116217 - Solid State Physics

Netanel Lindner

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Abstract

1 Introduction

Phase are distinguished by symmetries, e.g., liquid and solid have difference in transnational symmetry. Those phase transitions happens together with spontaneous symmetry breakage.For example, magnet "chooses" poles when transits to magnetic phase.

1.1 Heat capacity

Most of matereals have $C = 3k_B$, except diamond in room temperature and pressure. In low temperatures though, materials have $C = \alpha T + \gamma T^3$. Thus, most of materials get to saturation in room temperature, while diamond doesn't. The linear factor appears only in conductors, thus should come from electrons.

Equipartition theorem

$$\left\langle x_m \frac{\partial H}{\partial x_n} \right\rangle = \delta_{mn} k_B T$$

in particular, for quadratic degree of freedom we get $\frac{1}{2}k_B T$.
Thus, assuming each atom is harmonic oscillator, we have

$$\langle E \rangle = 3k_B T$$

and

$$c_V = 3k_B$$

Einstein model Now assume the oscillators are quantum:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

The partition function

$$Z = \sum_n e^{-\beta E_n} = \sum_n e^{-\beta\hbar\omega\left(n+\frac{1}{2}\right)} = e^{-\frac{\beta\hbar\omega}{2}} \frac{1}{1 - e^{-\beta\hbar\omega}} = \frac{e^{-\frac{\beta\hbar\omega}{2}}}{e^{-\frac{\beta\hbar\omega}{2}}\left[e^{\frac{\beta\hbar\omega}{2}} - e^{-\frac{\beta\hbar\omega}{2}}\right]} = \frac{1}{2\sinh\left(\frac{\beta\hbar\omega}{2}\right)}$$

$$\langle E \rangle = -\frac{\partial}{\partial\beta}\ln Z_N = -\frac{1}{Z_N}\frac{\partial}{\partial\beta}Z = N \cdot 2\sinh\left(\frac{\beta\hbar\omega}{2}\right) \cdot \frac{\hbar\omega}{2}\frac{\cosh\left(\frac{\beta\hbar\omega}{2}\right)}{\sinh^2\left(\frac{\beta\hbar\omega}{2}\right)} = \frac{N\hbar\omega}{2}\frac{1}{\tanh\left(\frac{\beta\hbar\omega}{2}\right)}$$

$$\langle E \rangle = N\hbar\omega\left(n_B(\beta\hbar\omega) + \frac{1}{2}\right)$$

$$n_B(x) = \frac{1}{r^x - 1}$$

Now

$$c_V = \frac{\partial \langle E \rangle}{\partial T} = 3Nk_B(\beta\hbar\omega)^2 \frac{e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega} - 1\right)^2}$$

$$\lim_{T\to\infty} c_V = 3k_B N$$

$$\lim_{T\to 0} c_V = 0$$

which is expected, however, we got exponential dependence on T and not T^3.

1.2 Debye model

Debye proposed to model atoms in solid as sound waves. Plank already quantized EM-waves, the only differences is number of polarization options and speed of wave.
We'll often use periodic bound conditions, since this preserves the symmetry of the system.
Now, for wave e^{ikx} we get $e^{ikx} = e^{ik(x+L)}$, thus we get a condition on wavenumber

$$k = \frac{2\pi}{L} n$$

We also want to switch to integral on k.
The connection between frequency and wavenumber is $\omega(\vec{\mathbf{k}}) = v \cdot \left|\vec{\mathbf{k}}\right|$. The energy per wavenumber

$$\langle E \rangle = 3 \sum_{\vec{\mathbf{k}}} \hbar\omega(\vec{\mathbf{k}}) \left(n_B(\beta\hbar\omega(\vec{\mathbf{k}})) + \frac{1}{2} \right)$$

$$\langle E \rangle = 3 \frac{L^3}{(2\pi)^3} \int \mathrm{d}^3k \, \hbar\omega(\vec{\mathbf{k}}) \left(n_B(\beta\hbar\omega(\vec{\mathbf{k}})) + \frac{1}{2} \right) = 3 \frac{4\pi L^3}{(2\pi)^3} \int \frac{\omega^2 \, \mathrm{d}\omega}{v^3} \hbar\omega \left(n_B(\beta\hbar\omega) + \frac{1}{2} \right)$$

Now,

$$g(\omega) = L^3 \cdot \frac{12\pi\omega^2}{(2\pi)^3 v^3} = N \frac{12\pi\omega^2}{(2\pi)^3 v^3 \rho}$$

is density of states.
Define $\omega_d^3 = 6\pi^2 \rho v^3$, acquiring $g(\omega) = N \frac{9\omega^2}{\omega_d^3}$

$$\langle E \rangle = \frac{9N\hbar}{\omega_d^3} \int \omega^3 \, \mathrm{d}\omega \, \frac{1}{e^{\beta\hbar\omega} - 1} + \text{const}$$

Substituting $\beta\hbar\omega = x$:

$$\langle E \rangle = \frac{9N\hbar}{\omega_d^3 (\beta\hbar)^4} \underbrace{\int \mathrm{d}x \, x^3 \frac{1}{e^x - 1}}_{\frac{\pi^4}{15}}$$

$$\frac{\partial \langle E \rangle}{\partial T} = \frac{12\pi^4}{5} \frac{n k_B (k_B T)^3}{(\hbar\omega_d)^3}$$