High-Symmetry Materials and Superconductivity

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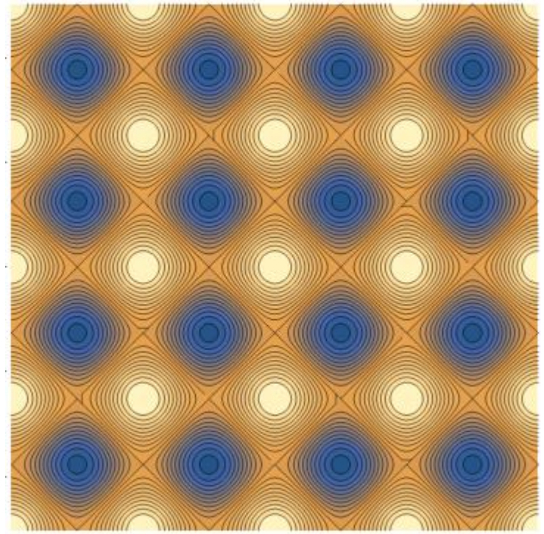
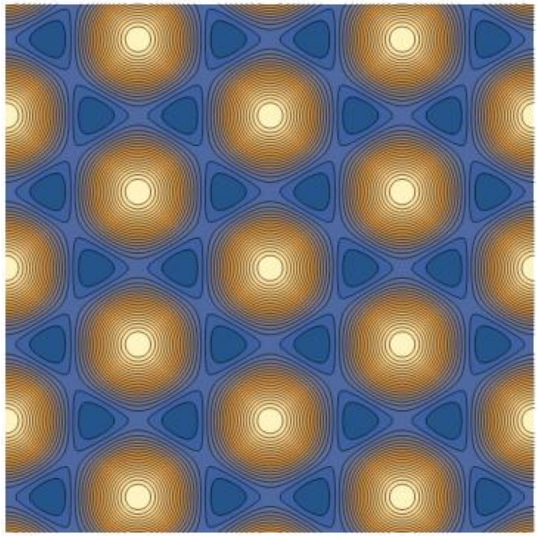
Materials can be Symmetric under rotations

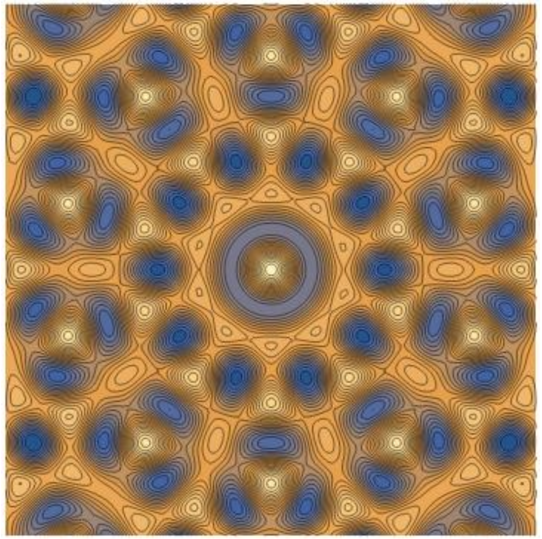
n = 4



n = 6

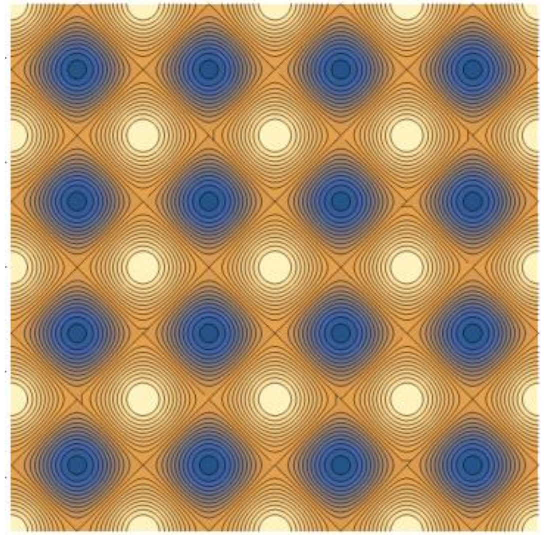


n = 10

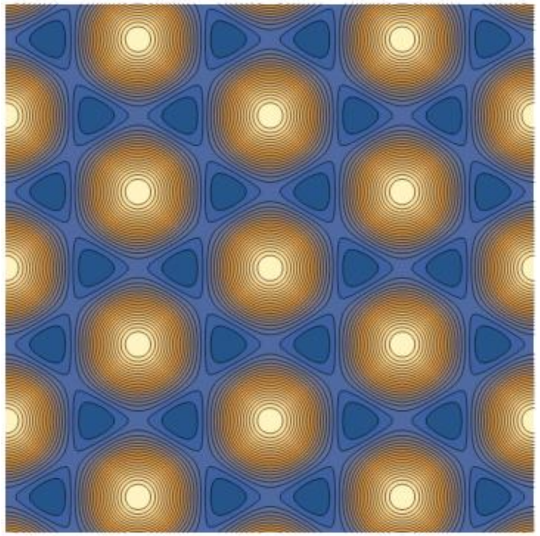


2, 3, and 4, and 6-fold rotationally symmetric materials repeat in space

n = 4

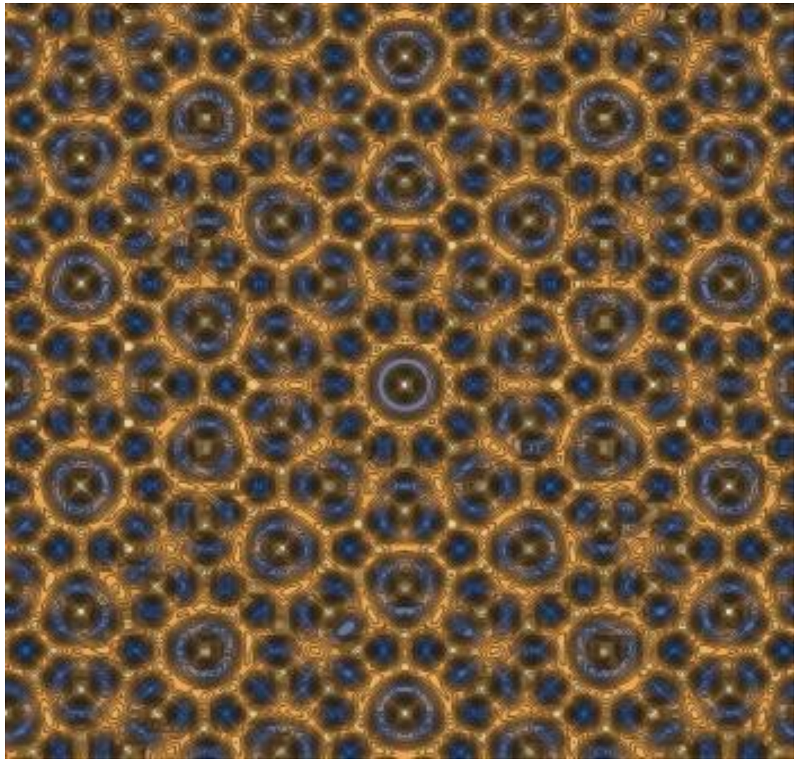


n = 6

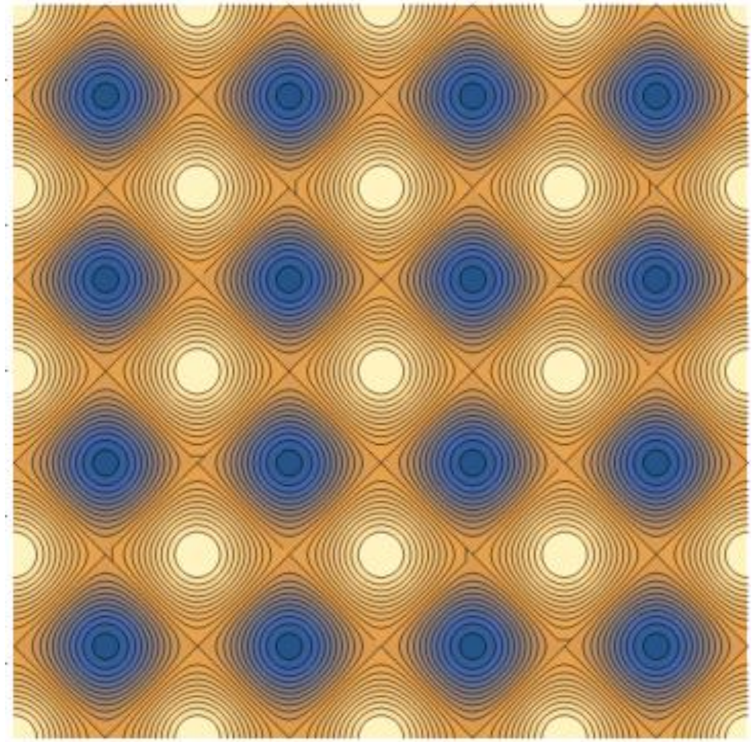


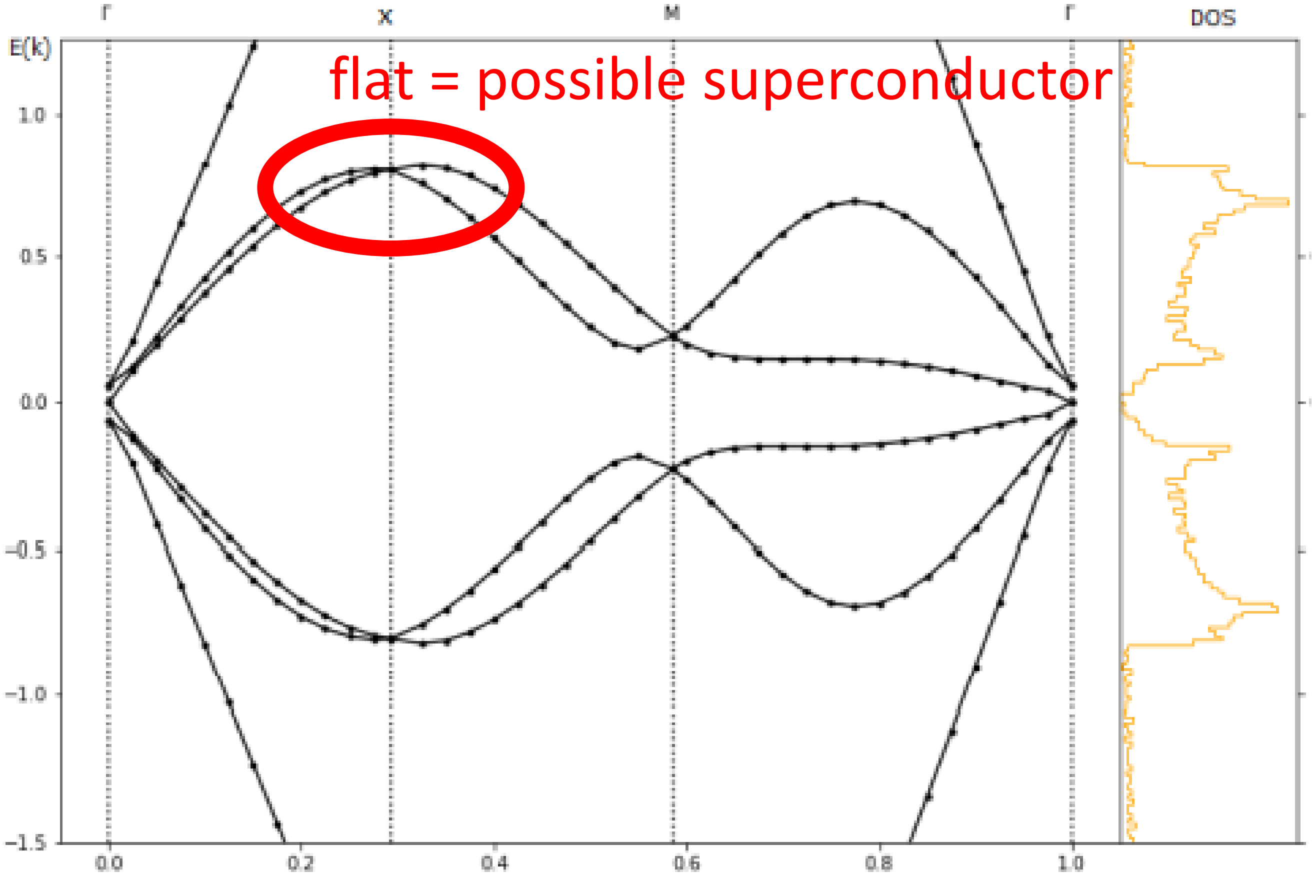
Other symmetries do not repeat in space

n = 10



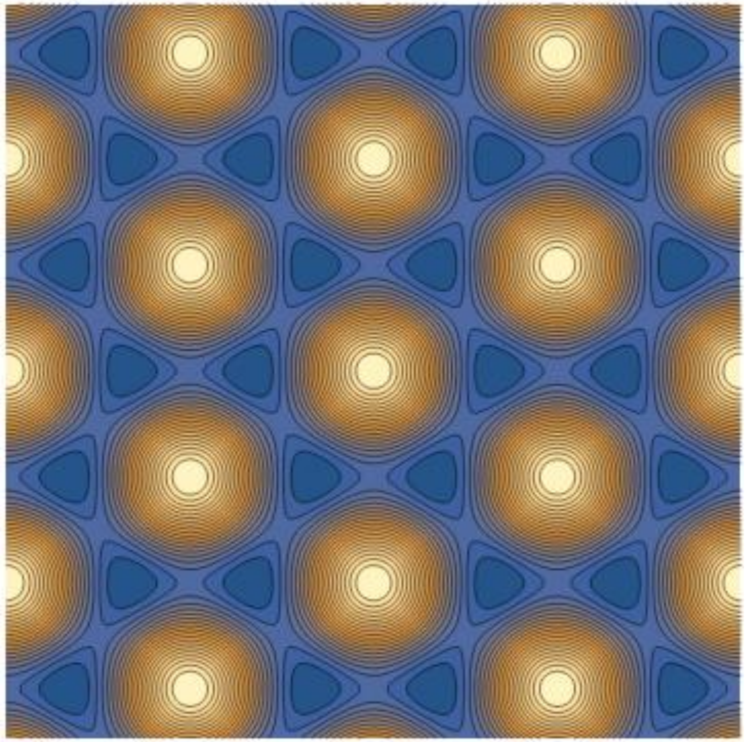
n = 4

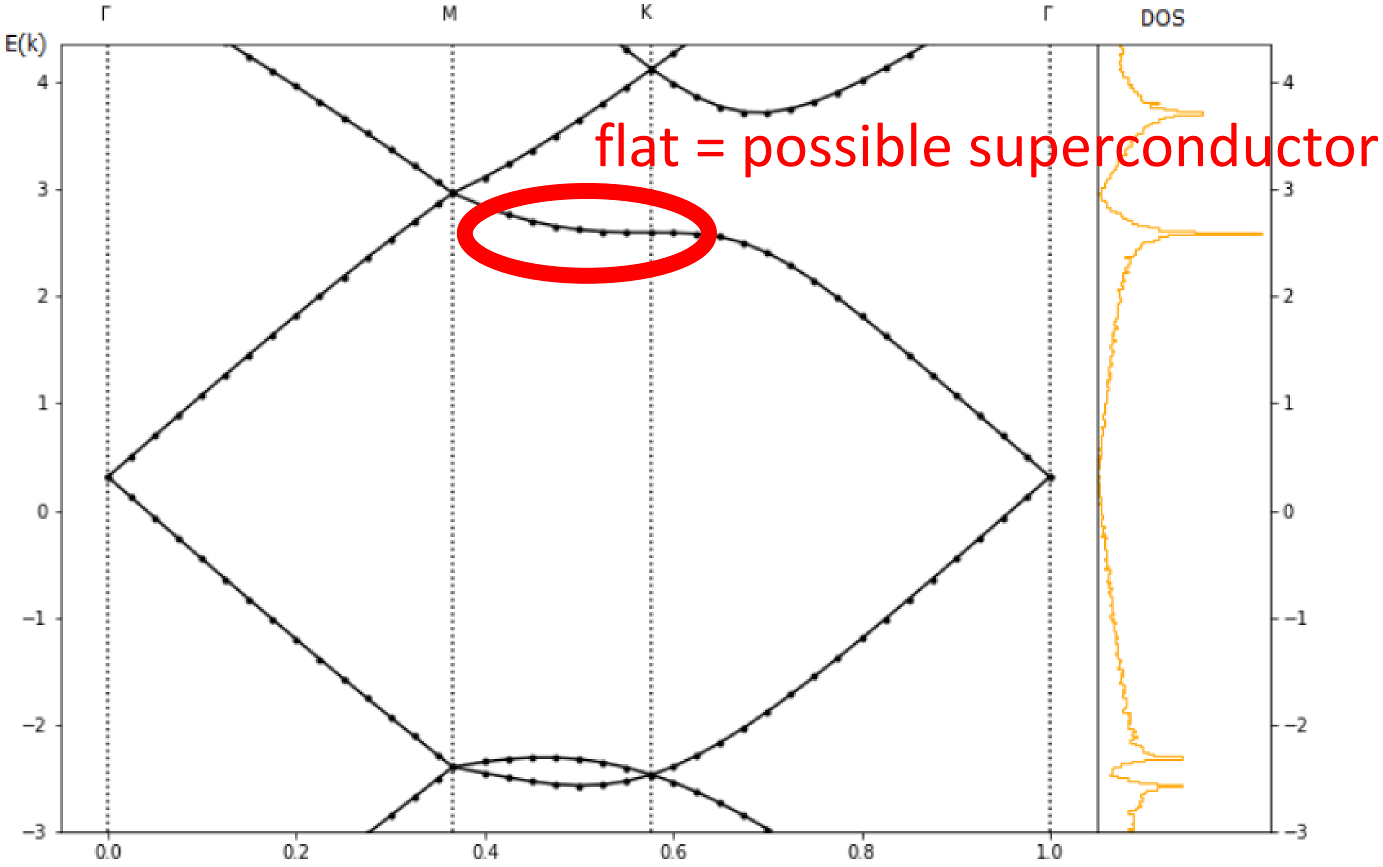




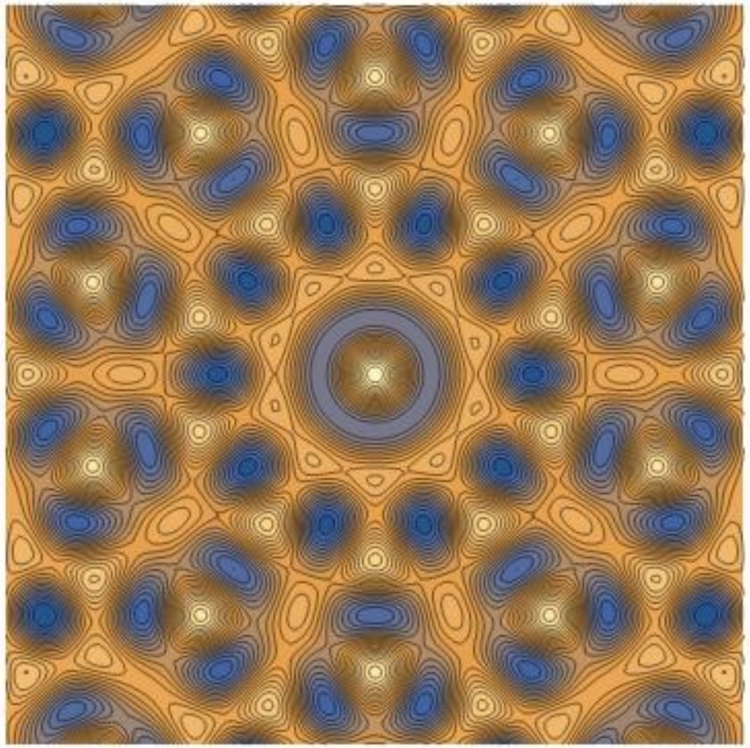
Γ
X
M
Γ
DOS
E(k)
flat = possible superconductor
1.0
0.5
0.0
−0.5
−1.0
−1.5
0.0
0.2
0.4
0.6
0.8
1.0

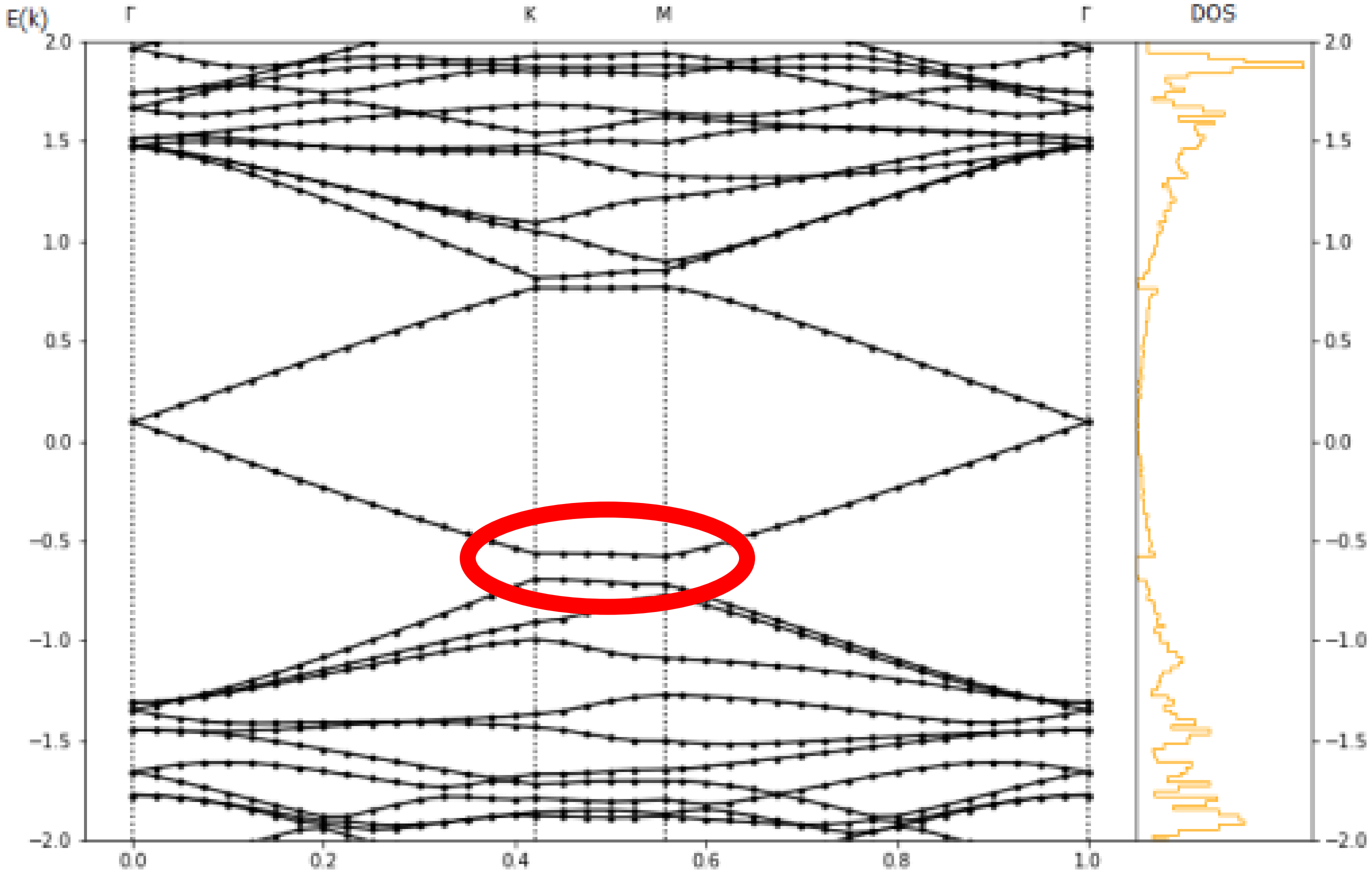
n = 6





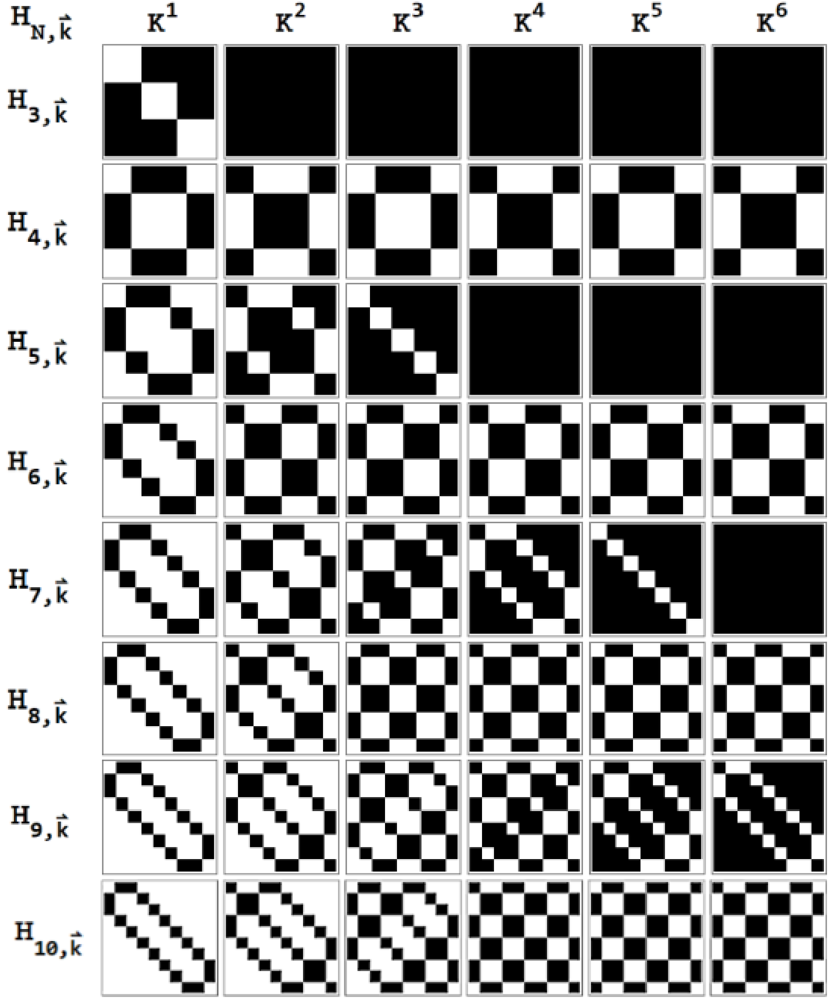
n = 10



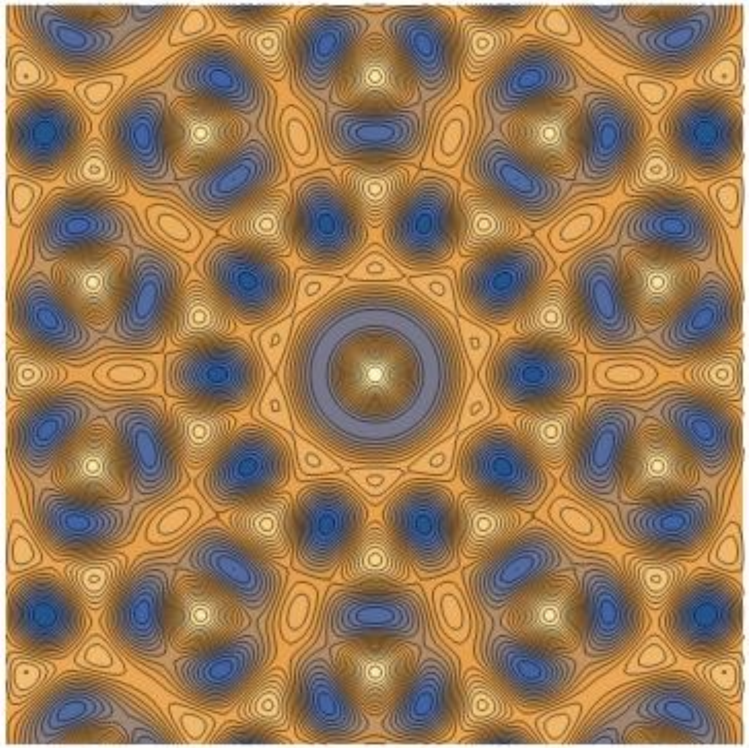


flat, but this computation is invalid, since there's a gap (not allowed by TR symmetry)

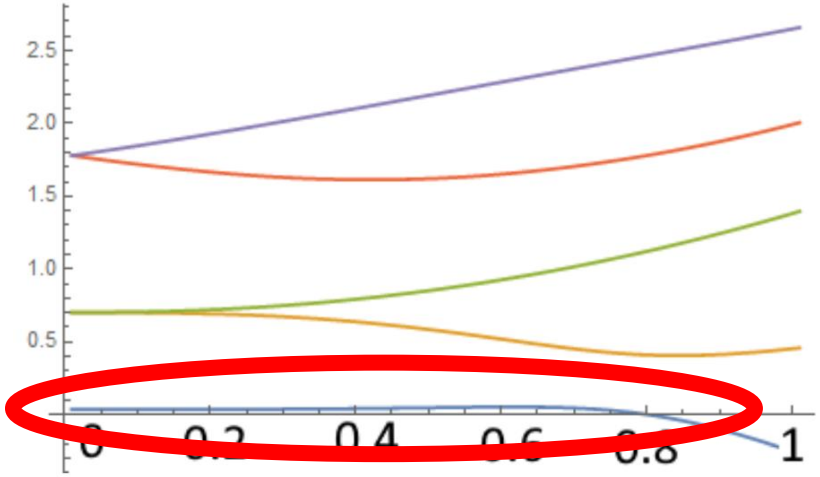
In order to compute the bands accurately, you need to use Perturbation Theory. This is very involved. Here’s a visualizationof the Hamiltonian for n = 6 :



n = 10



Do the analysis with perturbation instead (very involved calculation):



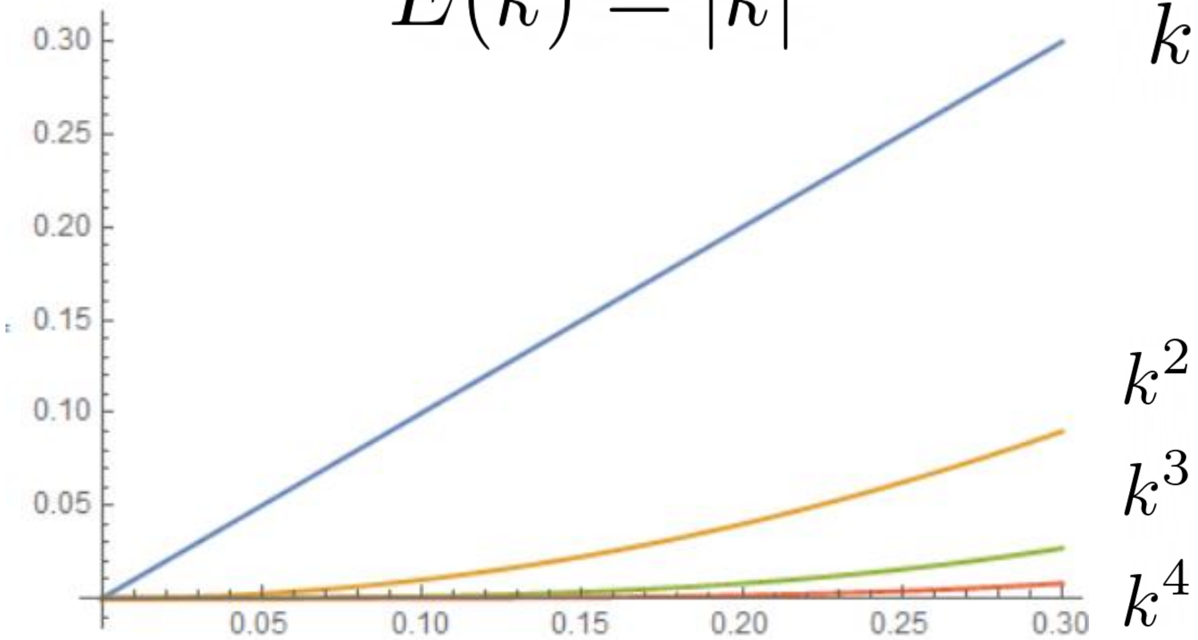
flat = possible superconductor

We found that High-Symmetry Materials can easily be made flat.

I.e. they might be superconductors.

Define flatness using different powers of k

$$E(\vec{k}) = |\vec{k}|^{\nu}$$



density of states in 2D ~ $E^{(2/\nu)-1}$

$\nu = 2$ Van Hove singularity

$\nu > 2$ High order Van Hove singularity

Bands in arbitrary materials have this form:

$$E(\vec{k}) = \Omega_x k_x + \Omega_y k_y + \alpha_{xx} k_x^2 + \alpha_{yy} k_y^2 + \alpha_{xy} k_x k_y + ...$$

Bands in N-Fold Rotationally Symmetric Materials have this form instead:

$$E_N(\vec{k}) = \alpha k^2 + \beta k^4 + \gamma k^6 + ... + \kappa k_x^N + \lambda k_x^{N-1} k_y + ...$$

N-Fold Rotationally Symmetric Materials have fewer terms, so you can more easily tune their parameters to make flat bands:

$$\alpha \to 0$$
$$\beta \to 0$$
$$\cdots$$