Light in honeycomb atomic lattice

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Who am I ?

Phd student working with **Sergey Skipetrov**:

In Grenoble at LPMMC:

Overview of the system

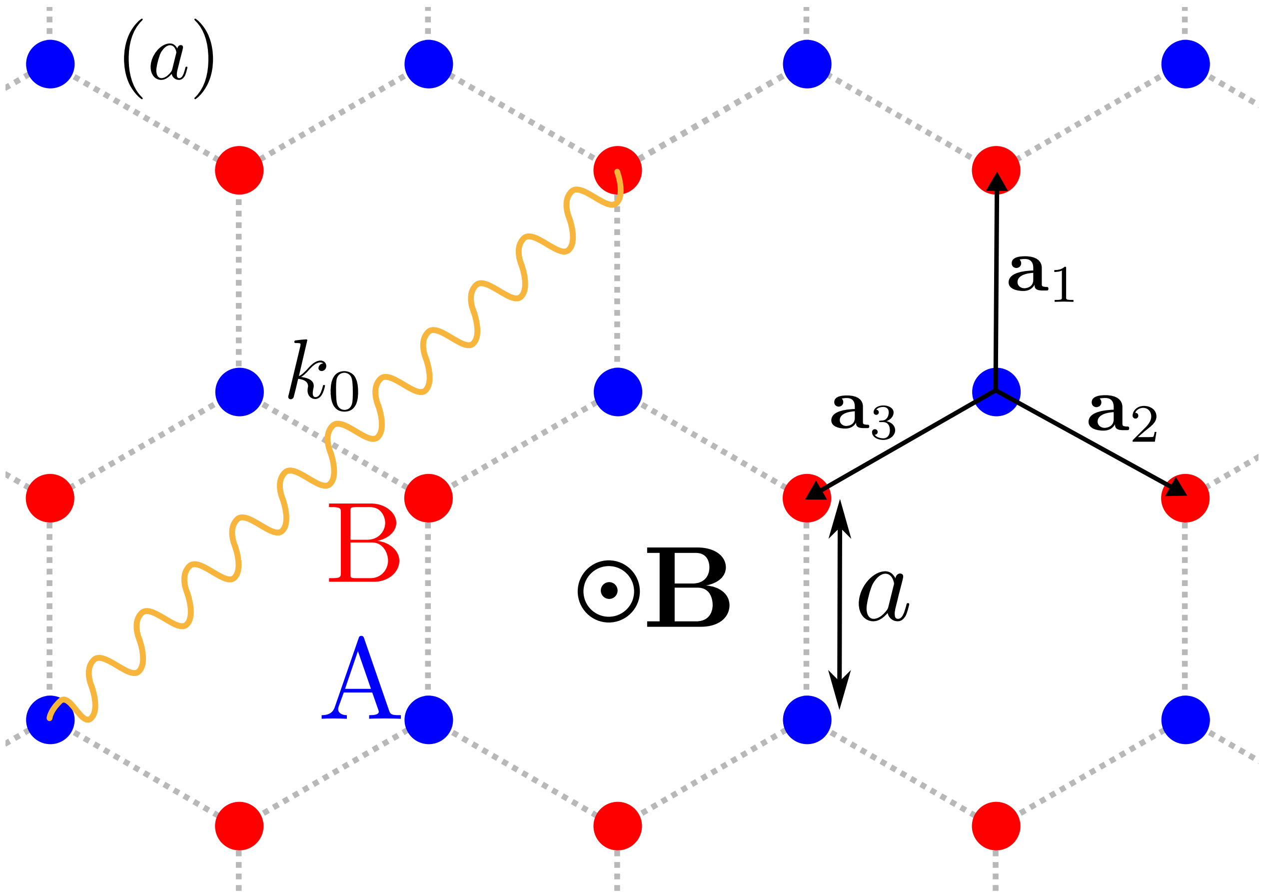


Figure 1.

Gaps into honeycomb lattice

- No nearest-neighbour model
- No crystal (no “bonds” between sites)
- Sites B and magnetic field $\mathbf{B}$ are two unrelated things

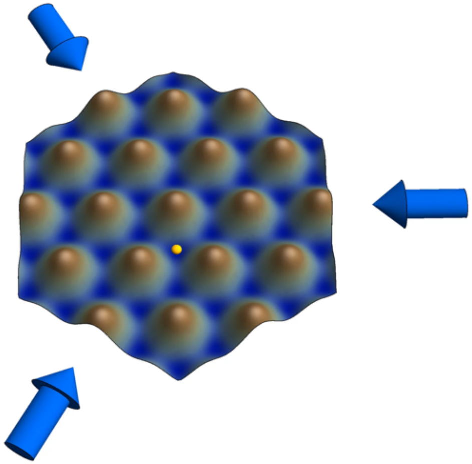
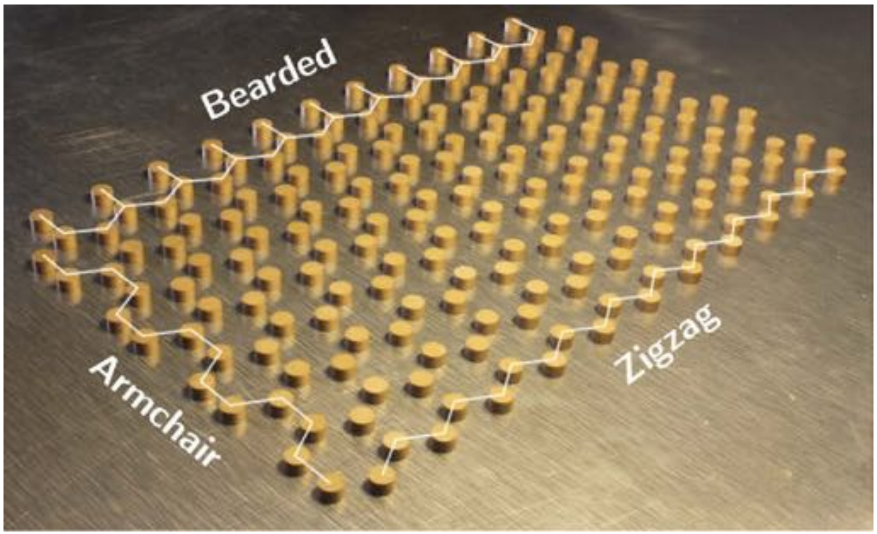


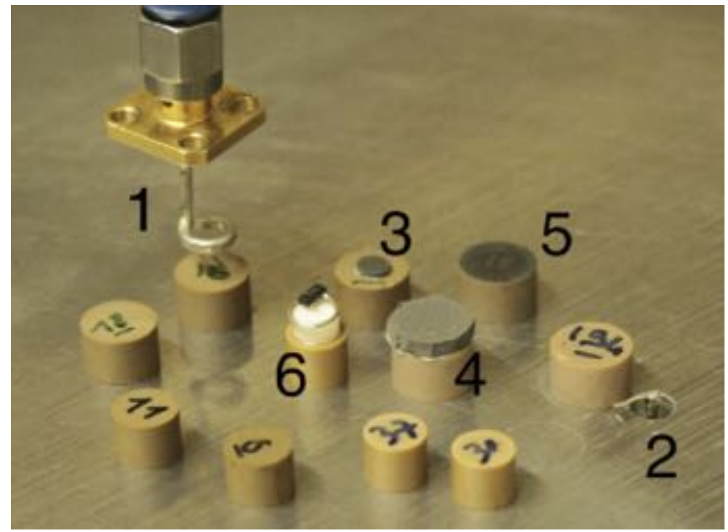
Figure 2. **Ultracold atoms in a honeycomb optical lattice**

https://www.quantum-munich.de/

Gaps into honeycomb lattice

Example by Mattis Reisner, Matthieu Bellec, Ulrich Kuhl, and Fabrice Mortessagne:

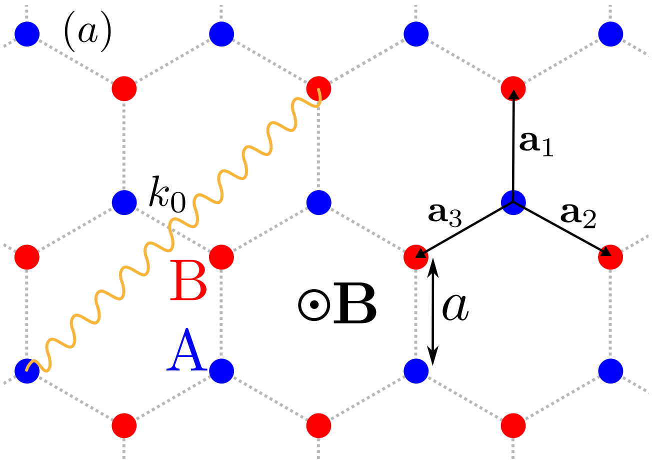




Gaps into honeycomb lattice

$$H = \hbar\sum_{n=1}^{N}\sum_{\alpha_n=\sigma_{\pm,0}}\left(\omega_0+\delta\omega_0^{(A,B)}+\mathrm{sgn}(\alpha_n)\mu_B B - i\frac{\Gamma_0}{2}\right)|\alpha_n\rangle\langle\alpha_n| + \frac{3\pi\hbar\Gamma_0}{k_0}\sum_{n\neq m}^{N}\sum_{\alpha_n,\beta_m=\sigma_{\pm},0}\mathcal{G}_{\alpha\beta}(\mathbf{r}_n-\mathbf{r}_m)|\alpha_n\rangle\langle\beta_m|$$

- N the number of identical two-levels atoms
- $\omega_0+\delta\omega_0^{(A,B)}$ resonance frequency of atoms of the sub-lattice A or B
- $\boldsymbol{B}$ the static magnetic field
- $\mathcal{G}_{\alpha\beta}$ the dyadic Green's function describing the coupling of atoms by EM waves
- σ reprents the three polarisations $\pm$ in the plane and 0 perpendicular



And we define a $3N\times 3N$ dimensionless matrix G made of 3×3 blocks: $G\mathbf{\Psi}=\Lambda\mathbf{\Psi}$

We define two very important parameters:

- $\Delta_{AB}=(\delta\omega_0^B-\delta\omega_0^A)/2\Gamma_0$ Frequency detuning
- $\Delta_{\mathbf{B}}=\mu B/\Gamma_0$ Zeeman Shift

Brillouin Zone

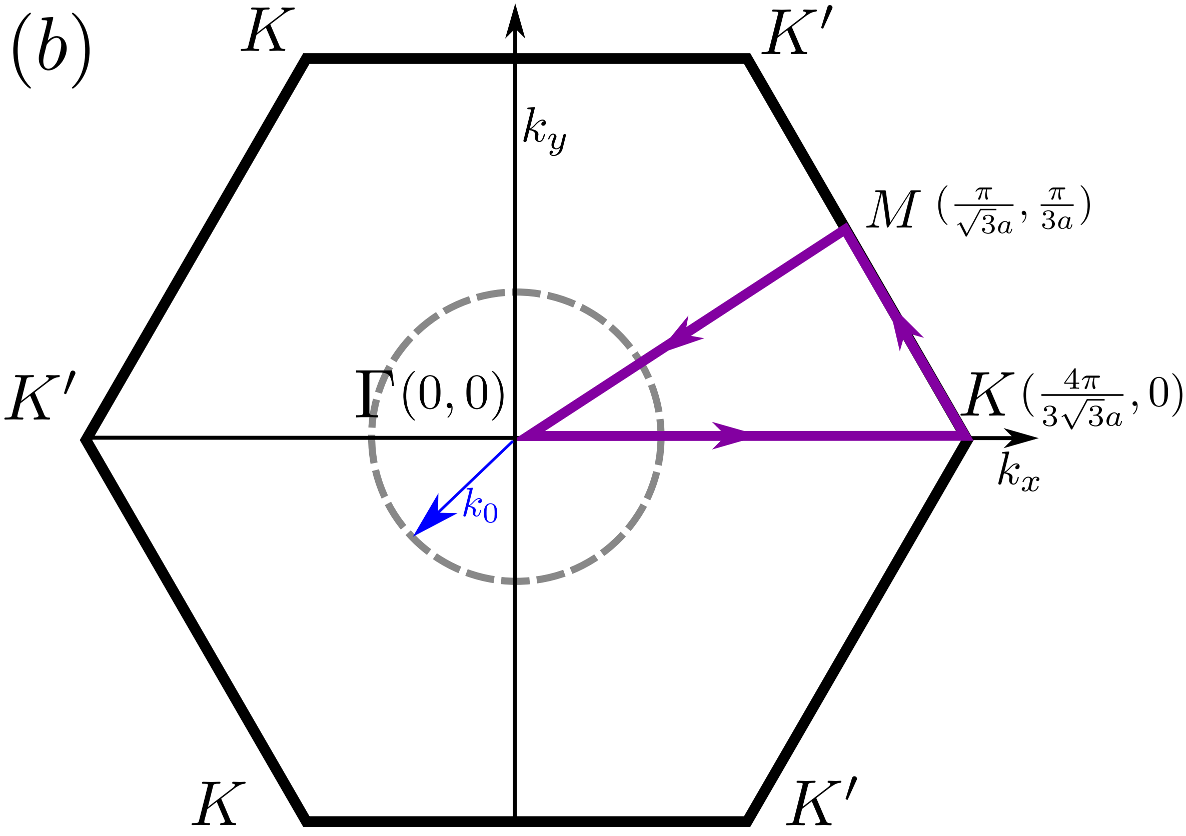


Figure 3. if $k_0 \gtrsim 1/a$ waves can escape

Gaps into honeycomb lattice

Periodicity + TE modes only:

$$\mathbf{\Psi}_n = \psi(\mathbf{k})\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_n}$$

Transforms the problem into:

$$G\mathbf{\Psi} = \Lambda\mathbf{\Psi} \quad \Rightarrow \quad M(\mathbf{k})\psi(\mathbf{k}) = \Lambda\psi(\mathbf{k})$$

Where M is a 4×4 matrix:

$$M(\mathbf{k}) = \begin{pmatrix} S_1^{\sigma+\sigma+} & S_1^{\sigma+\sigma-} & S_2^{\sigma+\sigma+} & S_2^{\sigma+\sigma-} \\ S_1^{\sigma-\sigma+} & S_1^{\sigma-\sigma-} & S_2^{\sigma-\sigma+} & S_2^{\sigma-\sigma-} \\ S_3^{\sigma+\sigma+} & S_3^{\sigma+\sigma-} & S_4^{\sigma+\sigma+} & S_4^{\sigma+\sigma-} \\ S_3^{\sigma-\sigma+} & S_3^{\sigma-\sigma-} & S_4^{\sigma-\sigma+} & S_4^{\sigma-\sigma-} \end{pmatrix}$$

$$\begin{aligned} S_1^{\alpha\beta} &= \sum_{\mathbf{r}_m\in A} G_{AA}^{\alpha\beta}(\mathbf{r}_m)\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_m} \\ S_2^{\alpha\beta} &= \sum_{\mathbf{r}_m\in A} G^{\alpha\beta}(\mathbf{r}_m+\mathbf{a}_1)\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_m} \\ S_3^{\alpha\beta} &= \sum_{\mathbf{r}_m\in A} G^{\alpha\beta}(\mathbf{r}_m-\mathbf{a}_1)\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_m} \\ S_4^{\alpha\beta} &= \sum_{\mathbf{r}_m\in A} G_{BB}^{\alpha\beta}(\mathbf{r}_m)\mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_m} \end{aligned}$$

Using Poisson summation formula:

$$\sum_{\substack{\mathbf{r}_m \in A \\ \mathbf{r}_m \neq 0}} G^{\alpha\beta}(\mathbf{r}_m) \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}_m} = \frac{1}{\mathcal{A}} \sum_{\mathbf{g}_m \in A'} g^{\alpha\beta}(\mathbf{g}_m - \mathbf{k}; 0) - G^{\alpha\beta}(\mathbf{0})$$

To ensure convergence of this integral we introduce a gaussian cut-off :

$$g^{\alpha\beta}(\mathbf{q}; \mathbf{r}') = -\frac{6\pi}{k_0} \frac{(k_0^2\,\delta_{\alpha\beta} - q_\alpha q_\beta)}{2\pi k_0^2} \mathrm{e}^{i\mathbf{q}\cdot\mathbf{r}'} \int \frac{1}{k_0^2 - \mathbf{q}^2 - q_z^2} \mathrm{d}q_z \rightarrow \int \frac{\mathrm{e}^{-a_{\mathrm{ho}}^2(\mathbf{q}^2 + q_z^2)/2}}{k_0^2 - \mathbf{q}^2 - q_z^2} \mathrm{d}q_z$$

Which can be expressed in a closed form:

$$\boxed{g^{\alpha\beta}(\mathbf{q}; 0) = -\frac{6\pi}{k_0} (\delta_{\alpha\beta} k_0^2 - q_\alpha q_\beta) \mathcal{I}(\mathbf{q})}$$

With:

$$\begin{aligned}
\mathcal{I}(\mathbf{q}) &= \chi(\mathbf{q}) \frac{\pi}{\Lambda(\mathbf{q})} (-i + \mathrm{erfi}(a_{\mathrm{ho}} \Lambda(\mathbf{q}) / \sqrt{2})) \\
\chi(\mathbf{q}) &= \frac{1}{2\pi k_0^2} \mathrm{e}^{-(k_0 a_{\mathrm{ho}})^2/2} \\
\Lambda(\mathbf{q}) &= \sqrt{k_0^2 - q^2}
\end{aligned}$$

And similarly we can compute $G^{\alpha\beta}(\mathbf{0})$ as the inverse Fourier transform of $g^{\alpha\beta}(\mathbf{q};0)$ where $\mathbf{q}=\mathbf{0}$

$$\boxed{G^{\alpha\beta}(\mathbf{0}) = -\left(\frac{\mathrm{erfi}(k_0 a_{\mathrm{ho}}/\sqrt{2}) - i}{\mathrm{e}^{k_0^2 a_{\mathrm{ho}}^2/2}} - \frac{-1/2 + (k_0 a_{\mathrm{ho}})^2}{\sqrt{\pi/2}(k_0 a_{\mathrm{ho}})^3}\right)\delta_{\alpha\beta}}$$

2017, *PRL 119, J. Perczel, and M. D. Lukin* 10.1103/PhysRevLett.119.023603

Only the imaginary part is convergent when $a_{\mathrm{ho}} \to 0$ and the real part is divergent (Lamb shift):

$$\mathrm{Im}(G^*_{\alpha\beta}(\mathbf{0})) \xrightarrow[a_{\mathrm{ho}}\to 0]{} 1$$

Band diagram

By considering eigenfrequencies $\omega = \omega_0 - \frac{\Gamma_0}{2}\Re(\Lambda)$ and decay rates $\Gamma = \Gamma_0 \Im(\Lambda)$ we can plot the band diagram by findings eigenvalues of $M(\mathbf{k})$

Video

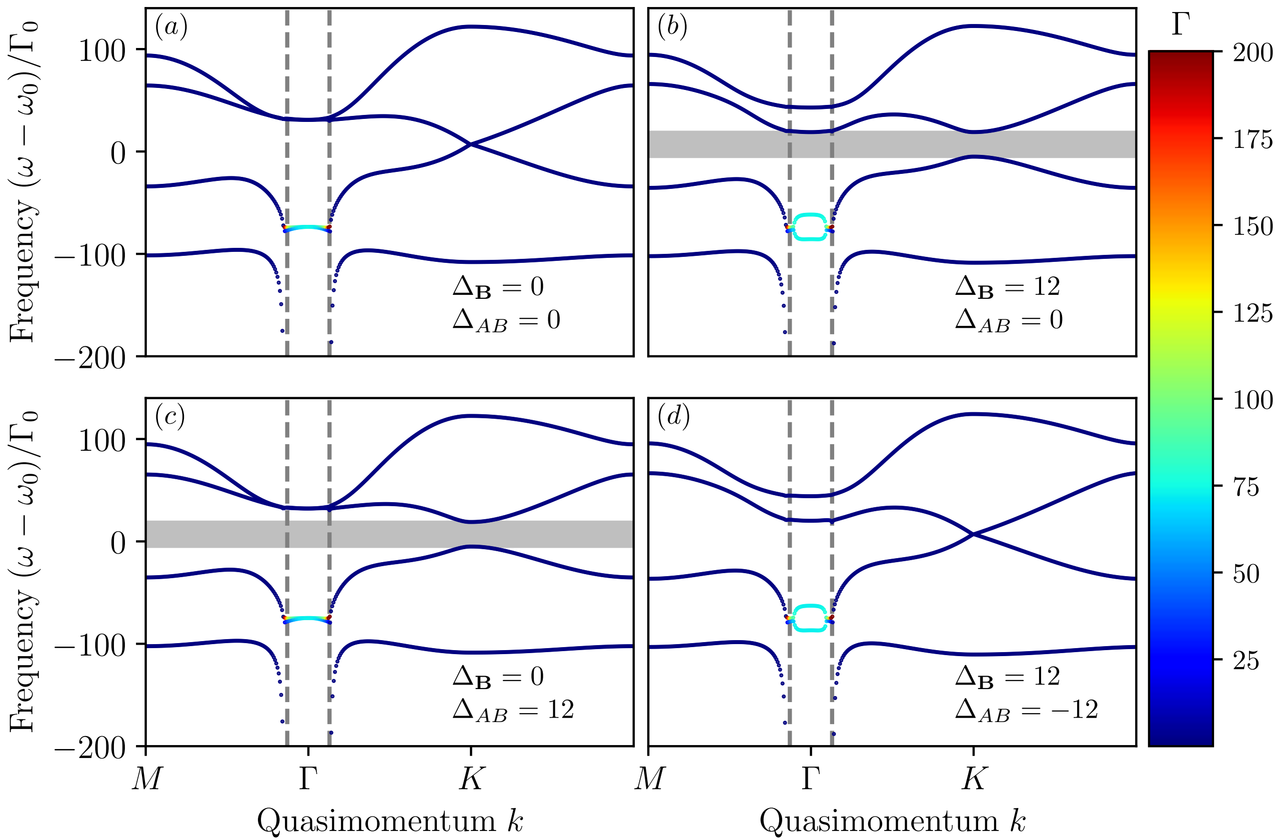


Figure 4. $k_0a = 2\pi \times 0.05$

A compact formula

$$\begin{aligned} W_{\text{gap}} &= 2\big||\Delta_{\mathbf{B}}| - |\Delta_{AB}|\big| && \text{if} \quad 0 < |\Delta_{\mathbf{B}}| < R_1 \\ &= \frac{1}{2}(c_0 - c_1 + S - |\Delta_{AB}|) && \text{if} \quad R_1 < |\Delta_{\mathbf{B}}| < R_2 \\ &= -2|\Delta_{\mathbf{B}}| + S && \text{if} \quad R_2 < |\Delta_{\mathbf{B}}| < R_3 \\ &= 0 && \text{elsewhere} \end{aligned}$$

Where:

$$S = 2\mathrm{Re}\left(\sqrt{4\Delta_{AB}^2 + \frac{1}{4}(c_2 + i\, c_3)^2}\right)$$

$$R_1 = \frac{1}{4}(c_0 - c_1 + S + 2|\Delta_{AB}|)$$

$$R_2 = \frac{1}{4}(c_0 - c_1 + S - 2|\Delta_{AB}|)$$

$$R_3 = S/2$$

c_0,c_1 and c_2 are elements of the matrix $M(\mathbf{k})$ and they only rely on $k_0 a$, the width of the gap is dependant of three parameters: $\Delta_{\mathbf{B}}$,Δ_{AB} and $k_0 a$.

Numerical confirmation

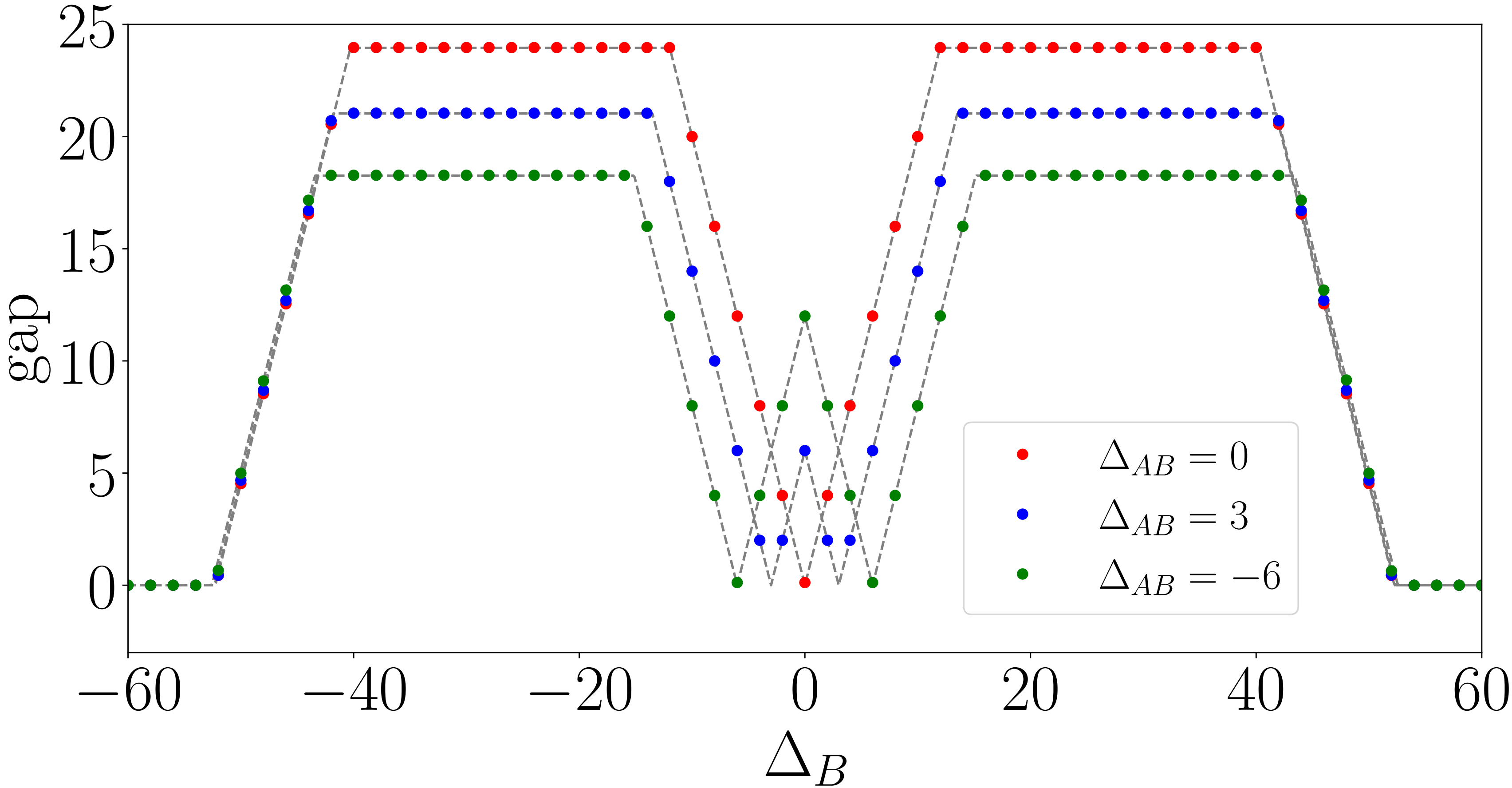
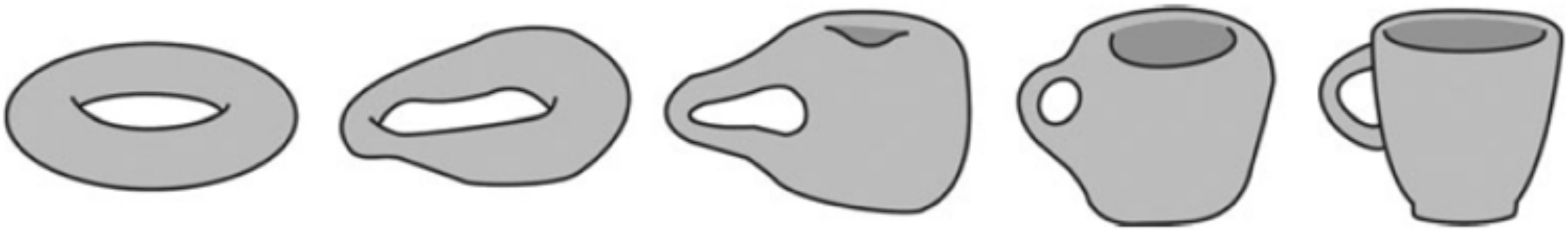


Figure 5. $k_0 a = 2\pi \times 0.05$

Topological properties



Topological properties

Topological properties

We define the Chern number as:

$$C = \frac{1}{2\pi}\int_{\mathrm{BZ}} \Omega(\mathbf{k}) d^2\mathbf{k}$$

Where $\Omega(\mathbf{k})$ is the Berry curvature such that:

$$\Omega(\mathbf{k}) = i\left[\left\langle \frac{\partial\psi(\mathbf{k})}{\partial k_x}\middle|\frac{\partial\psi(\mathbf{k})}{\partial k_y}\right\rangle - \left\langle \frac{\partial\psi(\mathbf{k})}{\partial k_y}\middle|\frac{\partial\psi(\mathbf{k})}{\partial k_x}\right\rangle\right]$$

To compute it faster we use the approach of *T. Fukui et al* by discretizing the Brillouin Zone. We define:

$$C_{\mathrm{gap}} = \sum_{b_i < \mathrm{gap}} c(b_i)$$

Which is the quantity we refer to when speaking about the Chern number of our system.

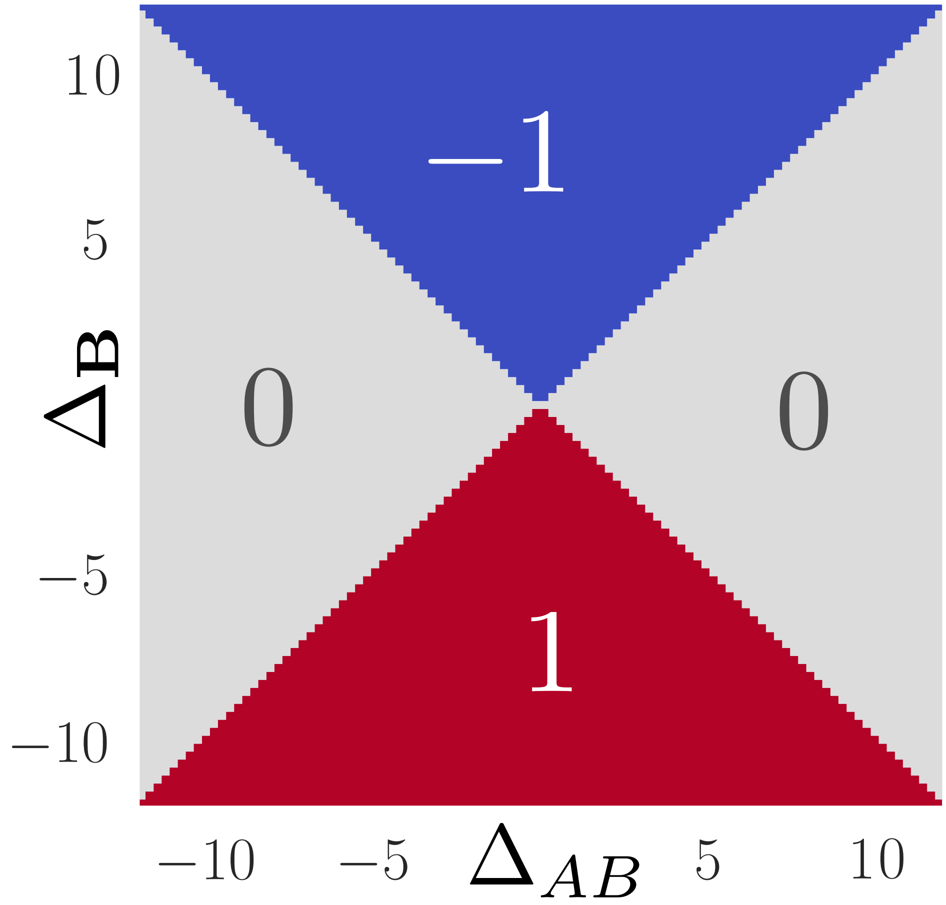


Figure 6. Chern number for $k_0 a = 2\pi \times 0.05$

Localization of modes

For a mode ψ_n we define the weight of the modes on sites A as:

$$P_A^n(\mathbf{k}) = \left|\psi_n^{(1)}(\mathbf{k})\right|^2 + \left|\psi_n^{(2)}(\mathbf{k})\right|^2$$

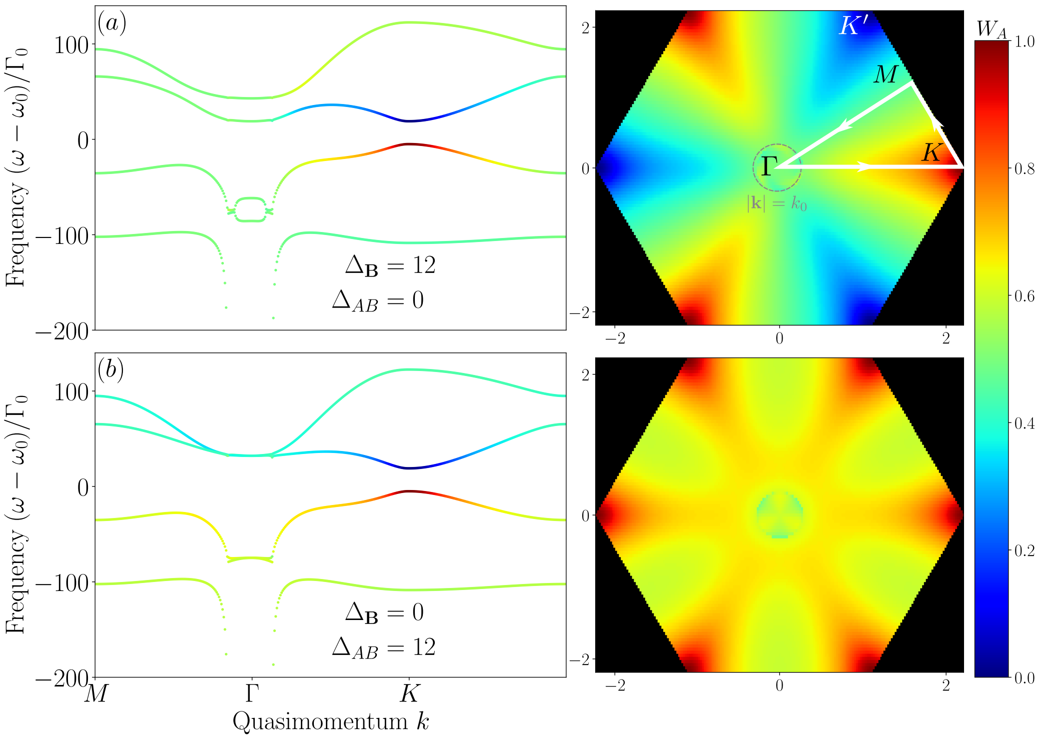


Figure 7.

Honeycomb lattice within a cavity

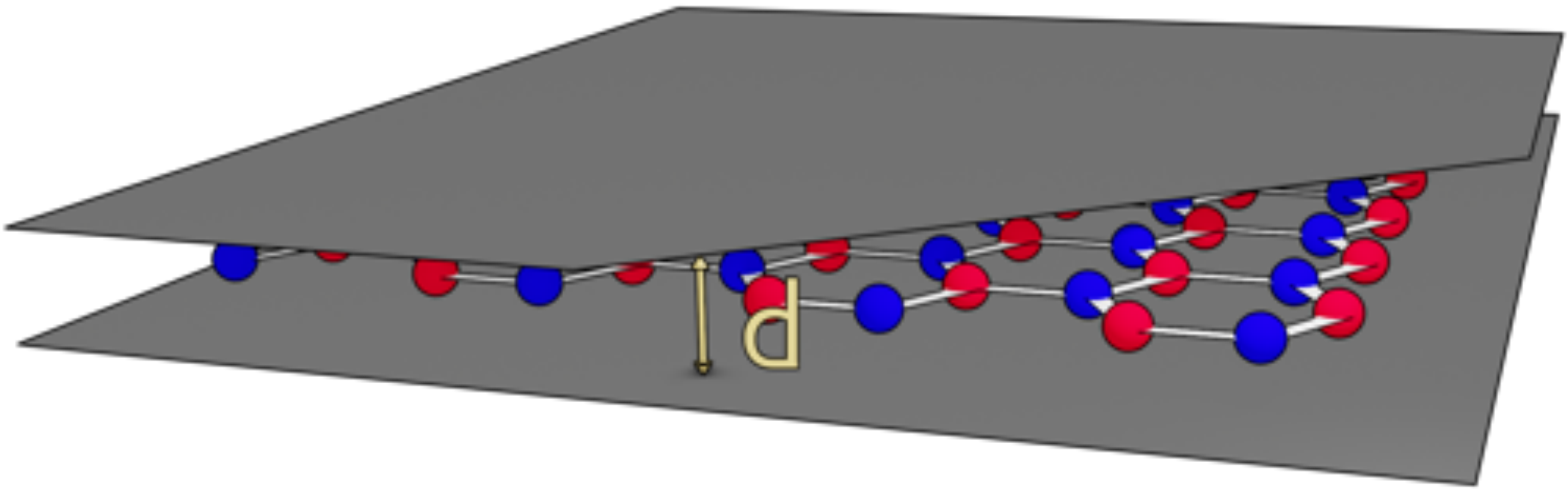


Figure 8.

It translates as the following boundary conditions:

$$\mathbf{B}\cdot\mathbf{n}=0$$

$$\mathbf{E}\times\mathbf{n}=\mathbf{0}$$

Method of images:

$$G^{\alpha\beta}(\mathbf{r}_m) \to \sum_{n=-\infty}^{+\infty} (-1)^n G^{\alpha\beta}_{\text{free}}(\mathbf{r}^n_m)$$

We then get:

$$\boxed{g^{\alpha\beta}(\mathbf{q};0) = -\frac{6\pi}{k_0}(\delta_{\alpha\beta}k^2 - q_\alpha q_\beta)\left(\mathcal{I}(\mathbf{q}) + \frac{i}{\sqrt{k_0^2-q^2}\,k_0^2}\frac{1}{1+\mathrm{e}^{-i\sqrt{k_0^2-q^2}d}}\right),\ \sqrt{k_0^2-q^2}d \neq \pi}$$

And:

$$\begin{aligned} G_{\text{plates}}(\mathbf{0}) &= -\left(\frac{\operatorname{erfi}(k_0 a/\sqrt{2}) - i}{\mathrm{e}^{k_0^2 a^2/2}} - \frac{-1/2 + (k_0 a)^2}{\sqrt{\pi/2}(k_0 a)^3}\right. \\ &\quad \left. - 3\left(\frac{\ln(1+\mathrm{e}^{ik_0 d})}{k_0 d} + i\frac{\mathrm{Li}_2(-\mathrm{e}^{ik_0 d})}{(k_0 d)^2} - \frac{\mathrm{Li}_3(-\mathrm{e}^{ik_0 d})}{(k_0 d)^3}\right)\right)\delta_{\alpha\beta} \end{aligned}$$

The imaginary part is simply the decay rate for one atom between two plates, this was already computed before in **1973**, *OPTICS COMMUNICATIONS, P. Milloni and P. Knight*

Honeycomb lattice within a cavity

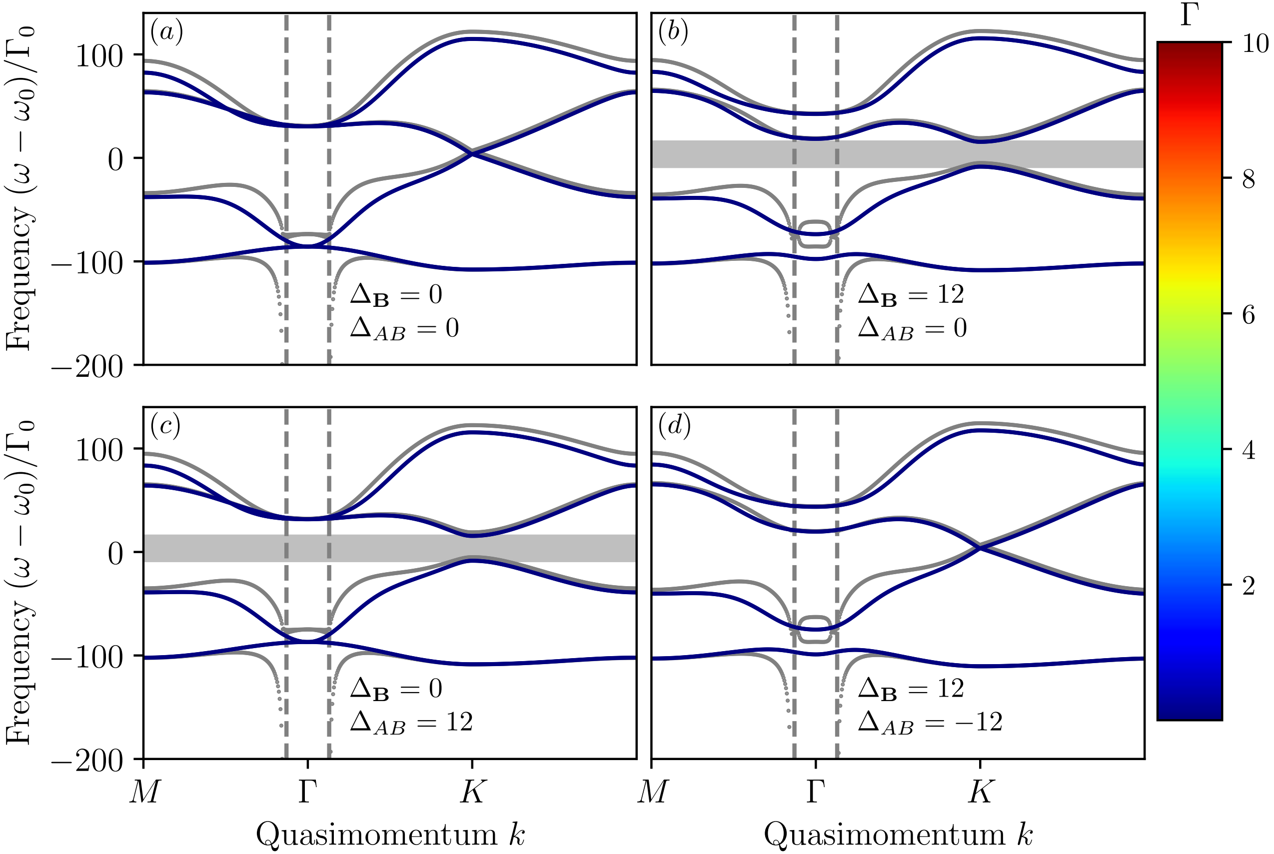


Figure 9. $k_0 d = 2 - k_0 a = 2\pi \times 0.05$

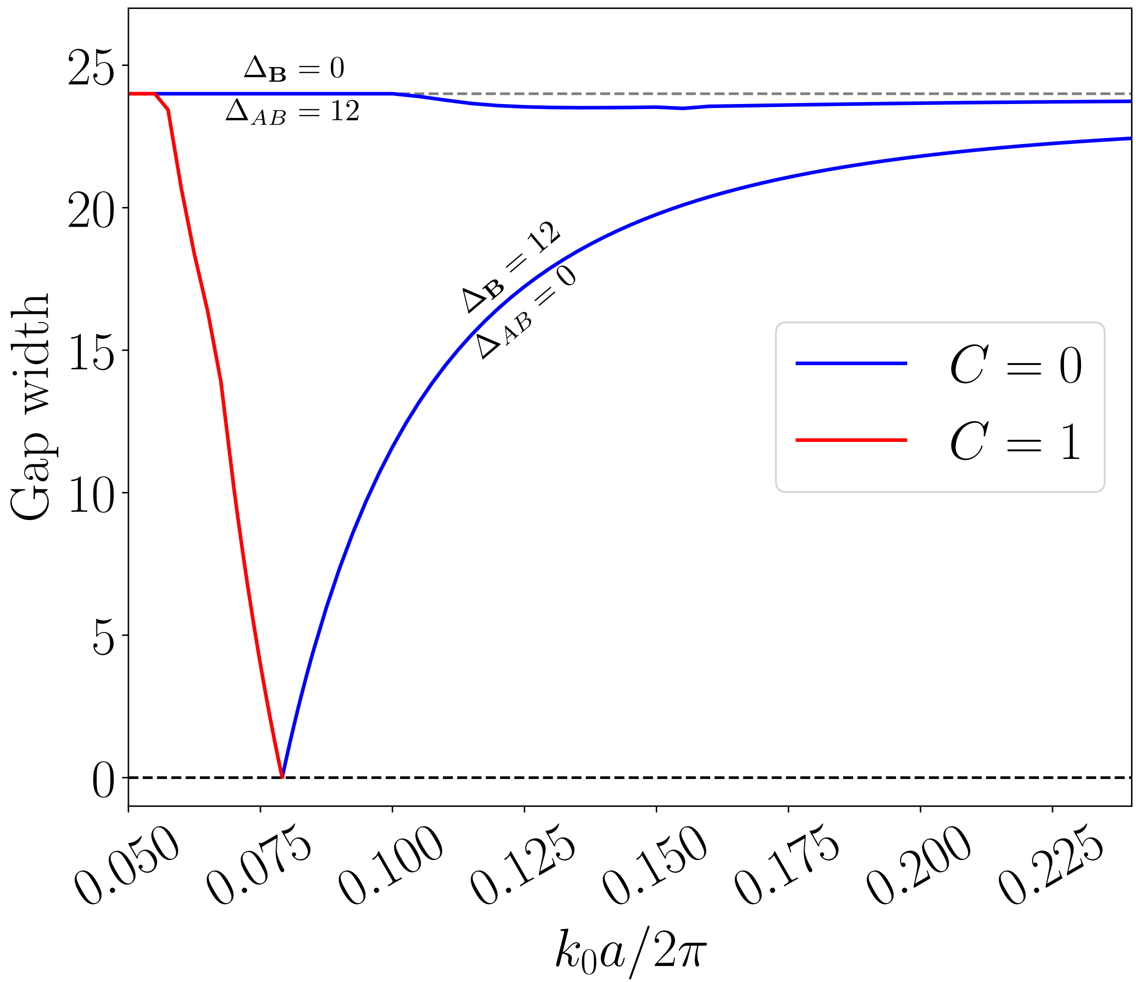

$\Delta_{\mathbf{B}} = 0$
$\Delta_{AB} = 12$
$\Delta_{\mathbf{B}} = 12$
$\Delta_{AB} = 0$
$C = 0$
$C = 1$
Gap width
0
5
10
15
20
25
0.050
0.075
0.100
0.125
0.150
0.175
0.200
0.225
$k_0 a / 2\pi$

Figure 10.

Conclusion

- Study of band diagram and topologcial properties of honeycomb atomic lattices
- General formula to describe the width of the gap in the optical spectrum of an honeycomb lattice with a magnetic field and two types of atoms
- Interesting topological properties occur only when $k_0 a \lesssim 0.1 \times 2\pi$
- Generalizing to the case of atomic lattice between reflecting plates

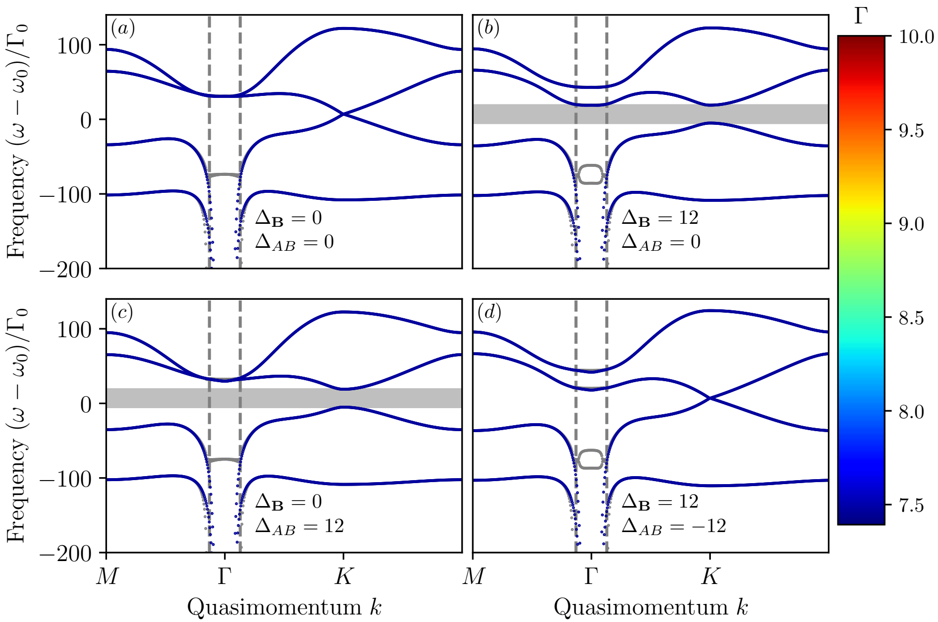


Figure 11. $k_0 d = 11$

We define a $3N \times 3N$ dimensionless matrix G made of 3×3 blocks:

$$G_{mn} = \delta_{mn}(i \pm 2\Delta_{AB} - 2\alpha\Delta_B)\mathbb{1}_{3\times 3} + (1 - \delta_{mn})d_{\mathrm{eg}}A_{mn}d_{\mathrm{eg}}^{\dagger}$$

With:

- $\Delta_{AB} = (\delta\omega_0^B - \delta\omega_0^A)/2\Gamma_0$
- $\Delta_{\mathbf{B}} = \mu B/\Gamma_0$ and α is -1,1, and 0 for the three diagonal elements.
- d_{eg} is a transformation matrix to go from cartesian to polar coordinates

And:

$$A_{mn} = (1 - \delta_{mn})\frac{3}{2}\frac{\mathrm{e}^{ik_0r}}{k_0r}\left(P(i\,k_0r)\mathbb{1} + Q(i\,k_0r)\frac{\mathbf{r}_{mn}\otimes\mathbf{r}_{mn}}{r_{mn}^2}\right)$$

Where:

- $k_0 = \omega_0/c$
- $\mathbf{r}_{mn} = \mathbf{r}_m - \mathbf{r}_n$
- $P(x) = 1 - 1/x + 1/x^2$ and $Q(x) = -1 + 3/x - 3/x^2$

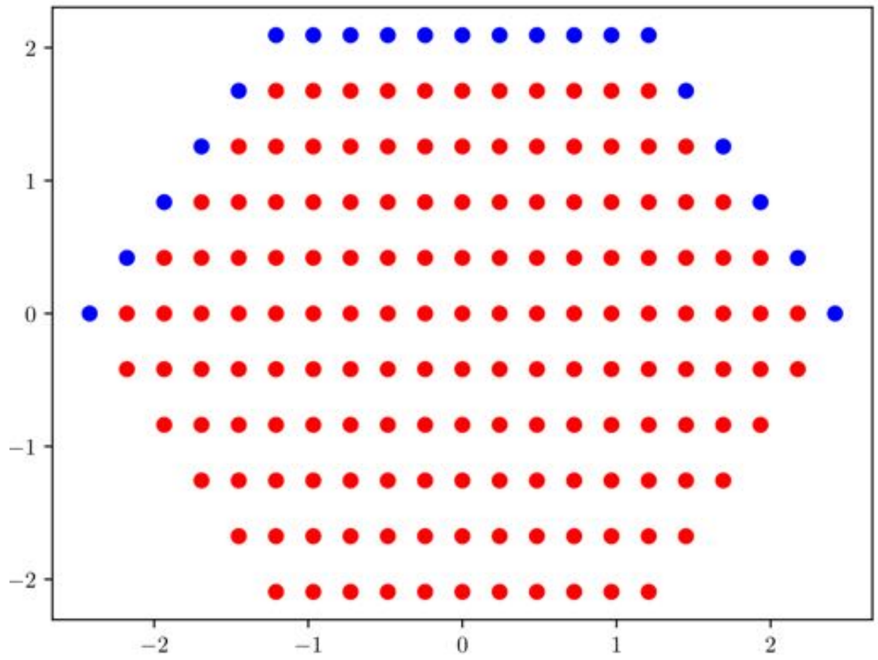


Figure 12.

Chern Numbers in Discretized Brillouin Zone: Efficient Method of Computing (Spin) Hall Conductances, J. Phys. Soc. Jpn. 74, *Takahiro Fukui, Yasuhiro Hatsugai and Hiroshi Suzuki*