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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September 8, 2022

Outline

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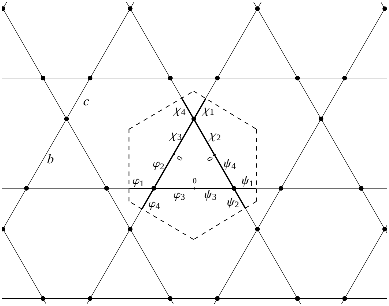
The operator to investigate here is the particle Hamiltonian acting as $\psi_j \mapsto -\psi_j''$ assuming $\hbar = 2m = 1$.



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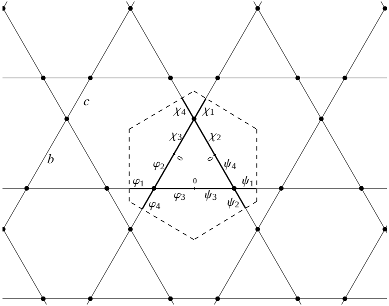

The coupling condition (P Exner and M Tater, Phys. Lett. A 382 (2018))

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

$$\psi_j(x) = B_j^+ \, e^{ikx} + B_j^- \, e^{-ikx}, \qquad x \in [0, \tfrac{1}{2}c], \qquad j = 1, 2,$$
$$\psi_j(x) = B_j^+ \, e^{ikx} + B_j^- \, e^{-ikx}, \qquad x \in [0, \tfrac{1}{2}b], \qquad j = 3, 4,$$
$$\varphi_j(x) = C_j^+ \, e^{ikx} + C_j^- \, e^{-ikx}, \qquad x \in [-\tfrac{1}{2}b, 0], \qquad j = 2, 3,$$
$$\varphi_j(x) = C_j^+ \, e^{ikx} + C_j^- \, e^{-ikx}, \qquad x \in [-\tfrac{1}{2}c, 0], \qquad j = 1, 4,$$
$$\chi_1(x) = D_1^+ \, e^{ikx} + D_1^- \, e^{-ikx}, \qquad x \in [0, \tfrac{1}{2}c],$$
$$\chi_2(x) = D_2^+ \, e^{ikx} + D_2^- \, e^{-ikx}, \qquad x \in [-\tfrac{1}{2}b, 0],$$
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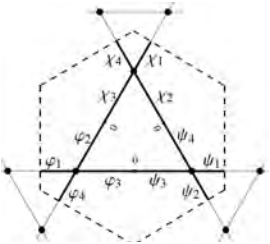

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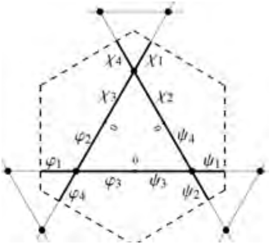

Floquet conditions at the free ends of the cell

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

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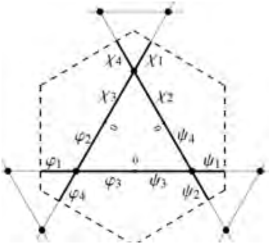

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$$\psi_2(\tfrac{c}{2}) = e^{i(\theta_2-\theta_1)}\chi_4(-\tfrac{c}{2}), \qquad \psi_2'(\tfrac{c}{2}) = e^{i(\theta_2-\theta_1)}\chi_4'(-\tfrac{c}{2}),$$

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

At the segment midpoints

$$\chi_2(0) = \psi_4(0), \qquad \chi_2'(0) = \psi_4'(0),$$
$$\varphi_3(0) = \psi_3(0), \qquad \varphi_3'(0) = \psi_3'(0),$$
$$\varphi_2(0) = \chi_3(0), \qquad \varphi_2'(0) = \chi_3'(0).$$

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

$$\psi_2(0) - \psi_1(0) + i\ell\left(\psi_2'(0) + \psi_1'(0)\right) = 0,$$
$$\psi_3(\tfrac{1}{2}b) - \psi_2(0) + i\ell\left(-\psi_3'(\tfrac{1}{2}b) + \psi_2'(0)\right) = 0,$$
$$\psi_4(\tfrac{1}{2}b) - \psi_3(\tfrac{1}{2}b) - i\ell\left(\psi_4'(\tfrac{1}{2}b) + \psi_3'(\tfrac{1}{2}b)\right) = 0,$$
$$\psi_1(0) - \psi_4(\tfrac{1}{2}b) + i\ell\left(\psi_1'(0) - \psi_4'(\tfrac{1}{2}b)\right) = 0,$$

$$\varphi_2(-\tfrac{1}{2}b) - \varphi_1(0) + i\ell\left(\varphi_2'(-\tfrac{1}{2}b) - \varphi_1'(0)\right) = 0,$$
$$\varphi_3(-\tfrac{1}{2}b) - \varphi_2(-\tfrac{1}{2}b) + i\ell\left(\varphi_3'(-\tfrac{1}{2}b) + \varphi_2'(-\tfrac{1}{2}b)\right) = 0,$$
$$\varphi_4(0) - \varphi_3(-\tfrac{1}{2}b) + i\ell\left(-\varphi_4'(0) + \varphi_3'(-\tfrac{1}{2}b)\right) = 0,$$
$$\varphi_1(0) - \varphi_4(0) - i\ell\left(\varphi_1'(0) + \varphi_4'(0)\right) = 0,$$

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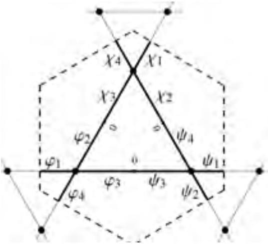

Spectral condition is obtained as

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

where

$$\lambda_1(k):=2(k^2\ell^2+1)(4(k^2\ell^2+1)^2\big(\cos k(c+d)+\cos k(c-2d)+2\cos kd+\cos 2kd\big)+\Big(3k^4\ell^4+18k^2\ell^2+3\Big)$$
$$+\Big(k^4\ell^4+14k^2\ell^2+1\Big)\,(2\cos kd+1)\cos k(2c-d)+\Big(5k^4\ell^4+22k^2\ell^2+5\Big)\,\big(\cos k(d-c)+\cos kc\big)\big),$$
$$\lambda_2(k):=8\left(k^2\ell^2+1\right)\left(k^2\ell^2-1\right)^2\cos\frac{k(d-c)}{2}\cos\frac{kc}{2}\Big(\cos\frac{k(2c-d)}{2}+2\cos\frac{kd}{2}\Big),$$
$$\lambda_3(k):=16k\ell\left(k^2\ell^2-1\right)^2\sin\frac{k(d-c)}{2}\sin\frac{kc}{2}\sin\frac{k(d-2c)}{2}.$$

and

$$f_\theta:=\cos\theta_1+\cos(\theta_1-\theta_2)+\cos\theta_2,\quad -\tfrac{3}{2}\le f_\theta\le 3,$$
$$g_\theta:=\sin\theta_2+\sin(\theta_1-\theta_2)-\sin\theta_1,\quad -\tfrac{3\sqrt{3}}{2}\le g_\theta\le\tfrac{3\sqrt{3}}{2}.$$

Positive spectrum: spectral conditions

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

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

$$4\big(k^2\ell^2+1\big)\big(2\cos kc+1\big)\sin kc\ \sin^2\tfrac{kc}{2}$$
$$\times\Bigg(\big(k^4\ell^4+14k^2\ell^2+1\big)\cos kc+2(\cos 2kc+\cos 3kc+\tfrac{1}{2})(k^2\ell^2+1)^2-(\cos kc+1)(k^2\ell^2-1)^2 f_\theta\Bigg)$$
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$$=0$$

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

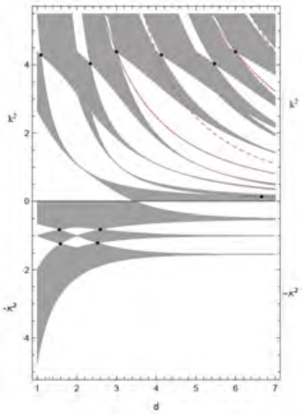
$$k \in \left\{k:\ \lambda^{\pm}(k) \le \lambda_1(k) \le \lambda^0(k) \quad \cup \quad \lambda^0(k) \le \lambda_1(k) \le \lambda^{\pm}(k)\right\}$$

where

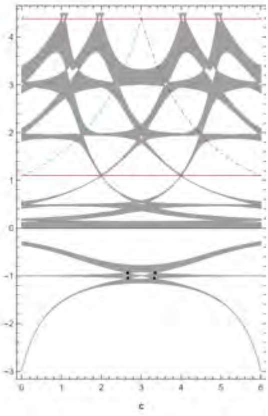
$$\lambda^0(k) := 3\,\lambda_2(k),$$
$$\lambda^{\pm}(k) := -\tfrac{3}{2}\left(\lambda_2(k) \pm \sqrt{3}\,\lambda_3(k)\right)$$

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

i. $c = \ell = 1$



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



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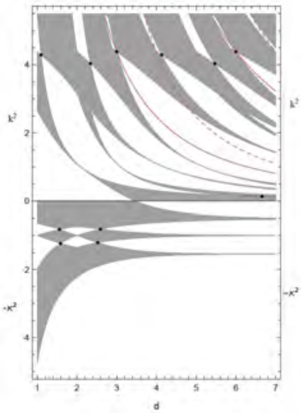

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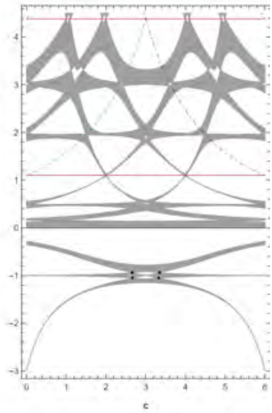

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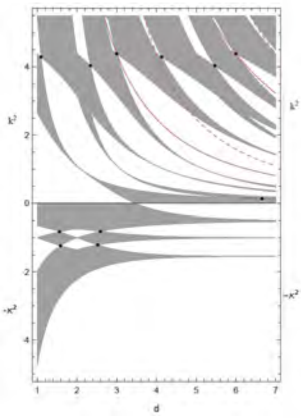

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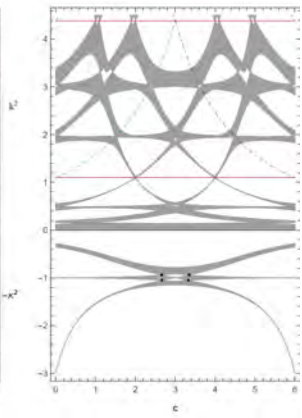

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- For $\{d - c, c, d\} = \ell\big((-1)^{n+1} + (6n-3)\big)\frac{\pi}{6}$ with $n \in \mathbb{N}$, the bands degenerate to ℓ^{-1}.

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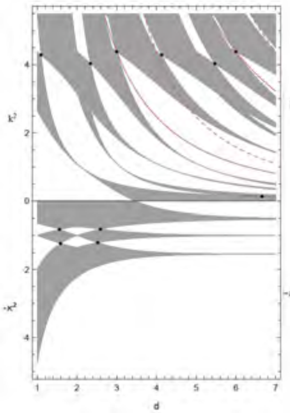

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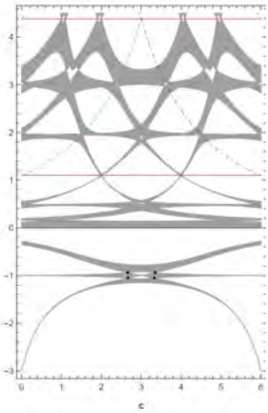

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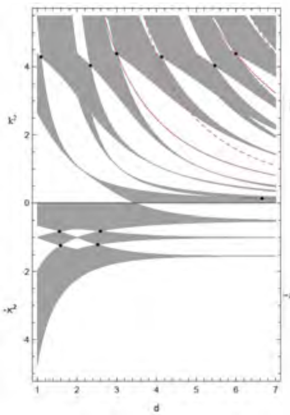

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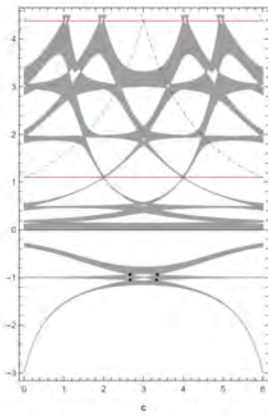

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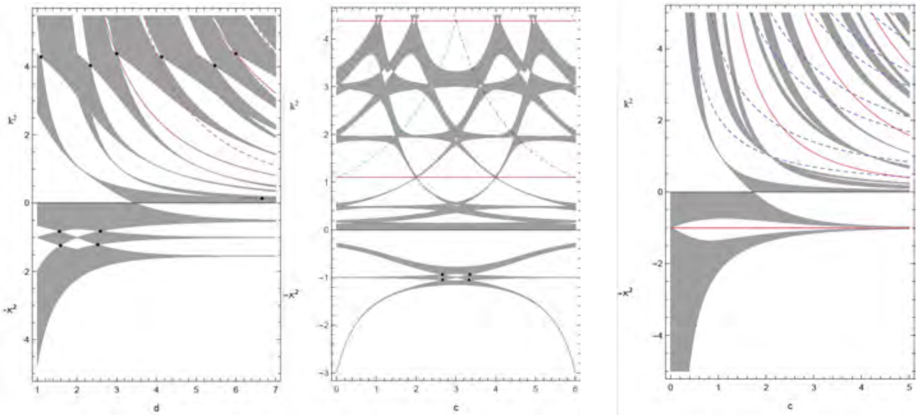

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Asymptotic behavior of the spectral bands at high energies

To take a look at the bands structure in the high-energy regime, $k \to \infty$, 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 $k \to \infty$, 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)]

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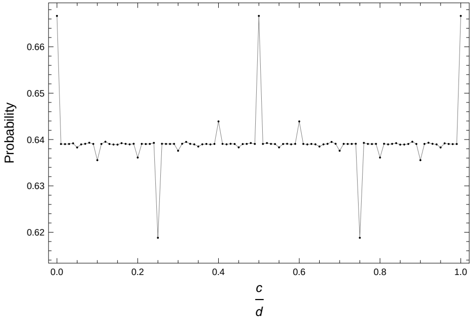
If $\frac{c}{d} \in \mathbb{Q}$, it takes different values



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)]

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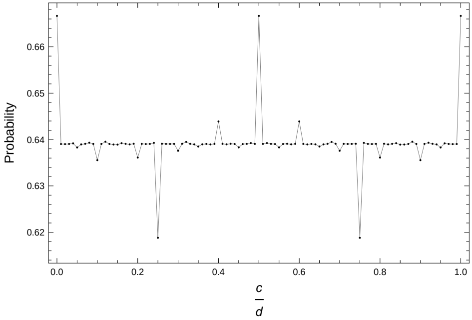
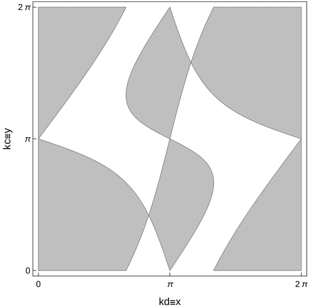


if $\frac{c}{d} \notin \mathbb{Q}$, the value is the same being ≈ 0.639



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 $k = \frac{1}{c}|2m\pi \pm \operatorname{arcsec} 4|$ 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 $\left(\frac{2\pi}{3c}, \frac{4\pi}{3c}\right)$ 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

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

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

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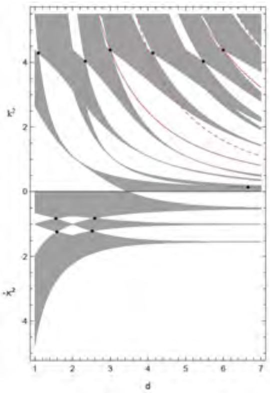
Flat bands: There exists flat band $-\ell^{-2}$ only in the equilateral case.

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

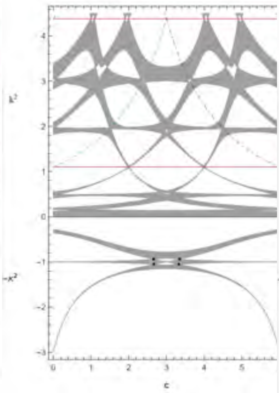
$$\kappa\in\left\{\kappa:\ \tilde{\lambda}^{\pm}(\kappa)\le\tilde{\lambda}_1(\kappa)\le\tilde{\lambda}^0(\kappa)\quad\cup\quad\tilde{\lambda}^0(\kappa)\le\tilde{\lambda}_1(\kappa)\le\tilde{\lambda}^{\pm}(\kappa)\right\}$$

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

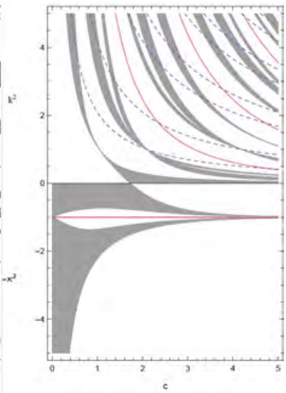
The general model



The general model

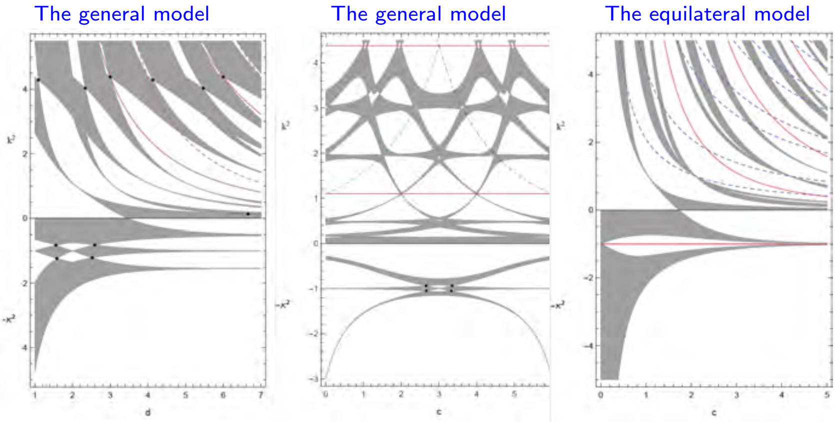


The equilateral model



- 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)



- 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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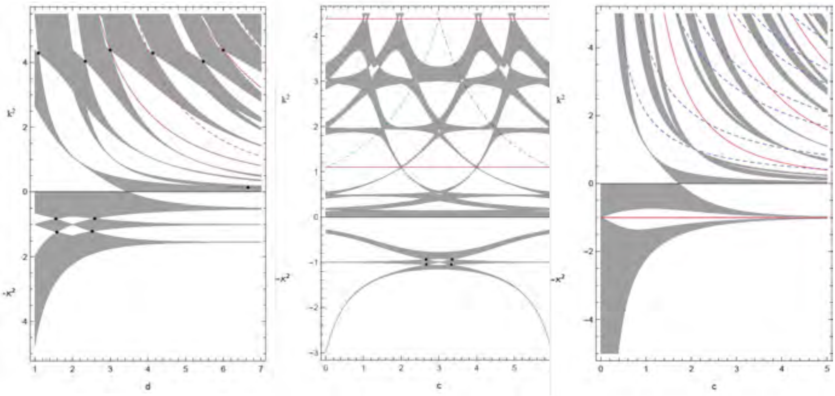
The general model | The general model | The equilateral model



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- 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 $d-c$.

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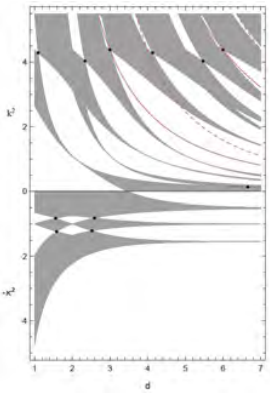
The general model



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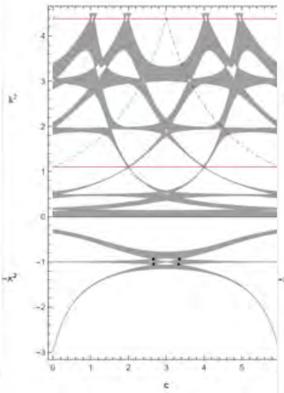
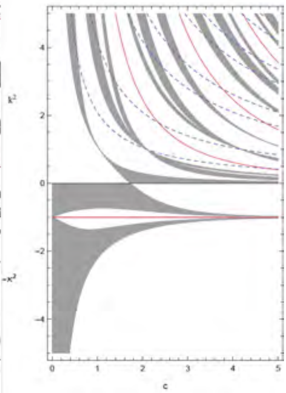


The equilateral model

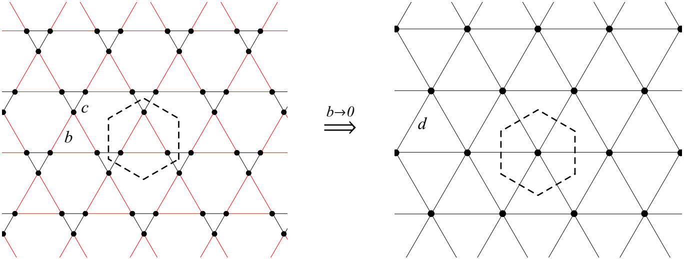


- There cannot be more than three negative bands [1, Theorem 2.6] which may merge into each other (only in the general case).
- The number $-\ell^{-2}$ belongs to the spectrum; as the edge lengths tend to infinity, the negative bands shrink to points below and above this energy.
- The negative bands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

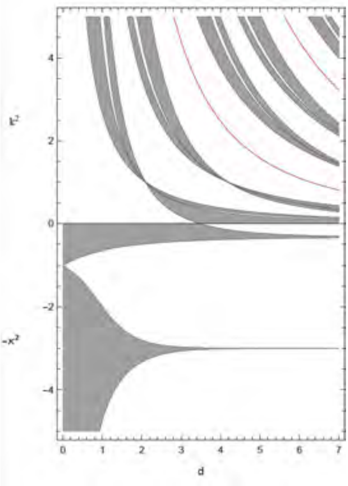
The kagome lattice degenerates to the triangular one when one of the edge lengths shrinks to zero; the elementary cell now contains a single vertex of degree six.



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

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

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).

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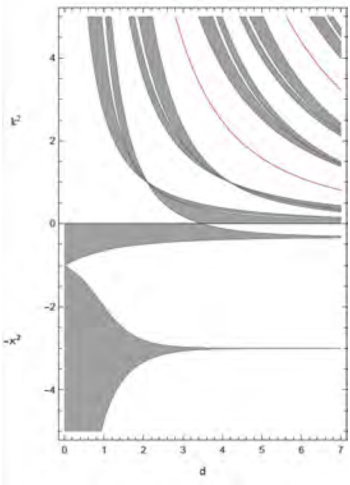
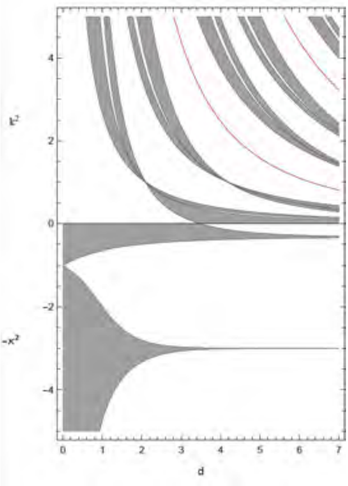


- For $k = \frac{2n\pi}{d}$ with $n \in \mathbb{N}$, the number k^2 belongs to the spectrum (flat bands).
- Positive bands degenerate to a point at $k = \ell^{-1}$ for $d = \ell\big((-1)^{n+1} + (6n-3)\big)\frac{\pi}{6}$ with $n \in \mathbb{N}$.

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



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- Positive bands degenerate to a point at $k = \ell^{-1}$ for $d = \ell\big((-1)^{n+1} + (6n-3)\big)\frac{\pi}{6}$ with $n \in \mathbb{N}$.
- In the high energy regime, the probability of belonging to the spectrum is $\frac{2}{3}$.

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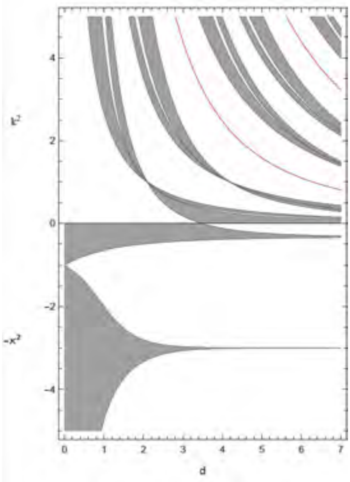

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- In the high energy regime, the probability of belonging to the spectrum is $\frac{2}{3}$.
- The negative spectrum consists of two bands, one negative band in each of the domains $\kappa \in (0, \ell^{-1})$ and (ℓ^{-1}, ∞); there is no flat band.

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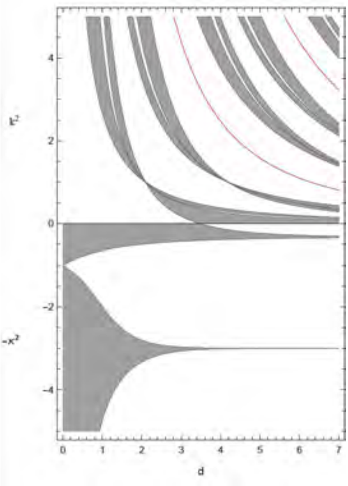

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- The negative spectrum consists of two bands, one negative band in each of the domains $\kappa \in (0, \ell^{-1})$ and (ℓ^{-1}, ∞); there is no flat band.
- For large values of d, the negative bends shrink to the energies $-3\ell^{-2}$ and $-\frac{1}{3}\ell^{-2}$.

Thank you for your attention!