Systems of interacting particles

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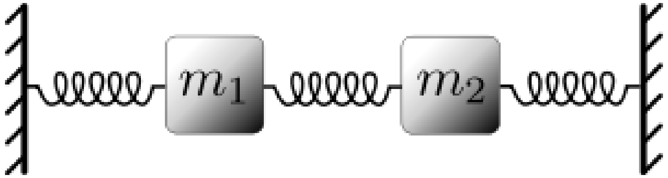
- Solids
  - Lattice vibrations and normal modes
  - Debye approximation
- Non-ideal classical gas
  - Calculation of the partition function for low densities
  - Equation of state and virial coefficients
- Ferromagnetism
  - Interaction between spins
  - Weiss molecular-field approximation

Normal mode

$$m\ddot{x}_1 = -kx_1 + k(x_2 - x_1) = -2kx_1 + kx_2$$

$$m\ddot{x}_2 = -kx_2 + k(x_1 - x_2) = -2kx_2 + kx_1$$



$$x_1(t) = A_1 e^{i\omega t} \qquad x_2(t) = A_2 e^{i\omega t}$$

$$-\omega^2 m A_1 e^{i\omega t} = -2kA_1 e^{i\omega t} + kA_2 e^{i\omega t} \longrightarrow (\omega^2 m - 2k)A_1 + kA_2 = 0$$

$$-\omega^2 m A_2 e^{i\omega t} = kA_1 e^{i\omega t} - 2kA_2 e^{i\omega t} \longrightarrow kA_1 + (\omega^2 m - 2k)A_2 = 0$$

$$\begin{bmatrix} \omega^2 m - 2k & k \\ k & \omega^2 m - 2k \end{bmatrix} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = 0 \longrightarrow (\omega^2 m - 2k)^2 - k^2 = 0$$

$$\omega_1 = \sqrt{\frac{k}{m}}, \qquad \omega_2 = \sqrt{\frac{3k}{m}}.$$

Lattice vibrations and normal modes

$$H_r = \frac{1}{2}\left(\dot{q}_r^2 + \omega_r^2 q_r^2\right) \longrightarrow \varepsilon_r = \left(nr + \frac{1}{2}\right)\hbar\omega_r$$

$$H = V_0 + \frac{1}{2}\sum_{r=1}^{3N}\left(\dot{q}_r^2 + \omega_r^2 q_r^2\right) \longrightarrow E_{n_1,\cdots n_{3N}} = -N\eta + \sum_{r=1}^{3N} n_r \hbar\omega_r$$

$$-N\eta \equiv V_0 + \frac{1}{2}\sum_r \hbar\omega_r$$

$$Z = \sum_{n_1,\cdots,n_{3N}} e^{-\beta[-N\eta + n_1\hbar\omega_1 + \cdots + n_{3N}\hbar\omega_{3N}]} = e^{\beta N\eta}\left(\sum_{n_1=0}^{\infty} e^{-\beta\hbar\omega_1 n_1}\right)\cdots\left(\sum_{n_{3N}=0}^{\infty} e^{-\beta\hbar\omega_{3N} n_{3N}}\right)$$

$$Z = e^{\beta N\eta}\left(\frac{1}{1-e^{-\beta\hbar\omega_1}}\right)\cdots\left(\frac{1}{1-e^{-\beta\hbar\omega_{3N}}}\right)$$

Lattice vibrations and normal modes

$$\ln Z = \beta N\eta - \sum_{r=1}^{3N} \ln(1 - e^{-\beta\hbar\omega_r})$$

$\sigma(\omega)d\omega$ The number of normal modes with angular frequency in the range between w and w+dw

$$\ln Z = \beta N\eta - \int_0^\infty \ln(1 - e^{-\beta\hbar\omega})\sigma(\omega)d\omega$$

$$\bar{E} = -\frac{\partial \ln \mathrm{Z}}{\partial \beta}$$

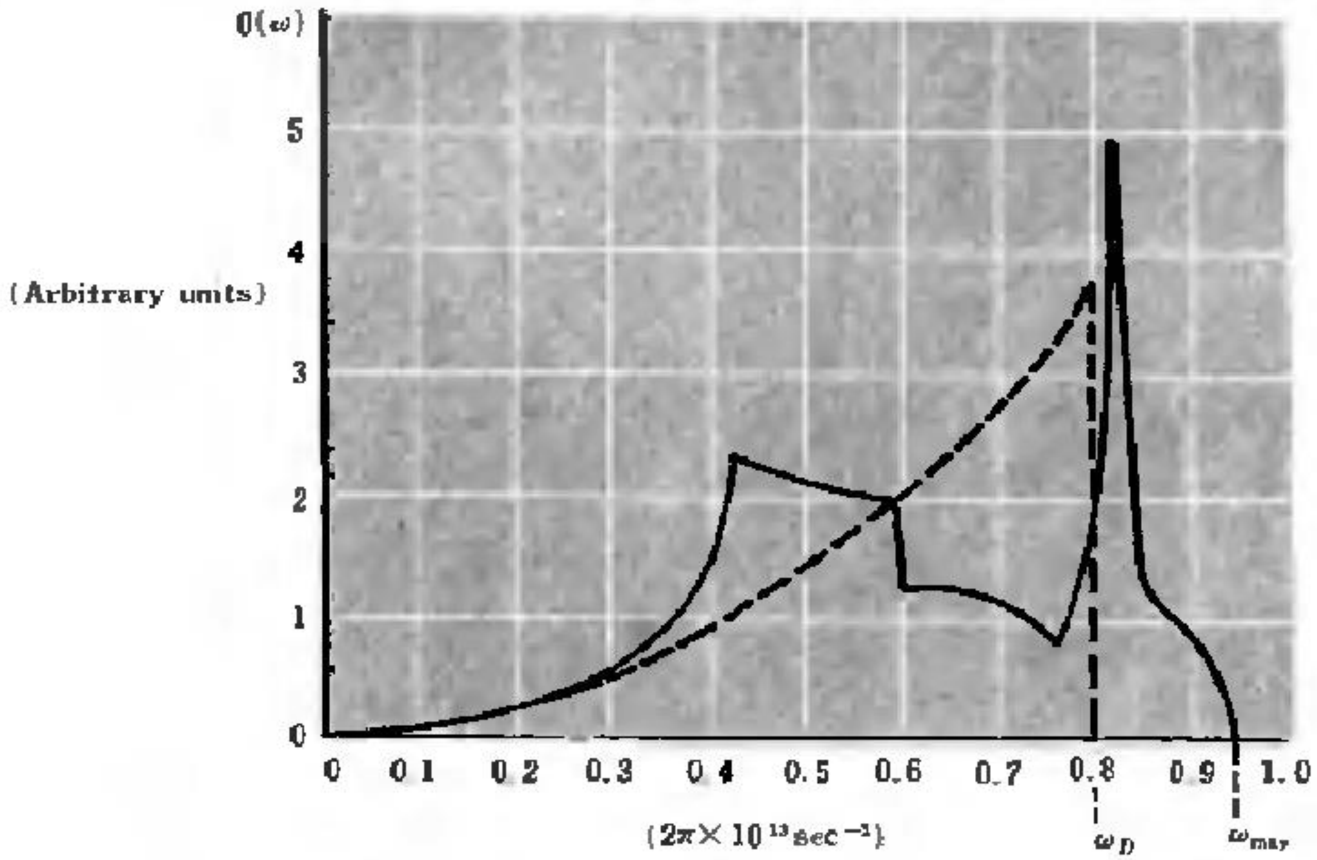
$$C_V = \left(\frac{\partial \bar{E}}{\partial T}\right)_V = -k\beta^2 \left(\frac{\partial \bar{E}}{\partial \beta}\right)_V$$

$$C_V = k\int_0^\infty \frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega} - 1)^2}(\beta\hbar\omega)^2 \sigma(\omega)d\omega$$

Debye approximation

Continuous elastic medium

$$\sigma_D(\omega) = \begin{cases} \sigma_c(\omega), \omega < \omega_D \\ 0, \omega > \omega_D \end{cases}$$



Debye approximation

$$\sigma_c(\omega)\,\mathrm{d}\omega = 3\frac{V}{(2\pi)^3}(4\pi\kappa^2 d\kappa) = 3\frac{V}{2\pi^2 c_s^3}\omega^2 d\omega$$ (Sec. 9-9)

$$\int_0^{\infty}\sigma_D(\omega)d\omega = \int_0^{\omega_D}\sigma_c(\omega)d\omega = 3N$$

$$\omega_D = c_s\left(6\pi^2\frac{N}{V}\right)^{\frac{1}{3}} \longrightarrow k\theta_D \equiv \hbar\omega_D$$

$$C_V = k\int_0^{\omega_D}\frac{e^{\beta\hbar\omega}}{(e^{\beta\hbar\omega}-1)^2}(\beta\hbar\omega)^2\frac{3V}{2\pi^2 c_s^3}\omega^2 d\omega$$

Debye approximation

$$C_V = 3Nkf_D\left(\frac{\theta_D}{T}\right)$$

$$f_D(\mathrm{y}) \equiv \frac{3}{y^3}\int_0^y \frac{e^x}{(e^x-1)^2}x^4dx, x \equiv \beta\hbar\omega$$

$$y \to 0, f_D(y) \to \frac{3}{y^3}\int_0^y x^2dx = 1 \longrightarrow C_V = 3Nk$$

$$y \gg 1, f_D(\mathrm{y}) = \frac{4\pi^4}{5}\frac{1}{y^3} \longrightarrow C_V = \frac{12\pi^4}{5}Nk\left(\frac{T}{\theta_D}\right)^3$$

Non-ideal classical gas

$$\bar{U} = -\frac{\partial}{\partial\beta}\ln Z_U$$

$$\text{Hence,} \ln Z_U(\beta) = N\ln V - \int_0^\beta \bar{U}(\beta')d\beta'$$

$$\bar{U} = \frac{1}{2}N(N-1)\bar{u} \approx \frac{1}{2}N^2\bar{u}$$

$$\bar{u} = -\frac{\partial}{\partial\beta}\ln\int e^{-\beta u}d^3\vec{R}$$

$$\int e^{-\beta u}d^3\vec{R} = \int[1+(e^{-\beta u}-1)]d^3\vec{R} = V + I = V\left(1+\frac{I}{V}\right)$$

$$I(\beta) \equiv \int(e^{-\beta u}-1)d^3\vec{R} = \int(e^{-\beta u}-1)4\pi R^2 dR$$

Non-ideal classical gas

$$\bar{u} = -\frac{\partial}{\partial\beta}\left[\ln V + \ln\left(1 + \frac{I}{V}\right)\right] \approx 0 - \frac{\partial}{\partial\beta}\left(\frac{I}{V} + \cdots\right) \quad ,(I \ll V)$$

$$Hence, \bar{u} = -\frac{1}{V}\frac{\partial I}{\partial\beta}$$

$$\ln Z_U(\beta) = N\ln V + \frac{1}{2}\frac{N^2}{V}I(\beta)$$

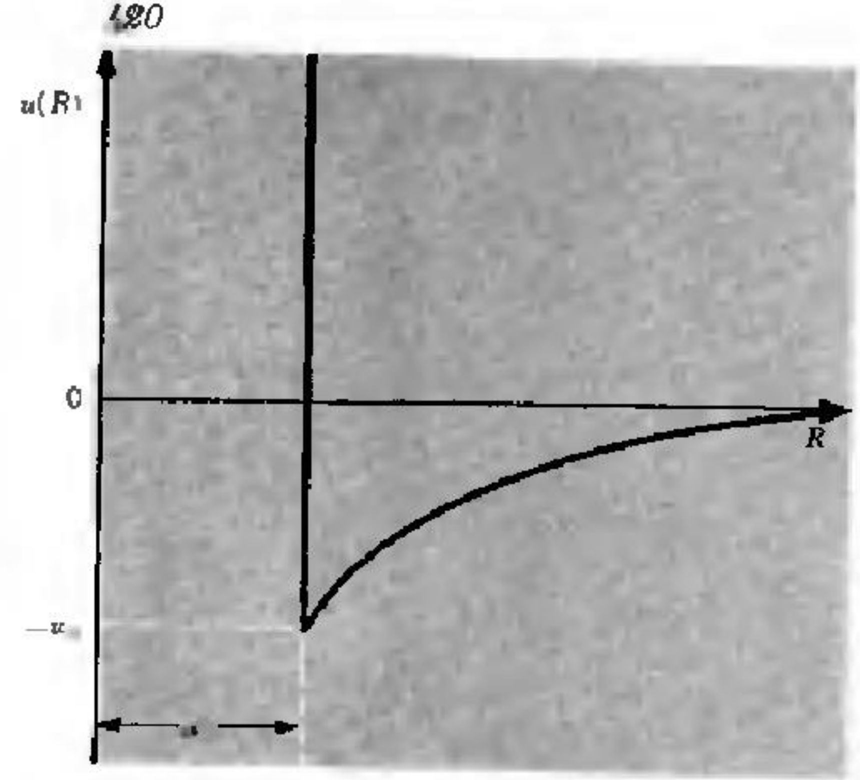
Non-ideal classical gas

$$\beta \bar{p} = \frac{\partial \ln Z_U}{\partial V} = \frac{N}{V} - \frac{1}{2}\frac{N^2}{V^2} I$$

The general form of pressure:

$$\frac{\bar{p}}{kT} = n + B_2(T)n^2 + B_3(T)n^3 + \cdots$$

$$\text{Hence, } B_2 = -\frac{1}{2} I = -2\pi \int (e^{-\beta u} - 1) R^2 dR$$



$$u(\mathrm{R}) = \begin{cases} \infty, R < R_0 \\ -u_0 \left(\frac{R_0}{R} \right)^s, R > R_0 \end{cases}$$

Non-ideal classical gas

The van der Waals equation

$$u(\mathrm{R}) = \begin{cases} \infty, R < R_0 \\ -u_0\left(\dfrac{R_0}{R}\right)^s, R > R_0 \end{cases}$$

$$B_2 = 2\pi\int_0^{R_0} R^2 dR - 2\pi\int_{R_0}^{\infty}(e^{-\beta u} - 1)R^2 dR$$

Assume that the temperature is high enough that: $\beta u_0 \ll 1$

$$B_2 = \frac{2\pi}{3}R_0^3 - 2\pi\beta u_0\int_{R_0}^{\infty}\left(\frac{R_0}{R}\right)^s R^2 dR = \frac{2\pi}{3}R_0^3\left(1 - \frac{3}{s-3}\frac{u_0}{kT}\right), (\mathrm{s} > 3)$$

We assume: $b' \equiv \frac{2\pi}{3}R_0^3, a' \equiv \left(\frac{3}{s-3}\right)b'u_0$

$$\text{Hence}, B_2 = b' - \frac{a'}{kT}$$

Non-ideal classical gas

$$\bar{p} = kTn + kT\left(b' - \frac{a'}{kT}\right)n^2 = nkT + \left(kTb' - a'\right)n^2$$

$$\bar{p} + a'n^2 = nkT(1 + b'n) \approx \frac{nkT}{1 - b'n}, (b'n \ll 1)$$

$$\left(\bar{p} + \frac{a}{v^2}\right)(v - b) = RT \qquad a \equiv N_a^2 a', b \equiv N_a b'$$

N_a : Avogadro’s number

Interaction between spins

- Two kinds of interaction between atoms:

  (1) magnetic interaction

  (2) exchange interaction

$$H_{jk} = -2J\vec{S}_j \cdot \vec{S}_k = -2JS_{jz}S_{kz}$$

Interaction between spins

$$H = H_0 + H'$$

$$H_0 = -g\mu_0 \sum_{j=1}^{N} \vec{S}_j \cdot \vec{H}_0 = -g\mu_0 H_0 \sum_{j=1}^{N} S_{jz}$$

$$\vec{m} = g\mu_0 \vec{S}$$

$$H' = \frac{1}{2}\left(-2J \sum_{j=1}^{N} \sum_{k=1}^{n} S_{jz} S_{kz} \right)$$

N: the number of atoms

n: the number of neighboring atoms

Weiss molecular-field approximation

- Focus attention on a particular atom j, then

$$H_j = -g\mu_0 H_0 S_{jz} - 2JS_{jz}\sum_{k=1}^{n} S_{kz}$$

$$2J < \sum_{k=1}^{n} S_{kz} >_n \equiv g\mu_0 H_m$$

$$H_j = -g\mu_0 (H_0 + H_m) S_{jz}$$

$$\bar{S}_{jz} = SB_S(\eta), \eta \equiv \beta g\mu_0 (H_0 + H_m)$$

Sec. 7.8

Weiss molecular-field approximation

- Then we get a self-consistent equation:

$$2JnSB_S(\eta) = g\mu_0 H_m$$

Expressing H_m in terms of η

$$B_S(\eta) = \frac{kT}{2nJS}\left(\eta - \frac{g\mu_0 H_0}{kT}\right)$$