Photonic Crystals \ Electrons

fcc

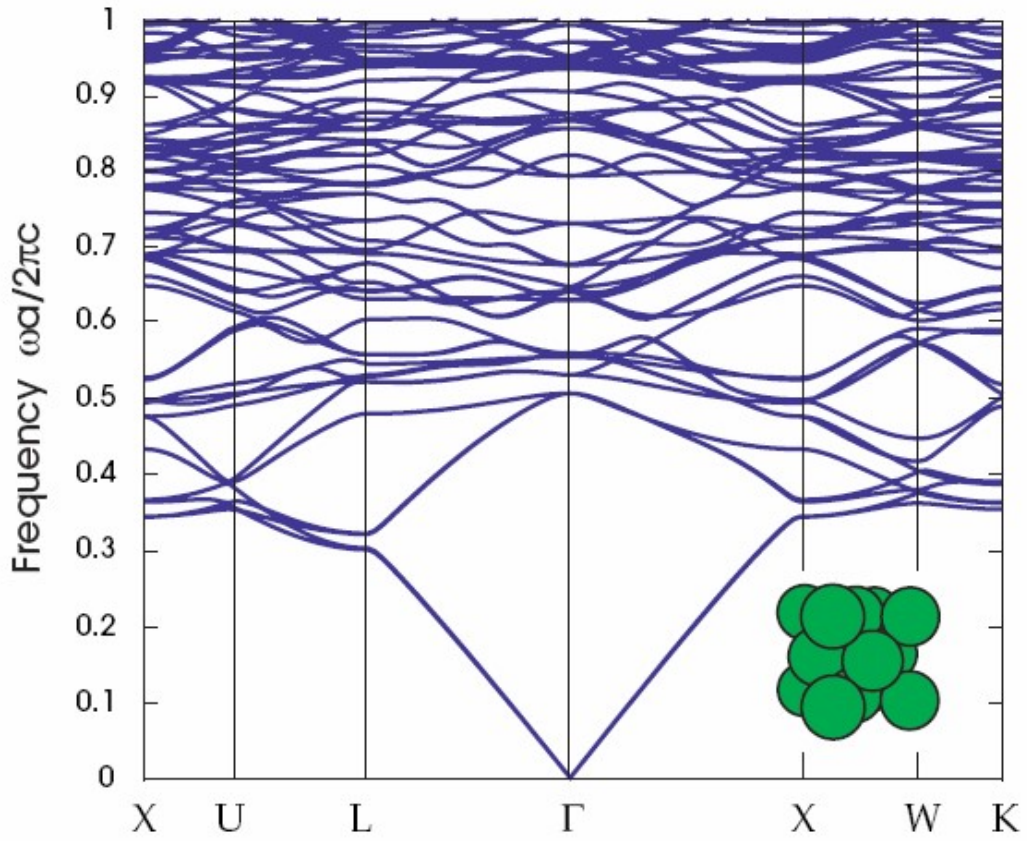

Figure 2: The photonic band structure for the lowest-frequency electromagnetic modes of a face-centered cubic (fcc) lattice of close-packed dielectric spheres ($\varepsilon = 13$) in air (inset). Note the *absence* of a complete photonic band gap. The wave vector varies across the irreducible Brillouin 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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diamond

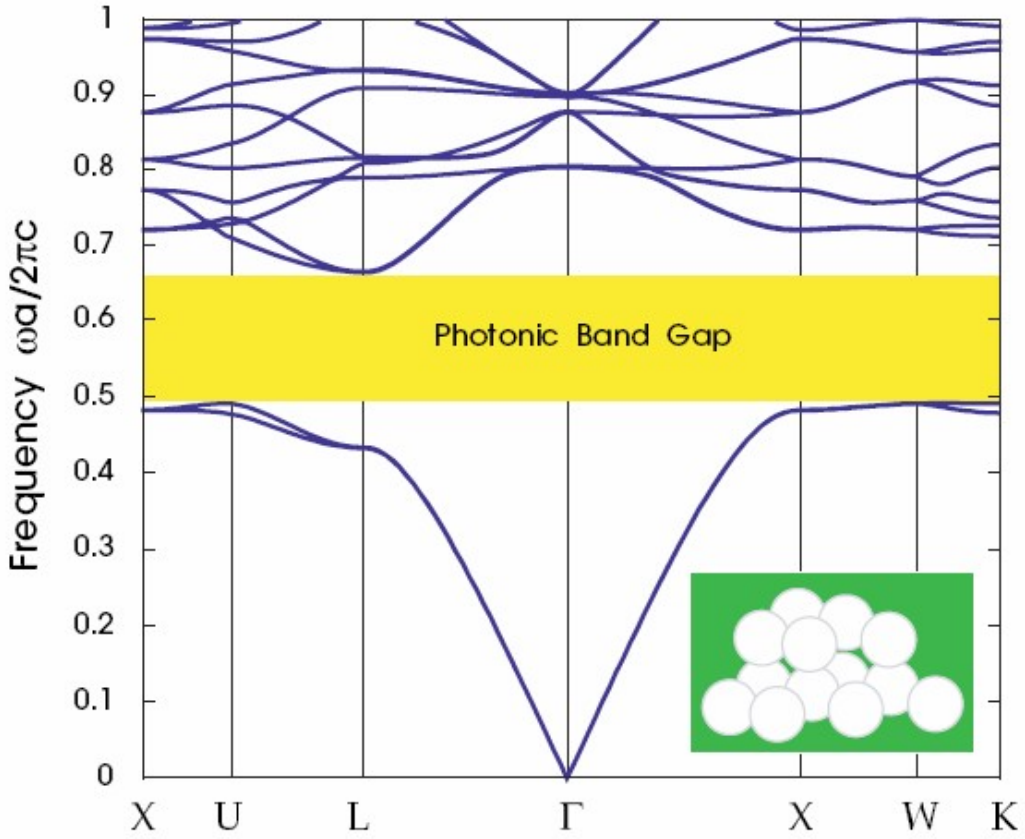

Figure 3: The photonic band structure for the lowest bands of a diamond lattice of air spheres in a high dielectric ($\varepsilon = 13$) material (inset). A complete photonic band gap is shown in yellow. The wave vector varies across the irreducible Brillouin zone between the labelled high-symmetry points; see appendix B for a discussion of the Brillouin zone of an fcc lattice.

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Yablonovite

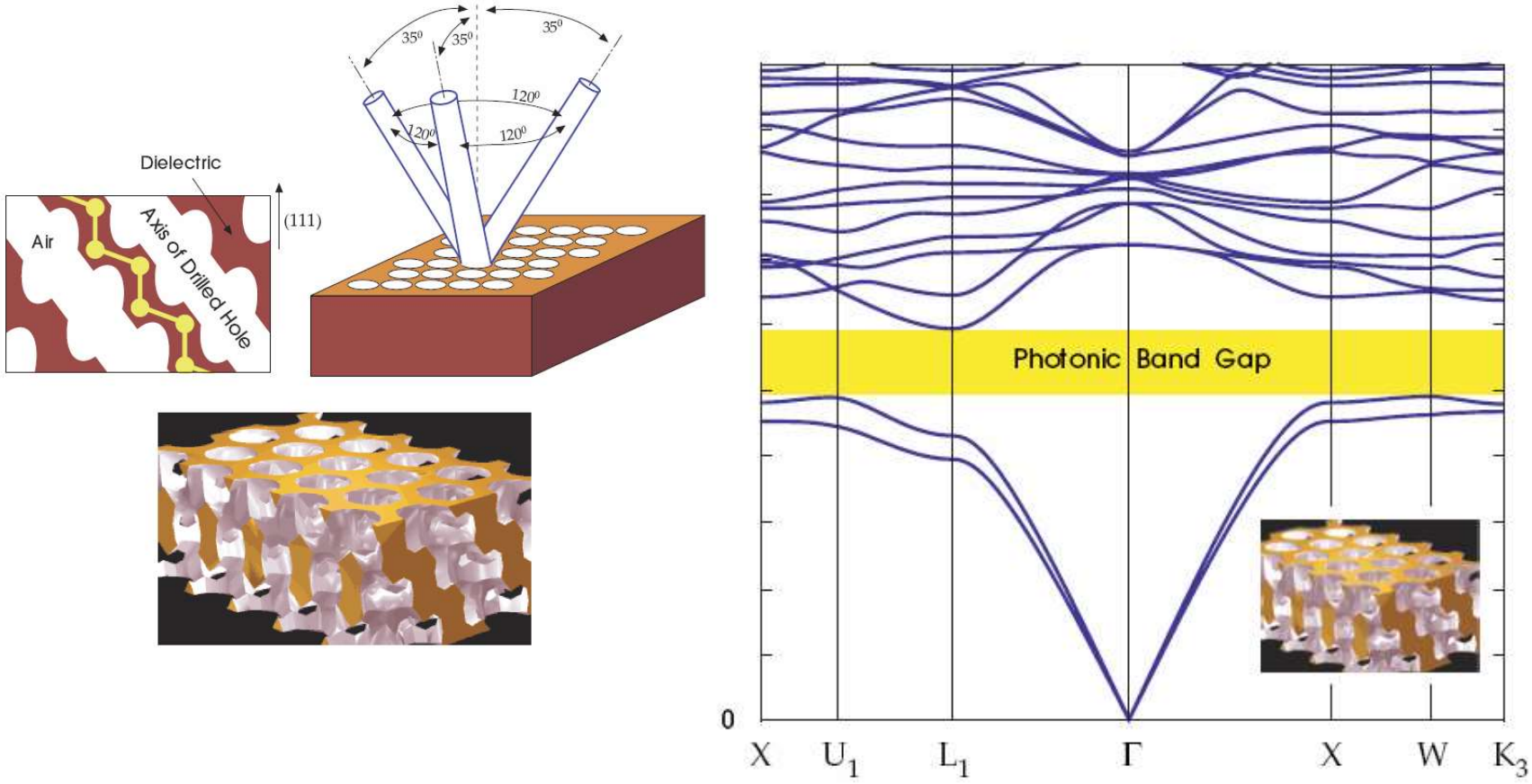

Figure 5: The photonic band structure for the lowest bands of Yablonovite (inset, from figure 4). Wave vectors are shown for a portion of the irreducible Brillouin zone that includes the edges of the complete gap (yellow). A detailed discussion of this band structure can be found in Yablonovitch et al. (1991*a*).

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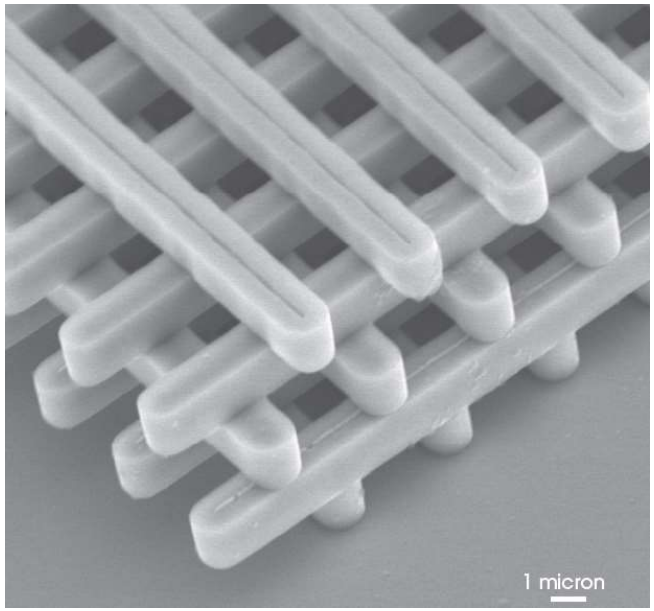
Woodpile



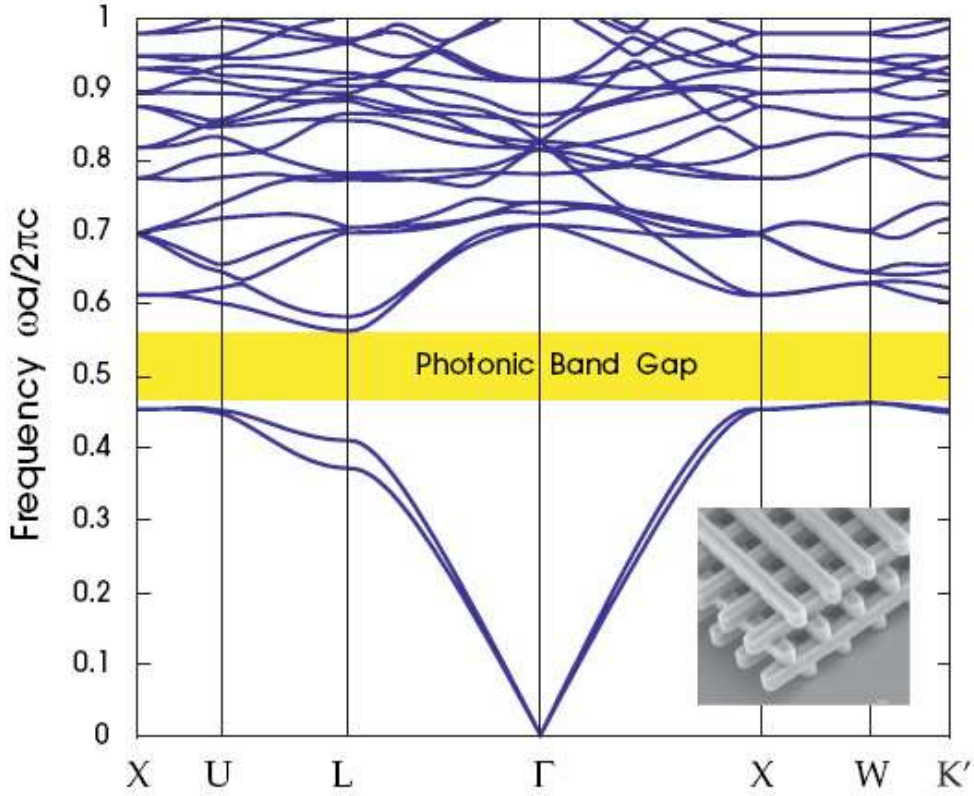


Figure 7: The photonic band structure for the lowest bands of the woodpile structure (inset, from figure 6) with $\varepsilon = 13$ logs in air. The irreducible Brillouin zone is larger than that of the fcc lattice described in appendix B, because of reduced symmetry—only a portion is shown, including the edges of the complete photonic band gap (yellow).

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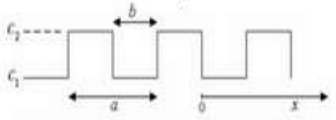
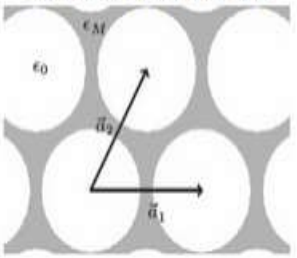
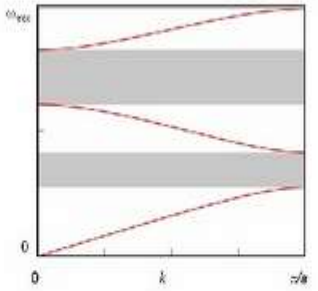
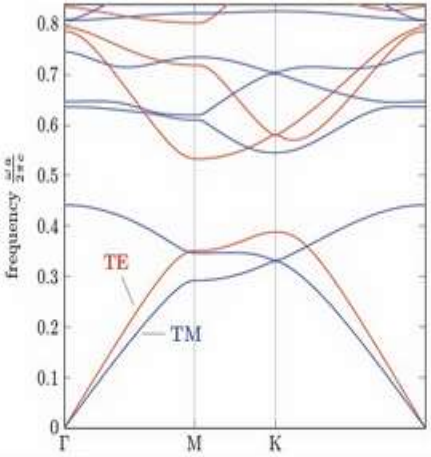
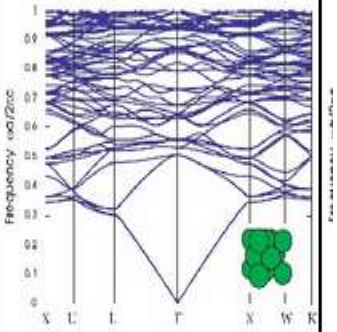
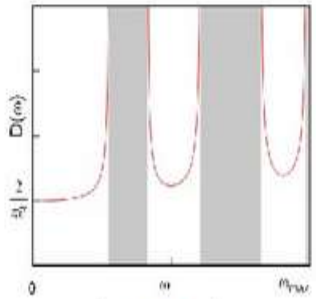
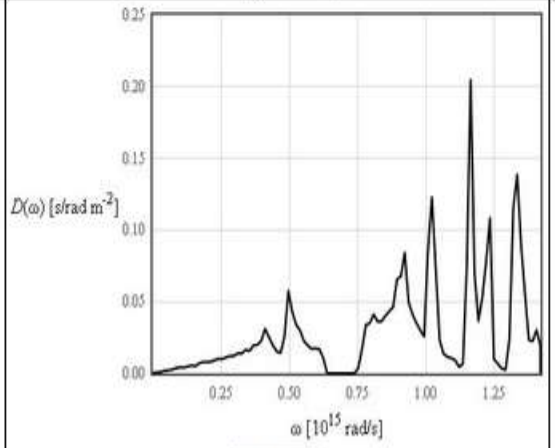
Photonic crystals

	1-D Multilayer film	2-D triangular array of air holes	fcc
	 1-D Multilayer film		 http://ab-initio.mit.edu/book
Dispersion relation	 Calculate ω(k)		 http://ab-initio.mit.edu/book
Density of states	 Calculate DoS	 Show DoS	

Student projects

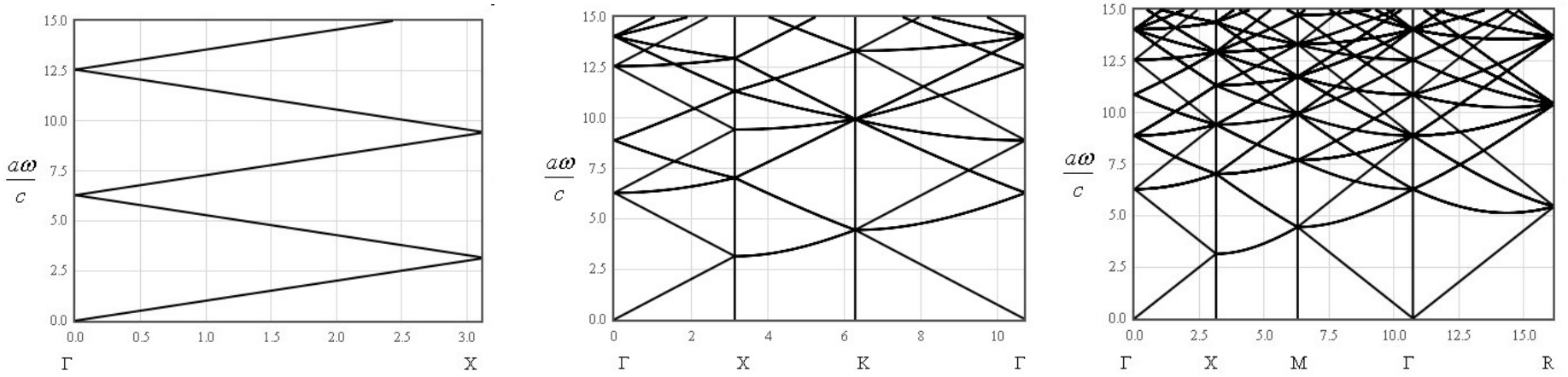
Describe the plane wave method for the web page.

Calculate the band structure and density of states for a photonic crystal.

Help complete the table of the empty lattice approximation

Write a program that calculates the photonic band structure of any 1-D crystal.

Plot the thermodynamic properties of some photonic crystal (you need the density of states)



Electrons

Thermodynamic properties

Free electrons

Fermi surfaces

Band structure calculations

- Empty lattice approximation
- Plane wave method
- Tight binding

Thermodynamic properties of non-interacting fermions

The grand canonical partition function is

$$Z_{gr} = \sum_q \exp\left(\frac{\mu}{k_B T}\right)^{N_q} \exp\left(-\frac{E_q}{k_B T}\right) = \sum_q \exp\left(-\frac{E_q - \mu N_q}{k_B T}\right)$$

Here q sums over the macro states. Only one fermion is allowed per microscopic quantum state.

$$N_q = \sum_i n_{qi} \qquad E_q = \sum_i n_{qi}\varepsilon_i \qquad n_{qi} \in 0,1$$

n_{qi} are occupation numbers that specify if microstate i is occupied in macrostate q

http://lamp.tu-graz.ac.at/~hadley/ss2/fermigas/thermo/thermo.php

Thermodynamic properties of non-interacting fermions

$$Z_{gr} = \sum_q \exp\left(-\frac{E_q - \mu N_q}{k_B T}\right) = \sum_q \exp\left(-\frac{\sum_i n_{qi}\left(\varepsilon_i - \mu\right)}{k_B T}\right) = \sum_q \prod_i \exp\left(-\frac{n_{qi}\left(\varepsilon_i - \mu\right)}{k_B T}\right)$$

The sum over all possible macrostates can also be written as the sum over all possible microstates.

$$Z_{gr} = \sum_{n_1=0}^{1}\sum_{n_2=0}^{1}\cdots\sum_{n_j=0}^{1}\cdots\prod_i \exp\left(-\frac{n_i\left(\varepsilon_i - \mu\right)}{k_B T}\right) = \prod_i\left(\exp\left(-\frac{\left(\varepsilon_i - \mu\right)}{k_B T}\right)+1\right)$$

Pull the n_i factors through the other sums then write out the sum over 0 and 1.

Thermodynamic properties of non-interacting fermions

Grand potential: $\Phi = U - TS - \mu N = -k_B T \ln(Z_{gr})$

$$\Phi = -k_B T \sum_i \ln\left(\exp\left(-\frac{(\varepsilon_i - \mu)}{k_B T} \right) + 1 \right)$$

Approximate the sum by an integral over the density of states.

$$\phi = \frac{\Phi}{V} = -k_B T \int_{-\infty}^{\infty} D(E) \ln\left(\exp\left(-\frac{(E - \mu)}{k_B T} \right) + 1 \right) dE$$

Differentiate to find the number density.

$$n = -\frac{\partial \phi}{\partial \mu} = \int_{-\infty}^{\infty} \frac{D(E)}{1 + \exp\left(\frac{E - \mu}{k_B T} \right)} dE$$

Fermi function

Thermodynamic properties

Grand potential density:

$$\phi = -k_B T \int_{-\infty}^{\infty} D(E) \ln\left(\exp\left(-\frac{(E-\mu)}{k_B T}\right)+1\right) dE$$

Helmholz free energy density:

$$f = \phi + \mu n = \int_{-\infty}^{\infty} D(E)\left(\frac{\mu}{1+\exp\left(\frac{E-\mu}{k_B T}\right)} - k_B T \ln\left(\exp\left(-\frac{(E-\mu)}{k_B T}\right)+1\right)\right) dE$$

Entropy density:

$$s = -\frac{\partial \phi}{\partial T} = \frac{1}{T}\int_{-\infty}^{\infty} D(E)\left(\frac{(E-\mu)}{1+\exp\left(\frac{(E-\mu)}{k_B T}\right)} - k_B T \ln\left(\exp\left(-\frac{(E-\mu)}{k_B T}\right)+1\right)\right) dE$$

http://lamp.tu-graz.ac.at/~hadley/ss2/fermigas/thermo/thermo.php

Thermodynamic properties

Chemical potential (implicitly defined by):

$$n = \int_{-\infty}^{\infty} \frac{D(E)}{1+\exp\left(\frac{(E-\mu)}{k_B T}\right)} dE$$

DoS → mu

Internal energy density:

$$u = \phi + Ts + \mu n = \int_{-\infty}^{\infty} \frac{ED(E)}{1+\exp\left(\frac{E-\mu}{k_B T}\right)} dE$$

DoS → u(T)

Energy spectral density:

$$u(E,T) = \frac{ED(E)}{1+\exp\left(\frac{E-\mu}{k_B T}\right)}$$

DoS → u(E)

Specific heat:

$$c_v = \frac{\partial u}{\partial T} = \int_{-\infty}^{\infty} \frac{ED(E)(E-\mu)\exp\left(\frac{E-\mu}{k_B T}\right)}{k_B T^2 \left(1+\exp\left(\frac{E-\mu}{k_B T}\right)\right)^2} dE$$

DoS → cv(T)

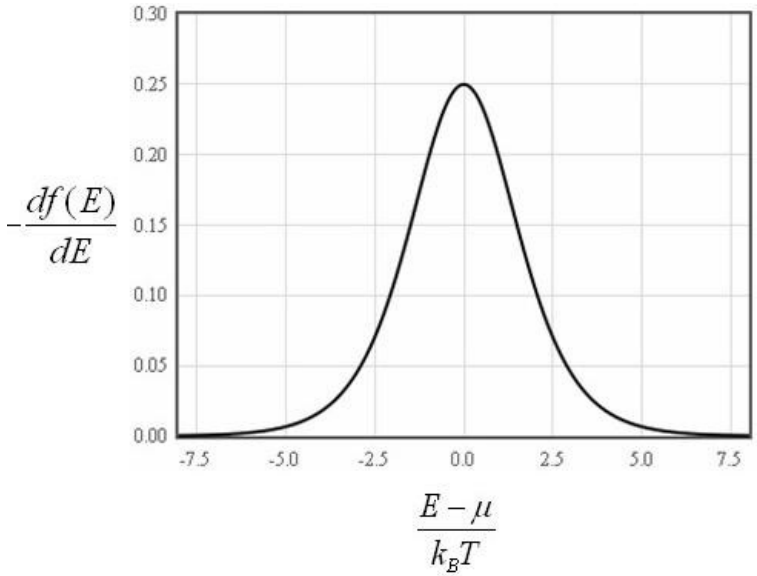
http://lamp.tu-graz.ac.at/~hadley/ss2/fermigas/thermo/thermo.php

Properties of metals depend mostly on the electron states at the Fermi surface

$$n = \int_{-\infty}^{\infty} D(E) f(E) dE = \int_{-\infty}^{\infty} \frac{D(E) dE}{\exp\left(\frac{E-\mu}{k_B T}\right)+1}.$$

$$K(E) = \int_{-\infty}^{E} D(E') dE'.$$

$$n = \int_{-\infty}^{\infty} D(E) f(E) dE = K(\infty) f(\infty) - K(-\infty) f(-\infty) - \int_{-\infty}^{\infty} K(E) \frac{f(E)}{dE} dE.$$



http://lampx.tugraz.at/~hadley/ss1/materials/thermo/dos2mu.html

Free electron Fermi gas 1-d

$$D(k) = \frac{2}{\pi}$$

$$E = \frac{\hbar^2 k^2}{2m} \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$dE = \frac{\hbar^2 k}{m}\, dk$$

$$D(k)dk = D(E)dE$$

$$D(E) = \sqrt{\frac{2m}{\hbar^2 \pi^2 E}} = \frac{n}{2\sqrt{E_F E}} \qquad \mathrm{J^{-1}m^{-1}}$$