Uncertainty Principle of Homogenization and Dispersion Relations near Higher-Order Gamma-Point Frequencies

Vadim A Markel

University of Pennsylvania (2003-present)

and University of Aix-Marseille (2015-2017)

joint work with

Igor Tsukerman

University of Akron

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A Historical Motivation

V.A.Markel, Correct definition of the Poynting vector in electrically and magnetically polarizable medium reveals that negative refraction is impossible
Opt. Expr. **16**, 19152 (2008)

Comment: R.Marques, *Opt. Expr.* **17**, 7322 (2009).
Reply: *Opt. Expr.* **17**, 7325 (2009)

Comment: A.Favaro, P.Kinsler and M.W.McCall , *Opt. Expr.* **17**, 15167 (2009).
Reply: *Opt. Expr.* **17**, 15170 (2009)

Comment: V.A.Markel, *J. Mod. Opt.* **57**, 2098 (2010)
Reply: M.W.McCall, P.Kinsler, A.Favaro, *J. Mod. Opt.* **57**, 2103 (2010)
Rejoinder: V.A.Markel, *J. Mod. Opt.* **57**, 2109 (2010)

Heating Rate in Material Media (Stationary Fields)

$q = \langle \mathbf{J} \cdot \mathbf{E} \rangle_{\text{time}}$ - Heating rate (per unit volum per unite time)

$\mathbf{J} = \partial \mathbf{P} / \partial t + \mathrm{c} \nabla \times \mathbf{M}$ - Total induced current created by all charges associated with the medium, including conductivity current.

There are no external or "free" currents overlapping with the medium

Heating rate is the "systematic influx of energy (per unit time per unit volume) from external sources of radiation."

LL, VIII

A) Non-Magnetic Medium

$$\mathbf{J} = \partial \mathbf{P} / \partial t$$

$$\mathbf{E}(\mathbf{r},t) = \mathrm{Re}[\mathbf{E}_\omega(\mathbf{r})e^{-i\omega t}]$$

$$\mathbf{P}(\mathbf{r},t) = \mathrm{Re}[\mathbf{P}_\omega(\mathbf{r})e^{-i\omega t}]$$

$$\mathbf{J}(\mathbf{r},t) = \mathrm{Re}[\mathbf{J}_\omega(\mathbf{r})e^{-i\omega t}]$$

$$\mathbf{P}_\omega(\mathbf{r}) = \frac{\varepsilon_\omega - 1}{4\pi}\mathbf{E}_\omega(\mathbf{r}) \; ; \; \mathbf{J}_\omega(\mathbf{r}) = -i\omega \mathbf{P}_\omega(\mathbf{r})$$

$$q = \frac{1}{2}\mathrm{Re}[\mathbf{J}_\omega^* \cdot \mathbf{E}_\omega] = \frac{\omega}{8\pi}\left|\mathbf{E}_\omega\right|^2 \mathrm{Im}(\varepsilon_\omega)$$

The conventional result

B) Magnetic Medium (The Volume Term)

(i) $\mathbf{r} \in V \ , \quad \nabla \mu_\omega = 0$

$$\mathbf{J} = \partial \mathbf{P} / \partial t + c \nabla \times \mathbf{M}$$

$$\mathbf{J}_\omega = -i\omega \frac{\varepsilon_\omega - 1}{4\pi} \mathbf{E}_\omega + c \nabla \times \frac{\mu_\omega - 1}{4\pi} \mathbf{H}_\omega$$

$$\mathbf{J}_\omega = -i\omega \frac{\varepsilon_\omega - 1}{4\pi} \mathbf{E}_\omega + c \frac{\mu_\omega - 1}{4\pi} \nabla \times \mathbf{H}_\omega$$

$$\nabla \times \mathbf{H}_\omega = -i \frac{\omega}{c} \mathbf{D}_\omega = -i \frac{\omega}{c} \varepsilon_\omega \mathbf{E}_\omega$$

$$\mathbf{J}_\omega = \frac{\omega}{4\pi i} \left[\mu_\omega \varepsilon_\omega - 1 \right] \mathbf{E}_\omega$$

$$q_V = \frac{\omega \left| \mathbf{E}_\omega \right|^2}{8\pi} \operatorname{Im}\left[\mu_\omega \varepsilon_\omega \right]$$

This is different from the conventional result

B) Magnetic Medium (The Surface Term)

$$\text{(ii)}\quad \mathbf{r} \in S = \partial V \ , \quad \nabla \mu_\omega(\mathbf{r}) = (\mu_\omega - 1)\hat{\mathbf{n}}_{\mathbf{R}}\,\delta\left(\hat{\mathbf{n}}_{\mathbf{R}} \cdot (\mathbf{r} - \mathbf{R})\right)$$

R - point on the surface

$\hat{\mathbf{n}}_{\mathbf{R}}$ - outward unit normal drawn at point **R**

$$q_S(\mathbf{R}) = \frac{\omega}{8\pi}\mathrm{Re}\left[\left(1 - \mu_\omega\right)\left(\mathbf{H}_\omega \times \mathbf{E}_\omega^*\right)\cdot \hat{\mathbf{n}}_{\mathbf{R}}\right]$$

$$Q = \underbrace{\int_V q_V(\mathbf{r})\,d^3 r}_{} + \underbrace{\int_{\partial V} q_s(\mathbf{R})\,d^2 R}_{}$$

$$= \quad Q_V \quad + \quad Q_S$$

(total heat absorbed by the body per unit time)

A Comparison of Results

The conventional result

$$q_{\text{conv}} = \frac{\omega}{8\pi}\left[\left|\mathbf{E}_\omega\right|^2 \varepsilon''_\omega + \left|\mathbf{H}_\omega\right|^2 \mu''_\omega\right]$$

$$Q_{\text{conv}} = \int q_{\text{conv}}\left(\mathbf{r}\right)d^3r \qquad \text{(volume term only)}$$

My result

$$q_{\text{my}}^{(V)} = \frac{\omega\left|\mathbf{E}_\omega\right|^2}{8\pi}\operatorname{Im}\left[\mu_\omega\varepsilon_\omega\right]$$

$$q_{\text{my}}^{(S)}\left(\mathbf{R}\right) = \frac{\omega}{8\pi}\operatorname{Re}\left[\left(1-\mu_\omega\right)\left(\mathbf{H}_\omega \times \mathbf{E}_\omega^*\right)\cdot\hat{\mathbf{n}}_{\mathbf{R}}\right]$$

$$Q_{\text{my}} = \int q_{\text{my}}^{(V)}(\mathbf{r})d^3r + \int q_{\text{my}}^{(S)}\left(\mathbf{R}\right)d^2R$$

It can be shown that

$$Q_{\text{my}} = Q_{\text{conv}}$$

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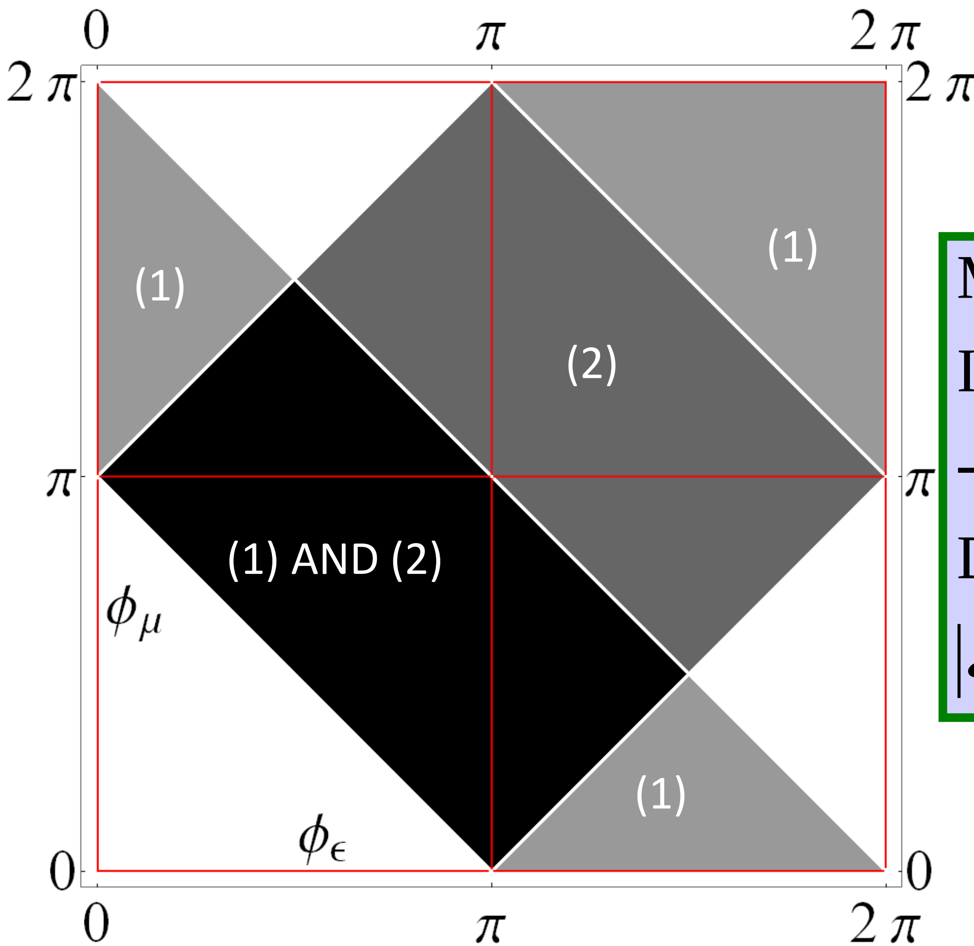
but

$$q_{\text{my}} \neq q_{\text{conv}}$$

Objections

1. The definition of NR is wrong. Use Depine-Lakhtakia definition.
2. My expressions violate energy conservation.
3. Low or zero-frequency apparent counter-examples.
4. Magnetic field can also do work, e.g., on magnetic moments. Otherwise, how do you explain ….” [choose your example]
5. The electric and magnetic currents are different in physical origin and the same laws of motion can not be applied to them.
6. NR is really obtained as the result of homogenization, and the fields vary strongly inside the sample. The quadratic combinations used in the derivation are not applicable. [A variant: A Composite material can be describable by local effective medium parameters while the fields inside strongly fluctuate.]



My condition:

$\mathrm{Im}(\varepsilon\mu)<0$ (1)

Depine-Lakhtakia

$|\varepsilon|\mathrm{Re}(\mu)+|\mu|\mathrm{Re}(\varepsilon)<0$ (2)

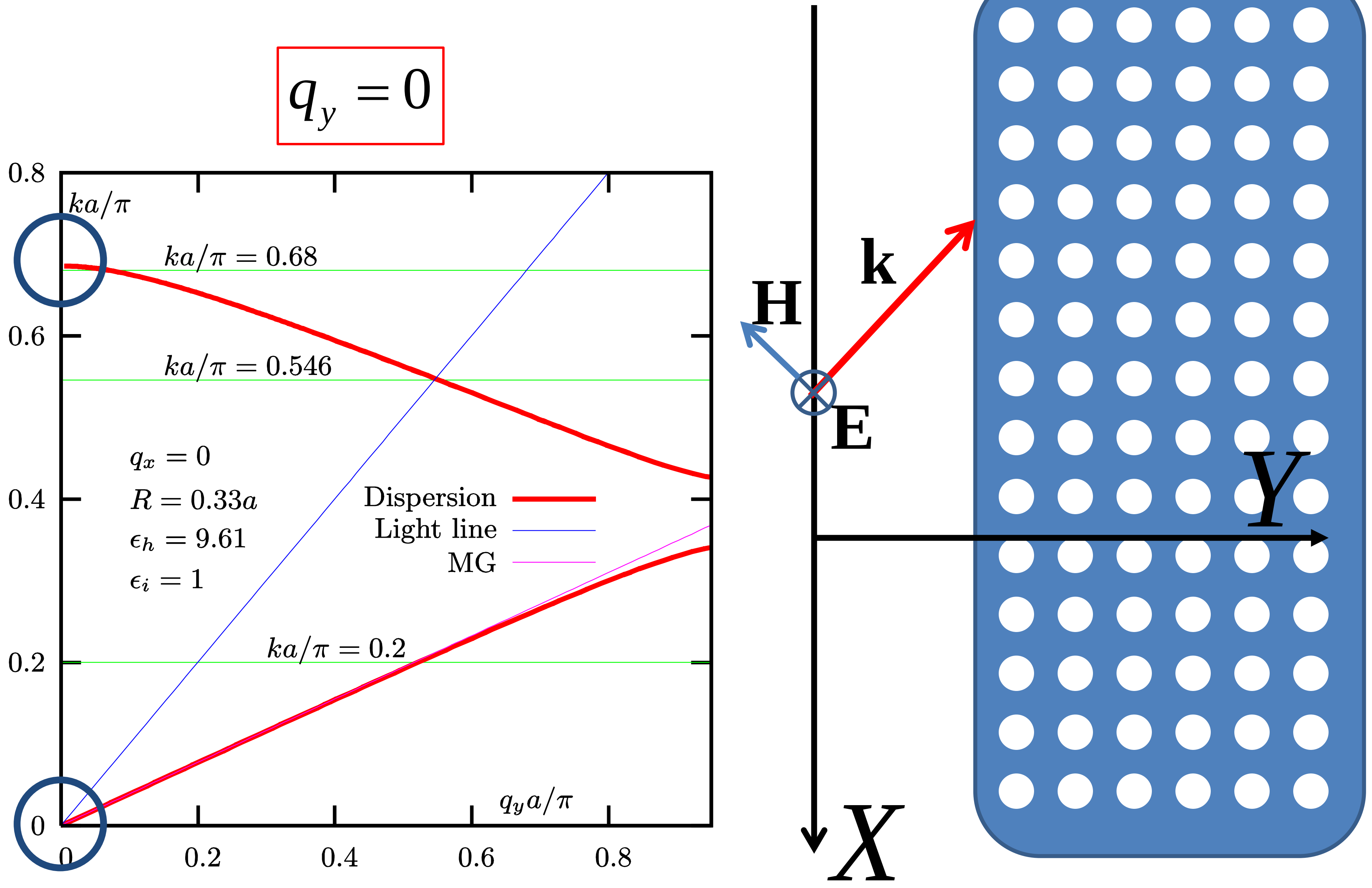
Are Photonic Crystals Homogenizable in Higher Bands?

Necessary condition: The dispersion relation in a photonic crystal should mimic that In a homogeneous material (we do not consider nonlocality).

This can be possible near the Γ-point frequencies

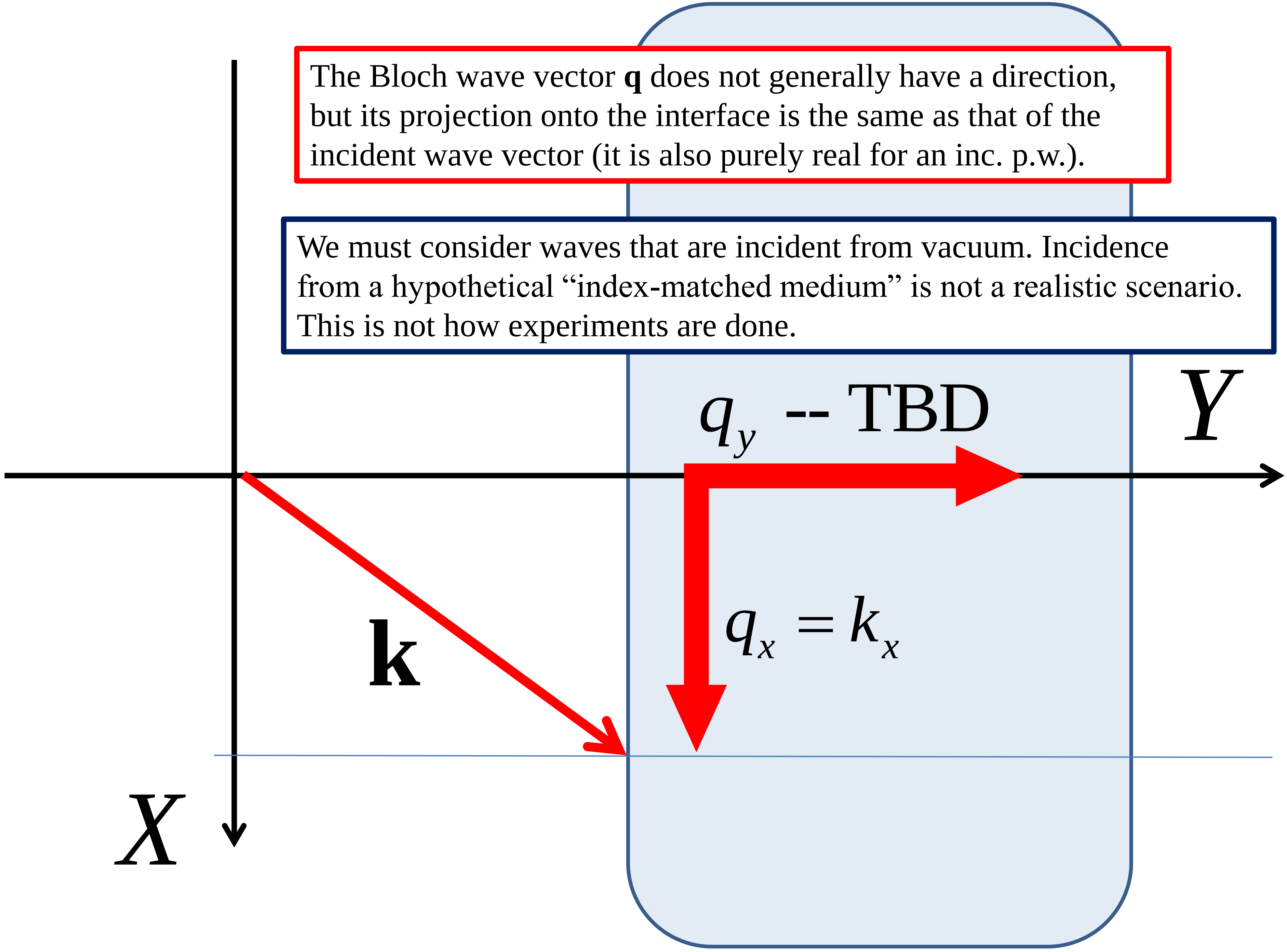
Long Bloch wavelengths $\Rightarrow$ a quasi-homogeneous medium

Example 1: 2D Cubic lattice, s-pol

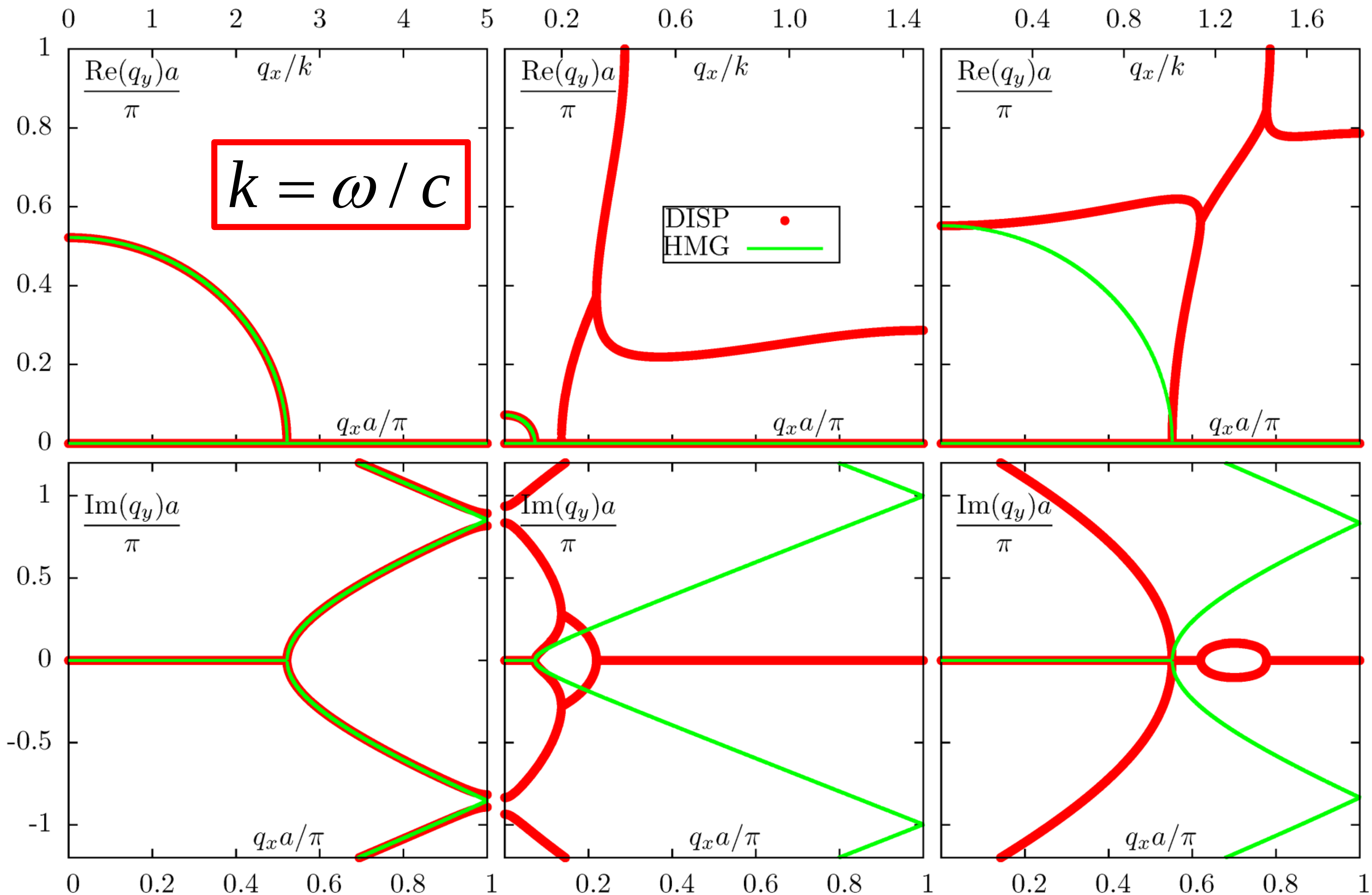


The Bloch wave vector **q** does not generally have a direction, but its projection onto the interface is the same as that of the incident wave vector (it is also purely real for an inc. p.w.).

We must consider waves that are incident from vacuum. Incidence from a hypothetical "index-matched medium" is not a realistic scenario. This is not how experiments are done.

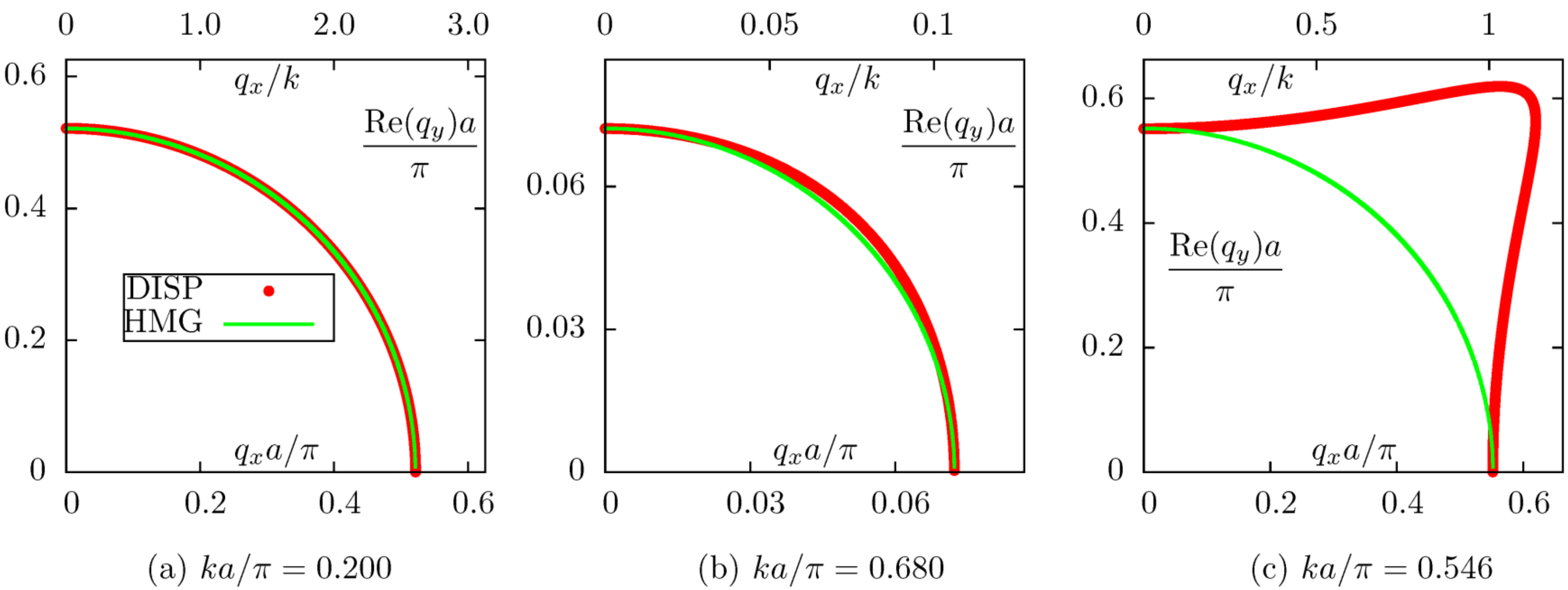


COMPLEX ISOFREQUENCY LINES AT DIFFERENT FREQUENCIES (SQUARE LATTICE)



(a) $ka/\pi = 0.200$ (b) $ka/\pi = 0.680$ (c) $ka/\pi = 0.546$

"CIRCULAR" PART (THE FIRST LOBE) OF THE ISOFREQUENCY LINE



First band; conventional (MG) homogenization theory is valid:

Perfect match to a circle.

The "circular" part of the iso-frequency line extends well into incident evanescent waves.

Truly "all-angle" effective refractive index (in fact, see next slide, it's even better!).

Second band; very close to 2^{nd} Γ-point frequency.

Visually looks like a circle, but the match is not perfect (and see the next slide, it's even worse!)

The circular part extends only to q_x/k~0.1 (max inc. angle 6deg).

Very far from being "all-angle".

Second band at the intersection with the light line. This is the frequency at which one would expect *n*~ -1.

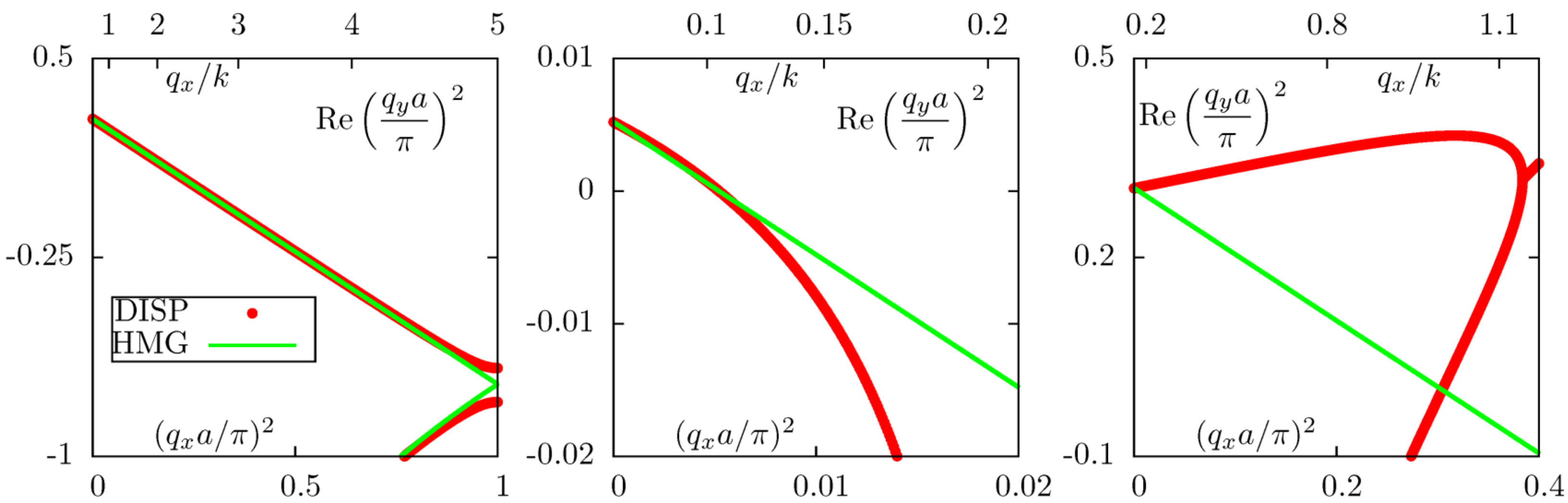
Forget about it….

In the case of "isotropic" effective material parameters, we expect

$$q_y^2 = \varepsilon_{\mathrm{eff}} \mu_{\mathrm{eff}} k^2 - q_x^2$$

Therefore, for a fixed k, q_y^2 should be a linear function of q_x^2 .

Lets check this....



(a) $ka/\pi = 0.200$ (b) $ka/\pi = 0.680$ (c) $ka/\pi = 0.546$

(a) The above observation is applicable up to fairly large ratios q_x/k .

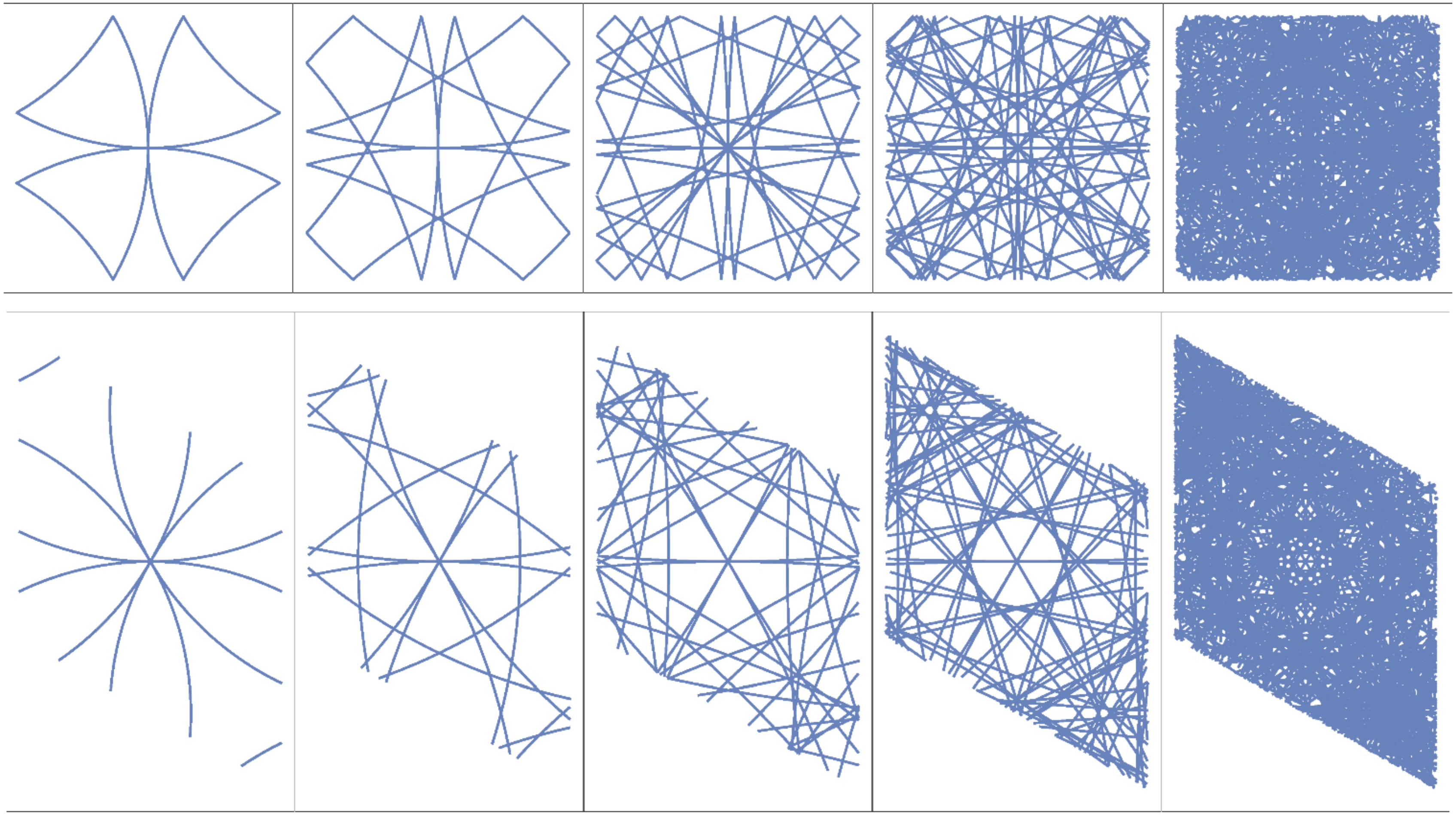
(The red dots in the lower-right corner are the higher-order imaginary wave numbers)

(b) Second band; very close to 2nd Γ-point.

The linear dependence is not perfect and breaks down very fast.

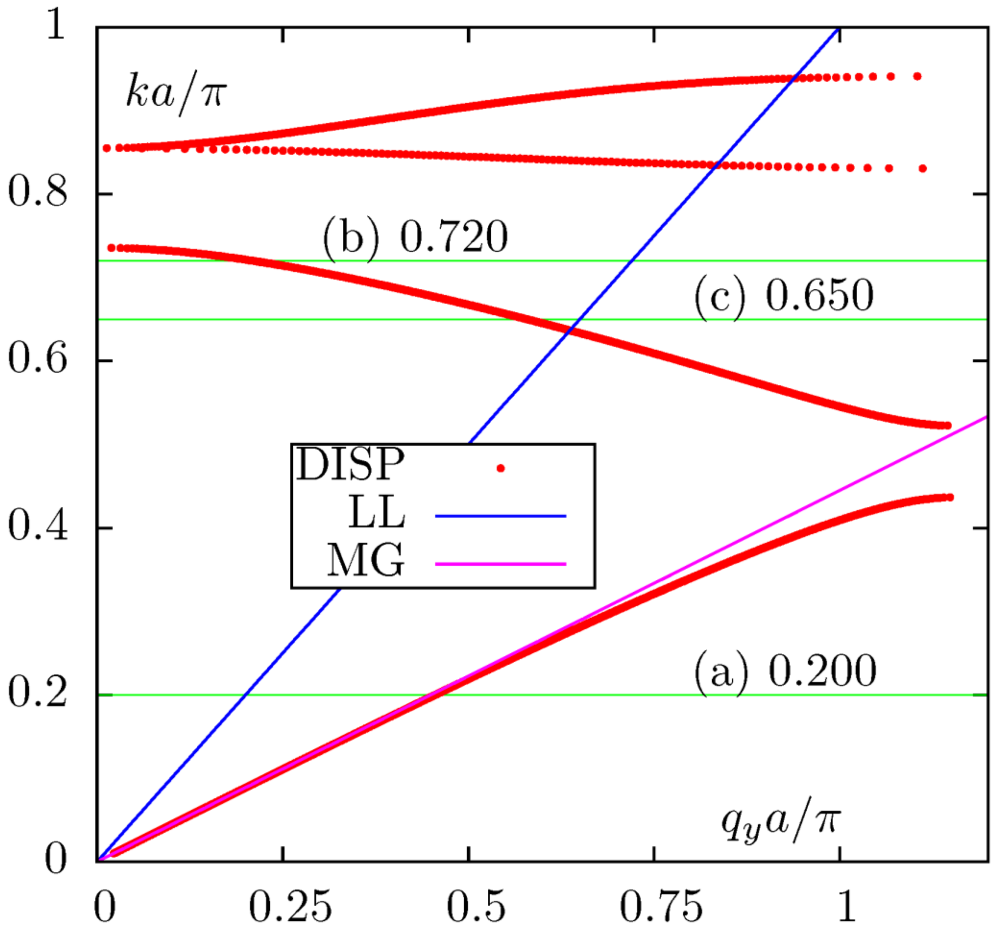
Effective parameters are very far from being “all-angle”.

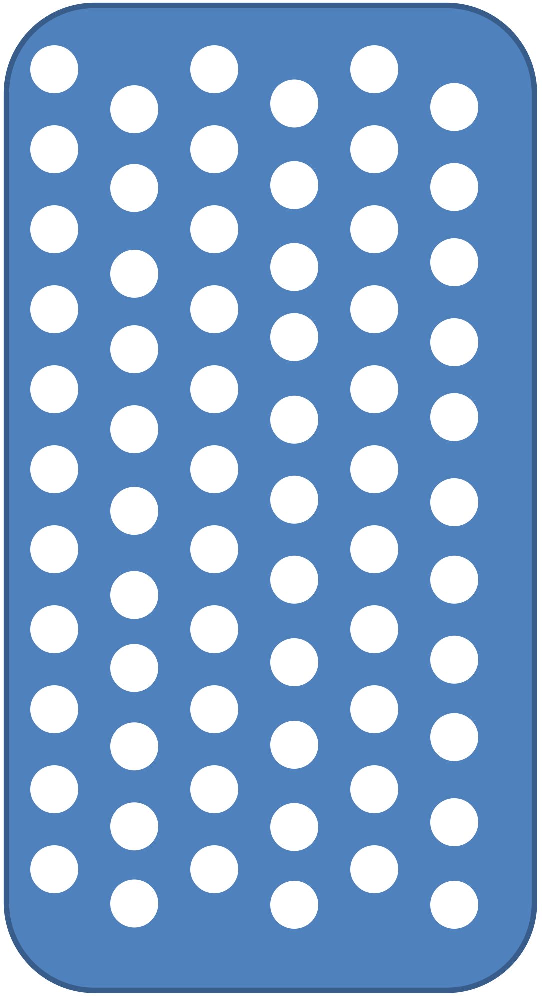
Isofrequency lines of an artificially folded homogeneous medium. No higher-order Gamma-point frequencies.



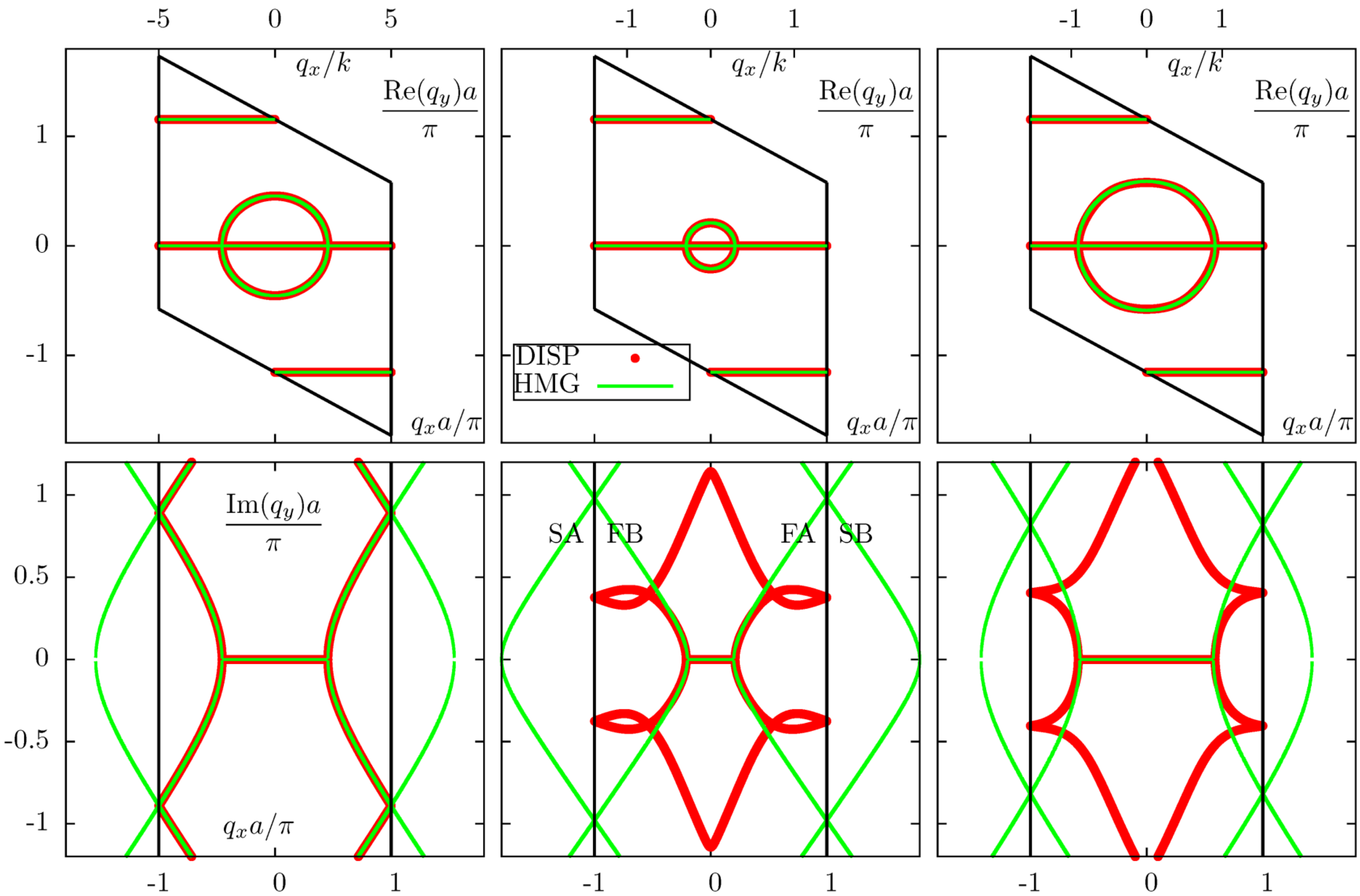
(a) $n = 1$ (b) $n = 2$ (c) $n = 5$ (c) $n = 10$ (d) $n = 50$

Example 2: 2D triangular lattice, s-pol



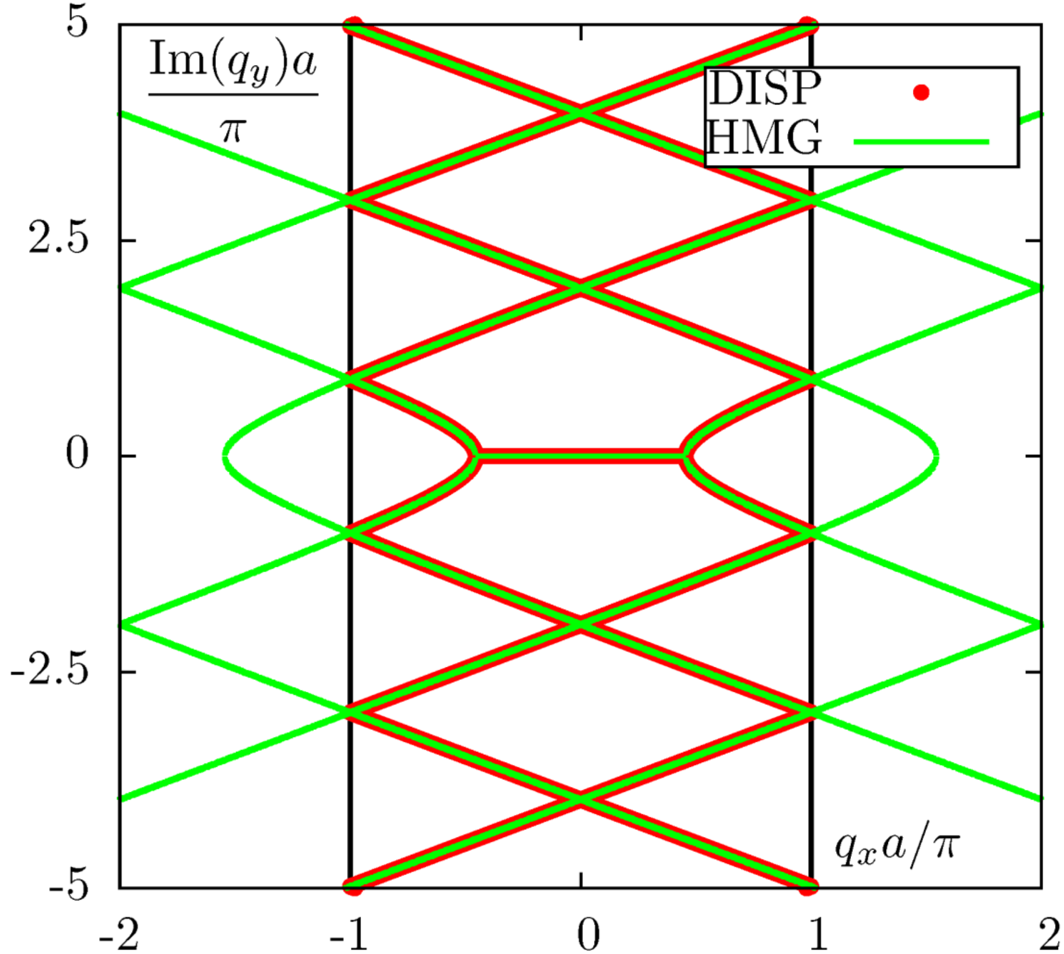


COMPLEX ISOFREQUENCY LINES AT DIFFERENT FREQUENCIES (TRIANGULAR LATTICE)

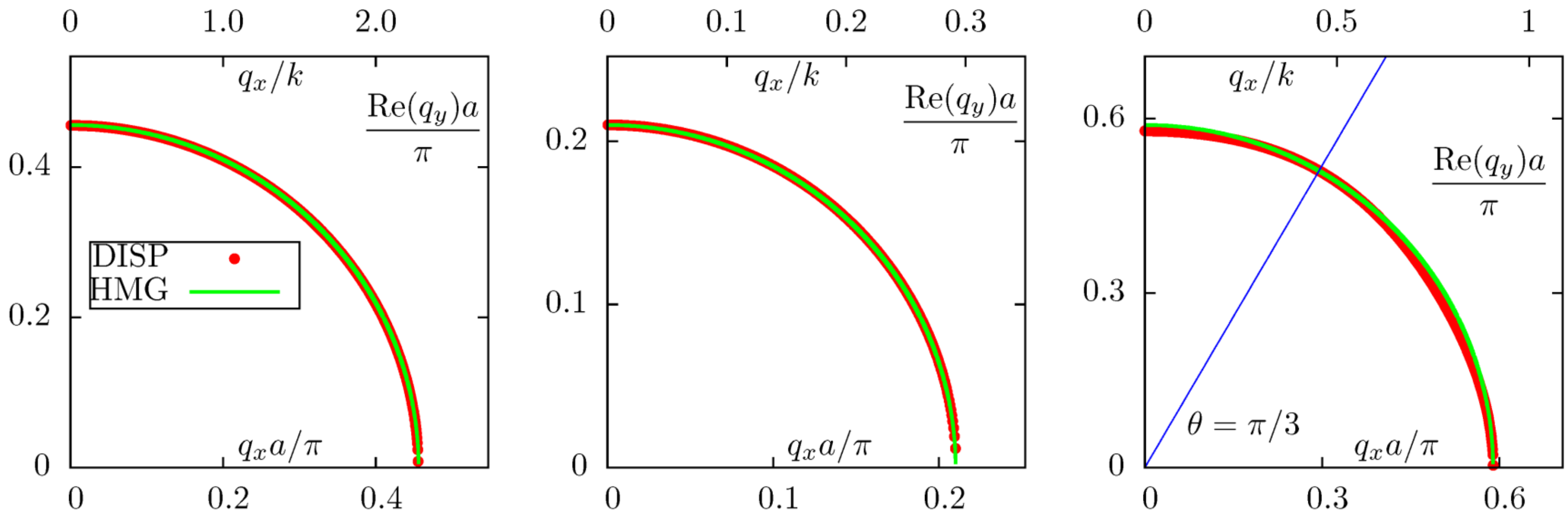


(a) $ka/\pi = 0.200$ (b) $ka/\pi = 0.720$ (c) $ka/\pi = 0.650$

EXPANDED VIEW FOR $ka = 0.2$

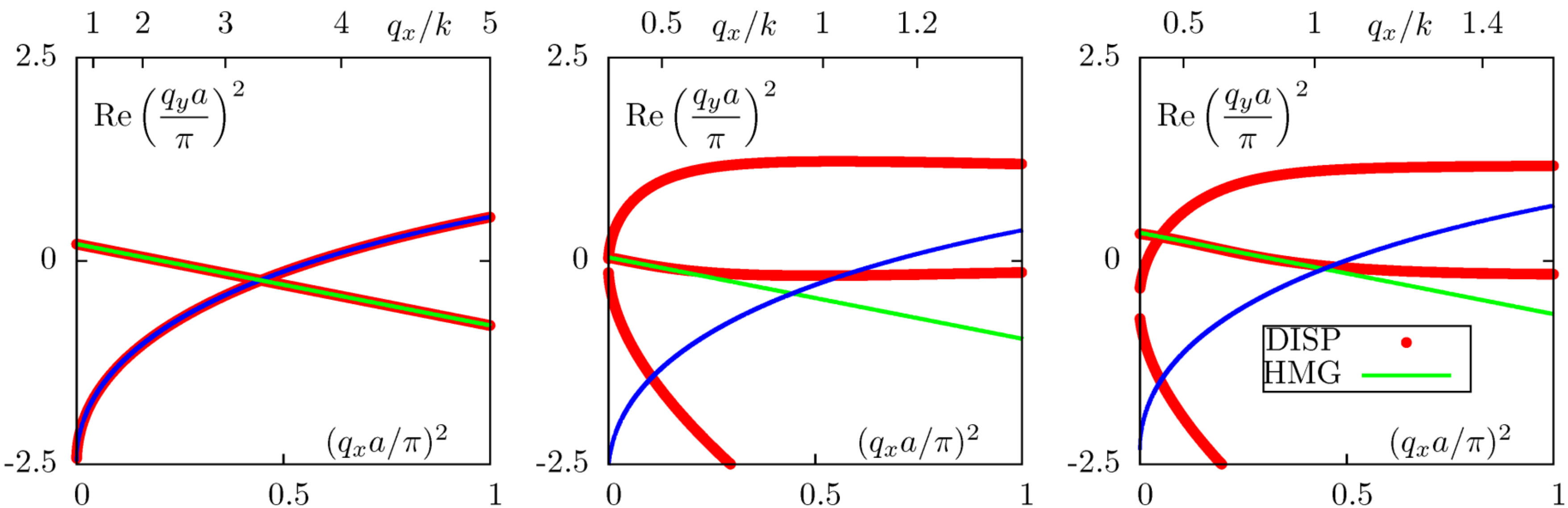


EXPANDED VIEW OF THE QUASI-CIRCULAR SEGMENTS



(a) $ka/\pi = 0.200$ (b) $ka/\pi = 0.720$ (c) $ka/\pi = 0.65$

SQUARES



(a) $ka/\pi = 0.200$ (b) $ka/\pi = 0.720$ (c) $ka/\pi = 0.650$

THEORETICAL EXPLANATION

The basic idea has been published by Pokrovsky and Efros in 2002:

A.L. Pokrovsky and A.L. Efros, Solid State Commun. **124**, 283 (2002).

It can be shown that the dispersion equation of an arbitrary photonic crystal can be written in the following form [1,2]:

$q^2 \equiv \mathbf{q} \cdot \mathbf{q} = k^2 \Sigma(k, \mathbf{q})$

$k = \dfrac{\omega}{c}$ -- free space wave number

$\mathbf{q}$ -- Bloch wave vector

$\Sigma(k, \mathbf{q})$ -- can be computed by matrix inversion for each pair $(k, \mathbf{q})$ given the geometry and composition of the PC

Near a Γ-point frequency, q^2 is small and we can expand $\Sigma(k, \mathbf{q})$ in powers of $\mathbf{q}$:

$$\Sigma(k, \mathbf{q}) = \Sigma_0 + \Sigma_2 \frac{q^2}{k^2} + \dots \quad \text{(for PCs with a center of symmetry } \Sigma_1 = \Sigma_3 = \dots = 0\text{)}$$

Then, by keeping only second-order terms, we obtain: $q^2 = \dfrac{\Sigma_0}{1 - \Sigma_2} k^2$

It can be seen that the index of refraction is ***isotropic***, that is, independent of the direction of **q**. Keeping only second-order terms in the above expansion IS NOT ESSENTIAL for arriving at this conclusion.

[1] V.A.Markel and J.C.Schotland, Homogenization of Maxwell's equations in periodic composites: Boundary effects and dispersion relations, ***PRE*** **85, 066603 (2012).**
[2] V.A.Markel and I.Tsukerman, Current-driven homogenization and effective medium parameters for finite samples ***PRB*** **88, 125131 (2013) .**

Assuming the approach of the previous slide is correct,

we have the isotropic dispersion of the form $q^2 = \frac{\Sigma_0}{1-\Sigma_2} k^2$.

It is typical to make the association:

$$\varepsilon = \Sigma_0 \quad , \qquad \mu = \frac{1}{1-\Sigma_2} \quad , \; n^2 = \varepsilon\mu = \frac{\Sigma_0}{1-\Sigma_2}$$

We do not discuss here the validity of this approach (what about boundary conditions, etc.?)

But is the conclusion about the isotropy of the refractive index near the higher Γ-point frequencies correct? Was the expansion valid? The answer is **NO**. And here is why.

The statement that q^2 is small is not equivalent to the satement that its Cartesian components are small.

Example:

$$q_x = A \, , \quad q_y = iA \, , \quad q^2 = q_x^2 + q_y^2 = 0 \, , \qquad A \to 0$$

We must consider more general vectors **q**, which do not necessarily have a well-defined direction. In fact, this consideration is absolutely essential if we want to assign a PC an index of refraction in the traditional sense, that is, applicable to a sufficiently broad range of illuminating conditions.

The expansion $\Sigma(k,\mathbf{q}) = \Sigma_0 + \Sigma_2\left(\frac{q}{k}\right)^2 + \Sigma_4\left(\frac{q}{k}\right)^4 \ldots$

is incorrect (or incomplete). It should contain individual Cartesian components of $\mathbf{q}$, which are not small near the 2nd (and higher) Γ-point frequencies.

SQUARE LATTICES: The lowest-order term that does not obey circular symmetry is

$$\text{Const} \times (ka)^4 \frac{q_x^2 q_y^2}{k^4}$$

Here Const is a dimensionless constant of the order of unity, which depends on the PC geometry and composition.

When we consider different incident angles, the ratios $\frac{q_x}{k}$ and $\frac{q_y}{k}$ are not necessarily small. So the non-circularly symmetric terms give a huge contribution.

However, near the first Γ-point frequency, the factor $(ka)^4$ is very small, so the non-symmetric terms do not spoil homogenization...

Near the 2nd (and higher) Γ-point frequencies, this is no longer so.

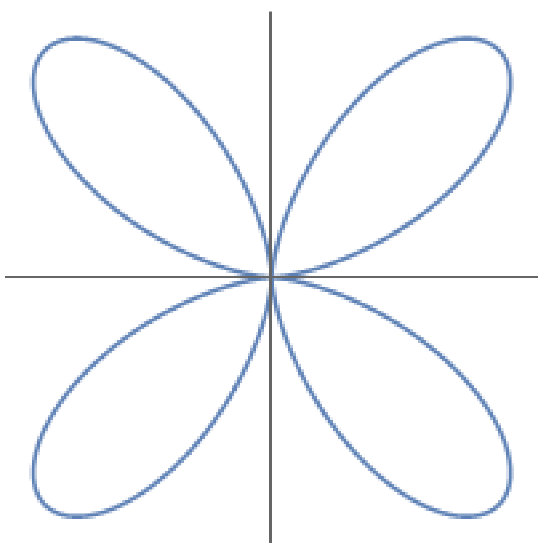
A complete diagramatic perturbation theory for Σ can be built... but this will only be useful to compute some dimensionless constants.

TRIANGULAR LATTICES: The lowest-order terms that do not obey circular symmetry are

$$\mathrm{Const}\ \times (ka)^6 \frac{q_x^2(q_x^4 - 6q_x^2 q_y^2 + 9q_y^4)}{k^6}$$

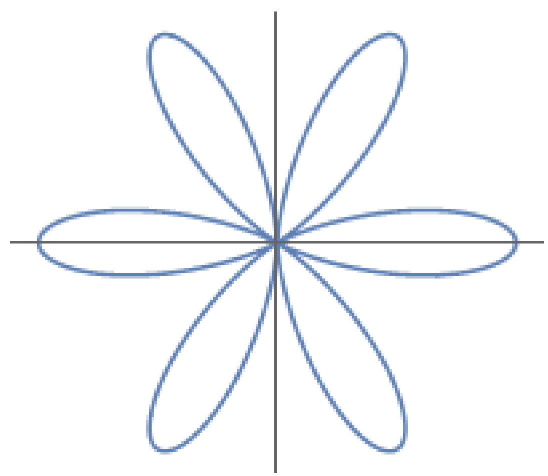
$$\mathrm{Const}\ \times (ka)^6 \frac{q_y^2(q_y^4 - 6q_x^2 q_y^2 + 9q_x^4)}{k^6}$$

Here Const is a dimensionless constant of the order of unity, which depends on the PC geometry and composition.



Square Lattice

Square Lattice



Triangular Lattice

Conclusions

- Nontrivial magnetic response of periodic structures composed of intrinsically nonmagnetic constituents has limitations and is subject to an "uncertainty principle".
- Namely, the stronger the magnetic response, the less accurate ("certain") predictions of the effective medium theory are.
- In practice, there is still room for engineering design, but the trade-offs between magnetic response and the accuracy of homogenization should be noted.

Conclusion (The Uncertainty Principle)

- For any homogenization theory, the more the predicted magnetic permeability deviates from unity, the less