

Institute of Solid State Physics

Review

We determined the normal modes of the electromagnetic field. Each normal mode can be labeled by \vec{k} and polarization.

We quantized the normal modes and found they have quantized energies

$$\hbar\omega(j+\frac{1}{2}) \qquad j=0,1,2,3\cdots$$

Thermodynamic properties of non-interacting bosons

Consider a system of non-interacting bosons that can occupy microscopic quantum states with energies ϵ_i . Since the bosons do not interact, the energy of one quantum state does not depend on the occupation of any of the other quantum states. A macrostate q of this system consists of N_q bosons. The total energy of this macrostate is E_q .

$$N_q = \sum_i n_{qi} \qquad E_q = \sum_i n_{qi} \epsilon_i \tag{1}$$

Here n_{qi} are occupation numbers that specify how many bosons occupy microstate *i* in macrostate *q*. An arbitrary number of bosons can occupy each microscopic quantum state.

$$n_{qi} \in 0, 1, \dots, \infty$$
 (2)

To calculate the thermodynamic properties, the grand canonical partition function Z_{gr} is constructed.

$$Z_{gr} = \sum_{q} \exp\left(\frac{\mu}{k_B T}\right)^{N_q} \exp\left(\frac{-E_q}{k_B T}\right) = \sum_{q} \exp\left(-\frac{E_q - \mu N_q}{k_B T}\right)$$
(3)

Here μ is the chemical potential, k_B is Boltzmann's constant, and T is the absolute temperature. The energy E_q and particle number N_q of the macrostates can be expressed in terms of the microscopic states.

$$Z_{gr} = \sum_{q} \exp\left(-\frac{\sum_{i} n_{qi}(\epsilon_i - \mu)}{k_B T}\right) = \sum_{q} \prod_{i} \exp\left(\frac{-n_{qi}(\epsilon_i - \mu)}{k_B T}\right)$$
(4)

The index q runs over all macrostates. The lowest energy macrostate has zero bosons in all of the microstates. There are macrostates with just one boson in one microstate and there are macrostates with many bosons in each of several microstates. The sum over all possible macrostates can be written as the sum over all possible microstates.

$$Z_{gr} = \sum_{n_1=0}^{\infty} \sum_{n_2=0}^{\infty} \cdots \sum_{n_{max}=0}^{\infty} \prod_i \exp\left(\frac{-n_i(\epsilon_i - \mu)}{k_B T}\right)$$
(5)

Here n_i are the number of bosons in energy state ϵ_i . The n_i are independent of each other and the factors can be pulled through the sums,

$$Z_{gr} = \left[\sum_{n_1=0}^{\infty} \exp\left(-\frac{n_1(\epsilon_1 - \mu)}{k_B T}\right)\right] \left[\sum_{n_2=0}^{\infty} \exp\left(-\frac{n_2(\epsilon_2 - \mu)}{k_B T}\right)\right] \cdots \left[\sum_{n_{max}=0}^{\infty} \exp\left(-\frac{n_{max}(\epsilon_{max} - \mu)}{k_B T}\right)\right]$$
(6)

All of the factors in square brackets are the same. This can be rewritten as a product where the indices are not necessary anymore,

$$Z_{gr} = \prod_{i} \left[\sum_{n=0}^{\infty} \exp\left(-\frac{n(\epsilon_{i}-\mu)}{k_{B}T}\right) \right].$$
(7)

$$Z_{gr} = \prod_{i} \left[\sum_{n=0}^{\infty} \exp\left(-\frac{n(\epsilon_i - \mu)}{k_B T}\right) \right].$$
⁽⁷⁾

At low particle densities and high temperatures, the average number of bosons in all of the microscopic states will be less than one. Thus the chemical potential will be less than the lowest microscopic energy level, $\mu < \epsilon$. In this case, the sum over n is a geometric series " $1 + x + x^2 + \cdots = \frac{1}{1-x}$ " where $x = \exp\left(-\frac{\epsilon_i - \mu}{k_B T}\right) < 1$. Summing this series yields,

$$Z_{gr} = \prod_{i} \left[1 - \exp\left(-\frac{\epsilon_i - \mu}{k_B T}\right) \right]^{-1}.$$
(8)

As the temperature decreases or the particle density increases, the chemical potential will increase. As $\mu \to \epsilon_0$ the occupation of the lowest energy level becomes large and the bosons undergo a Bose-Einstein condensation. Here, we will only consider the case where $\mu < \epsilon_0$.

The thermodynamic grand potential can be determined from the grand canonical partition function, $\Phi = U - TS - \mu N = -k_B T \ln(Z_{gr})$. Here U is the internal energy, S is the entropy, and N is the average number of bosons in the system.

$$\Phi = -k_B T \ln(Z_{gr}) = k_B T \sum_i \ln\left[1 - \exp\left(\frac{\mu - \epsilon_i}{k_B T}\right)\right]$$
(9)

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(9)

This sum can be approximated by an integral over the density of states D(E). The density of states is defined per unit volume V so the grand potential density is,

$$\phi = \frac{\Phi}{V} = k_B T \int_{-\infty}^{\infty} D(E) \ln\left[1 - \exp\left(\frac{\mu - E}{kBT}\right)\right] dE$$
(10)

The particle density is minus the derivative of the grand potential density with respect to the chemical potential.

$$n = \frac{\partial \phi}{\partial \mu} = k_B T \int_{-\infty}^{\infty} D(E) \frac{1}{1 - \exp\left(\frac{\mu - E}{k_B T}\right)} \exp\left(\frac{\mu - E}{k_B T}\right) \cdot \frac{1}{k_B T} dE$$
$$= \int_{-\infty}^{\infty} D(E) \frac{1}{\exp\left(\frac{E - \mu}{k_B T}\right) - 1} dE \quad (11)$$
$$\underbrace{\exp\left(\frac{E - \mu}{k_B T}\right) - 1}_{F_{BE}(E)} dE$$

Bose-Einstein function
$$F_{BE}(E) = \frac{1}{\exp(E - \mu/k_B T) - 1}$$

$$f = \phi + \mu n = \int_{-\infty}^{\infty} D(E) \Biggl\{ k_B T \Biggl[1 - \exp \Biggl(\frac{\mu - E}{k_B T} \Biggr) \Biggr] + \frac{\mu}{\exp \Bigl(\frac{E - \mu}{k_B T} \Bigr) - 1} \Biggr\} dE$$

$$s = -\frac{\partial \phi}{\partial T} = \frac{1}{T} \int_{-\infty}^{\infty} D(E) \Biggl\{ -k_B T \ln \biggl[1 - \exp \biggl(\frac{\mu - E}{k_B T} \biggr) \biggr] + \frac{E - \mu}{\exp \Bigl(\frac{E - \mu}{k_B T} \Bigr) - 1} \Biggr\} dE$$

$$u=f+Ts=\int\limits_{-\infty}^{\infty}rac{ED(E)}{\exp\left(rac{E-\mu}{k_BT}
ight)-1}\,dE$$

$$c_v = rac{\partial u}{\partial T} = \int\limits_{-\infty}^{\infty} rac{ED(E)(E-\mu)\exp\left(rac{E-\mu}{k_BT}
ight)}{k_BT^2\left[\exp\left(rac{E-\mu}{k_BT}
ight) - 1
ight]^2} dE$$

Normal modes

For an electromagnetic field in a cubic region of length L with periodic boundary conditions, the vector potential has the form:

$$\vec{A}_{\perp} \sin\left(k_{x}x + k_{y}y + k_{z}z\right)$$
 $k_{x}, k_{y}, k_{z} = \dots -\frac{4\pi}{L}, -\frac{2\pi}{L}, 0, \frac{2\pi}{L}, \frac{4\pi}{L}$...





polarizations

Density of states

$$D(k)dk = \frac{k^2}{\pi^2}dk = D(\omega)d\omega$$

use the dispersion relation to convert D(k) to $D(\omega)$

 $\omega = ck$ $d\omega = cdk$ $D(\omega) = \frac{\omega^2}{c^3 \pi^2}$

$$D(E) = \frac{E^2}{\pi^2 c^3 \hbar^3}$$

Summary of the results for the quantization of the wave equation in 1,2, and 3 dimensions

	1-D	2-D
Wave Equation $c =$ speed of light $A_j = j^{\text{th}}$ component of the vector potential	$c^2 \frac{d^2 A_j}{dx^2} = \frac{d^2 A_j}{dt^2}$	$c^{2}\left(\frac{d^{2}A_{j}}{dx^{2}} + \frac{d^{2}A_{j}}{dy^{2}}\right) = \frac{d^{2}A_{j}}{dt^{2}}$
Eigenfunction solutions k = wavenumber $\omega =$ angular frequency	$A_{j} = \exp\left(i\left(kx - \alpha t\right)\right)$	$A_{j} = \exp\left(i\left(\vec{k}\cdot\vec{r} - \alpha t\right)\right)$
Dispersion relation	$\omega = ck$	$\omega = c \left \vec{k} \right $
Density of states	$D(k) = \frac{2}{\pi}$	$D(k) = \frac{k}{\pi} \qquad [\mathbf{m}^{-1}]$
Density of states $D(\omega) = D(k) \frac{dk}{d\omega}$	$D(\omega) = \frac{2}{\pi c}$ [s/m]	$D(\omega) = \frac{\omega}{\pi c^2}$ [s/m ²]
Density of states $D(\lambda) = D(k) \frac{dk}{d\lambda}$	$D(\lambda) = \frac{4}{\lambda^2} [\mathbf{m}^{-2}]$	$D(\lambda) = \frac{4\pi}{\lambda^3} [\mathbf{m}^{-3}]$
$\lambda = \text{wavelength}$ Density of states $D(E) = D(\omega) \frac{d\omega}{dE}$	$D(E) = \frac{2}{\pi \hbar c} \qquad [\mathbf{J}^{-1}\mathbf{m}^{-1}]$	$D(E) = \frac{E}{\pi \hbar^2 c^2} \qquad [\mathbf{J}^{-1}\mathbf{m}^{-2}]$
Chemical potential	$\mu = 0$	μ=0
Intensity spectral density $k_B = 1.3806504 \times 10^{-23} \text{ [J/K] Boltzmann's}$ constant $h = 6.62606896 \times 10^{-34} \text{ [J s] Planck's constant}$	$I(\lambda) = \frac{2hc^2}{\lambda^3 \left(\exp\left(\frac{hc}{\lambda k_B T}\right) - 1 \right)} \qquad [J \text{ m}^{-1} \text{s}^{-1}]$	$I(\lambda) = \frac{4hc^2}{\lambda^4 \left(\exp\left(\frac{hc}{\lambda k_B T}\right) - 1 \right)} [J \text{ m}^{-2}\text{s}^{-1}]$
$\frac{d I(\lambda)}{d \lambda} \bigg _{\lambda = \lambda_{\max}} = 0$	$\lambda_{\rm max} = \frac{0.0050994367}{\rm T}$ [m]	$\lambda_{\rm max} = \frac{0.0036696984}{\rm T}$ [m]
Stefan - Boltzmann law $I = \int_{0}^{\infty} I(\lambda) d\lambda$ $\zeta(3) \approx 1.202 \text{ Riemann } \zeta \text{ function}$ $\sigma = 5.67 \times 10^{-8} \text{ Stefan-Boltzmann constant}$	$I = \frac{\pi^2 k_B^2 T^2}{3h} \qquad [J \text{ s}^{-1}]$	$I = \frac{8\zeta(3)k_B^{3}T^{3}}{h^2c} \qquad [J m^{-1} s^{-1}]$

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.



Plane wave:

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

Diffraction condition



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



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

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

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

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

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

Eigen function solutions of the translation operator have Bloch form.

Photonic bands

