

Spectrum of Kagome and triangular networks with time-reversal non-invariant vertex coupling

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in collaboration with Prof. Pavel Exner

Based on: [M. Baradaran, and P. Exner: J. Math. Phys. 63, 083502 \(2022\)](#)

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- Kagome lattice: the spectral condition
 - Positive spectrum: flat bands and continuous spectrum
 - Asymptotic behavior of the spectral bands at high energies
 - Negative spectrum
- Triangular lattice: the spectral condition
 - Positive spectrum: flat bands and continuous spectrum
 - Asymptotic behavior of the spectral bands at high energies
 - Negative spectrum

Kagome lattice: the spectral condition

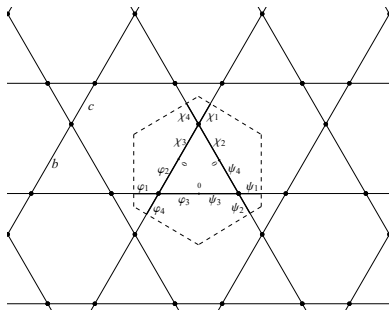
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The operator to investigate here is the particle Hamiltonian acting as $\psi_j \mapsto -\psi_j''$ assuming $\hbar = 2m = 1$.

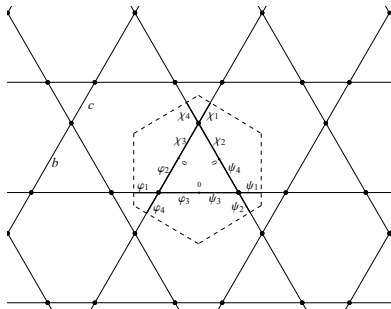


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The coupling condition (P Exner and M Tater, Phys. Lett. A 382 (2018))

We assume the coupling condition $(\psi_{j+1} - \psi_j) + i\ell(\psi'_{j+1} + \psi'_j) = 0$ which, obviously, violates the time-reversal invariance; we use the symbols ψ_j (ψ'_j) for the boundary value of the function ψ_j (respectively, ψ'_j) at the given vertex.

Seeking a solution at energy $E = k^2 > 0$, we employ the following Ansatz

$$\psi_j(x) = B_j^+ e^{ikx} + B_j^- e^{-ikx}, \quad x \in [0, \tfrac{1}{2}c], \quad j = 1, 2,$$

$$\psi_j(x) = B_j^+ e^{ikx} + B_j^- e^{-ikx}, \quad x \in [0, \tfrac{1}{2}b], \quad j = 3, 4,$$

$$\varphi_j(x) = C_j^+ e^{ikx} + C_j^- e^{-ikx}, \quad x \in [-\tfrac{1}{2}b, 0], \quad j = 2, 3,$$

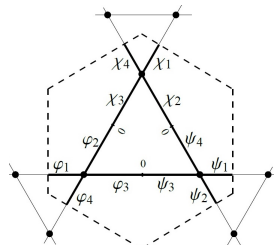
$$\varphi_j(x) = C_j^+ e^{ikx} + C_j^- e^{-ikx}, \quad x \in [-\tfrac{1}{2}c, 0], \quad j = 1, 4,$$

$$\chi_1(x) = D_1^+ e^{ikx} + D_1^- e^{-ikx}, \quad x \in [0, \tfrac{1}{2}c],$$

$$\chi_2(x) = D_2^+ e^{ikx} + D_2^- e^{-ikx}, \quad x \in [-\tfrac{1}{2}b, 0],$$

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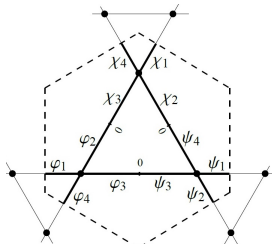
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Floquet conditions at the free ends of the cell

$$\chi_1(\tfrac{c}{2}) = e^{i\theta_1} \varphi_4(-\tfrac{c}{2}), \quad \chi_1'(\tfrac{c}{2}) = e^{i\theta_1} \varphi_4'(-\tfrac{c}{2}),$$

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for some $\theta_1, \theta_2 \in [-\pi, \pi)$

Seeking a solution at energy $E = k^2 > 0$, we employ the following Ansatz

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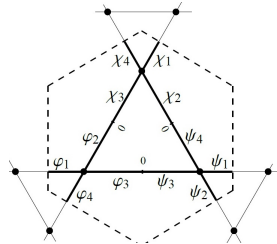
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$$\begin{aligned} \chi_1(\tfrac{c}{2}) &= e^{i\theta_1} \varphi_4(-\tfrac{c}{2}), & \chi_1'(\tfrac{c}{2}) &= e^{i\theta_1} \varphi_4'(-\tfrac{c}{2}), \\ \psi_1(\tfrac{c}{2}) &= e^{i\theta_2} \varphi_1(-\tfrac{c}{2}), & \psi_1'(\tfrac{c}{2}) &= e^{i\theta_2} \varphi_1'(-\tfrac{c}{2}), \\ \psi_2(\tfrac{c}{2}) &= e^{i(\theta_2 - \theta_1)} \chi_4(-\tfrac{c}{2}), & \psi_2'(\tfrac{c}{2}) &= e^{i(\theta_2 - \theta_1)} \chi_4'(-\tfrac{c}{2}), \end{aligned}$$

for some $\theta_1, \theta_2 \in [-\pi, \pi]$

At the segment midpoints

$$\begin{aligned} \chi_2(0) &= \psi_4(0), & \chi_2'(0) &= \psi_4'(0), \\ \varphi_3(0) &= \psi_3(0), & \varphi_3'(0) &= \psi_3'(0), \\ \varphi_2(0) &= \chi_3(0), & \varphi_2'(0) &= \chi_3'(0). \end{aligned}$$

Imposing the matching conditions at each vertex of the graph cell, taking into account that the derivatives are taken in the outward direction, we get

$$\psi_2(0) - \psi_1(0) + i\ell (\psi'_2(0) + \psi'_1(0)) = 0,$$

$$\psi_3(\tfrac{1}{2}b) - \psi_2(0) + i\ell (-\psi'_3(\tfrac{1}{2}b) + \psi'_2(0)) = 0,$$

$$\psi_4(\tfrac{1}{2}b) - \psi_3(\tfrac{1}{2}b) - i\ell (\psi'_4(\tfrac{1}{2}b) + \psi'_3(\tfrac{1}{2}b)) = 0,$$

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$$\varphi_2(-\tfrac{1}{2}b) - \varphi_1(0) + i\ell (\varphi'_2(-\tfrac{1}{2}b) - \varphi'_1(0)) = 0,$$

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$$\varphi_4(0) - \varphi_3(-\tfrac{1}{2}b) + i\ell (-\varphi'_4(0) + \varphi'_3(-\tfrac{1}{2}b)) = 0,$$

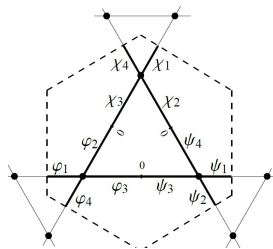
$$\varphi_1(0) - \varphi_4(0) - i\ell (\varphi'_1(0) + \varphi'_4(0)) = 0,$$

$$\chi_2(-\tfrac{1}{2}b) - \chi_1(0) + i\ell (\chi'_2(-\tfrac{1}{2}b) + \chi'_1(0)) = 0,$$

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$$\chi_4(0) - \chi_3(\tfrac{1}{2}b) - i\ell (\chi'_4(0) + \chi'_3(\tfrac{1}{2}b)) = 0,$$

$$\chi_1(0) - \chi_4(0) + i\ell (\chi'_1(0) - \chi'_4(0)) = 0.$$



Spectral condition is obtained as

$$\sin \frac{kc}{2} \sin \frac{kd}{2} \sin \frac{k(d-c)}{2} \left(\lambda_1(k) - \lambda_2(k) f_\theta - \lambda_3(k) g_\theta \right) = 0$$

where

$$\begin{aligned} \lambda_1(k) := & 2(k^2 \ell^2 + 1) (4(k^2 \ell^2 + 1)^2 (\cos k(c+d) + \cos k(c-2d) + 2 \cos kd + \cos 2kd) + (3k^4 \ell^4 + 18k^2 \ell^2 + 3) \\ & + (k^4 \ell^4 + 14k^2 \ell^2 + 1) (2 \cos kd + 1) \cos k(2c-d) + (5k^4 \ell^4 + 22k^2 \ell^2 + 5) (\cos k(d-c) + \cos kc)), \end{aligned}$$

$$\lambda_2(k) := 8 (k^2 \ell^2 + 1) (k^2 \ell^2 - 1)^2 \cos \frac{k(d-c)}{2} \cos \frac{kc}{2} \left(\cos \frac{k(2c-d)}{2} + 2 \cos \frac{kd}{2} \right),$$

$$\lambda_3(k) := 16k\ell (k^2 \ell^2 - 1)^2 \sin \frac{k(d-c)}{2} \sin \frac{kc}{2} \sin \frac{k(d-2c)}{2}.$$

and

$$f_\theta := \cos \theta_1 + \cos(\theta_1 - \theta_2) + \cos \theta_2, \quad -\frac{3}{2} \leq f_\theta \leq 3,$$

$$g_\theta := \sin \theta_2 + \sin(\theta_1 - \theta_2) - \sin \theta_1, \quad -\frac{3\sqrt{3}}{2} \leq g_\theta \leq \frac{3\sqrt{3}}{2}.$$

Positive spectrum: spectral conditions

$$\sin \frac{kc}{2} \sin \frac{kd}{2} \sin \frac{k(d-c)}{2} \left(\lambda_1(k) - \lambda_2(k) f_\theta - \lambda_3(k) g_\theta \right) = 0$$

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For $d = 2c$, i.e. the **equilateral** graph, the spectral condition reduces to

$$\begin{aligned} & 4(k^2 \ell^2 + 1) (2 \cos kc + 1) \sin kc \sin^2 \frac{kc}{2} \\ & \times \left((k^4 \ell^4 + 14k^2 \ell^2 + 1) \cos kc + 2(\cos 2kc + \cos 3kc + \frac{1}{2})(k^2 \ell^2 + 1)^2 - (\cos kc + 1)(k^2 \ell^2 - 1)^2 f_\theta \right) \\ & = 0 \end{aligned}$$

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i. Infinitely degenerate eigenvalues (flat bands)

- In the general case, the number k^2 belongs to the spectrum for $k = \frac{2n\pi}{l}$ with $l = \{d - c, c, d\}$ and $n \in \mathbb{N}$; in the equilateral case, they merge into $k^2 = (\frac{n\pi}{c})^2$.
- In the general case, for $\{d - c, c, d\} = \ell((-1)^{n+1} + (6n - 3)) \frac{\pi}{6}$ with $n \in \mathbb{N}$, the bands degenerate to the point $k = \ell^{-1}$; in the equilateral case, this happens for $c = \ell((-1)^{n+1} + (6n - 3)) \frac{\pi}{12}$.
- In the equilateral case, the number k^2 belongs to the spectrum for $k = ((-1)^{n+1} + (6n - 3)) \frac{\pi}{6c}$ with $n \in \mathbb{N}$.

ii. Continuous bands

Continuous spectrum is determined by the condition

$$\lambda_1(k) = \lambda_2(k) f_\theta + \lambda_3(k) g_\theta$$

Using the Hessian method of determining extrema of multivariate functions as well as checking the boundaries of our rectangular domain, we find that:

A number k^2 belongs to a spectral band if and only if

$$k \in \{k : \lambda^\pm(k) \leq \lambda_1(k) \leq \lambda^0(k) \quad \cup \quad \lambda^0(k) \leq \lambda_1(k) \leq \lambda^\pm(k)\}$$

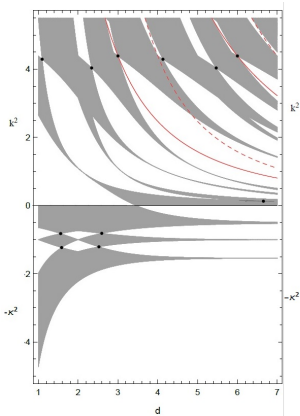
where

$$\lambda^0(k) := 3 \lambda_2(k),$$

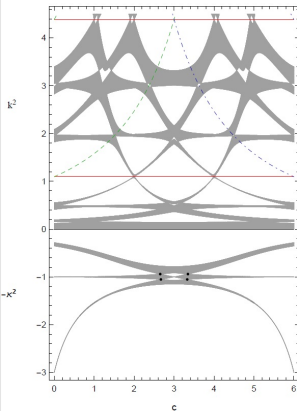
$$\lambda^\pm(k) := -\frac{3}{2} (\lambda_2(k) \pm \sqrt{3} \lambda_3(k))$$

The band-and-gap pattern for particular values of parameters

i. $c = \ell = 1$

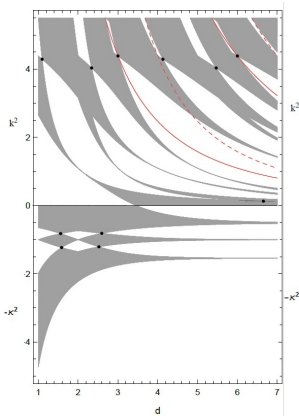


ii. $d = 6, \ell = 1$

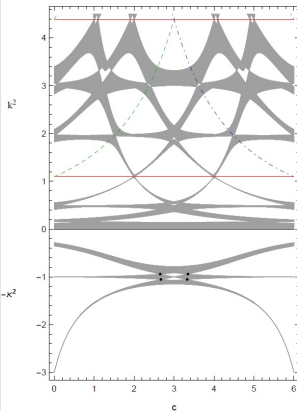


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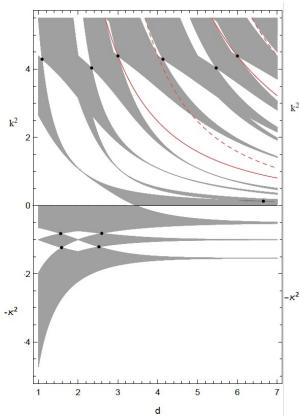
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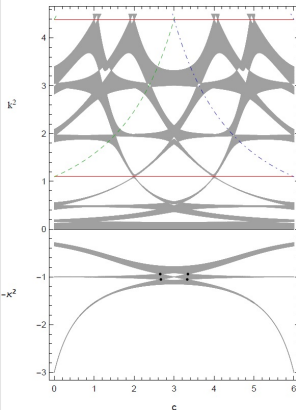
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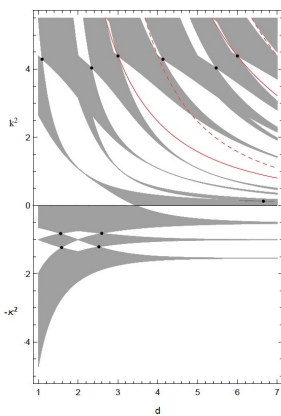
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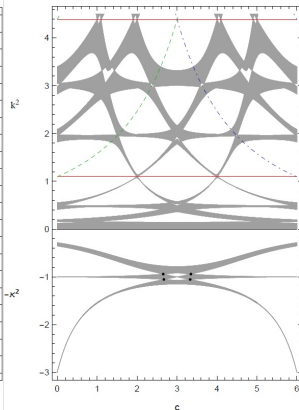
- For $d \geq 2\sqrt{3}\ell$, the positive spectrum starts at zero.
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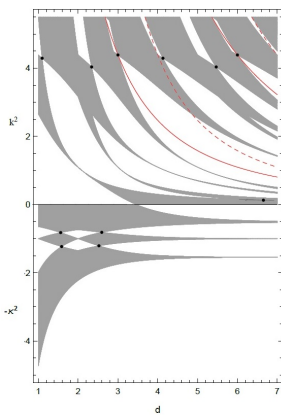
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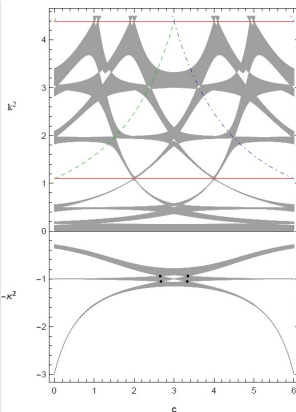
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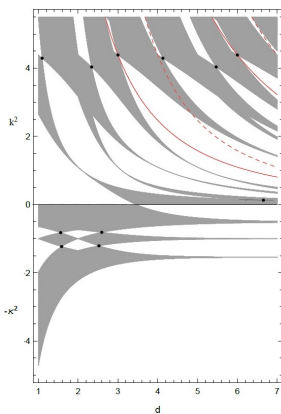
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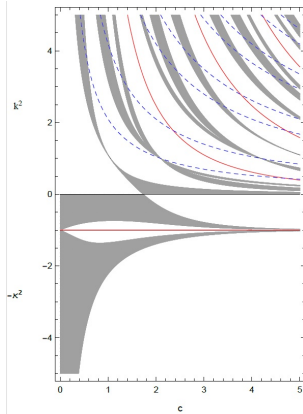
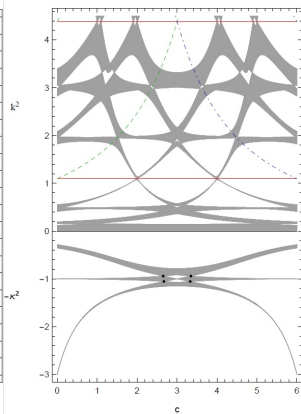
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Asymptotic behavior of the spectral bands at high energies

To take a look at the bands structure in the high-energy regime, $k \rightarrow \infty$, we rewrite the spectral condition $\lambda_1(k) - \lambda_2(k) f_\theta - \lambda_3(k) g_\theta = 0$ in the form $\alpha(k) \cdot k^6 + \mathcal{O}(k^5) = 0$ where

$$\alpha(k) = 4 \left(\cos \frac{k(2c-d)}{2} + 2 \cos \frac{kd}{2} \right) \\ \times \left((2 \cos k(c-d) + 4 \cos kd - 1) \cos \frac{kd}{2} + \cos \frac{k(2c+d)}{2} - 2 f_\theta \cos \frac{kc}{2} \cos \frac{k(c-d)}{2} \right).$$

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Hence, as $k \rightarrow \infty$, the function $\alpha(k)$ should be close to zero which results in two types of spectral bands:

- Pairs of narrow bands in the vicinity of the points k which solve the equation $\cos \frac{k(2c-d)}{2} + 2 \cos \frac{kd}{2} = 0$.
- Wide bands which grow asymptotically; they correspond to those values of k for which the function in the second bracket is close to zero.

In the high energy regime, a number k belongs to the spectral bands if

$$0 \leq \frac{5}{4} + \frac{\cos kd \cos \frac{k(2c-d)}{2} + \cos \frac{3kd}{2}}{\cos \frac{k(2c-d)}{2} + \cos \frac{kd}{2}} \leq \frac{9}{4},$$

with a relative error $\mathcal{O}(k^{-1})$ from which we can calculate the probability of being in the spectrum [R. Band, G. Berkolaiko, Phys. Rev. Lett. 113 (2013)]

$$P_\sigma(H) := \lim_{K \rightarrow \infty} \frac{1}{K} |\sigma(H) \cap [0, K]|$$

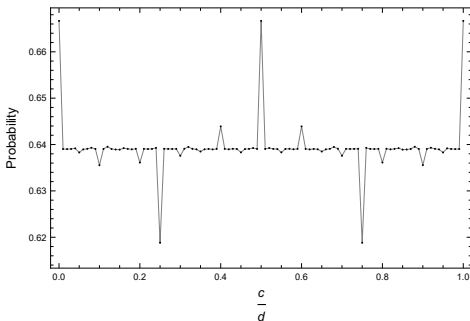
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If $\frac{c}{d} \in \mathbb{Q}$, it takes different values



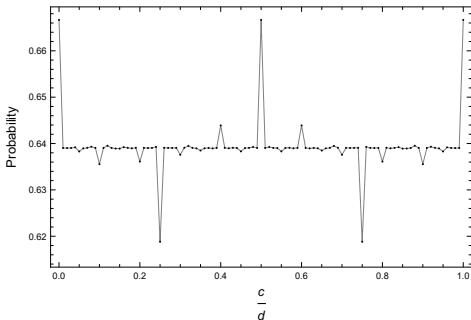
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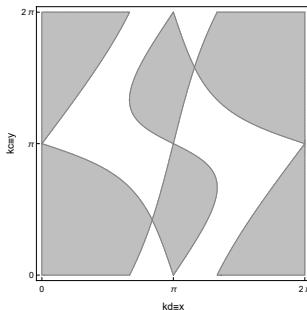
with a relative error $\mathcal{O}(k^{-1})$ from which we can calculate the probability of being in the spectrum [R. Band, G. Berkolaiko, Phys. Rev. Lett. 113 (2013)]

$$P_\sigma(H) := \lim_{K \rightarrow \infty} \frac{1}{K} |\sigma(H) \cap [0, K]|$$

If $\frac{c}{d} \in \mathbb{Q}$, it takes different values



if $\frac{c}{d} \notin \mathbb{Q}$, the value is the same being ≈ 0.639



In the equilateral case, i.e. $d = 2c$, the condition of belonging to the spectral bands in the high energy regime reduces to

$$0 \leq \xi(k) \leq \frac{9}{8} ; \quad \xi(k) := \cos kc - \cos 2kc.$$

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The function $\xi(k)$ is periodic with period $T = \frac{2\pi}{c}$ and reaches its maximum value, $\frac{9}{8}$, at $k = \frac{1}{c}|2m\pi \pm \text{arcsec } 4|$ with $m \in \mathbb{Z}$; then, it remains to calculate the probability that $\xi(k)$ is positive for a randomly chosen value of k .

By elementary calculus, one easily finds that $\xi(k)$ is negative over the domain $(\frac{2\pi}{3c}, \frac{4\pi}{3c})$ and thus, the probability of belonging to the spectrum, for any c , is equal to

$$P_{\sigma}(H) = 1 - \frac{1}{T} \left(\frac{4\pi}{3c} - \frac{2\pi}{3c} \right) = \frac{2}{3}$$

The negative spectrum

Replacing k by $i\kappa$ with $\kappa > 0$ in the positive spectrum, we obtain the spectral condition

$$\sinh \frac{\kappa c}{2} \sinh \frac{\kappa d}{2} \sinh \frac{\kappa(d-c)}{2} \left(\tilde{\lambda}_1(\kappa) - \tilde{\lambda}_2(\kappa) f_\theta - \tilde{\lambda}_3(\kappa) g_\theta \right) = 0$$

where

$$\begin{aligned} \tilde{\lambda}_1(\kappa) &:= 2(1 - \kappa^2 \ell^2) \left(4(\kappa^2 \ell^2 - 1)^2 \left(\cosh \kappa(c+d) + \cosh \kappa(c-2d) + 2 \cosh \kappa d + \cosh 2\kappa d \right) + \left(3\kappa^4 \ell^4 - 18\kappa^2 \ell^2 + 3 \right) \right. \\ &\quad \left. + \left(\kappa^4 \ell^4 - 14\kappa^2 \ell^2 + 1 \right) (2 \cosh \kappa d + 1) \cosh \kappa(2c-d) + \left(5\kappa^4 \ell^4 - 22\kappa^2 \ell^2 + 5 \right) (\cosh \kappa(d-c) + \cosh \kappa c) \right), \\ \tilde{\lambda}_2(\kappa) &:= 8(1 - \kappa^2 \ell^2) \left(\kappa^2 \ell^2 + 1 \right)^2 \left(\cosh \frac{\kappa(2c-d)}{2} + 2 \cosh \frac{\kappa d}{2} \right) \cosh \frac{\kappa(d-c)}{2} \cosh \frac{\kappa c}{2}, \\ \tilde{\lambda}_3(\kappa) &:= 16\kappa \ell \left(\kappa^2 \ell^2 + 1 \right)^2 \sinh \frac{\kappa(d-c)}{2} \sinh \frac{\kappa c}{2} \sinh \frac{\kappa(d-2c)}{2}. \end{aligned}$$

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Flat bands: There exists flat band $-\ell^{-2}$ only in the equilateral case.

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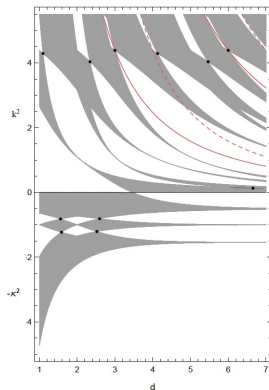
Flat bands: There exists flat band $-\ell^{-2}$ only in the equilateral case.

Continuous bands: A number $-\kappa^2$ belongs to a spectral band if

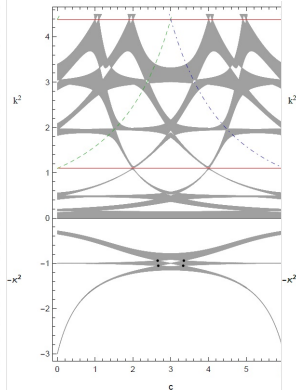
$$\kappa \in \left\{ \kappa : \tilde{\lambda}^\pm(\kappa) \leq \tilde{\lambda}_1(\kappa) \leq \tilde{\lambda}^0(\kappa) \quad \cup \quad \tilde{\lambda}^0(\kappa) \leq \tilde{\lambda}_1(\kappa) \leq \tilde{\lambda}^\pm(\kappa) \right\}$$

where $\tilde{\lambda}^0(\kappa) := 3\tilde{\lambda}_2(\kappa)$ and $\tilde{\lambda}^\pm(\kappa) := -\frac{3}{2} \left(\tilde{\lambda}_2(\kappa) \pm \sqrt{3} \tilde{\lambda}_3(\kappa) \right)$.

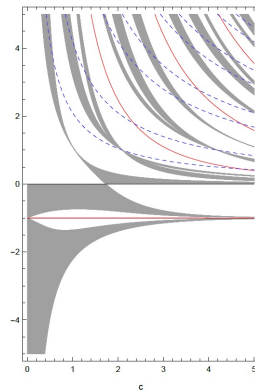
The general model



The general model



The equilateral model

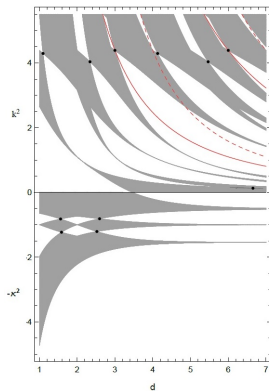


- There cannot be more than three negative bands [1, Theorem 2.6] which may merge into each other (only in the general case).

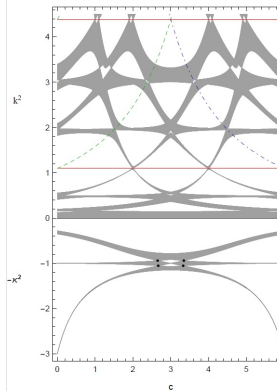


[1]. M. Baradaran, P. Exner, and M. Tater, Ann. Phys. 433, 168992 (2022)

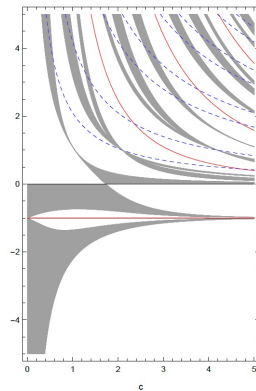
The general model



The general model



The equilateral model

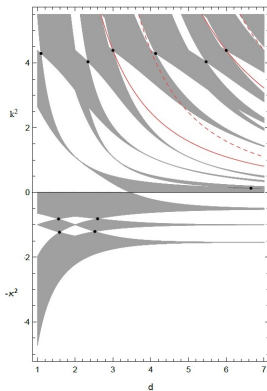


- There cannot be more than three negative bands [1, Theorem 2.6] which may merge into each other (only in the general case).
- The number $-\ell^{-2}$ belongs to the spectrum; as the edge lengths tend to infinity, the negative bands shrink to points below and above this energy.

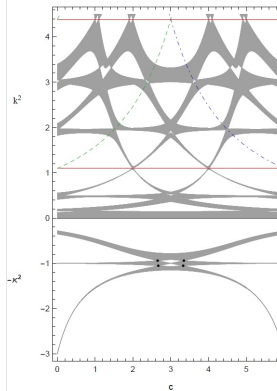


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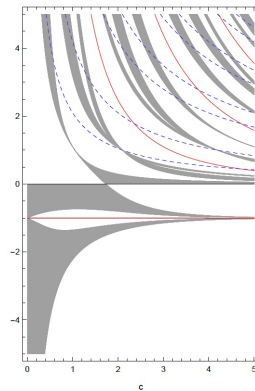
The general model



The general model



The equilateral model

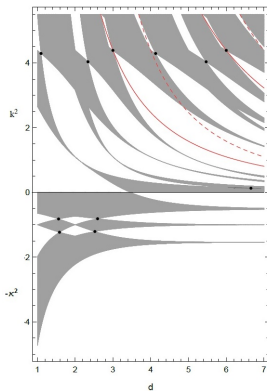


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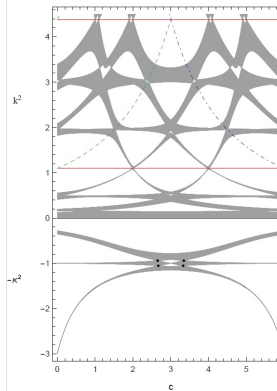


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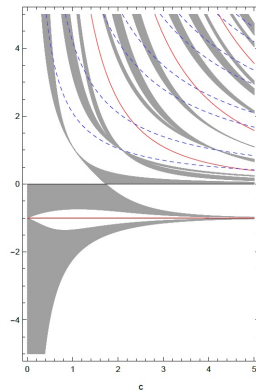
The general model



The general model



The equilateral model



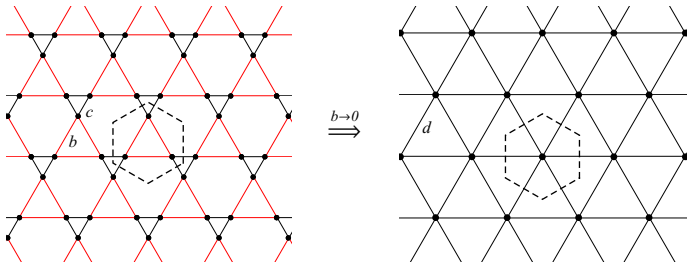
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- The number $-\ell^{-2}$ belongs to the spectrum; as the edge lengths tend to infinity, the negative bands shrink to points below and above this energy.
- The negative bands are symmetric with respect to the interchange of c and $d - c$.
- For $d \leq 2\sqrt{3}\ell$, the first negative band reaches zero.



[1]. M. Baradaran, P. Exner, and M. Tater, Ann. Phys. 433, 168992 (2022)

Triangula lattice

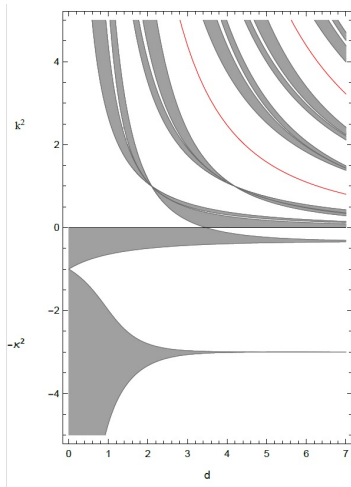
The kagome lattice degenerates to the triangular one when one of the edge lengths shrinks to zero; the elementary cell now contains a single vertex of degree six.



The spectral condition can be derived in the same way as in the kagome lattice case or by taking the limit $c \rightarrow d$ in the spectral condition of the kagome lattice; this yields

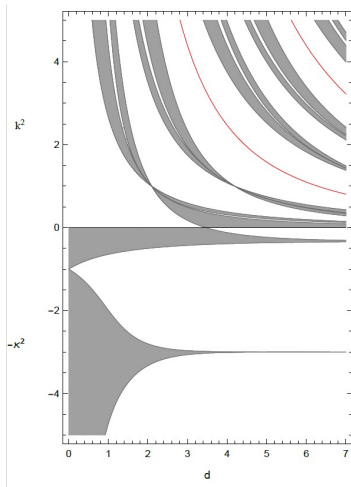
$$\begin{aligned}
 & (k^2 \ell^2 + 1) \sin^2 \frac{kd}{2} \\
 & \times \left(3(k^4 \ell^4 + 6k^2 \ell^2 + 1) + (3k^4 \ell^4 + 10k^2 \ell^2 + 3)(2 \cos kd + \cos 2kd) - 4(k^2 \ell^2 - 1)^2 \cos^2 \frac{kd}{2} f_\theta \right) \\
 & = 0
 \end{aligned}$$

The band-and-gap pattern for $\ell = 1$



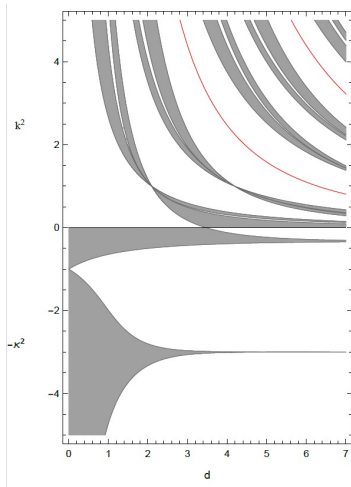
- For $k = \frac{2n\pi}{d}$ with $n \in \mathbb{N}$, the number k^2 belongs to the spectrum (flat bands).

The band-and-gap pattern for $\ell = 1$



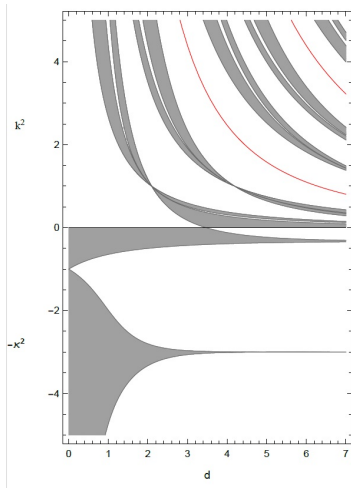
- For $k = \frac{2n\pi}{d}$ with $n \in \mathbb{N}$, the number k^2 belongs to the spectrum (flat bands).
- Positive bands degenerate to a point at $k = \ell^{-1}$ for $d = \ell((-1)^{n+1} + (6n - 3)) \frac{\pi}{6}$ with $n \in \mathbb{N}$.

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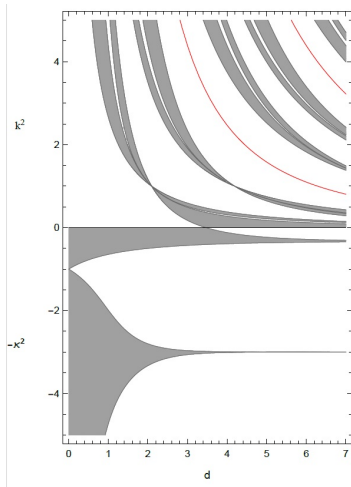
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- For large values of d , the negative bands shrink to the energies $-3\ell^{-2}$ and $-\frac{1}{3}\ell^{-2}$.

Thank you for your attention!