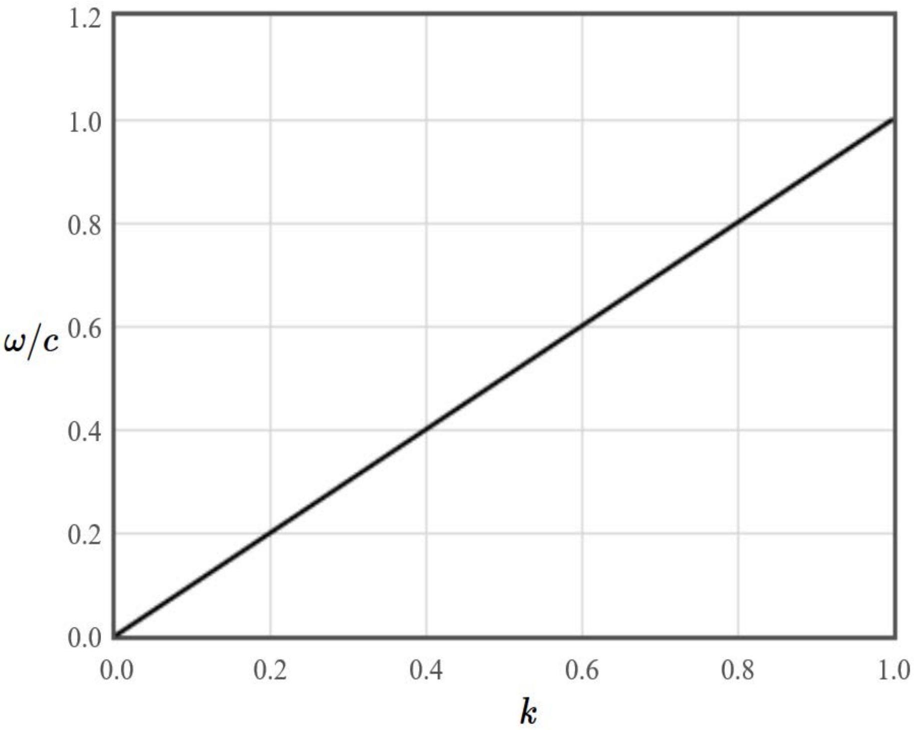
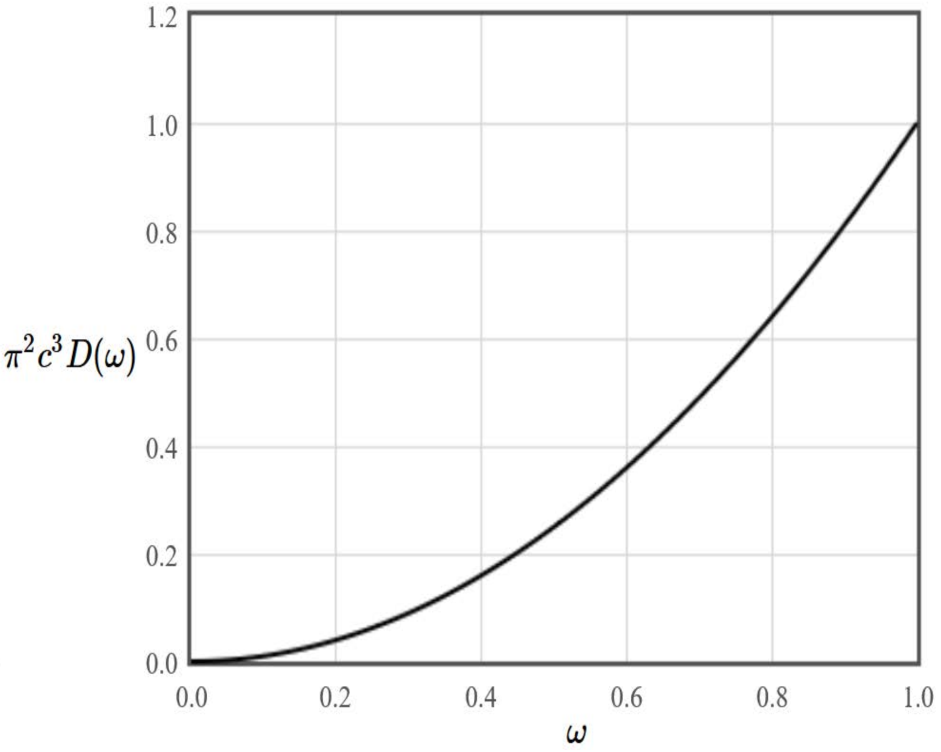
Photonic Crystals

Light in vacuum



Dispersion relation

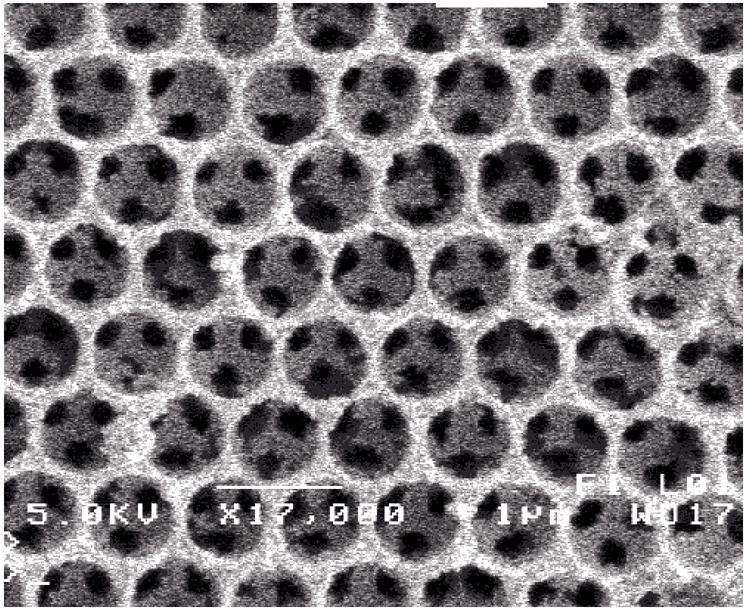


Density of states

Light in a crystal

Light moving in a periodic structure will be diffracted when the diffraction condition is satisfied.

$$\Delta\vec{k} = \vec{G}$$



Any periodic function can be represented as a Fourier series

$$f(\vec{r}) = \sum_{\vec{G}} f_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$$

G = reciprocal lattice vector (depends on the Bravais lattice)

For real functions: $f_G^* = f_{-G}$

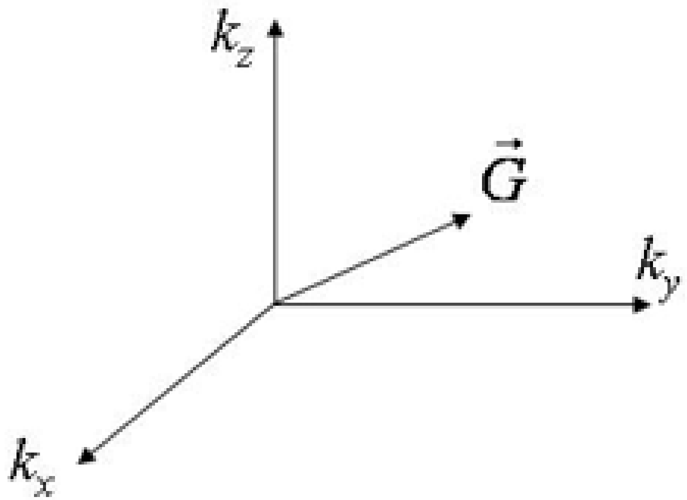
Every Bravais lattice has a reciprocal lattice.

Reciprocal space

K-space is a space of plane waves.

A k-vector points in the direction that the wave is moving.

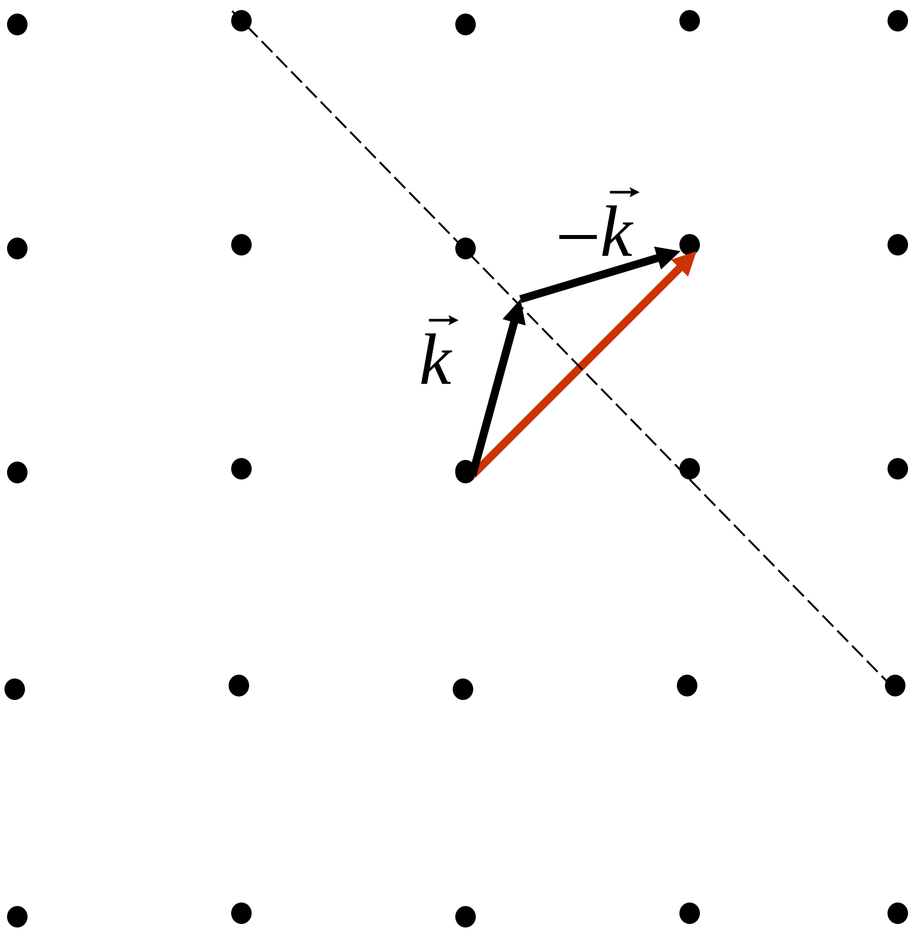
$$\lambda = \frac{2\pi}{\left|\vec{k}\right|}$$



Plane wave:

$$\exp(-i\vec{G}\cdot\vec{r}) = \cos(G_x x + G_y y + G_z z) + i\sin(G_x x + G_y y + G_z z)$$

Diffraction condition



$$\vec{k}' - \vec{k} = \vec{G}$$

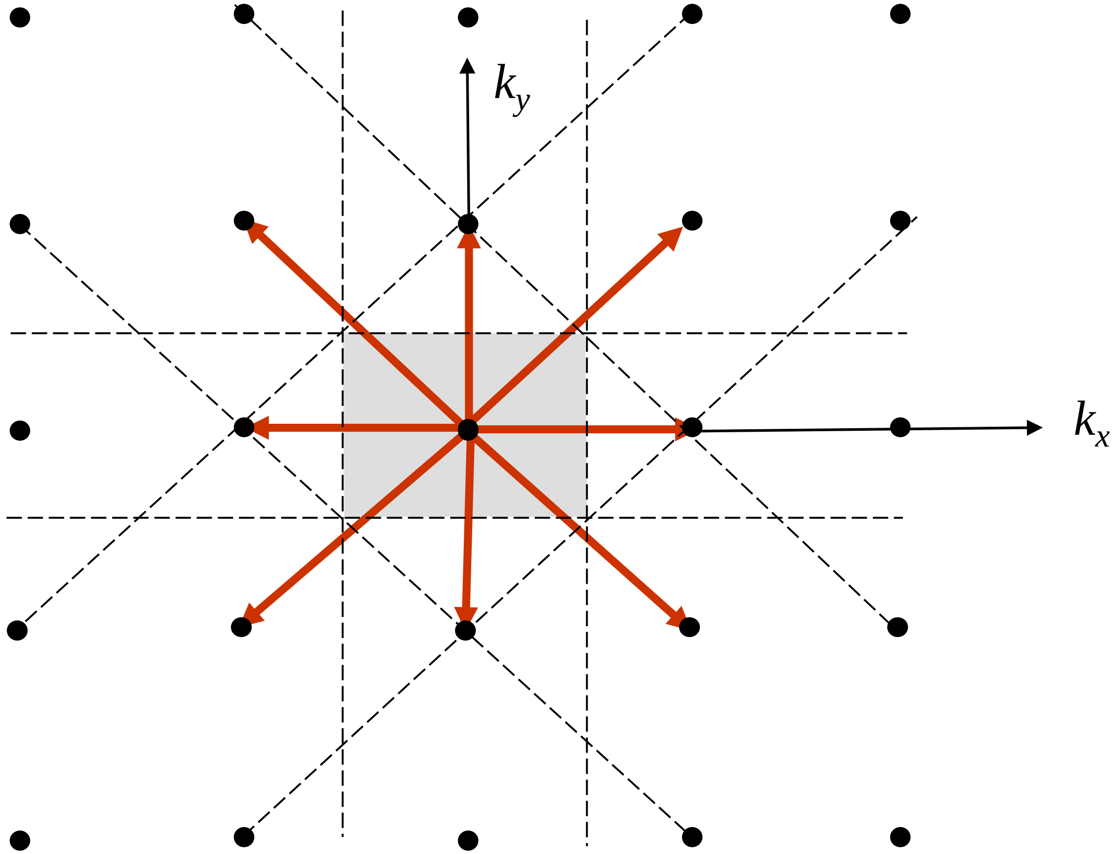
For every *G* there is a -*G* so the diffraction condition can also be written as

$$\vec{k} - \vec{k}' = \vec{G}$$

a wave will be diffracted if the wave vector ends on one of the planes

Brillouin zones

Leon Brillouin



1st Brillouin zone consists of the *k*-states around the origin that can be reached without crossing a plane.

Bloch Theorem

$$f(\vec{r}) = \sum_{\vec{k}} C_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$$ ← Any wave function that satisfies periodic boundary conditions

$$f(\vec{r}) = \sum_{\vec{k}\in 1Bz} \sum_{\vec{G}} C_{\vec{k}+\vec{G}} e^{i\left(\vec{k}+\vec{G}\right)\cdot\vec{r}}$$

These *k*'s label the symmetries

$$f_{\vec{k}}(\vec{r}) = \sum_{\vec{G}} C_{\vec{k}+\vec{G}} e^{i(\vec{k}+\vec{G})\cdot\vec{r}} = e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}} C_{\vec{k}+\vec{G}} e^{i\vec{G}\cdot\vec{r}} = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$$

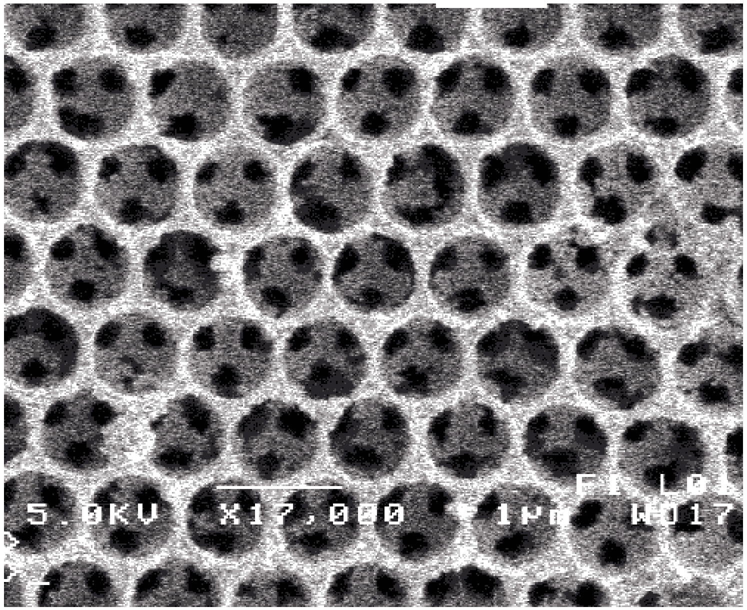
periodic function

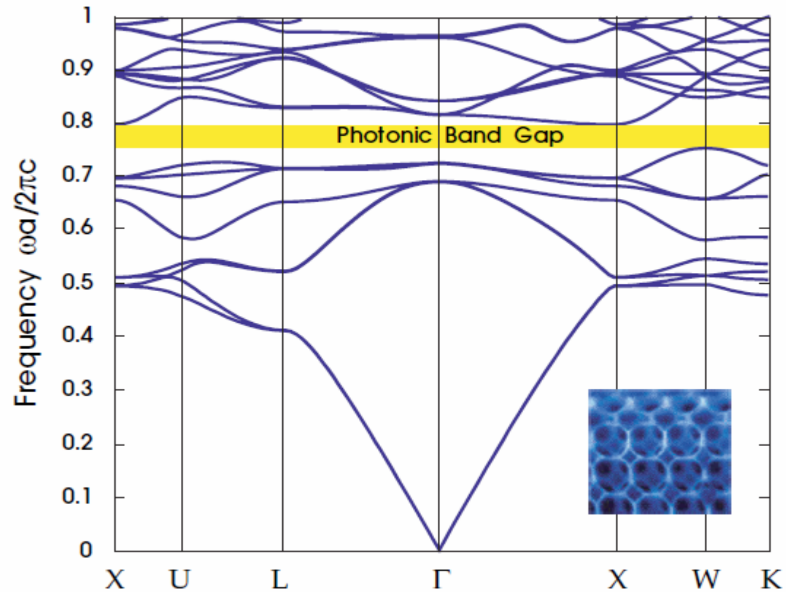
Bloch form $f_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$

$$T_{mnl} f_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot(\vec{r}+m\vec{a}_1+n\vec{a}_2+l\vec{a}_3)} u_{\vec{k}}(\vec{r}+m\vec{a}_1+n\vec{a}_2+l\vec{a}_3) = e^{i\vec{k}\cdot(m\vec{a}_1+n\vec{a}_2+l\vec{a}_3)} f_{\vec{k}}(\vec{r})$$

Eigen function solutions of the translation operator have Bloch form.

Inverse opal photonic crystal





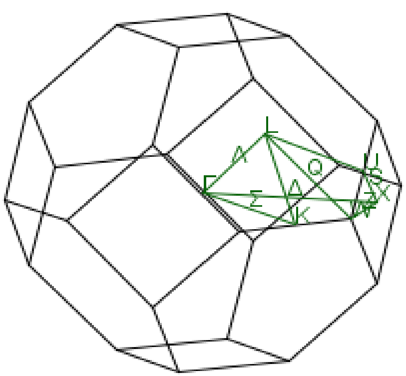


Figure 8: The photonic band structure for the lowest bands of an "inverse opal" structure: a face-centered cubic (fcc) lattice of close-packed air spheres in dielectric ($\varepsilon = 13$). (Inset shows fabricated structure from figure 9.) There is a complete photonic band gap (yellow) between the eighth and ninth bands. The wave vector varies across the irreducible Brillouin zone between the labelled high-symmetry points; see appendix B for a discussion of the Brillouin zone of an fcc lattice.

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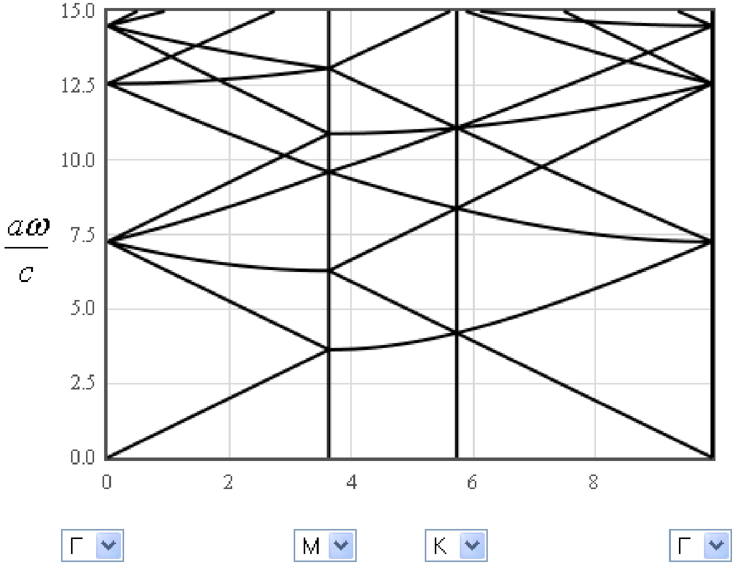
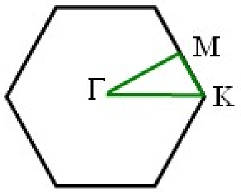
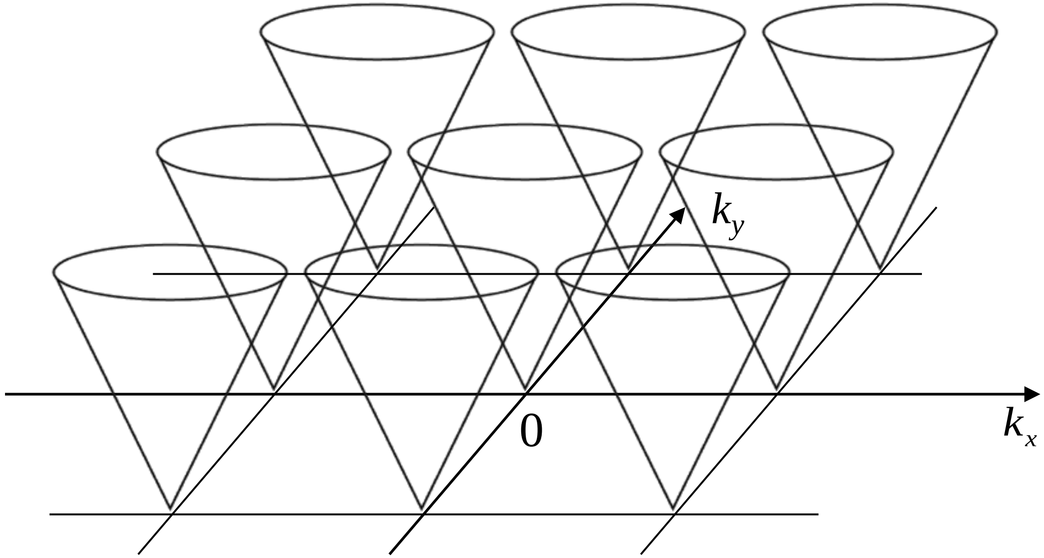
Empty lattice approximation



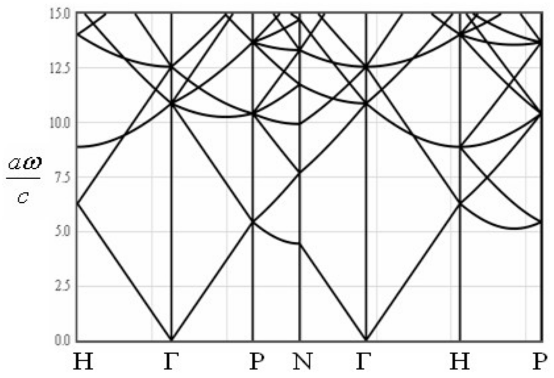




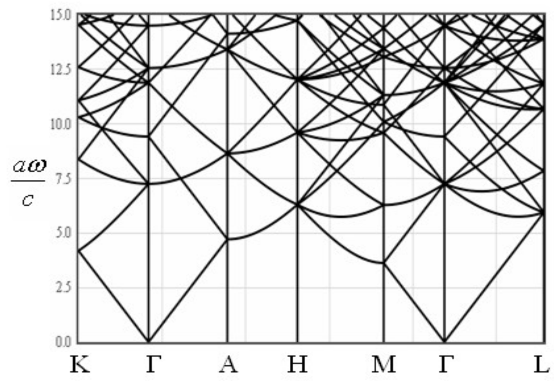
$$\omega = c\left|\vec{k}\right|$$

Empty lattice approximation

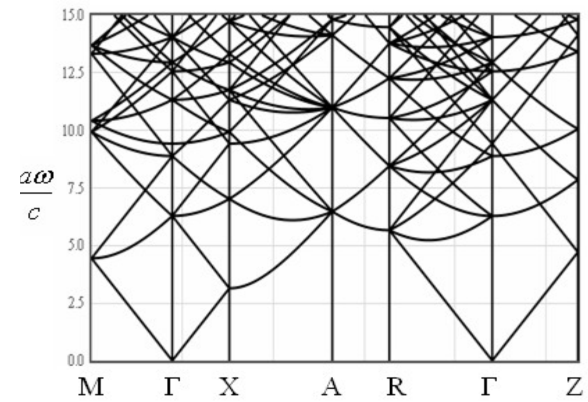
Body centered cubic

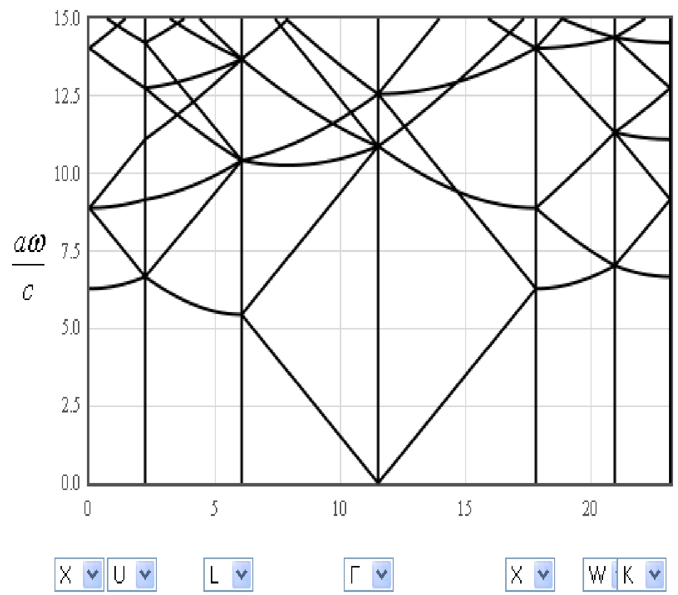


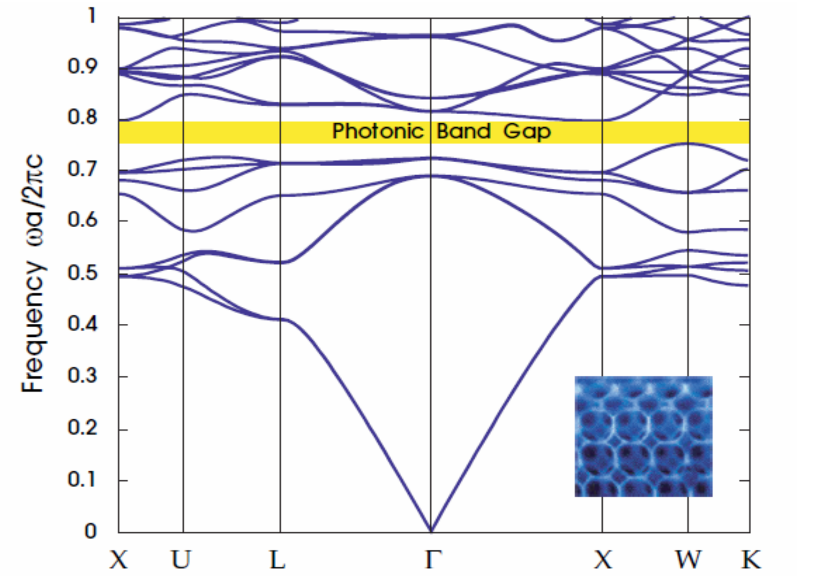
Hexagonal



Tetragonal







Plane wave method

$$c(\vec{r})^2 \nabla^2 A_j = \frac{d^2 A_j}{dt^2}$$

$$c(\vec{r})^2 = \sum_{\vec{G}} b_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \qquad A_j = \sum_{\vec{k}} A_{\vec{k}} e^{i\left(\vec{k}\cdot\vec{r}-\omega t\right)}$$

$$\sum_{\vec{G}} b_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} \sum_{\vec{\kappa}} \left(-\kappa^2\right) A_{\vec{\kappa}} e^{i\left(\vec{\kappa}\cdot\vec{r}-\omega t\right)} = -\omega^2 \sum_{\vec{k}} A_{\vec{k}} e^{i\left(\vec{k}\cdot\vec{r}-\omega t\right)}$$

$$\sum_{\vec{\kappa}} \sum_{\vec{G}} \left(-\kappa^2\right) b_{\vec{G}} A_{\vec{\kappa}} e^{i\left(\vec{G}\cdot\vec{r}+\vec{\kappa}\cdot\vec{r}-\omega t\right)} = -\omega^2 \sum_{\vec{k}} A_{\vec{k}} e^{i\left(\vec{k}\cdot\vec{r}-\omega t\right)}$$

collect like terms: $\vec{G}+\vec{\kappa}=\vec{k} \quad \Rightarrow \quad \vec{\kappa}=\vec{k}-\vec{G}$

Central equations: $$\sum_{\vec{G}} \left(\vec{k}-\vec{G}\right)^2 b_{\vec{G}} A_{\vec{k}-\vec{G}} = \omega^2 A_{\vec{k}}$$

Plane wave method

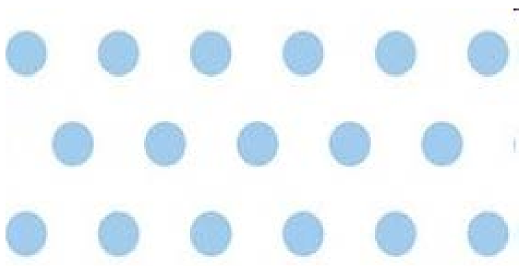
Central equations: $$\sum_{\vec{G}}\left(\vec{k}-\vec{G}\right)^2 b_{\vec{G}} A_{\vec{k}-\vec{G}} = \omega^2 A_{\vec{k}}$$

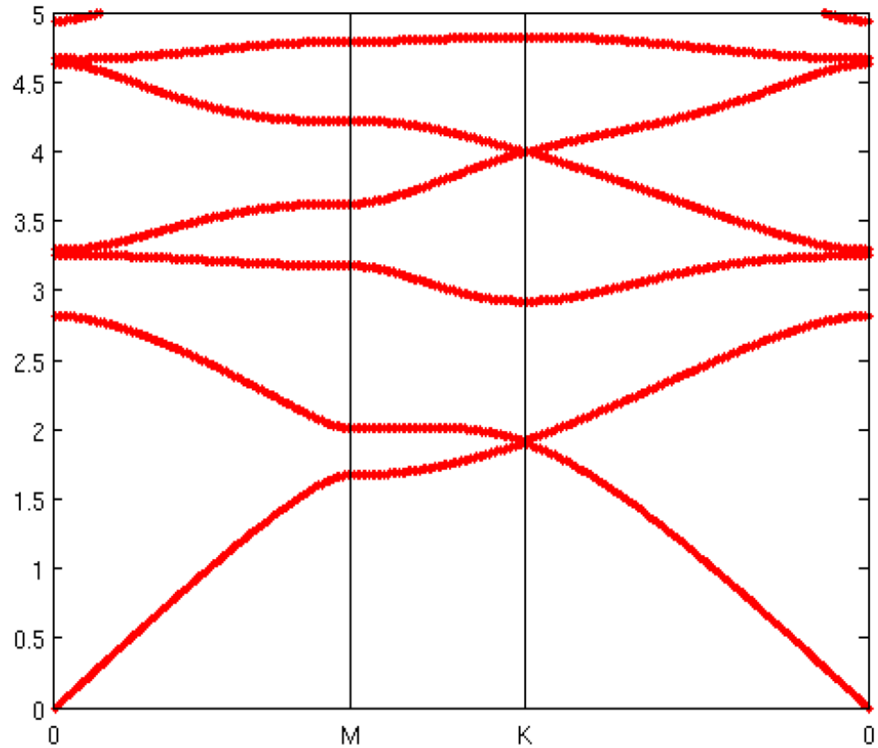
Choose a k value inside the 1st Brillouin zone. The coefficient A_k is coupled by the central equations to coefficients A_k outside the 1st Brillouin zone. Write these coupled equations in matrix form.

$$\begin{bmatrix} \left(\vec{k}+\vec{G}_2\right)^2 b_0 & \left(\vec{k}+\vec{G}_2-\vec{G}_1\right)^2 b_{\vec{G}_1} & k^2 b_{\vec{G}_2} & \left(\vec{k}+\vec{G}_2-\vec{G}_3\right)^2 b_{\vec{G}_3} & \left(\vec{k}+\vec{G}_2-\vec{G}_4\right)^2 b_{\vec{G}_4} \\ \left(\vec{k}+2\vec{G}_1\right)^2 b_{-\vec{G}_1} & \left(\vec{k}+\vec{G}_1\right)^2 b_0 & k^2 b_{\vec{G}_1} & \left(\vec{k}+\vec{G}_1-\vec{G}_2\right)^2 b_{\vec{G}_2} & \left(\vec{k}+\vec{G}_1-\vec{G}_3\right)^2 b_{\vec{G}_3} \\ \left(\vec{k}+\vec{G}_2\right)^2 b_{-\vec{G}_2} & \left(\vec{k}+\vec{G}_1\right)^2 b_{-\vec{G}_1} & k^2 b_0 & \left(\vec{k}-\vec{G}_1\right)^2 b_{\vec{G}_1} & \left(\vec{k}-\vec{G}_2\right)^2 b_{\vec{G}_2} \\ \left(\vec{k}-\vec{G}_1+\vec{G}_3\right)^2 b_{-\vec{G}_3} & \left(\vec{k}-\vec{G}_1+\vec{G}_2\right)^2 b_{-\vec{G}_2} & k^2 b_{-\vec{G}_1} & \left(\vec{k}-\vec{G}_1\right)^2 b_0 & \left(\vec{k}-2\vec{G}_1\right)^2 b_{\vec{G}_1} \\ \left(\vec{k}-\vec{G}_2+\vec{G}_4\right)^2 b_{-\vec{G}_4} & \left(\vec{k}-\vec{G}_2+\vec{G}_3\right)^2 b_{-\vec{G}_3} & k^2 b_{-\vec{G}_2} & \left(\vec{k}-\vec{G}_2+\vec{G}_1\right)^2 b_{-\vec{G}_1} & \left(\vec{k}-\vec{G}_2\right)^2 b_0 \end{bmatrix} \begin{bmatrix} A_{k+G_2} \\ A_{k+G_1} \\ A_k \\ A_{k-G_1} \\ A_{k-G_2} \end{bmatrix} = \omega^2 \begin{bmatrix} A_{k+G_2} \\ A_{k+G_1} \\ A_k \\ A_{k-G_1} \\ A_{k-G_2} \end{bmatrix}$$

There is a matrix like this for every k value in the 1st Brillouin zone.

Close packed circles in 2-D

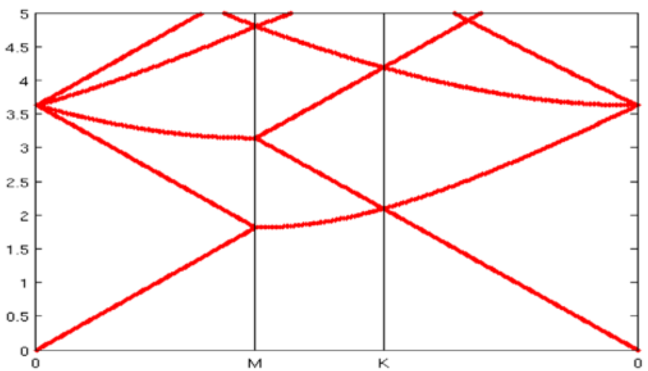


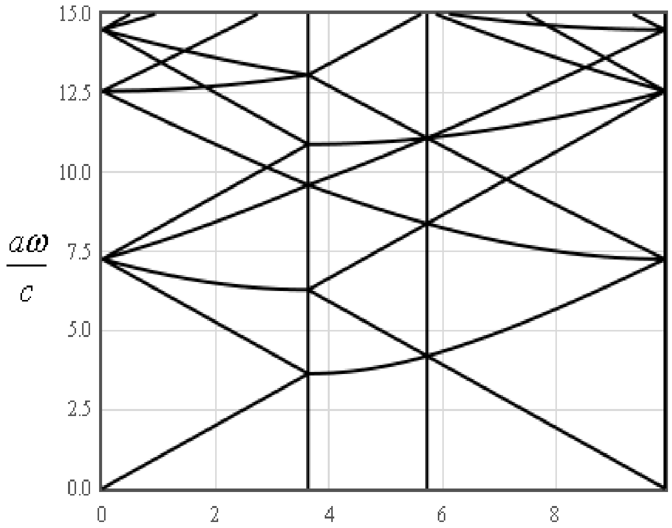


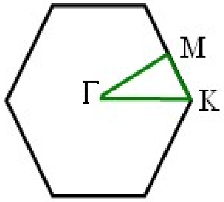
Solved by a student with the plane wave method

Uniform speed of light

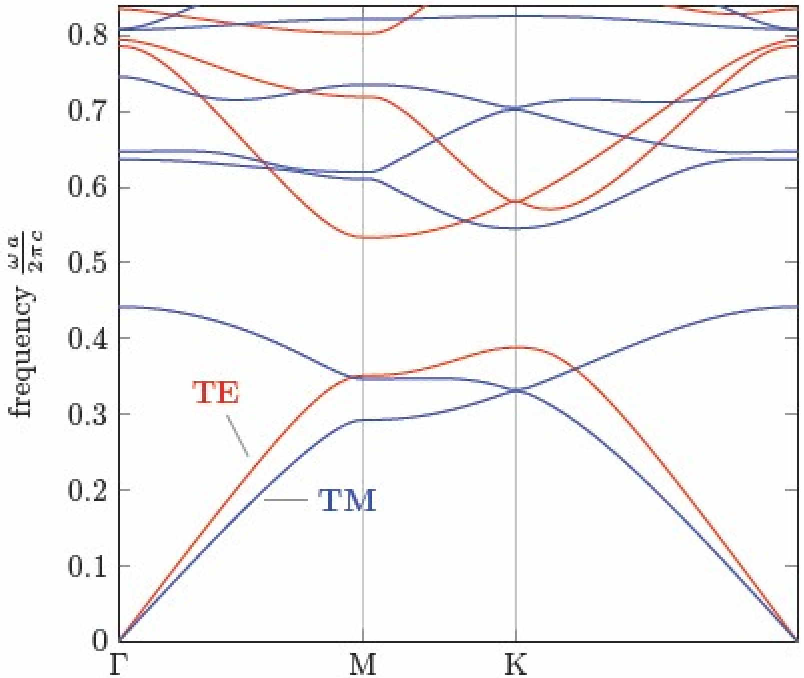
$$\begin{bmatrix} (\vec{k}+\vec{G}_2)^2 b_0-\omega^2 & 0 & 0 & 0 & 0 \\ 0 & (\vec{k}+\vec{G}_1)^2 b_0-\omega^2 & 0 & 0 & 0 \\ 0 & 0 & k^2 b_0-\omega^2 & 0 & 0 \\ 0 & 0 & 0 & (\vec{k}-\vec{G}_1)^2 b_0-\omega^2 & 0 \\ 0 & 0 & 0 & 0 & (\vec{k}-\vec{G}_2)^2 b_0-\omega^2 \end{bmatrix} \begin{bmatrix} A_{k+G_2} \\ A_{k+G_1} \\ A_k \\ A_{k-G_1} \\ A_{k-G_2} \end{bmatrix} = 0$$



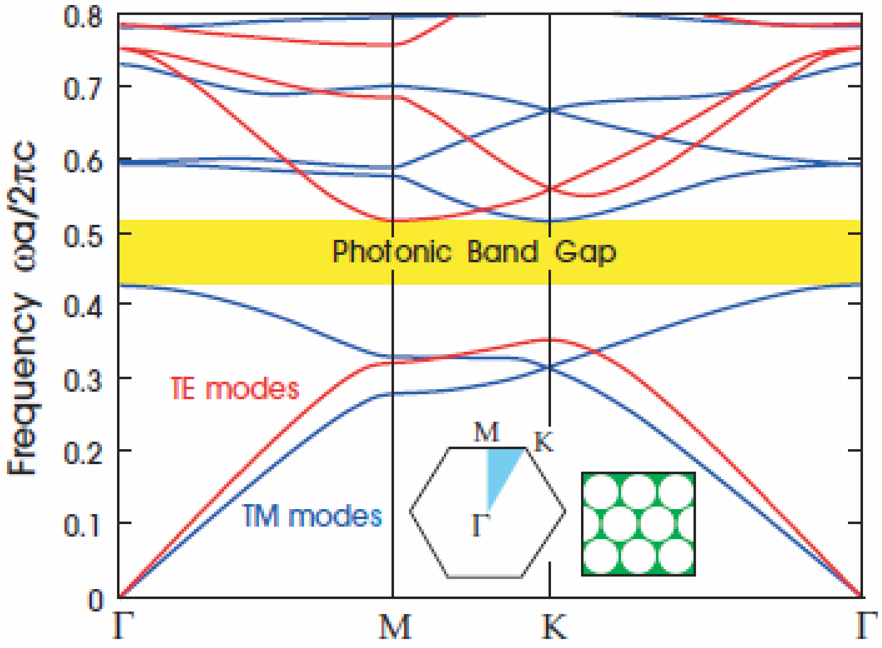




2-D array of air columns



Student project



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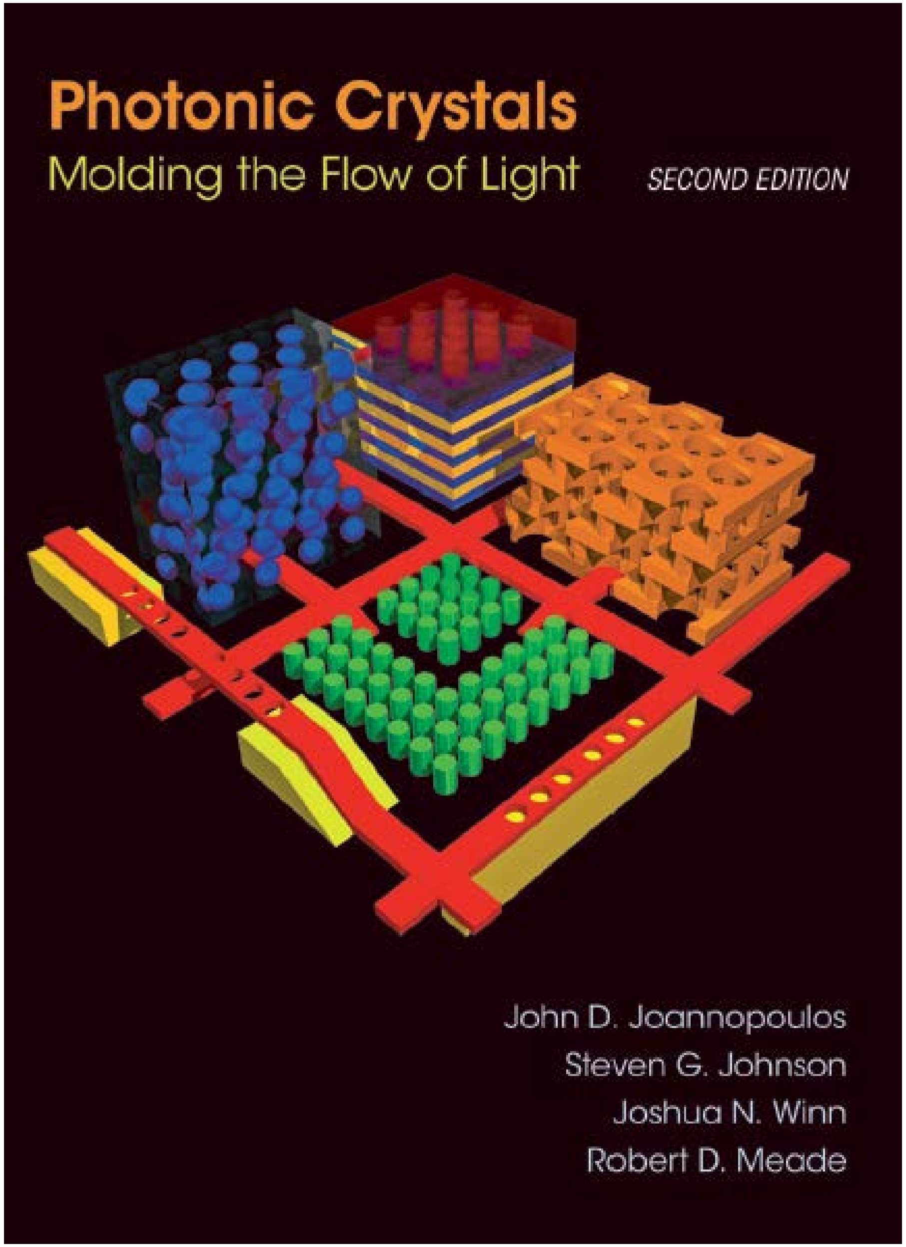
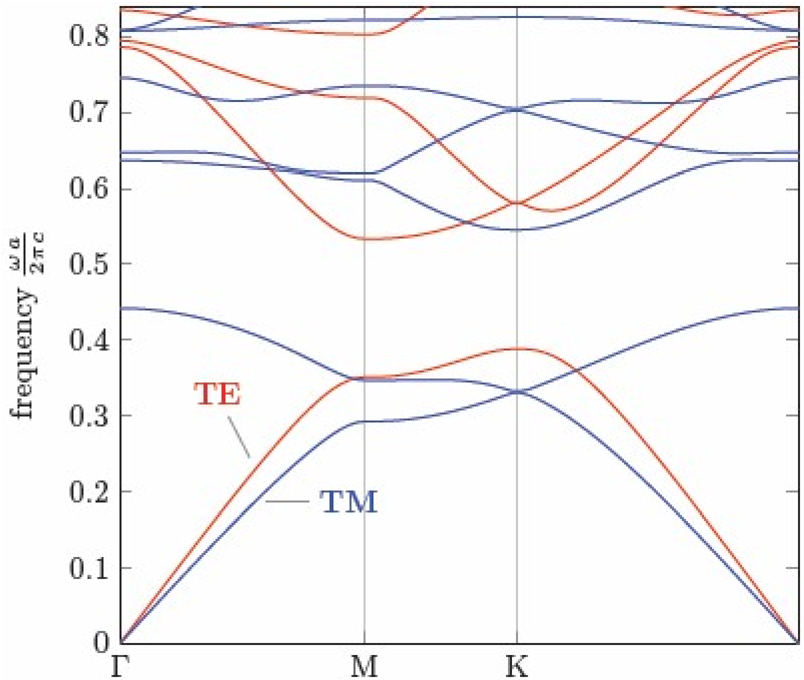
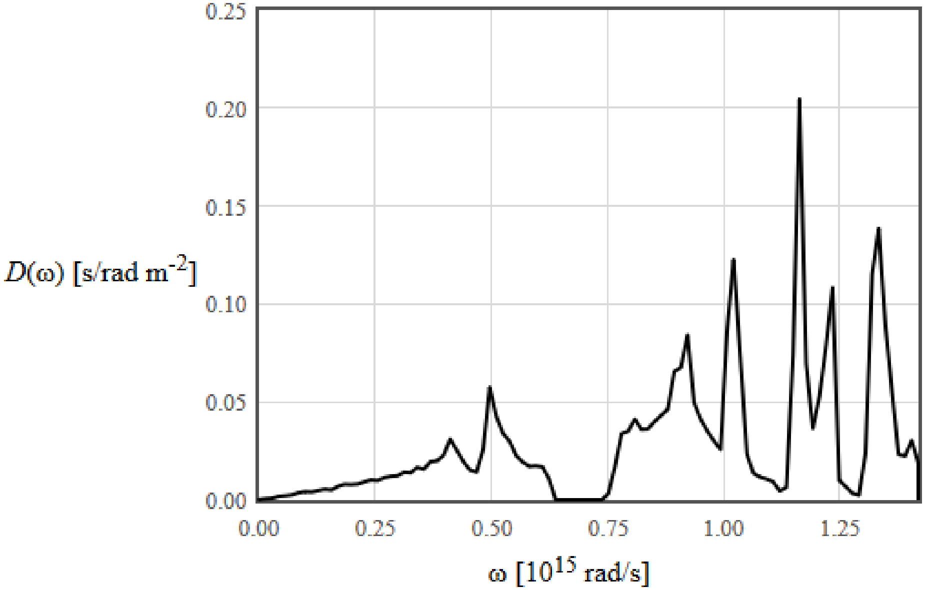


Use the plane wave method to calculate photon dispersion relations and densities of states.

2-D array of air columns





ω [rad/s]	$D(\omega)$ [rad/s m^{-2}]
0.0000	0.0000
1.4193e+11	0.00013904
1.4335e+13	0.00055617
2.8528e+13	0.00083426
4.2721e+13	0.0018076
5.6914e+13	0.0020856
7.1107e+13	0.0025028
8.5299e+13	0.0036151
9.9492e+13	0.0041713
1.1369e+14	0.0040322
1.2788e+14	0.0047275

Density of states → Specific heat

The specific heat is the derivative of the internal energy with respect to the temperature.

$$c_v = \left(\frac{\partial u}{\partial T}\right)_{V,N}$$

This can be expressed in terms of an integral over the frequency ω.

$$c_v = \frac{\partial}{\partial T}\int u(\omega)d\omega = \frac{\partial}{\partial T}\int \hbar\omega D(\omega)\frac{1}{e^{\frac{\hbar\omega}{k_BT}}-1}d\omega$$

The Leibniz integral rule can be used to bring the differentiation inside the integral. If the photon density of states $D(\omega)$ is temperature independent, the result is,

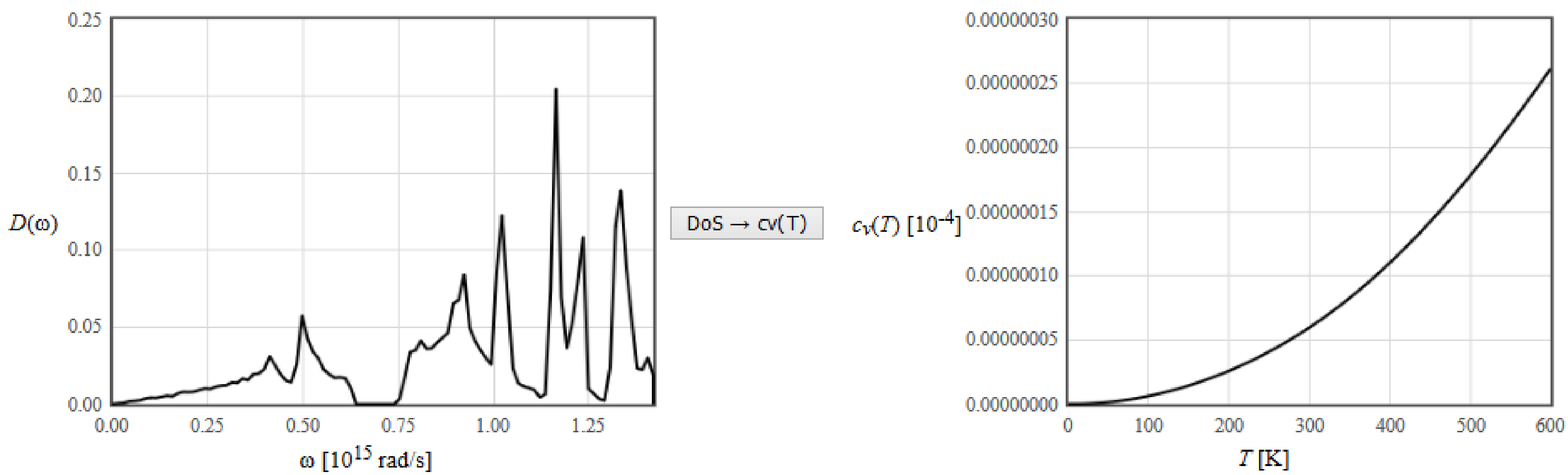
$$c_v = \int \hbar\omega D(\omega)\frac{\partial}{\partial T}\left(\frac{1}{e^{\frac{\hbar\omega}{k_BT}}-1}\right)d\omega$$

Since only the Bose-Einstein factor depends on temperature, the differentiation can be performed analytically and the expression for the specific heat is,

$$c_v = \int \left(\frac{\hbar\omega}{T}\right)^2 \frac{D(\omega)e^{\frac{\hbar\omega}{k_BT}}}{k_B\cdot\left(e^{\frac{\hbar\omega}{k_BT}}-1\right)^2}d\omega$$

The form below uses this formuula to calculate the temperature dependence of the specific heat from tabulated data for the density of states. The density of states data is input as two column at the lower left. The first column is the angular-frequency ω in rad/s. The second column is the density of states. The units of the density of states depends on the dimensionality: s/m for 1d, s/m³ for 3d.

After the 'DoS → cv(T)' button is pressed, the density of states is plotted on the left and $c_v(T)$ is plotted from temperature T_{min} to temperature T_{max} on the right. The data for the $c_v(T)$ plot als tabular form in the lower right textbox. The first column is the temperature in Kelvin and the second column is the specific heat in units of J K^{-1} m^{-1}, J K^{-1} m^{-2}, or J K^{-1} m^{-3} depending on the dimensionality.



http://lampx.tugraz.at/~hadley/ss1/dbr/dos2cv.html