Wave Propagation through Photonic Crystal Slabs
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Chapter 6

Control of spontaneous emission in photonic crystals

In chapters 4 and 5 we have studied the phenomena of negative refraction and the focusing of light by two-dimensional photonic crystals. In this chapter we focus on another interesting optical property of photonic crystals, namely their ability to control the spontaneous emission of defects inside the photonic crystal.

6.1 Spontaneous emission of light

Spontaneous emission of light is a widely studied phenomenon, both due to its importance in the fundamental understanding of light-matter interactions and in the applications, such as for example transistors, optical switches, microlasers, solar cells, . . ., which depend on it. As early as in 1946, it was noticed that spontaneous emission can be controlled with cavity structures [210]. Theoretically, the spontaneous emission rate can be obtained from Fermi’s golden rule containing the local radiative density of states (LRDOS) [211]. For relatively simple cavity structures, the modification of the spontaneous emission rate can be calculated analytically using either a classical [212–218] or a quantum mechanical approach [219–232]. It has been shown that the classical and quantum mechanical results for the spontaneous emission are equivalent [212–213, 215, 217, 218, 232]. This equivalence allows the calculation of the spontaneous emission rate [233, 235], the external quantum efficiency [235] and the spontaneous emission factor [235, 236] in a microcavity of arbitrary geometry, using a finite-difference time domain (FDTD) algorithm [20].
Control of spontaneous emission is also one of the main applications of photonic crystals [4]. It was suggested that complete photonic band gaps allow complete inhibition of spontaneous emission for frequencies deep inside the photonic band gap [4]. Also photonic band gap materials that do not possess complete photonic band gaps but pseudogaps are of interest, since they can allow for a substantially suppressed spontaneous emission. In the early experimental studies on the variation of spontaneous emission in photonic crystals [237–242], the light sources were dye molecules. Theoretical calculations have shown that the effect of the photonic band gap on the fluorescence lifetime of the dye molecules in these structures was very small and that the experimentally measured variations in lifetime were mainly caused by other processes such as electronic/chemical interactions between the molecules and the medium [243]. In 2002, Koenderink et al. made the first observation of the inhibition of spontaneous emission in a photonic crystal consisting of a FCC crystal of air spheres in Titania [244]. They demonstrated that in their experiment the reduction in the emitted power was not due to chemical interactions of the dye with its environment. An experiment in the same spirit showed the inhibition of spontaneous emission of a light emitting Indium-Gallium-Arsenide-Phosphide (InGaAsP) multiple quantum well in a GaAs woodpile structure [245]. The first experiment showing true control of spontaneous emission (by changing the lifetime of the excited state) made use of semiconductor quantum dots in inverse opal photonic crystals [246]. Subsequent experiments demonstrating the suppression of light emission caused by the defect of the photonic band gap are described in [247–250].

In this chapter, we present a simple procedure to determine the spontaneous emission rate from short-time FDTD simulation data of the electromagnetic energy field. We validate this procedure by computing the LRDOS of two-dimensional photonic crystals, employing the unconditionally stable FDTD method described in Chapter 2. Although this computation is more expensive than the procedure based on the electromagnetic field energy data, this FDTD based method does not require a solution of the eigenvalue problem nor integrations over the first Brillouin zone.

### 6.2 The emission rate

As discussed in Chapter 2, we can write the time-dependent Maxwell equations for the electromagnetic fields in linear, isotropic, nondispersive, lossless dielectric materials without electric charges and magnetic current sources as

$$\frac{\partial}{\partial t} \Psi(t) = \mathcal{H} \Psi(t) - \mathcal{S}(t),$$  \hspace{1cm} (6.1)
6.2. The emission rate

where \( \Psi(t) = (\sqrt{\mu(r)} H(r, t), \sqrt{\varepsilon(r)} E(r, t))^T \), \( \mathcal{H} \) denotes the operator

\[
\begin{pmatrix}
0 & -\frac{1}{\sqrt{\mu(r)}} \nabla \times \frac{1}{\sqrt{\varepsilon(r)}} \\
\frac{1}{\sqrt{\varepsilon(r)}} \nabla \times \frac{1}{\sqrt{\mu(r)}} & 0
\end{pmatrix},
\]

(6.2)

and \( \mathcal{S}(t) = (0, J(r, t)/\sqrt{\varepsilon(r)})^T \) denotes the source term.

From the definition of \( \Psi(t) \) it follows that

\[
\langle \Psi(t) | \Psi(t) \rangle = \int_V [\varepsilon(r)(E^2(r, t) + \mu(r)H^2(r, t))] d\mathbf{r},
\]

(6.3)

relating the length (norm) of vector \( \Psi(t) \) to the energy density \( w(r, t) = \varepsilon(r)E^2(r, t) + \mu(r)H^2(r, t) \) of the electromagnetic fields. Here \( V \) denotes the volume of the enclosing box. The energy emitted by the point source can thus be defined as \( U(t) = \langle \Psi(t) | \Psi(t) \rangle \). The emission rate can be obtained by differentiation of \( U(t) \): \( P(t) = \partial U(t)/\partial t \).

As mentioned earlier, the emission properties can also be investigated by calculating the LRDOS. Here we demonstrate that there is a simple relation between the emitted energy and the LRDOS. The formal solution of Eq. (6.1) is given by

\[
\Psi(t) = e^{t\mathcal{H}} \Psi(0) - \int_0^t e^{(t-u)\mathcal{H}} \mathcal{S}(u) du.
\]

(6.4)

We assume that the electric current density of a unit point source located at \( \mathbf{r} = \mathbf{r}_0 \) is given by

\[
J(r, t) = \mathbf{O} \theta(t) \delta(\mathbf{r} - \mathbf{r}_0) \sin \Omega t,
\]

(6.5)

where \( \Omega \) is the angular frequency of the source and \( \mathbf{O} \) defines the direction of the electric current. As indicated by the step function \( \theta(t) \) in Eq. (6.5), the source is turned on at \( t = 0 \). Making use of Eq. (6.4) and Eq. (6.5) and assuming that \( \Psi(r, t = 0) = 0 \), we find

\[
U(t) = \langle \Psi(t) | \Psi(t) \rangle = \frac{1}{\varepsilon(\mathbf{r}_0)} \int_0^t \int_0^t \langle \mathbf{S}_0 | e^{(u'-u)\mathcal{H}} \mathbf{S}_0 \rangle \sin \Omega u \sin \Omega u' du du'
\]

\[
= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_0^t \int_0^t N_{\text{rad}}(\mathbf{S}_0, \mathbf{O}, \omega) \cos \omega(u' - u) \sin \omega u \sin \omega u' dudud\omega,
\]

(6.6)

where \( \mathbf{S}_0 = (0, \hat{\mathbf{S}}_0) \) and \( \langle \mathbf{r} | \hat{\mathbf{S}}_0 \rangle = \mathbf{O} \delta(\mathbf{r} - \mathbf{r}_0) \). The LRDOS is defined by \( N_{\text{rad}}(\mathbf{S}_0, \mathbf{O}, \omega) = \varepsilon(\mathbf{r}_0)^{-1} N(\mathbf{S}_0, \mathbf{O}, \omega) \) (see Eq. (2.51)), where

\[
N(\mathbf{S}_0, \mathbf{O}, \omega) \equiv \int_{-\infty}^{+\infty} e^{i\omega t} \langle \mathbf{S}_0 | e^{t\mathcal{H}} \mathbf{S}_0 \rangle dt,
\]

(6.7)

denotes the local density of states (LDOS) for frequency \( \omega \) and direction \( \mathbf{O} \) at the position
6. Control of spontaneous emission in photonic crystals

We carry out the time integration to obtain

\[
U(t) = \frac{1}{\pi} \int_{-\infty}^{+\infty} N_{rad}(S_0, O, \omega) \left[ \frac{\sin^2 t(\omega - \Omega)/2}{(\omega - \Omega)^2} - \frac{\sin t(\omega - \Omega)/2 \sin t(\omega + \Omega)/2}{\omega - \Omega - \Omega} \cos t\Omega \right] d\omega. \tag{6.8}
\]

In the limit \( t \to \infty \) the contribution of the second term in Eq. (6.8) vanishes, yielding for the emission rate

\[
\lim_{t \to \infty} P(t) = \lim_{t \to \infty} \frac{\partial U(t)}{\partial t} = \lim_{t \to \infty} \int_{-\infty}^{+\infty} N_{rad}(S_0, O, \omega) \frac{\sin t(\omega - \Omega)}{2\pi(\omega - \Omega)} d\omega = \frac{N_{rad}(S_0, O, \Omega)}{2}, \tag{6.9}
\]

which, apart from some constants, agrees with Eq. (26) in [217] and with the expression obtained by using Fermi’s Golden Rule [211].

For microcavities of arbitrary geometry, \( U(t) \) is most easily calculated by solving the time-dependent Maxwell equations by means of an FDTD method [20]. We employ an algorithm that, in the absence of external currents, conserves the energy exactly (see Chapter 2). This property ensures that the time-dependence of \( U(t) \) is due to the presence of the source only. In our numerical work, we use square simulation areas completely filled with the photonic crystal and having boundaries that are perfect reflecting conductors. We measure distances in units of the wavelength \( \lambda \) of light in air. Time and frequency are then expressed in units of \( \lambda/c \) and \( c/\lambda \), respectively, where \( c \) denotes the velocity of light in air. For photonic crystals with lattice constant \( a \), \( f = \omega a/2\pi c \) is the dimensionless frequency.

6.3 Spontaneous emission in two-dimensional photonic crystals

We study the emission properties of a point source embedded in a two-dimensional photonic crystal. The photonic crystal consists of a triangular lattice of air holes drilled in a dielectric material with \( \varepsilon = 12.96 \) and \( \mu = 1 \). We study two cases, the holes having a diameter \( d = 0.80a \) and \( d = 0.96a \), respectively. For reference, we use the MIT Photonic-Bands package [190] to compute the photonic band structure diagram for the TM mode. The results are shown in Fig. 6.1. For \( d = 0.80a \), no gap is observed for the TM mode, but a gap extending from \( f = 0.24 \) to \( f = 0.40 \) is observed for the TE mode. For \( d = 0.96a \), the photonic crystal has a complete photonic band gap. For the TM mode the gap extends from \( f = 0.43 \) to \( f = 0.52 \) and for the TE mode from \( f = 0.36 \) to \( f = 0.53 \).
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Figure 6.1: Photonic band structure diagram of TM (top) and TE (bottom) modes for a triangular lattice of air holes drilled in a dielectric medium ($\varepsilon = 12.96, \mu = 1, \sigma = 0$). The holes have a diameter $d$. (a): TM mode, $d = 0.80a$. (b): TM mode, $d = 0.96a$. (c): TE mode, $d = 0.80a$. (d): TE mode, $d = 0.96a$. $f = \omega a/2\pi c$ is the dimensionless frequency. The first Brillouin zone of a triangular lattice and the symmetry points are shown in the inset (see Appendix A).

6.3.1 TM mode

To compute the emitted energy we put a point source with a current density specified by Eq. (6.5) at different locations $r_0$ near the center of the simulation area. The locations are chosen such that the source is located at one of the $E_z$-points of the two-dimensional Yee grid (see Fig. 2.2, TM mode). The emitted energy $U(t)$ is trivially obtained from the solution for the electromagnetic fields, see Eq. (6.3). In order to have a reference value for the emitted energy, we first compute $U(t)$ for a point source located in the middle of a square.

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area completely filled with air. In what follows, we refer to this setup as the empty area. The result is shown in Fig. 6.2 (crosses). The slope of the line that can be drawn through the data for \( t \leq 20 \) gives a measure for the emission rate (up to a scaling factor). For larger times the data deviates from a straight line. This is due to reflections at the boundaries of the simulation area. The solid symbols in Fig. 6.2 denote the results for a point source embedded in the triangular-lattice photonic crystal with \( d = 0.80a \). We show three results for a source emitting light with a frequency \( f = 0.30 \). If the source is located in the center of a hole (solid squares) the emitted energy is very small and almost constant as a function of time. Hence, light emission is strongly suppressed and for all practical purposes inhibited. If we move the source away from the center of the hole, but so that it is still located in the air region (solid triangles), light emission is enhanced compared to the case for which the source was placed in the centre of the hole (solid squares), but strongly suppressed compared to the empty area case (crosses). Placing the source in a region with \( \varepsilon = 12.96 \) leads to an emission enhancement (solid circles) compared to the empty area case. Changing the frequency of the emitted light to \( f = 0.53 \) and putting the source in the center of a hole also leads to a suppression of the light emission (solid diamonds), but not to an inhibition of the emission, as in the case of \( f = 0.3 \). From these results, it can be concluded that the emission rate strongly depends on the location of the source and on the frequency of the emitted light: Emission enhancement as well as emission suppression can be observed. Even if the photonic crystal has no photonic...
6.3. Spontaneous emission in two-dimensional photonic crystals

Figure 6.3: LRDOS (TM mode) for various source locations $r_0$ in the triangular-lattice photonic crystal with $d = 0.80a$. (a): $r_0 = (0, 0)$; (b): $r_0 = a(0.20, 0.23)$; (c): $r_0 = a(\sqrt{3}/3, 0)$. $f = \omega a/2\pi c$ is the dimensionless frequency.

band gap, the emission of a point source can be almost completely suppressed [52].

Fig. 6.2 also shows the results of the energy emitted by a point source embedded in the triangular-lattice photonic crystal with $d = 0.96a$, a photonic crystal having a photonic band gap. For $f = 0.48$, a frequency inside the photonic band gap, and sources located in the center of a hole (open squares) or in the dielectric material (open circles), light emission is inhibited for all practical purposes. Note that the values for $U(t)$ for these two cases are comparable to the value of $U(t)$ for the case of a source emitting light with a frequency $f = 0.3$ and located in the center of a hole in the photonic crystal with $d = 0.80a$. Increasing the frequency of the light emitted by a source, located at the center of a hole, to $f = 0.56$ (open triangles) leads to a strong emission enhancement compared to the empty area case.

We validate the conclusions based on the behavior of the results for $U(t)$ by computing the LRDOS. We use the following procedure: We first set the electromagnetic fields at the point $r_0$ on the two-dimensional Yee grid so that $E_z(r_0, t) = 1$ and so that all other (components of the) electromagnetic fields are zero at all other points of the grid. We then solve the
time-dependent Maxwell equations and store the values of \( f(t) = \varepsilon(r_0)^{-1} \langle S_0 | e^{iHt} S_0 \rangle \). The (fast) Fourier transform of \( f(t) \) then yields the LRDOS. By using an unconditionally stable algorithm (see Chapter 2) we do not have to solve the eigenvalue problem for \( H \). This is an important advantage over methods that compute the L(R)DOS by integrating the modulus of the electric field in the first Brillouin zone. Not only does the diagonalization require a lot of computer time, also all points of the entire first Brillouin zone should be included in the calculation of the L(R)DOS [251]. As pointed out in [251], this integral was often performed incorrectly within an irreducible first Brillouin zone [252–255] by using a linear tetrahedron method.

Figures 6.3 and 6.4 show the results for the LRDOS for the same source positions as the ones used to obtain the results depicted in Fig. 6.2. The height of the peaks in the LRDOS have a physical meaning: from Eq. (2.52) it follows that the height of the peak in the LRDOS at frequency \( \omega \) is proportional to the electromagnetic field intensity of the corresponding eigenmode. For practical purposes, we consider the LRDOS to exhibit a gap if for a certain frequency range the electromagnetic field intensity is below the threshold of numerical noise, which in our numerical simulations is approximately \( 10^{-10} \). Figure 6.3 shows the LRDOS for sources embedded in a triangular-lattice photonic crystal with \( d = 0.80a \). If the source is located in the center of a hole (see Fig. 6.3a), then the LRDOS shows a small gap around \( f = 0.30 \). In this frequency range there are no electromagnetic modes. Hence, light with a frequency \( f = 0.30 \) emitted by a source positioned in the center of a hole cannot propagate into the photonic crystal. Note however, that the photonic crystal has no photonic band gap and hence the DOS has no gaps around \( f = 0.30 \). Increasing the frequency of the source to for example \( f = 0.53 \) allows the light to propagate through the system. Moving the source away from the center of a hole, but in a way that it is still located in the air region, results in an increase of the density of states around \( f = 0.30 \) (see Fig. 6.3b). Although the LRDOS is

\[ \text{Figure 6.4: LRDOS (TM mode) for various source locations } r_0 \text{ in the triangular-lattice photonic crystal with } d = 0.96a. \text{ (a): } r_0 = (0, 0); \text{ (b): } r_0 = a(\sqrt{3}/3, 0). \text{ } f = \omega a/2\pi c \text{ is the dimensionless frequency.} \]
6.3. Spontaneous emission in two-dimensional photonic crystals

still rather low at \( f = 0.30 \), light can now propagate into the photonic crystal. From Fig. 6.3, it can be seen that placing the source in a region with \( \varepsilon = 12.96 \) leads to a further increase of the LRDOS around \( f = 0.3 \). Comparing the results of Fig. 6.2 with the results of Fig. 6.3 indicates that the number of modes at a given frequency gives a rough quantitative measure of the emission rate. Fig. 6.4 depicts the LRDOS for the case \( d = 0.96a \). For frequencies inside the photonic band gap, no modes are available, independent of the position of the source. Hence, for \( f = 0.48 \) emission is inhibited, as was also concluded from Fig. 6.2. For \( f = 0.56 \), a frequency in a pass band, no gaps in the LRDOS are seen for source positions in a hole. Note that in the low frequency domain the LRDOS depicted in Figs. 6.3 and 6.4 shows several small gaps. These gaps probably correspond to finite-size gaps. However, at these low frequencies it is very difficult to make a distinction between a finite-size gap and a real gap. This is a drawback of methods that use the LRDOS to study the emission rate.

6.3.2 TE mode

We now repeat the calculations for the TE mode instead of the TM mode. For this purpose, we replace the source term in Eq. (6.1) by

\[
S(t) = (0, M(r, t)/\sqrt{\mu(t)})^T,
\]

where \( M(r, t) \) denotes the magnetic current source and we replace the operator \( \mathcal{H} \) by

\[
\begin{pmatrix}
0 & -\frac{1}{\sqrt{\mu(r)}} \nabla \times \frac{1}{\sqrt{\varepsilon(r)}} \\
\frac{1}{\sqrt{\varepsilon(r)}} \nabla \times \frac{1}{\sqrt{\mu(r)}} & 0
\end{pmatrix},
\]

(6.11)

We assume that the magnetic current density of a unit point source located at \( r = r_0 \) has a similar form as the electric current density given in Eq. (6.5). Hence, we take

\[
M(r, t) = \Theta(t) \delta(r - r_0) \sin \Omega t.
\]

(6.12)

The expression for the energy emitted by the magnetic source is still given by Eqs. (6.3) and (6.8), but the LRDOS is now defined as

\[
N_{rad}(S_0, O, \omega) = \mu(r_0)^{-1} N(S_0, O, \omega).
\]

(6.13)

Note that for the photonic crystal \( \mu(r) = 1 \), so that for the TE mode the LRDOS equals the LDOS. To compute the emitted energy, we put a point source with a current density specified by Eq. (6.12) at different locations \( r_0 \) near the center of the simulation area. The locations are chosen such that the magnetic current source is located at one of the \( H_z \)-points of the two-dimensional Yee grid (see Fig. 2.2 TE-mode). The emitted energy is again obtained from the
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Figure 6.5: Emitted energy $U$ (TE mode) as a function of time $t$ for a point source embedded in air (crosses) and for a point source located at position $r_0$ in a two-dimensional photonic crystal. The photonic crystal consists of a triangular lattice of air holes with diameter $d$ drilled in a dielectric material ($\varepsilon = 12.96, \mu = 1$). The inset shows the triangular lattice network with spacing $a$ in real space. The crosses indicate the source positions $r_0$. Solid squares: $r_0 = (0, 0), f = 0.30, d = 0.80a$; Solid circles: $r_0 = a(\sqrt{3}/3, 0), f = 0.30, d = 0.80a$; Open triangles: $r_0 = (0, 0), f = 0.48, d = 0.96a$.

solution for the electromagnetic fields (see Eq. (6.3)). We first compute $U(t)$ for the empty area, which again serves as a reference value for the emitted energy in a photonic crystal. The result is shown in Fig. 6.5 (crosses). The solid (open) symbols in Fig. 6.5 denote the results for a point source embedded in the triangular-lattice photonic crystal with $d = 0.80a$ ($d = 0.96a$). For the TE mode, we only consider sources emitting frequencies in the photonic band gap. Hence, we expect that the emission of the point source is completely suppressed. For photonic crystals with $d = 0.80a$ we show two results for a source emitting light with a frequency $f = 0.3$. If the source is located in the center of a hole (solid squares) the emitted energy is very small and almost constant as a function of time. Hence, light emission is for all practical purpose inhibited. If we place the source in a region with $\varepsilon = 12.96$ (solid circles), the emitted energy is slightly enhanced and oscillates more compared to the case for which the source was placed in the center of a hole (solid squares), but on average the emission rate
is zero. Changing the frequency of the emitted light to \( f = 0.48 \) and putting the source in the center of a hole (open triangles) also leads to an inhibition of the emission, as in the case of \( f = 0.3 \). From these results, it can be concluded that the emission rate is zero for frequencies in the photonic band gap.

We validate the conclusions based on the behavior of the results for \( U(t) \) by computing the LRDOS. In the case of the TE mode we use the following procedure: We first set the electromagnetic fields at the point \( r_0 \) on the two-dimensional Yee grid so that \( H_z(r_0, t = 0) = 1 \) and so that all other (components of the) electromagnetic fields are zero at all other points of the grid. We then solve the time-dependent Maxwell equations and store the values of \( f(t) = \mu(r_0)^{-1}\langle S_0 | e^{tH} S_0 \rangle = \langle S_0 | e^{tH} S_0 \rangle \). The (fast) Fourier transform of \( f(t) \) then yields the LRDOS, which in this case is equal to the LDOS.

Figure 6.6 shows the results for the LRDOS for the same source positions as the ones used to obtain the results depicted in Fig. 6.5. Figures 6.6a and 6.6b show the LRDOS for sources embedded in a triangular-lattice photonic crystal with \( d = 0.80a \). If the source is located...
in the center of a hole or in a region with $\varepsilon = 12.96$, then the LRDOS shows a gap around $f = 0.3$. The gap corresponds to the photonic band gap. In this frequency range there are no electromagnetic modes. Hence, light with a frequency $f = 0.3$ emitted by a point source positioned in the center of a hole or in a region with $\varepsilon = 12.96$ cannot propagate into the photonic crystal, as was also concluded from Fig. 6.5. Figure 6.6c depicts the LRDOS for the case $d = 0.96a$. Also for this case, the photonic crystal has a photonic band gap for the TE mode. For frequencies inside the photonic band gap, no modes are available, independent of the position of the source. Hence, for $f = 0.48$ emission is inhibited, as was concluded from Fig. 6.5.

### 6.4 Conclusions

In this chapter we have presented a simple and efficient procedure to extract the spontaneous emission rate from short-time FDTD simulation data of the electromagnetic field energy in microcavities of arbitrary geometry. We demonstrated its validity by comparison with L(R)DOS calculations for two-dimensional triangular-lattice photonic crystals.

By using an unconditionally stable algorithm to compute the L(R)DOS we do not have to solve an eigenvalue problem. This is an important advantage over methods that compute the L(R)DOS by integrating the modulus of the electric field in the first Brillouin zone. However, computing the LRDOS gives only qualitative information about the emission rate, while computing the emitted energy gives quantitative information about the emission rate. By using the unconditionally stable method to compute the emitted energy, we are guaranteed that, in the absence of external currents, the algorithm conserves the energy exactly. This ensures that the time-dependence of the emitted energy is due to the presence of the source only. Hence, extracting the spontaneous emission rate from short-time FDTD simulation data of the electromagnetic field energy, obtained by an unconditionally stable method to solve the time-dependent Maxwell equations, is the most simple and efficient method to study spontaneous emission in arbitrary microcavities.
Appendix A

The Brillouin zone

In this appendix we explain the concept of first (irreducible) and higher Brillouin zones for the two-dimensional square and triangular lattice closely following [191]. A fundamental concept in the description of a crystalline solid, or in general a periodic structure, is the Bravais lattice, which specifies the periodic array in which the repeated units of the structure (such as the crystal) are arranged [191]. A Bravais lattice consists of all points with position vectors \( \mathbf{R} \) of the form

\[
\mathbf{R} = \sum_i n_i \mathbf{a}_i,
\]

(A.1)

where \( \mathbf{a}_i \) are linear independent vectors, and \( n_i \) range through all integers. The vectors \( \mathbf{a}_i \) are called primitive vectors and are said to generate or span the lattice. A Bravais lattice is thus an infinite array of discrete points with an arrangement and orientation that appears exactly the same, from whichever of the points the array is viewed [191].

Consider a set of points \( \mathbf{R} \) constituting a Bravais lattice, and a plane wave \( e^{i \mathbf{k} \cdot \mathbf{r}} \). Wave vectors \( \mathbf{K} \), which satisfy the relation

\[
e^{i \mathbf{K} \cdot (\mathbf{r} + \mathbf{R})} = e^{i \mathbf{K} \cdot \mathbf{r}},
\]

(A.2)

for any \( \mathbf{r} \) and for any \( \mathbf{R} \), belong to the reciprocal lattice of a Bravais lattice of points \( \mathbf{R} \). Factoring out \( e^{i \mathbf{K} \cdot \mathbf{r}} \), the reciprocal lattice can be characterized as the set of wave vectors \( \mathbf{K} \) satisfying

\[
e^{i \mathbf{K} \cdot \mathbf{R}} = 1, \quad \text{i.e.} \quad \mathbf{K} \cdot \mathbf{R} = N \cdot 2\pi,
\]

(A.3)

where \( N \) is an integer. A reciprocal lattice is defined with reference to a particular Bravais lattice, which is called the direct lattice. The reciprocal lattice is itself a Bravais lattice. The reciprocal lattice of a reciprocal lattice is just the original direct lattice. In three-dimensional space, if \( \mathbf{a}_i, i = 1, 2, 3 \) are a set of primitive vectors of the direct lattice, the reciprocal lattice
A. The Brillouin zone

Figure A.1: The two-dimensional square lattice. (a): Square lattice network with spacing $a$ in real space. The lattice vectors are denoted by $\mathbf{a}_1$ and $\mathbf{a}_2$. (b): Corresponding reciprocal lattice, a square lattice with spacing $2\pi/a$. The reciprocal lattice vectors are denoted by $\mathbf{b}_1$ and $\mathbf{b}_2$. The dotted lines are the perpendicular bisectors to the reciprocal lattice vectors connecting the origin ($\Gamma$ point) to its nearest neighbor reciprocal lattice points. The region enclosed by these lines and containing the origin is the first Brillouin zone (solid square). The shaded area is the irreducible first Brillouin zone. The symmetry points $\Gamma$, $M$ and $X$ are also shown.

can be generated by the primitive vectors $\mathbf{b}_i$, $i = 1, 2, 3$

$$\begin{align*}
\mathbf{b}_1 &= 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \\
\mathbf{b}_2 &= 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}, \\
\mathbf{b}_3 &= 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}. 
\end{align*} \tag{A.4}$$

In reciprocal space we can construct a region that surrounds the origin such that all $k$-points enclosed are closer to the origin than to any other reciprocal lattice point. This set of points in $k$-space is called the first Brillouin zone. As is geometrically evident, the first Brillouin zone is the region enclosed by the sets of planes that are perpendicular bisectors to the lattice vectors connecting the origin in $k$-space to its nearest neighbor reciprocal lattice points. In general, planes that are perpendicular bisectors of a line joining the origin of $k$-space of a reciprocal lattice points are called Bragg planes. Hence, the first Brillouin zone can also be defined as the set of points in $k$-space that can be reached from the origin without crossing any Bragg plane. Due to symmetry reasons, most of the time we only need to analyze a part of the first Brillouin zone. This part is called the irreducible first Brillouin zone. Higher Brillouin zones are simply other regions bounded by the Bragg planes. The second Brillouin zone is
defined as the set of points that can be reached from the first Brillouin zone by crossing only one Bragg plane. Similarly, the \( n \)th Brillouin zone is the set of points that can be reached from the \((n - 1)\)th zone by crossing one and only one Bragg plane. Alternatively, the \( n \)th Brillouin zone can be defined as the set of points that can be reached from the origin by crossing \( n - 1 \) Bragg planes, but no fewer.

We now consider the two mostly used two-dimensional lattices, namely the square and the triangular lattice (often mistakenly called hexagonal lattice). For a square lattice with spacing \( a \), the simplest lattice vectors are

\[
a_1 = a \hat{x} \quad \text{and} \quad a_2 = a \hat{y},
\]

(A.5)

where \( \hat{x} \) and \( \hat{y} \) denote unit vectors along the \( x \) and \( y \) axis, respectively. In order to use (A.4), we can use a third basis vector in the \( z \)-direction of any length. The results are

\[
b_1 = (2\pi/a) \hat{x} \quad \text{and} \quad b_2 = (2\pi/a) \hat{y}.
\]

(A.6)

It is easily seen that the reciprocal lattice of the square lattice is also a square lattice, but with spacing \( 2\pi/a \) instead of \( a \). The original lattice, the reciprocal lattice, the first Brillouin zone and the irreducible first Brillouin zone of the square lattice are depicted in Fig. A.1 The high symmetry \( k \)-points, which are the three corners of the irreducible first Brillouin zone, are
A. The Brillouin zone

Figure A.3: The Brillouin zones for (a): the square lattice and (b): the triangular lattice. The solid circles are the lattice points and the dashed lines are the Bragg lines. The first four Brillouin zones are marked with different gray scales.

given by

\[ \Gamma : \quad k_x = 0, \quad k_y = 0, \quad (A.7a) \]
\[ M : \quad k_x = \pi/a, \quad k_y = \pi/a, \quad (A.7b) \]
\[ X : \quad k_x = \pi/a, \quad k_y = 0. \quad (A.7c) \]

For a triangular lattice with spacing \( a \), the lattice vectors can be chosen as

\[ a_1 = a(\sqrt{3}\hat{x} + \hat{y})/2 \quad \text{and} \quad a_2 = a\hat{y}, \quad (A.8) \]
as shown in Fig. Fig. A.2 Using (A.4), we obtain the reciprocal lattice vectors

\[ b_1 = \frac{4\pi}{\sqrt{3}a} \hat{x} \quad \text{and} \quad b_2 = \frac{4\pi}{\sqrt{3}a}(-\frac{\sqrt{3}}{2}\hat{x} + \frac{1}{2}\hat{y}). \quad (A.9) \]

The reciprocal lattice is again a triangular lattice. Fig. A.2 shows the original lattice, the reciprocal lattice, the first Brillouin zone and the irreducible first Brillouin zone. The three corners of the irreducible first Brillouin zone, the high symmetry \( k \)-points, are defined as
follows

\( \Gamma : \quad k_x = 0, \quad k_y = 0, \quad \)  
(A.10a)

\( \text{M : } \quad k_x = \frac{2\pi}{\sqrt{3}a}, \quad k_y = 0, \quad \)  
(A.10b)

\( \text{K : } \quad k_x = \frac{2\pi}{\sqrt{3}a}, \quad k_y = \frac{2\pi}{3a}. \quad \)  
(A.10c)

In Fig. A.3 we show the Bragg planes (dashed lines) and the first four Brillouin zones for the two-dimensional square lattice and triangular lattice space.