostly work by Ulrich Koschella.

Binary Tiling Models



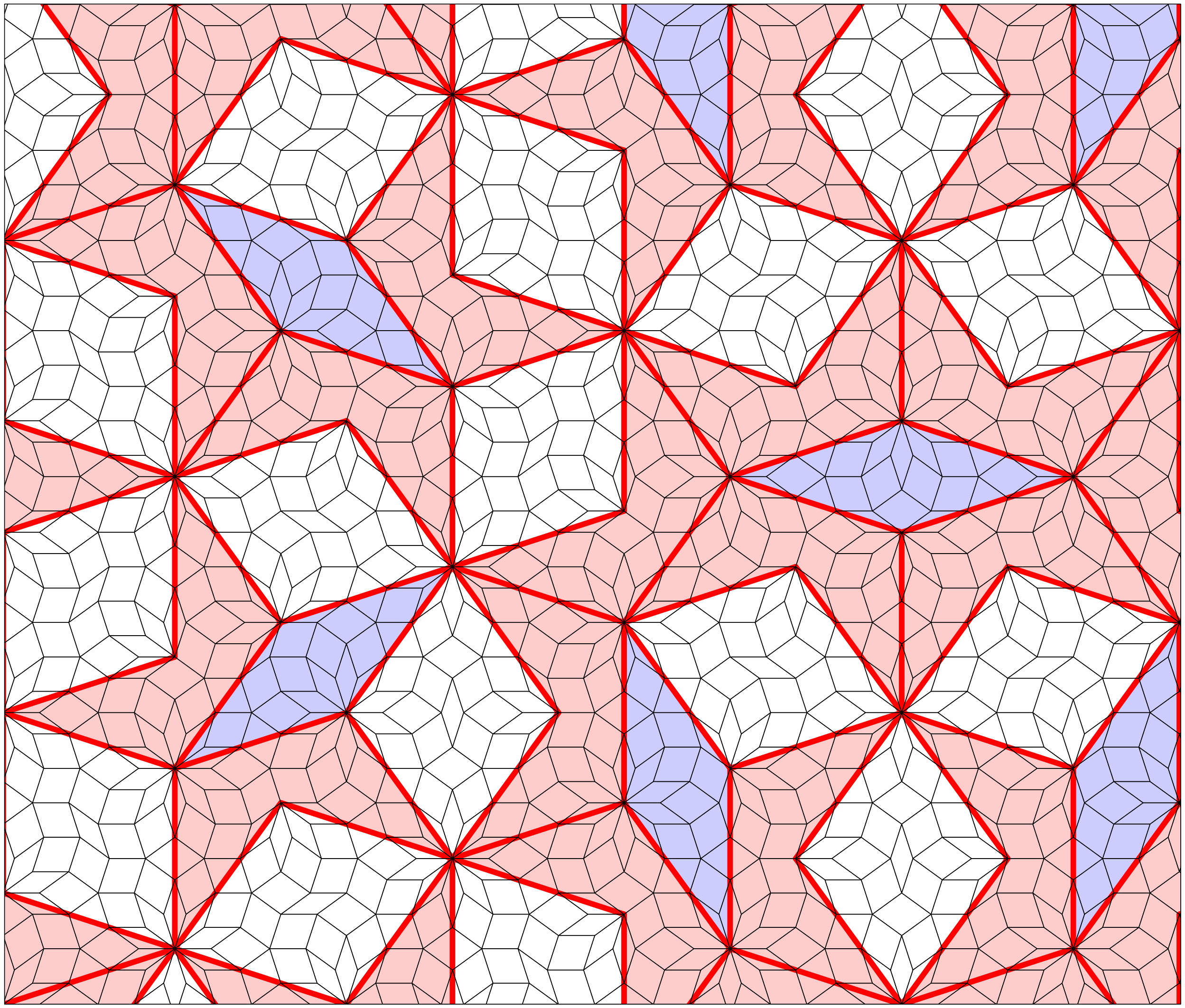
Binary tiling decoration of the Tübinge Triangle Tiling. Due to a matching constraint, binary tilings admit a simple decoration with two types of atoms.

Acceptance Domains

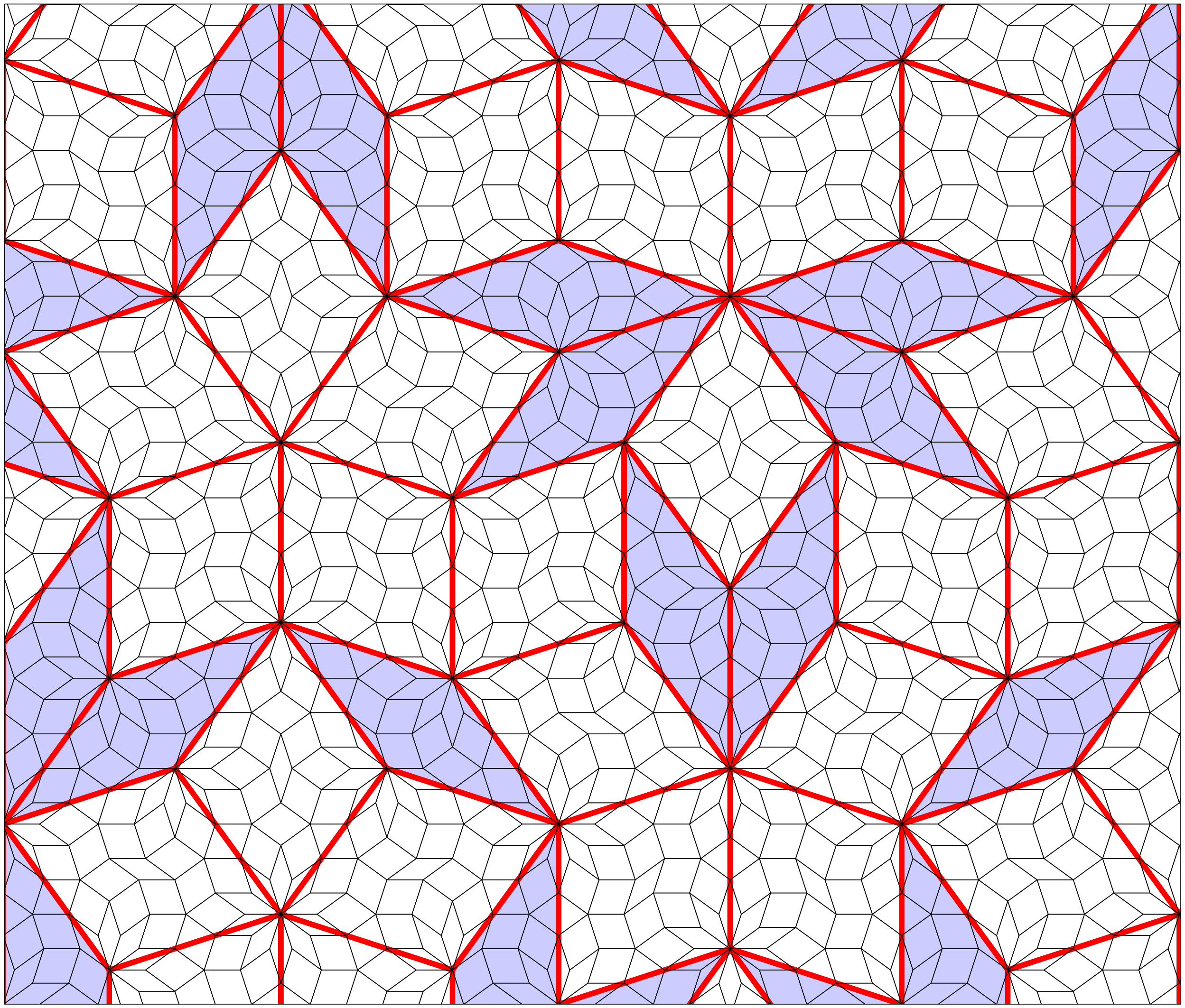


Three acceptance domains: the decagon for the large atoms, the two stars for the small atoms.

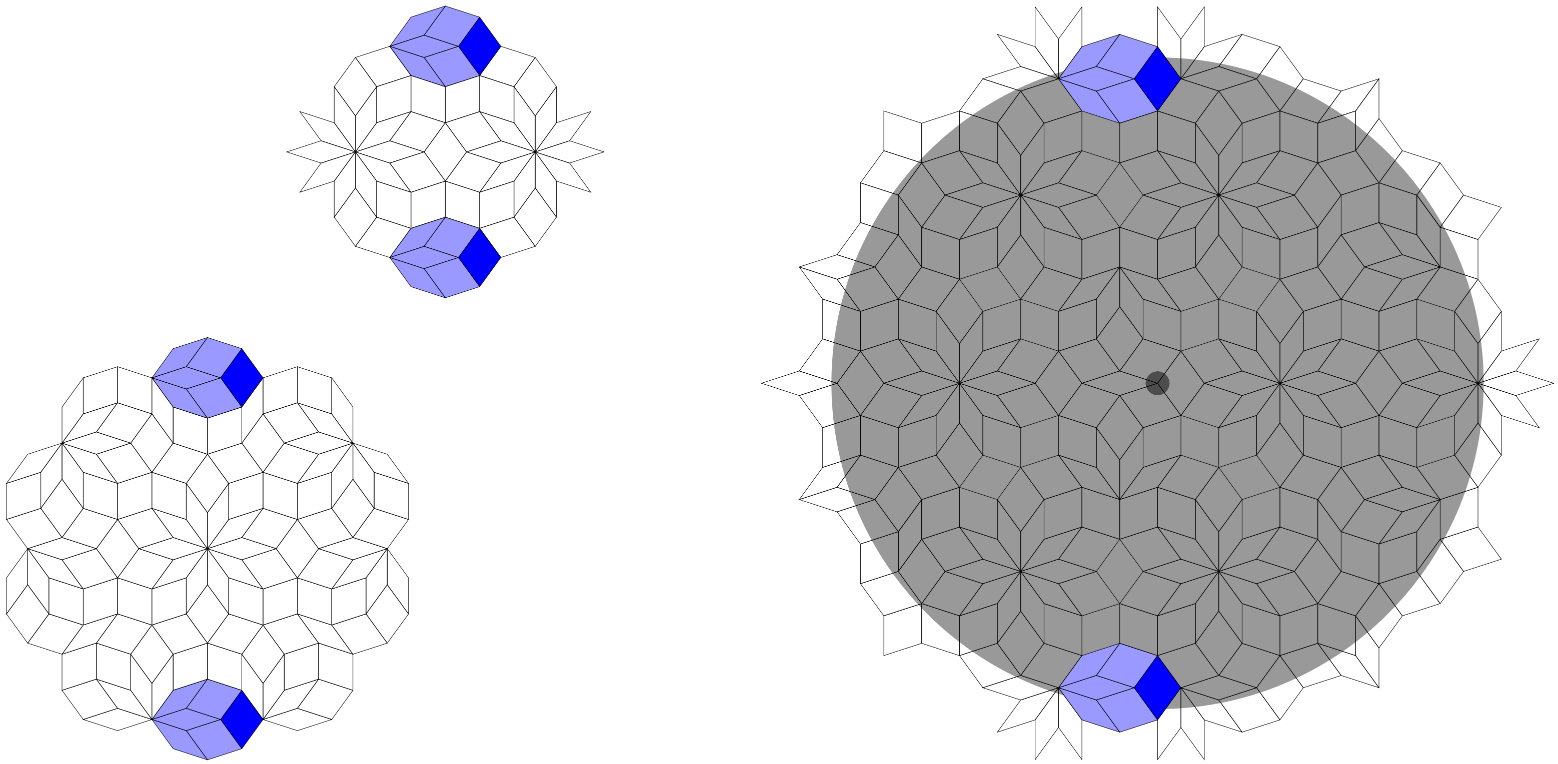
Large Scale Structure



Variant Based on Penrose Tiling



Matching Rule Radius



Being MLD to the Tübingen Trinangle Tiling, the binary tiling admits matching rules, but the matching rule radius is large....

Elastic Energy Density

Phonon strain: $\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i^{\|}}{\partial x_j^{\|}} + \frac{\partial u_j^{\|}}{\partial x_i^{\|}}\right)$

Phason strain: $\chi_{ij} = \frac{\partial u_i^{\perp}}{\partial x_j^{\|}}$

Elastic energy density:

$$f(\varepsilon, \chi) = \tfrac{1}{2} C^{\|}_{ij,kl} \varepsilon_{ij} \varepsilon_{kl} + \tfrac{1}{2} C^{\perp}_{ij,kl} \chi_{ij} \chi_{kl} + C^{\|,\perp} \varepsilon_{ij} \chi_{kl} + O((\varepsilon, \chi)^3)$$

Elastic Energy Density

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Phason strain: $\chi_{ij} = \frac{\partial u_i^{\perp}}{\partial x_j^{\parallel}}$

Elastic energy density:

$$f(\varepsilon, \chi) = \tfrac{1}{2}C^{\parallel}_{ij,kl}\varepsilon_{ij}\varepsilon_{kl} + \tfrac{1}{2}C^{\perp}_{ij,kl}\chi_{ij}\chi_{kl} + C^{\parallel,\perp}\varepsilon_{ij}\chi_{kl} + O((\varepsilon,\chi)^3)$$

Matching rule violations should lead to non-analytic terms:

$$f_{MR}(\chi) \propto \sum_{g\in D_{10}} |\chi_{01}|$$

Irreducible Components

Elastic energy in terms of irreducible strain components:

$$
\begin{aligned}
f = f_0 + \mu_1 \varepsilon^{(1)} & + \frac{1}{2}\lambda_3 (\varepsilon^{(1)})^2 \\
& + \frac{1}{2}\lambda_5 ((\varepsilon_1^{(6)})^2 + (\varepsilon_2^{(6)})^2) \\
& + \frac{1}{2}\lambda_7 ((\chi_1^{(6)})^2 + (\chi_2^{(6)})^2) \\
& + \frac{1}{2}\lambda_9 ((\chi_1^{(8)})^2 + (\chi_2^{(8)})^2) \\
& + \lambda_6 (\varepsilon_1^{(6)} \chi_1^{(6)} + \varepsilon_2^{(6)} \chi_2^{(6)}) + O((\varepsilon, \chi)^3)
\end{aligned}
$$

There are two phason elastic constants, and one phason-phonon coupling.

Relaxation Simulations

For samples with various phonon and phason strains, the atom positions are relaxed (with Lennard-Jones potentials), and the ground state energy is measured.

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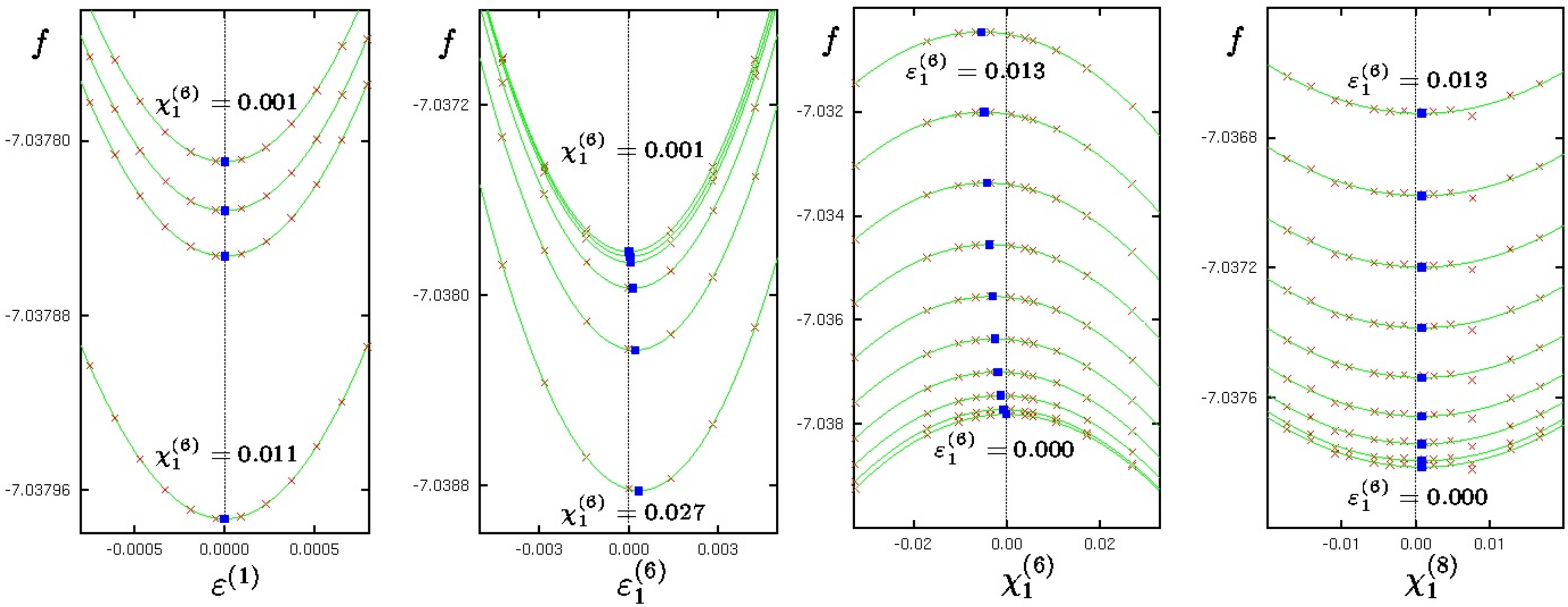
A variety on approximants is used to explore all directions in phason space.

Tübingen Trinangle Tiling admits many different approximants.

Relaxation Simulations – Results

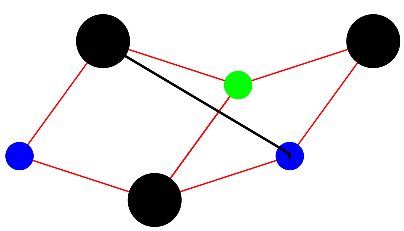


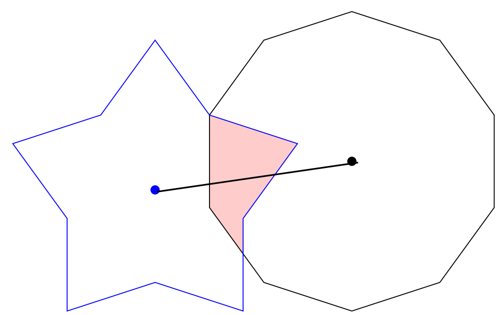
- all elastic constants are measured
- elastic energy has quadratic form
- there is one unstable mode

Energies From Patch Frequencies

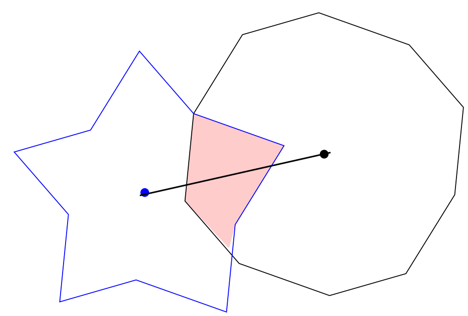
$$f(\chi;\phi) = \frac{1}{2V}\sum_{i\neq j}\phi_{ij}(r_{ij}) = \frac{1}{2V^*}\sum_{a,b,r^\perp} A_{ab,r^\perp}\cdot\phi_{ab}(r^{\|})$$

$r^{\|} = 1.54$





$A_{AB,r^\perp}(\chi = 0)$



$A_{AB,r^\perp}(\chi_2^{(6)} = 0.14)$

Phason Elastic Constants ($R_c = 1.92$)

$$f(\chi;\phi) = A_{BB,\mathbf{r}_1^\perp}(\chi)\,\phi_{\mathrm{BB}}(r_1^\parallel) + A_{AB,\mathbf{r}_2^\perp}(\chi)\,\phi_{\mathrm{AB}}(r_2^\parallel) + \ldots$$

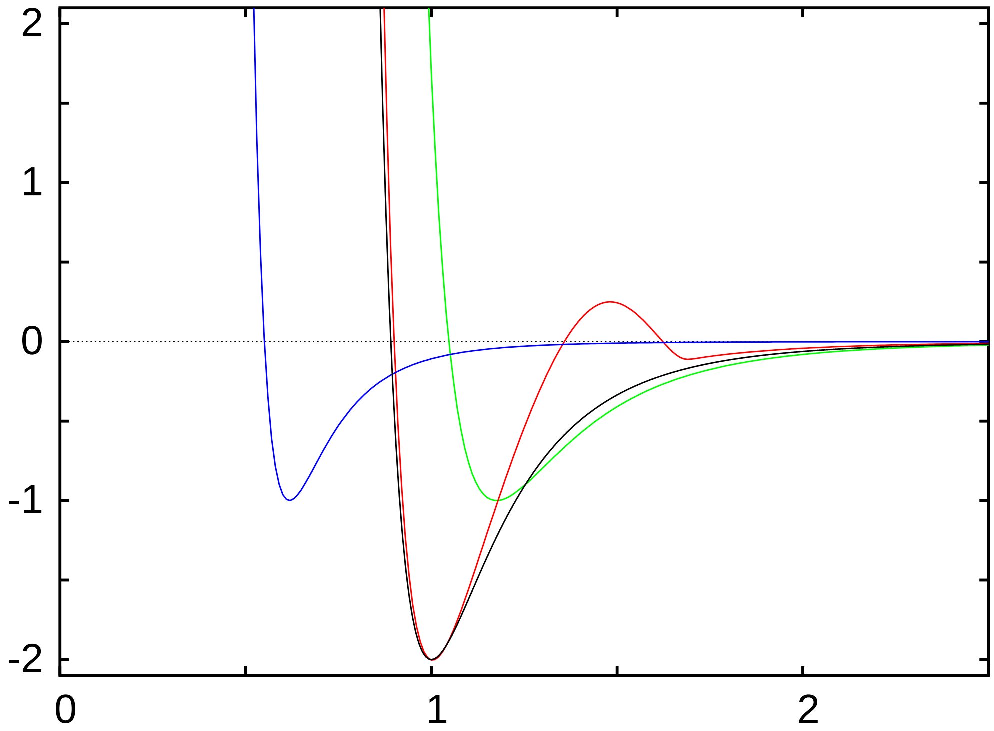
$$f(\chi;\phi) = f_0(\phi) + \tfrac{1}{2}\lambda_7(\phi)\left(\chi_1^{(6)^2} + \chi_2^{(6)^2}\right) + \tfrac{1}{2}\lambda_9(\phi)\left(\chi_1^{(8)^2} + \chi_2^{(8)^2}\right) + \mathrm{O}(\chi^3)$$

$$\begin{aligned}\lambda_7(\phi) = {} & -0.47\,\phi_{\mathrm{AA}}(1.18) - 2.38\,\phi_{\mathrm{AA}}(1.90)\\ & +0.76\,\phi_{\mathrm{BB}}(0.62) - 0.68\,\phi_{\mathrm{BB}}(1.18) - 3.47\,\phi_{\mathrm{BB}}(1.62) - 0.91\,\phi_{\mathrm{BB}}(1.90)\\ & +0.58\,\phi_{\mathrm{AB}}(1.00) + 4.40\,\phi_{\mathrm{AB}}(1.54)\end{aligned}$$

$$\begin{aligned}\lambda_9(\phi) = {} & \quad 0.47\,\phi_{\mathrm{AA}}(1.18) - 1.02\,\phi_{\mathrm{AA}}(1.90)\\ & -0.76\,\phi_{\mathrm{BB}}(0.62) - 2.72\,\phi_{\mathrm{BB}}(1.18) - 4.22\,\phi_{\mathrm{BB}}(1.62) - 4.27\,\phi_{\mathrm{BB}}(1.90)\\ & -0.58\,\phi_{\mathrm{AB}}(1.00) + 2.40\,\phi_{\mathrm{AB}}(1.54)\end{aligned}$$

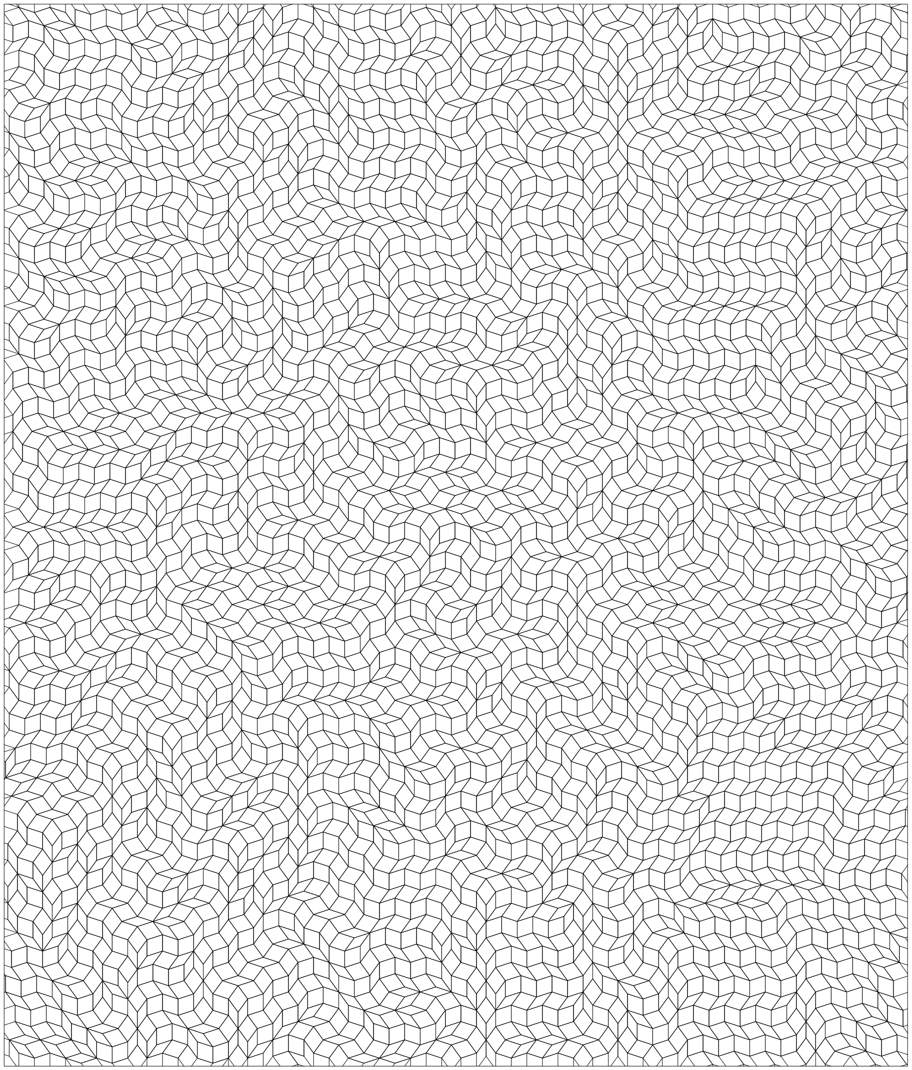
Terms at $r^\parallel = 1.54$ lead to instability ($\phi(r^\parallel = 1.54) < 0$).

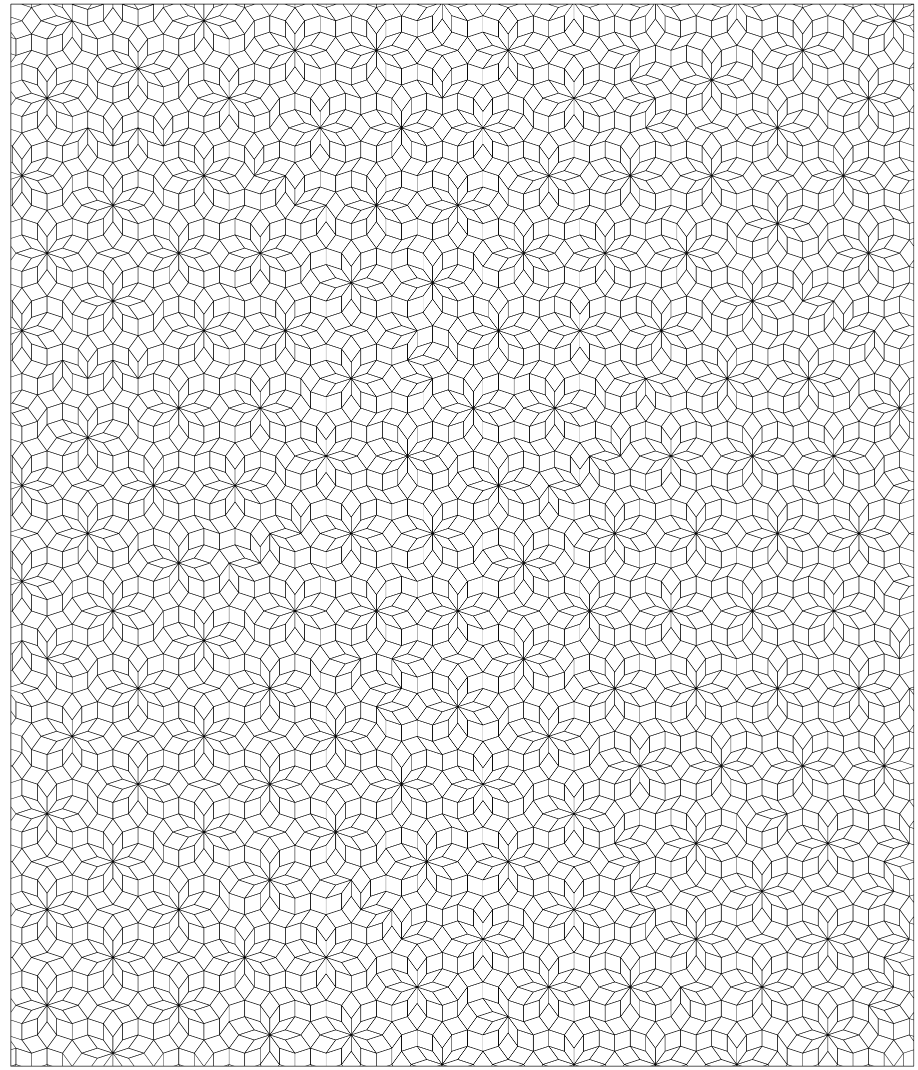
Modified Potentials to Avoid Instability



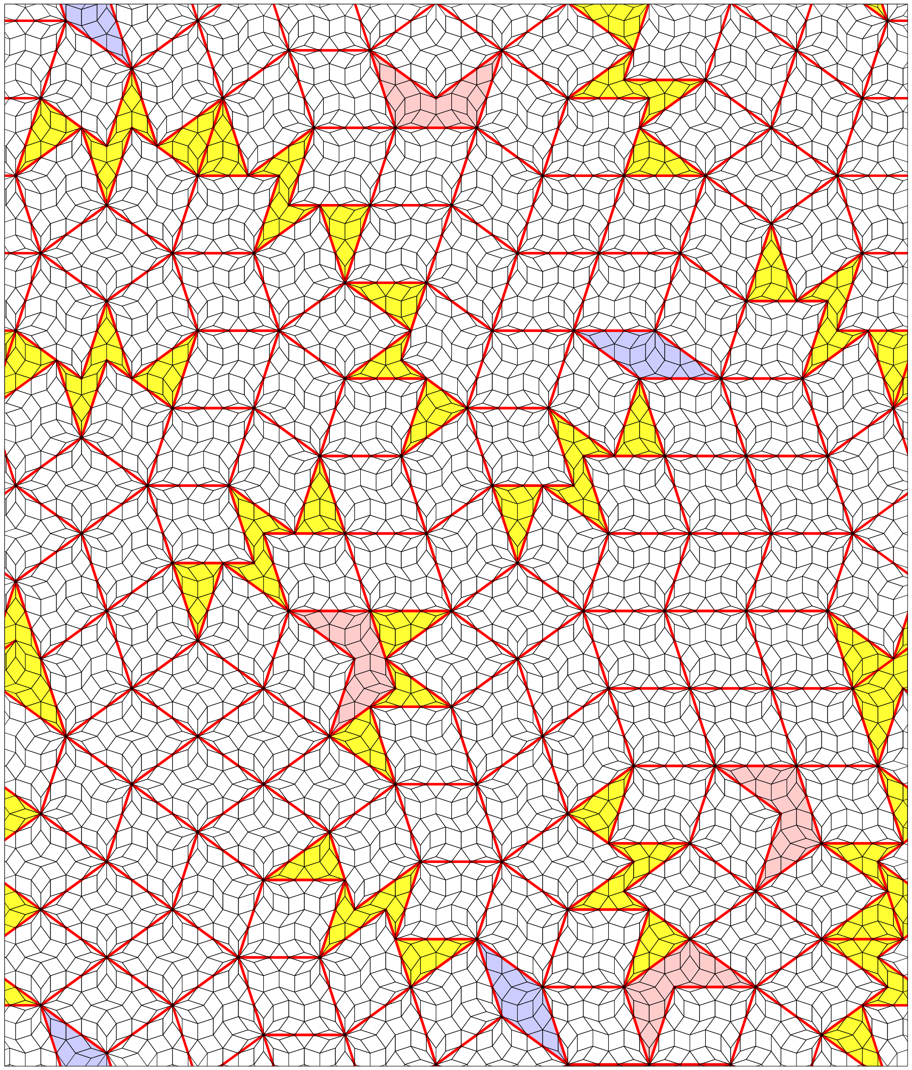
	LJ-Potential		Mod. Potential	
Elast. Const.	Devel.	MD	Devel.	MD
λ_7	-2.40	-2.70	-0.31	-0.88
λ_9	1.03	0.80	2.17	1.34
$(\lambda_7 + \lambda_9)/2$	-0.69	-0.95	0.93	0.23

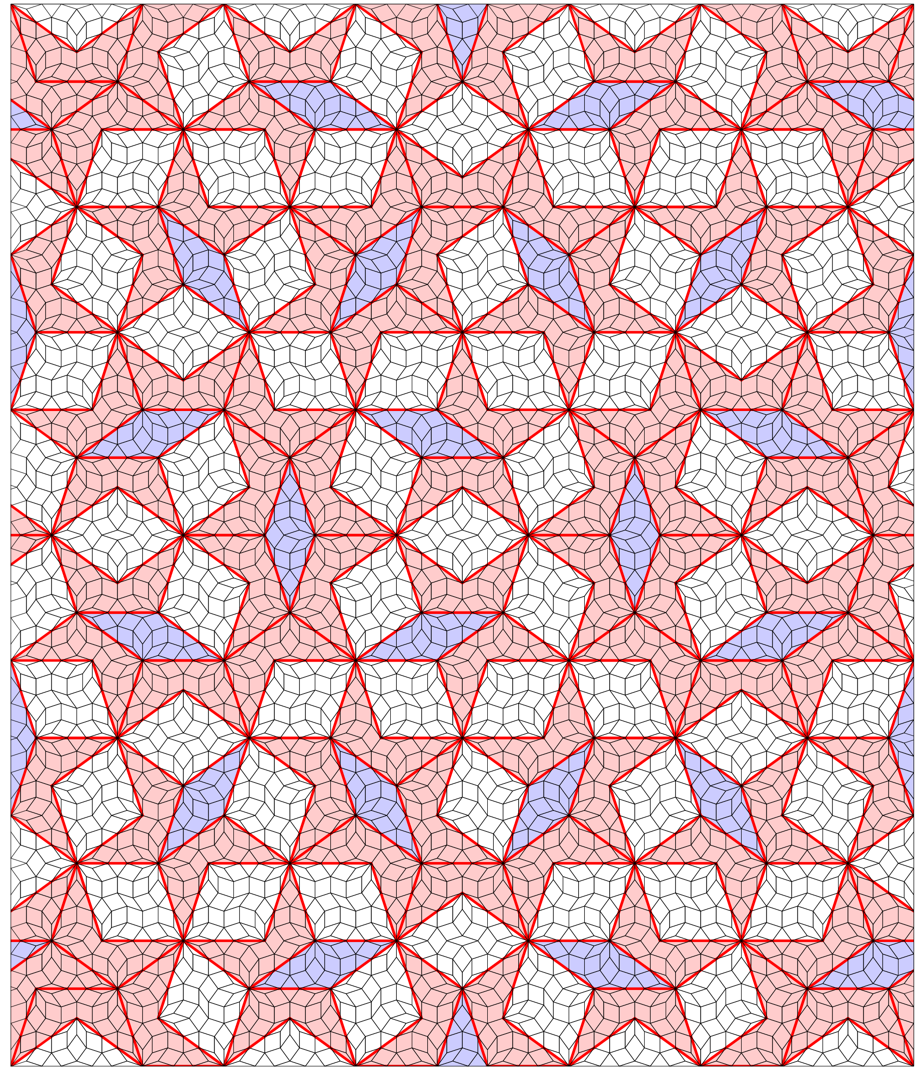
Lennard-Jones vs. Modified Potentials



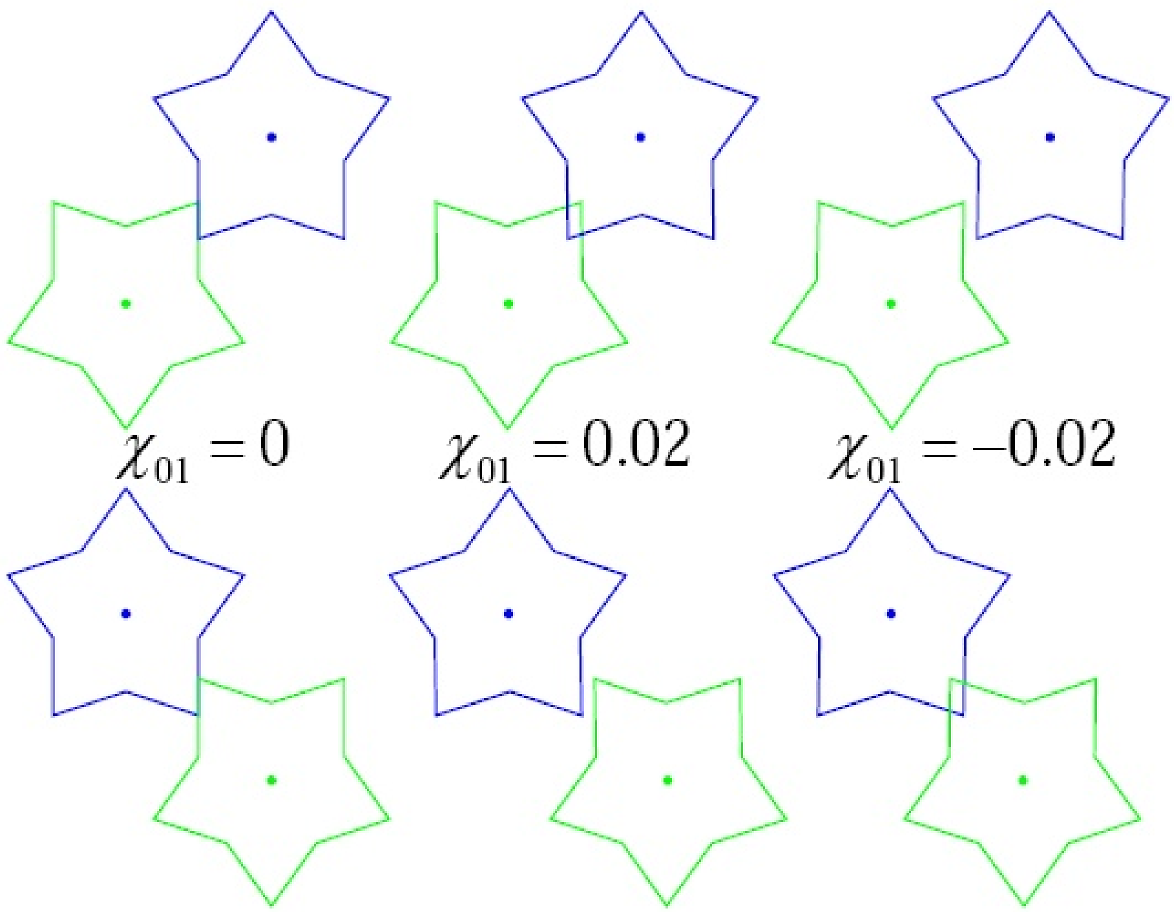


Modified Potentials vs. Perfect Structure





Degenerate Acceptance Domains



Due do matching rule violations, degeneracy of certain acceptance domains is lifted $\rightarrow$ non-analytic behaviour.

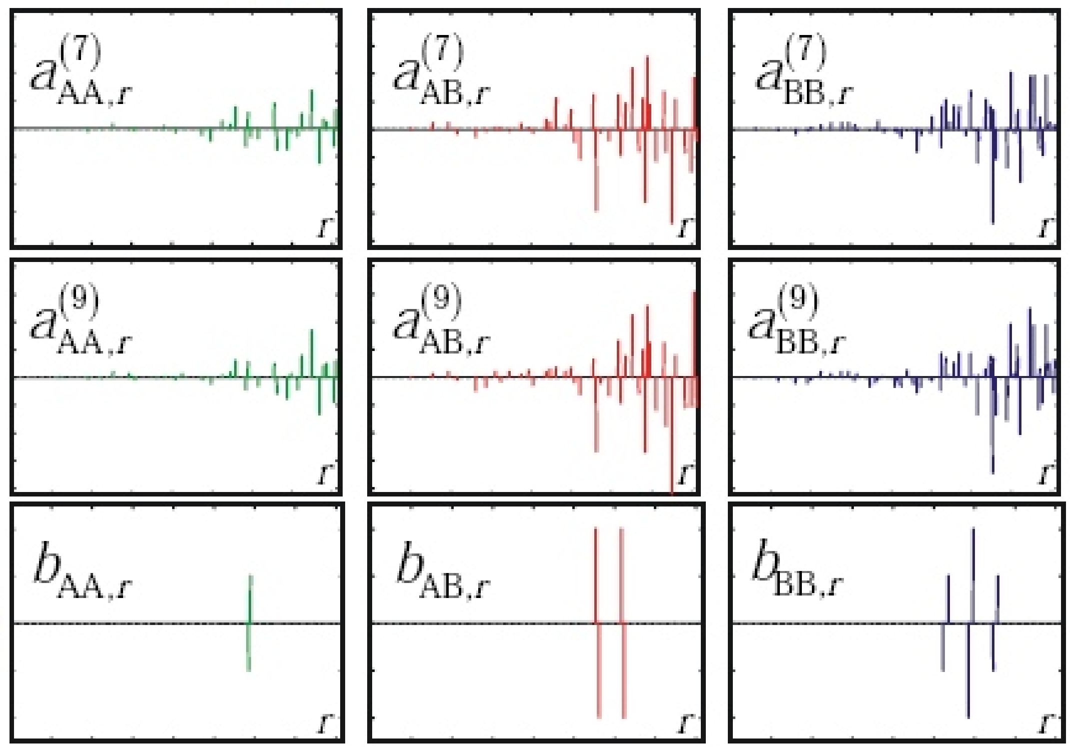
Phason Elastic Energy ($R_c = 8$)

$$f(\chi;\phi) = f_0(\phi) + \tfrac{1}{2}\lambda_7(\phi)\left(\chi_1^{(6)^2} + \chi_2^{(6)^2}\right) + \tfrac{1}{2}\lambda_9(\phi)\left(\chi_1^{(8)^2} + \chi_2^{(8)^2}\right)$$
$$+\mu_1(\phi)\,\tfrac{1}{20}\sum_{g\in D_{10}} g\left|\chi_{01}\right|$$
$$+\mu_2(\phi)\,\tfrac{1}{20}\sum_{g\in D_{10}} g\left(\chi_{11}\cdot\left|\chi_{01}\right|\right)$$

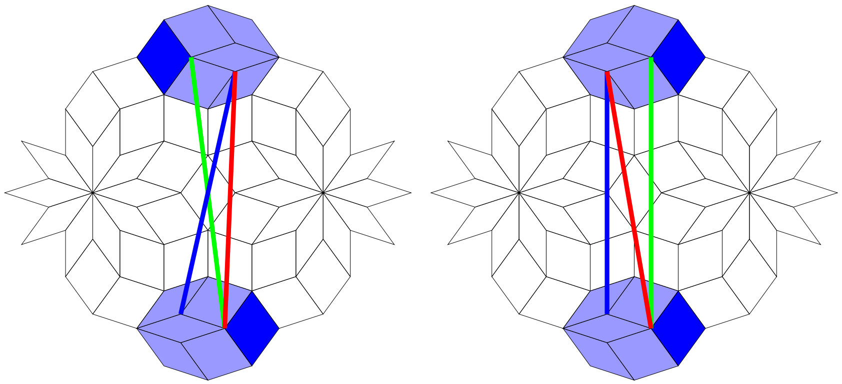
$$\lambda_7(\phi) = \sum_{ij,r} a_{ij,r}^{(7)}\,\phi_{ij}(r)$$

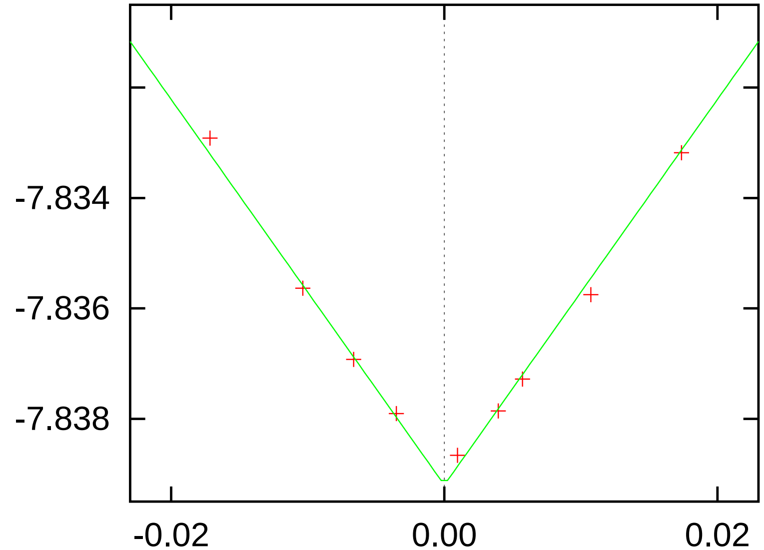
$$\lambda_9(\phi) = \sum_{ij,r} a_{ij,r}^{(9)}\,\phi_{ij}(r)$$

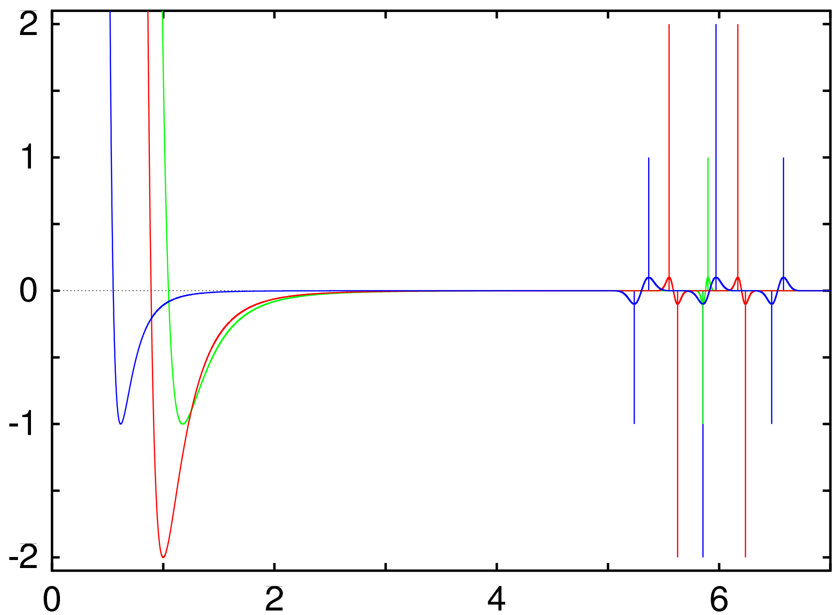
$$\mu_{1/2}(\phi) = c_{1/2}\sum_{ij,r} b_{ij,r}\,\phi_{ij}(r)$$

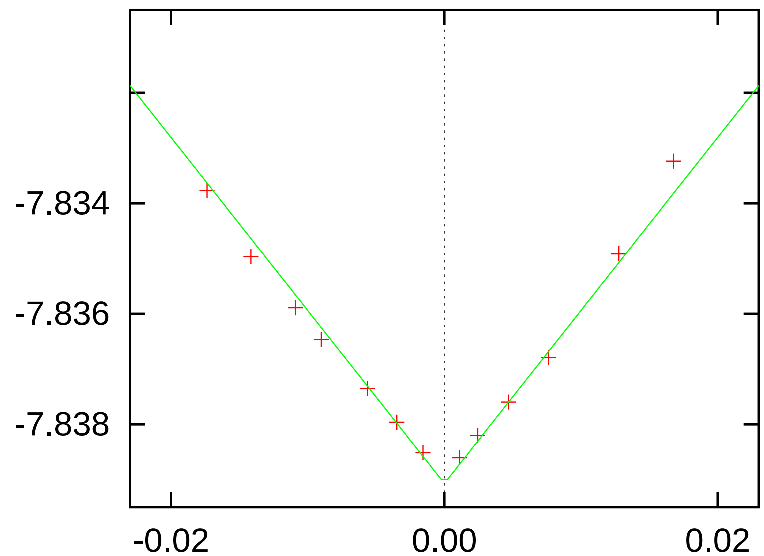


Non-Analytic Behaviour









Conclusions

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The binary tiling based on the Tübingen Trinangle Tiling is a particularly bad example in this respect.