Statistical Physics – PHYS 704 Course summary

Andréas Sundström

2016-12-12

1 Some Thermodynamic relations

- Energy: E, $dE = TdS PdV + \mu dN$. Min. in equilibrium when S and V are const.
- Helmholtz free energy: F = E TS, $dF = -SdT PdV + \mu dN$. Min. in equil. when T and V are const.
- Enthalph: W = E + PV, $dW = TdS + VdP + \mu dN$. Min. in equil. when S (adiabatic) and P are const.
- Gibbs free energy: $\Phi = E + PV TS$, $d\Phi = -SdT + VdP + \mu dN$. Min. in equil. when T and P are const.
- Grand potential: $\Omega = -PV$, $d\Omega = -SdT + PdV + Nd\mu$.

Derivative relations

$$\begin{split} &+\left(\frac{\partial T}{\partial V}\right)_{S}=-\left(\frac{\partial P}{\partial S}\right)_{T}=+\frac{\partial^{2} E}{\partial S \partial V}\\ &+\left(\frac{\partial T}{\partial P}\right)_{S}=+\left(\frac{\partial V}{\partial S}\right)_{P}=+\frac{\partial^{2} W}{\partial S \partial P}\\ &+\left(\frac{\partial S}{\partial V}\right)_{T}=+\left(\frac{\partial P}{\partial T}\right)_{V}=-\frac{\partial^{2} F}{\partial T \partial V}\\ &-\left(\frac{\partial S}{\partial P}\right)_{T}=+\left(\frac{\partial V}{\partial T}\right)_{P}=+\frac{\partial^{2} \Phi}{\partial T \partial P} \end{split} \tag{1}$$

Temperature

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{VN} \tag{2}$$

Heat-capacity

$$C_V = \left(\frac{\mathrm{d}E}{\mathrm{d}T}\right)_V = T\left(\frac{\partial S}{\partial T}\right)_V = -T\left(\frac{\partial^2 F}{\partial T^2}\right)_V$$
$$C_P = \left(\frac{\mathrm{d}W}{\mathrm{d}T}\right)_P = \left(\frac{\partial E}{\partial T}\right)_P + P\left(\frac{\partial V}{\partial T}\right)_P$$

Compressibility

$$\kappa_X = -\frac{1}{V} \left(\frac{\partial V}{\partial P} \right)_X \tag{4}$$

1.1 Some def. in stat. mech.

Definition of entropy

$$S := -\sum_{n,(N)} \rho_{n,(N)} \ln(\rho_{n,(N)}), \tag{5}$$

where ρ is the density function or distribution function. Canonical distribution (N constant)

$$\rho_n = \frac{1}{Z} e^{-E_n/T}, \quad Z = \sum_n e^{-E_n/T}.$$
(6)

$$F = -T \ln Z \tag{7}$$

Grand canonical distribution

$$\rho_{n,N} = \frac{1}{Z} e^{-(E_n - \mu N)/T}, \quad \mathcal{Z} = \sum_n e^{-(E_n - \mu N)/T}. \quad (8)$$

$$\Omega = -T \ln \mathcal{Z} \tag{9}$$

2 Theory of ideal gases

Ideal gas means that there is no interaction between particles, $\varepsilon = \hbar^2 k^2/(2m)$. In 3 dim.

$$\frac{1}{V} \sum_{k} \to \int \frac{\mathrm{d}^{3} k}{(2\pi)^{3}} = \int \mathrm{d}\varepsilon \, g(\varepsilon),\tag{10}$$

$$\frac{\mathrm{d}^3 k}{(2\pi)^3} = \mathrm{d}\varepsilon \, g(\varepsilon), \quad g(\varepsilon) = \frac{m^{3/2}}{\sqrt{2}\pi\hbar^3} \sqrt{\varepsilon}. \tag{11}$$

See assignment 3 for other dim.

(3)

2.1 Ideal Fermi gases

$$n^{(\text{F.D.})} = \frac{1}{e^{(\varepsilon - \mu)/T} + 1} \tag{12}$$

$$-\Omega = PV = \frac{2}{3}E = \frac{Vg_{s}T}{\lambda^{3}}f_{5/2}(z)$$
 (13)

$$N = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V} = \frac{Vg_{\rm s}}{\lambda^3} f_{3/2}(z) \tag{14}$$

$$\frac{PV}{NT} = \frac{f_{5/2}(z)}{f_{3/2}(z)} \tag{15}$$

Thermal wavelength $\lambda = h/\sqrt{2\pi mT} =: \Lambda/\sqrt{T}, \Lambda$ is a constant.

Fermi functions

$$f_{\nu}(z) = \frac{1}{\Gamma(\nu)} \int_{0}^{\infty} dx \frac{x^{\nu-1}}{z^{-1}e^{x} + 1}$$
 (16)

Fugacity $z = e^{\mu/T}$.

$$z\frac{\partial f_{\nu}(z)}{\partial z} = \frac{\partial f_{\nu}(z)}{\partial (\ln z)} = f_{\nu-1}(z)$$
 (17)

Fermi energy As $T \to 0$, the ccamical potential will go to

$$\mu(T \to 0) =: \varepsilon_{\rm F} = \frac{\hbar^2}{2m} \left(\frac{6}{q_{\rm s}} \pi^2 n\right)^{2/3},$$
 (18)

where $g_{\rm s}$ is the spin deganareacy, and n=N/V. In a regular metal, $\varepsilon_{\rm F}\sim 10^4\,{\rm K}$. For $T\ll \varepsilon_{\rm F}$

$$n^{(\mathrm{F.D.})}(\varepsilon) \approx \begin{cases} 1, & \varepsilon < \varepsilon_{\mathrm{F}} \\ 0, & \varepsilon > \varepsilon_{\mathrm{F}} \end{cases}$$
 (19)

and $\int_{0}^{\infty} d\varepsilon \, n^{(F.D.)}(\varepsilon) \dots \to \int_{0}^{\varepsilon_{F}} d\varepsilon \dots$

The internal energy

$$E(T \ll \varepsilon_{\rm F}) = \frac{3}{5} N \varepsilon_{\rm F} \tag{20}$$

2.2 Ideal Bose gases

$$n^{(\text{B.E.})} = \frac{1}{e^{(\varepsilon - \mu)/T} - 1} \tag{21}$$

$$-\Omega = PV = \frac{2}{3}E = \frac{Vg_{\rm s}T}{\lambda^3}g_{5/2}(z)$$
 (22)

$$N_{\rm e} = -\left(\frac{\partial \Omega}{\partial \mu}\right)_{T,V} = \frac{Vg_{\rm s}}{\lambda^3}g_{3/2}(z) \tag{23}$$

$$\frac{PV}{NT} = \frac{g_{5/2}(z)}{g_{3/2}(z)} \tag{24}$$

Thermal wavelength $\lambda = h/\sqrt{2\pi mT} =: \Lambda/\sqrt{T}, \Lambda$ is a constant.

Bose functions

$$g_{\nu}(z) = \frac{1}{\Gamma(\nu)} \int_{0}^{\infty} dx \frac{x^{\nu-1}}{z^{-1}e^{x} - 1}$$
 (25)

For bosons $\mu \leq 0$, meaning that $z = e^{\mu/T} \leq 1$.

$$z\frac{\partial g_{\nu}(z)}{\partial z} = \frac{\partial g_{\nu}(z)}{\partial(\ln z)} = g_{\nu-1}(z)$$
 (26)

At
$$z = 1$$
, $g_{\nu}(z = 1) = \zeta(\nu)$.

Critical temperature Critical temperature for ideal Bose gas (3 dim.)

$$T_{\rm c} = \frac{2\pi\hbar^2}{m} \left(\frac{N}{V q_{\rm s} \zeta(3/2)}\right)^{3/2} \tag{27}$$

Number of condensed particles

$$N_0 = N \left[1 - \left(\frac{T}{T_c} \right)^{3/2} \right], \quad T \le T_c.$$
 (28)

$$\lambda = \frac{h}{\sqrt{2\pi mT}}, \quad \lambda_{c} = \left[v\zeta(3/2)\right]^{1/3}$$

$$v = \frac{1}{n} = \frac{V}{N}, \quad v_{c} = \frac{\lambda^{3}}{\zeta(3/2)}$$
(29)

2.2.1 Photons

Photons are bosons with $\mu = 0$.

$$n^{\text{(photons)}} = \frac{1}{e^{\hbar\omega/T} - 1}.$$
 (30)

Number of photons in the interval ω to $\omega + d\omega$:

$$dN_{\omega} = \frac{V}{\pi^2 c^3} \frac{\omega^2 d\omega}{e^{\hbar \omega/T} - 1}.$$
 (31)

Energy in the same interval:

$$dE_{\omega} = \hbar\omega \, dN_{\omega} = V u_{\omega} \, d\omega, \tag{32}$$

where u_{ω} is the radiation energy density. Total radiation energy

$$E = \int_{0}^{\infty} dE_{\omega} = \frac{4\sigma}{c} V T^{4}, \qquad (33)$$

where $\sigma = \pi^2/(60\hbar^3c^2)$

2.2.2 Phonons

Chain of N particles connected with springs, mean distance a. Hamiltonian

$$H = \sum_{s=0}^{N-1} \left[\frac{p_s^2}{2m} + \frac{\kappa}{2} (q_{s+1} - q_s)^2 \right]$$
 (34)

Also periodoc boundary conditions: $q_{s+N} = q_s$ and $p_{s+N} = p_s$.

Fourier transform (momentum space)

$$H = \sum_{k=0}^{N-1} \left[\frac{1}{2m} p_{-k} p_k + \frac{m\omega_k^2}{2} q_{-k} q_k \right].$$
 (35)

This is a Hamiltonian for N harmonic oscillators:

$$H = \sum_{k=0}^{N-1} \hbar \omega_k \left(\hat{n}_k + \frac{1}{2} \right). \tag{36}$$

The frequency

$$\omega_{k} = \sqrt{\frac{2\kappa}{m}(1 - \cos(ka))}$$

$$\stackrel{ka \ll 1}{\approx} |ka| \sqrt{\frac{\kappa}{m}}.$$
(37)

Speed of sound

$$c_{\rm s} = \sqrt{\frac{\kappa a^2}{m}}. (38)$$

For $|ka| \ll 1$,

$$C_V = \frac{2\pi^2}{5\hbar^3 c_c^3} V T^3. (39)$$

3 Second quantaization

Main idea: use a Bogoliubov transformation to transform the Hamiltonian to to a hamiltonian of an ideal gas of quasi-particles.

Harmonic oscillator interpretation in momentum space Occupation number representation:

$$|\psi\rangle = |n_{k_1}, n_{k_2}, \dots, n_{k_i}, \dots\rangle \tag{40}$$

$$\hat{n}_{k_i} | n_{k_1}, \dots, n_{k_i}, \dots \rangle = n_{k_i} | n_{k_1}, \dots, n_{k_i}, \dots \rangle$$
 (41)

For bosons:

$$\left[a_k, a_{k'}^{\dagger}\right] = \delta_{k,k'},\tag{42}$$

whereas for fermions

$$\left\{c_k, c_{k'}^{\dagger}\right\} = \delta_{k,k'}.\tag{43}$$

The Hamiltonian for interacting bosons

(34)
$$H = \sum_{k}^{\text{non-interating}} \varepsilon_k a_k^{\dagger} a_k + \frac{1}{2V} \sum_{k,k',q} U(q) a_{k+q}^{\dagger} a_{k'-q}^{\dagger} a_{k'} a_k \quad (44)$$

and for fermions

(35)
$$H = \sum_{k,\sigma}^{\text{non-interating}} \varepsilon_k c_{k,\sigma}^{\dagger} c_{k,\sigma} + \frac{1}{2V} \sum_{k,k',q,\sigma,\sigma'} U(q) c_{k+q,\sigma}^{\dagger} c_{k'-q,\sigma}^{\dagger} c_{k',\sigma'} c_{k,\sigma}.$$
(45)

The inteaction, U(q), is given by

$$U(\mathbf{r} - \mathbf{r'}) = \frac{1}{V} \sum_{q} U(\mathbf{q}) e^{i\mathbf{q} \cdot (\mathbf{r} - \mathbf{r'})}, \quad (46)$$

or

$$U(\mathbf{q}) = \int d^3 r U(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}}.$$
 (47)

We can also talk about annihilation and creation operators in real space: $\psi^{\dagger}(\mathbf{r})$ creates a particle at position \mathbf{r} .

$$\int d^3r \, \varphi^{\dagger}(\mathbf{r}) \varphi(\mathbf{r}) = \sum_k a_k^{\dagger} a_k = \hat{N}$$
 (48)

These operators favolw the same commutation relations as the momentum space equivalence.

3.1 Superfluidity in ⁴He

At low enough temperatures most atoms will be in the ground state. Our goual is to bring the Hamiltonian to a form:

$$H = \sum_{k} E_k \xi_k^{\dagger} \xi_k + \text{const.}$$
 (49)

Mean-field theory:

$$a_0 a_0^{\dagger} \approx a_0^{\dagger} a_0 = |a_0| = N_0$$
 (50)

meaning that

$$a_0 = \sqrt{N_0} e^{i\varphi}. (51)$$

Bogoliubov transformation

$$\begin{cases} \xi_{k} = u_{k} a_{k} + v_{k} a_{-k}^{\dagger} \\ \xi_{k}^{\dagger} = u_{k} a_{k}^{\dagger} + v_{k} a_{-k} \end{cases}$$
 (52)

We still want the commutation relation $\left[\xi_k, \xi_k^{\dagger}\right] = 1$, which gives

$$u_k = \cosh \theta_k, \quad v_k \sinh \theta_k.$$
 (53)

And

$$\cosh 2\theta_k = \frac{A_k}{\sqrt{A_k^2 - B_k^2}}, \quad \sinh 2\theta_k = \frac{B_k}{\sqrt{A_k^2 - B_k^2}},$$
(54)

where

$$A_k = \varepsilon_k + nU(k), \quad B_k = nU(k).$$
 (55)

Energy of the quasi-particles

$$E_k = A_k \cosh 2\theta_k - B_k \sinh 2\theta_K$$

$$= \sqrt{A_k^2 - B_k^2} = \sqrt{\varepsilon_k [\varepsilon_k + 2nU(k)]}$$
(56)

Long wavelength limit $(k \approx 0)$

$$E_k \approx \hbar |k| \sqrt{\frac{nU(0)}{m}} \tag{57}$$

same form as phonons, and $c_s = \sqrt{nU(0)/m}$. The super fluid behaves more like a solid than a liquid.

As long as some disturbance is slower than $c_{\rm s}$, there can not be any dissipation of energy into the super fluid.

Spontaneously broken symmetry We can choose φ in the mean-field theory description of a_0 freely. And the particles curren will be

$$\boldsymbol{j} = \frac{\hbar n}{m} \boldsymbol{\nabla} \varphi \tag{58}$$

But if the geomery has holes, we must have a periodically varying φ , meaning that $\nabla \varphi = \ell 2\pi$ becomes quantized.

3.2 BCS theory of superconductivity

The BCS (mean-field) equation:

$$\Delta = \frac{U}{2V} \sum_{k} \frac{\Delta}{\sqrt{\xi_{k}^{2} + \Delta^{2}}} \left[1 - 2n^{(\text{F.D.})}(E_{k}) \right]
= \frac{U}{2V} \sum_{k} \frac{\Delta}{\sqrt{\xi_{k}^{2} + \Delta^{2}}} \tanh\left(\frac{E_{k}}{2T}\right).$$
(59)

Here $E_k = \sqrt{\xi_k^2 + \Delta^2}$, and $\xi_k = (\varepsilon_k - \varepsilon_F)$ varies from $-\varepsilon_F$ to ∞ .

Sums transfroms according to

$$\frac{1}{V} \sum_{k} \to g(\varepsilon_{\rm F}) \int_{-\hbar\omega_{\rm D}}^{\hbar\omega_{\rm D}} \mathrm{d}\xi, \tag{60}$$

where $\omega_{\rm D}$ is the Debye frequency, and $\hbar\omega_{\rm D} \ll \varepsilon_{\rm F}$ (typ. values $\hbar\omega_{\rm D} \sim 10^2\,{\rm K}$, while $\varepsilon_{\rm F} \sim 10^4\,{\rm K}$). Only the states around $\varepsilon = \varepsilon_{\rm F}$ ($\xi = 0$) affects superconductivity.

3.3 Ginsburg-Landau theory of superconductivity

4 Second order phase transitions

- 4.1 Ising model
- 4.2 Landau theory of cont. phase transitions

A Special functions

A.1 Gamma function

$$\Gamma(\nu) = \int_{0}^{\infty} x^{\nu - 1} e^{-x} dx$$
 (61)

$$\Gamma(n) = (n-1)!, \quad n \in \mathbb{Z}^+$$
 (62)

| | · / | / | 5/2 | 7/2 | 9/2 |
|-------------|--------------|----------------|-----------------|------------------|--------------------|
| $\Gamma(x)$ | $\sqrt{\pi}$ | $\sqrt{\pi}/2$ | $3\sqrt{\pi}/4$ | $15\sqrt{\pi}/8$ | $105\sqrt{\pi}/16$ |

A.2 Zeta function

The Riemann zeta function

$$\zeta(\nu) = \sum_{n=1}^{\infty} \frac{1}{n^{\nu}} = \int_{0}^{\infty} \frac{x^{\nu-1}}{e^{x} - 1} dx$$
 (63)

| x | 2 | 4 | 6 |
|------------|-----------|------------|-------------|
| $\zeta(x)$ | $\pi^2/6$ | $\pi^4/90$ | $\pi^6/945$ |
| x | 3/2 | 5/2 | 7/2 |
| $\zeta(x)$ | 2.61238 | 1.34149 | 1.12673 |
| x | 3 | 5 | 7 |
| $\zeta(x)$ | 1.20206 | 1.03693 | 1.00835 |

B The harmonic oscillator