NOTES ON IDEAL QUANTUM GASES[7]

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I. GRAN CANONICAL POTENTIAL

Many-body theory is based on second-quantisation, a formalism where the basic operators create or destroy particles, acting on a Fock-space. Thermal equilibrium is then suitably described by the grand-canonical formalism. The system is in contact with a thermal reservoir at temperature T, and exchanges particles with it. The total energy and the particle numbers are not fixed a priori, but their average values depend on the temperature T and the chemical potentials μ_i of the various species. The thermal state is:

$$\boxed{\hat\rho_{gc} = \frac{1}{Z_{gc}} e^{-\beta(\hat H - \sum \mu_i \hat N_i)}} \tag{1}$$

$\beta = 1/(k_B T)$. The normalization constant

$$Z_{gc} = \operatorname{tr} \exp[-\beta(\hat H - \sum \mu_i \hat N_i)]$$

is the partition function. It is a function of T, μ_i and of the parameters in the Hamiltonian (such as the volume V, external fields). If the different species do not interact, the Hamiltonian is the sum of commuting Hamiltonians of the single species, and the partition function factors.

The thermal average of an operator is:

$$O = \langle \hat O \rangle = \operatorname{tr}(\hat\rho_{gc} \hat O)$$

Certain averages define important thermodynamic variables: $N_i = \langle \hat N_i \rangle$ (*number of particles of type i*), $E = \langle \hat H \rangle$ (*internal energy*). They may be obtained[8] as:

$$N_i = \frac{1}{\beta}\frac{\partial}{\partial \mu_i} \log Z_{gc}$$

$$E - \sum \mu_i N_i = -\frac{\partial}{\partial \beta} \log Z_{gc}$$

The connection between the microscopic description and thermodynamics is established via the *gran canonical potential*:

$$\boxed{\Omega =: -k_B T \log Z_{gc}} \tag{2}$$

$$N_i = -\frac{\partial \Omega}{\partial \mu_i}, \quad E - \sum_i \mu_i N_i = \frac{\partial(\beta\Omega)}{\partial \beta} = \Omega - T\frac{\partial \Omega}{\partial T} \tag{3}$$

The Von Neumann entropy of a state $\hat\rho$ is

$$S = -k_B \operatorname{tr}(\hat\rho \log \hat\rho)$$

The entropy of a thermal state is $S = k_B\beta(E - \sum \mu_i N_i - \Omega)$. This is rewritten as

$$\boxed{\Omega = E - TS - \sum \mu_i N_i} \tag{4}$$

Eq.(3) shows that

$$S = -\frac{\partial \Omega}{\partial T} \tag{5}$$

The first principle of thermodynamics states that the variation of the internal energy in a reversible transformation is

$$dE = TdS - dW + \sum \mu_i dN_i$$

where TdS is the input of heat, dW is the mechanical work done by the system, $\mu_i dN_i$ is the variation of energy due to the variation of the number of particles. Then:

$$d\Omega = -SdT - dW - \sum N_i d\mu_i$$

Exercise I.1 *Show that*

$$1) \quad \langle N_i^2 \rangle - \langle N_i \rangle^2 = -k_B T \frac{\partial^2 \Omega}{\partial \mu_i^2} \tag{6}$$

$$2) \quad \langle K^2 \rangle - \langle K \rangle^2 = -\frac{\partial^2}{\partial \beta^2}(\beta\Omega) \tag{7}$$

where $K = H - \sum \mu_i N_i$.

Exercise I.2 *Show that the specific heat with* $dW = 0$ *may be evaluated from the entropy:*

$$C =: \frac{\partial E}{\partial T}\Big|_N = T\frac{\partial S}{\partial T}\Big|_N$$

When work produces a variation of the volume, $d\Omega = -SdT - pdV - \sum N_i d\mu_i$. The bulk pressure is

$$p = -\frac{\partial \Omega}{\partial V}$$

Since in this case only $\Omega(T, V, \mu)$ and V are extensive, a scaling gives: $\Omega(T, \lambda V, \mu_i) = \lambda \Omega(T, V, \mu_i)$. Derivative in $\lambda = 1$ gives:

$$\boxed{\Omega(T, V, \mu_i) = -pV} \tag{8}$$

This is the equation of state after replacing μ_i with $\mu_i(T, V, N)$, obtained by inversion of $N_i = -\partial\Omega/\partial\mu_i$.

The relation $\Omega = -pV$ and the expression for $d\Omega$ imply the *Gibbs-Duhem* relation:

$$-SdT + Vdp - \sum N_i d\mu_i = 0 \tag{9}$$

Therefore for isothermal or isobaric transformations:

$$\frac{\partial p}{\partial \mu_i}\Big|_T = \frac{N_i}{V}, \quad \frac{\partial \mu_i}{\partial T}\Big|_p = -\frac{S}{N_i} \tag{10}$$

Besides E and Ω, two other thermodynamic potentials are the Helmholtz free energy and the Gibbs potential:

$$dF = -SdT - pdV + \sum \mu_i dN_i \tag{11}$$

$$dG = -SdT + Vdp + \sum \mu_i dN_i \tag{12}$$

As G depends on the extensive variables N_i, it is $G(T, p, \lambda N_i) = \lambda G(T, p, N_i)$, which implies (9) and $G = \sum \mu_i N_i$.

Exercise I.3 *Write the scaling of the free energy and get* $F = \Omega + \sum \mu_i N_i$.

In presence of a surface: $dW = pdV - \gamma dA$, where γ is the surface tension (the work done per unit area to change the area without changing the volume). The pressure normal to the surface does not coincide with p:

$$p_n = -\frac{\partial\Omega}{\partial V} + \gamma\frac{dA}{dV} = p + \gamma\left(\frac{1}{r_1} + \frac{1}{r_2}\right)$$

r_1 and r_2 are the principal radii of curvature of the surface (Laplace).

The following identity, for a one-species system, shows that the relative fluctuation of the particle number vanishes in the thermodynamic limit:

$$\frac{\langle N^2\rangle - \langle N\rangle^2}{\langle N\rangle^2} = \frac{k_BT}{V}B_T, \quad B_T = -\frac{1}{V}\frac{\partial V}{\partial p}\Big|_T \tag{13}$$

$B_T > 0$ is the isothermal bulk modulus[9].

Ornstein-Zernike relation. The density-density thermal correlator is

$$\rho(\mathbf{x}, \mathbf{x}') = \langle \sum\nolimits_{i\neq j} \delta^3(\mathbf{x} - \mathbf{x}_i)\delta^3(\mathbf{x}' - \mathbf{x}_j)\rangle \tag{14}$$

Integration gives: $\int d^3x\, d^3x'\, \rho(\mathbf{x}, \mathbf{x}') = \langle N^2\rangle - N$. If the system is homogeneous and isotropic, the density is n and $\rho(\mathbf{x}, \mathbf{x}') =: n^2 g(|\mathbf{x} - \mathbf{x}'|)$, where g is the *pair distribution function.* Then

$$\langle N^2\rangle - N^2 = N + n^2 V \int_V d^3x[g(x) - 1]$$

The *Ornstein-Zernike relation (1914)* is obtained:

$$\boxed{k_BTB_T = \frac{1}{n} + \int_V d^3x[g(x) - 1]}$$

For uncorrelated particles $g(x) = 1$ one derives $pV = Nk_BT$. For a gas pf hard spheres $g(x) = \theta(x - x_0)$, and one obtains the van der Waals law[3].

II. INDEPENDENT PARTICLES[4,5]

We consider a single species of non-interacting identical particles with $\hat{H} - \mu\hat{N} = \sum_r(\epsilon_r - \mu)\hat{c}_r^\dagger\hat{c}_r$. The evaluation of the partition function in the occupation number basis gives the thermodynamic potential:

$$\Omega = \pm\, k_BT\sum_r \log\left[1 \mp e^{-\beta(\epsilon_r - \mu)}\right] \tag{15}$$

The mean occupation number of a state is

$$n_r = \langle\hat{c}_r^\dagger\hat{c}_r\rangle = \frac{\partial\Omega}{\partial\epsilon_k} = \frac{1}{e^{\beta(\epsilon_r - \mu)} \mp 1} \tag{16}$$

For bosons, $\mu \leq \epsilon_0$ to have $n_r \geq 0$. Hereafter, the chemical potential is chosen such that the ground-state energy is zero, $\epsilon_0 = 0$.
All thermal averages may be expressed in terms of n_r (Wick's theorem):

$$N = \sum\nolimits_r n_r, \quad E = \sum\nolimits_r \epsilon_r\, n_r, \tag{17}$$

$$\Omega = \mp k_BT\sum\nolimits_r \log\left(1 \pm n_r\right) \tag{18}$$

Sums on states may be converted to integrals with the counting function of states $N(\epsilon) = \sum_r \theta(\epsilon - \epsilon_r)$ and the density $\rho(\epsilon) = N'(\epsilon)$. Eqs.(18) and (15) (after an integration by parts) become:

$$N = \int_0^\infty d\epsilon\rho(\epsilon)n(\epsilon) \tag{19}$$

$$E = \int_0^\infty d\epsilon\rho(\epsilon)n(\epsilon)\epsilon \tag{20}$$

$$\Omega = -\int_0^\infty d\epsilon N(\epsilon)n(\epsilon) \tag{21}$$

Exercise II.1 *Evaluate the entropy (Landau):*

$$S = k_B\sum\nolimits_r (n_r \pm 1)\log(1 \pm n_r) - n_r\log n_r$$

Exercise II.2 $\langle\hat{c}_r^\dagger\hat{c}_r\hat{c}_s^\dagger\hat{c}_s\rangle - n_rn_s = \delta_{rs}\, n_r(1 \pm n_r)$.

Exercise II.3 *Show that in* $d = 3$ *the counting functions of states with energy below* ϵ *for the free particle, the relativistic particle, the massless particle with dispersion law* $\epsilon_\lambda(\mathbf{k}) = c_\lambda k$ *(*$\lambda = 1, 2, 3$ *are polarization states) are:*

$$N(\epsilon) = V\frac{2s+1}{6\pi^2}\left[\frac{2m\epsilon}{\hbar^2}\right]^{3/2} \tag{22}$$

$$N(\epsilon) = V\frac{2s+1}{6\pi^2}\left[\frac{\epsilon^2 - m^2c^4}{\hbar^2c^2}\right]^{3/2} \tag{23}$$

$$N(\epsilon) = V\frac{1}{6\pi^2}\frac{\epsilon^3}{\hbar^3}\left[\frac{1}{c_1^2} + \frac{1}{c_2^2} + \frac{1}{c_3^2}\right]^{3/2} \tag{24}$$

The examples show that it is of interest to study the case $N(\epsilon) = C\epsilon^\alpha$, where C and α are constants[10]. Hereafter, we restrict to this situation. First of all:

$$\Omega = -\frac{1}{\alpha}E \tag{25}$$

With $\beta\mu = \log z$, eqs.(19) and (20) are:

$$N = \frac{C\alpha}{\beta^\alpha}\int_0^\infty dx\frac{x^{\alpha-1}}{\frac{1}{z}e^x \mp 1} \tag{26}$$

$$E = k_BT\frac{C\alpha}{\beta^\alpha}\int_0^\infty dx\frac{x^\alpha}{\frac{1}{z}e^x \mp 1} \tag{27}$$

Upper sign refers to bosons, and lower sign to fermions.

Exercise II.4 *(massless ideal boson gas). Show that* $p = \frac{1}{3}(E/V)$, $E/V \sim T^4$ *and the specific heat per particle* $c_V \sim T^3$. *For phonons, the Debye cutoff strongly modifies the results.*

III. IDEAL FERMI GAS

We consider free electrons. The starting equations are:

$$N = 2V\int \frac{d\mathbf{k}}{(2\pi)^3}\frac{1}{e^{\beta(\epsilon_k-\mu)}+1} \tag{28}$$

$$E = 2V\int \frac{d\mathbf{k}}{(2\pi)^3}\frac{\epsilon_k}{e^{\beta(\epsilon_k-\mu)}+1} \tag{29}$$

Set $z = e^{\beta\mu}$ (fugacity), $x = \beta\epsilon_k$ and introduce the functions:

$$f_\alpha(z) = \frac{1}{\Gamma(\alpha)}\int_0^\infty dx \frac{x^{\alpha-1}}{\frac{1}{z}e^x+1}, \quad \alpha > 0 \tag{30}$$

The thermodynamic equations are parametric in z:

$$\frac{1}{2s+1}\frac{N}{V}\lambda^3 = f_{3/2}(z), \tag{31}$$

$$\frac{E}{N} = \frac{3}{2}k_BT\,\frac{f_{5/2}(z)}{f_{3/2}(z)} \tag{32}$$

$$pV = Nk_BT\,\frac{f_{5/2}(z)}{f_{3/2}(z)} \tag{33}$$

They contain a basic parameter: the thermal length

$$\boxed{\lambda(T) = \left(\frac{2\pi\hbar^2}{mk_BT}\right)^{1/2}}$$

It is the de Broglie length for a particle with energy $\approx k_BT$. The ratio $(N/V)^{1/3} \approx k_F$ measures the inverse of the typical distance among particles.
$z \ll 1$ corresponds to $k_F\lambda \ll 1$ (classical regime)
$z \gtrsim 1$ corresponds to $k_F\lambda \gtrsim 1$ (quantum regime).

We need the expansions for small and large z;

$$f_\alpha(z) = \sum_{k=1}^\infty (-1)^{k+1}\frac{z^k}{k^\alpha} = z - \frac{z^2}{2^\alpha} + \frac{z^3}{3^\alpha} - \ldots \tag{34}$$

$$f_\alpha(z) = \frac{(\log z)^\alpha}{\Gamma(\alpha+1)}\left[1 + 2\frac{\alpha(\alpha-1)}{(\log z)^2}\,f_2(1) + 2\frac{\alpha(\alpha-1)(\alpha-2)(\alpha-3)}{(\log z)^4}\,f_4(1) + \ldots\right] \tag{35}$$

$f_\alpha(1) = \zeta(\alpha)(1-2^{1-\alpha})$. The large z expansion is due to Sommerfeld and is shown in the appendix.

Inversion of $N(z)$ respectively gives ($s = 1/2$):

$$z = \frac{1}{2}\frac{N}{V}\lambda^3\left[1 + \frac{1}{4\sqrt{2}}\frac{N}{V}\lambda^3 + \ldots\right] \tag{36}$$

$$\log z = \beta E_F\left[1 - \frac{\pi^2}{12}\frac{1}{(\beta E_F)^2} + \ldots\right] \tag{37}$$

In the classical regime the chemical potential $\mu = k_BT\log z$ is negative. In the quantum regime it is positive with maximum value E_F.

In the classical (small z) regime, the equation of state of a perfect gas is obtained, with the first quantum correction:

$$pV = Nk_BT\left[1 + \frac{1}{8\sqrt{2}}\frac{N}{V}\lambda^3 + \ldots\right]. \tag{38}$$

The correction increases the pressure as a signature of the Pauli principle, which forbids particles with same spin to occupy the same position.

In the quantum regime (large z):

$$\frac{E}{N} = \frac{3}{5}E_F\left[1 + \frac{5\pi^2}{12}\frac{1}{(\beta E_F)^2} + \ldots\right] \tag{39}$$

The low T linear behaviour of the specific heat per particle, and the pressure of the degenerate gas are obtained:

$$c = \frac{\pi^2}{2}\frac{1}{E_F}k_B^2T + \ldots, \quad p = \frac{2}{5}\frac{N}{V}E_F + \ldots$$

Exercise III.1 *Evaluate the ratio* T/T_F *for free electrons at* $\mu = 0$ *(answer:* ≈ 0.5*).*

Exercise III.2 *Study the 2D ideal electron gas.*

IV. THE IDEAL BOSE GAS

For non interacting bosons, the equations (26) and (27) require the following functions:

$$g_\alpha(z) = \frac{1}{\Gamma(\alpha)}\int_0^\infty dx \frac{x^{\alpha-1}}{\frac{1}{z}e^x-1} \tag{40}$$

The small z expansion is

$$g_\alpha(z) = \sum_{k=1}^\infty \frac{z^k}{k^\alpha} = z + \frac{z^2}{2^\alpha} + \frac{z^3}{3^\alpha} + \ldots \tag{41}$$

Note that $zg'_\alpha(z) = g_{\alpha-1}(z)$ and the special value $g_\alpha(1) = \zeta(\alpha)$. The $z \to 1$ behaviour is given by the Taylor expansion $g_\alpha(z) = \zeta(\alpha) + (z-1)\zeta(\alpha-1) + \ldots$.
For $1 < \alpha < 2$ another expansion is needed (see appendix).

For non-interacting bosons $\mu \le 0$ (the energy scale is fixed such that $\epsilon_0 = 0$). When $\mu \to 0^-$, the B-E statistics allows the possibility for the occupation number of the ground state to be macroscopically large.

$$n_0 = \frac{1}{e^{-\beta\mu}-1} = \frac{z}{1-z} \tag{42}$$

($\beta\mu = \log z$, $0 < z \le 1$). The occupation n_0 is of order N if $z \approx 1 - \text{cost}/N$. When this occurs, the ground state must be singled out in the basic equations.
Free bosons in $d = 3$ undergo Bose-Einstein condensation at finite T. The equations for the ideal gas are ($s = 0$):

$$\frac{N-n_0}{V}\lambda^3 = g_{3/2}(z), \tag{43}$$

$$E = \frac{3}{2}k_BT\,\frac{V}{\lambda^3}g_{5/2}(z) \tag{44}$$

Exercise IV.1 *Show that the pressure of the ideal Bose gas is always smaller than the pressure of the ideal gas at same density and temperature:* $p < (N/V)k_BT$.

A. The Bose condensate

The Bose condensate is a phase with $n_0/N \neq 0$ in the thermodynamic limit. Necessarily $z \to 1^-$ ($\mu \to 0$) as $N \to \infty$. The equation for $N - n_0$ is expanded near $z = 1$ with (61), and z is expressed in terms of n_0 by (42):

$$1 - \frac{n_0}{N} = \frac{V\zeta(3/2)}{N\lambda^3}\left[1 - \frac{2\sqrt{\pi}}{\zeta(3/2)}\frac{1}{\sqrt{n_0}} + \dots\right] \tag{45}$$

In the thermodynamic limit, n_0 is of order N and the correction vanishes. Then (45) becomes:

$$\boxed{\frac{n_0}{N} = 1 - \left(\frac{T}{T_c}\right)^{3/2}} \quad T < T_c \tag{46}$$

where the critical temperature is defined by the identity

$$1 = \frac{V\zeta(3/2)}{N\lambda^3} \quad \text{i.e.} \quad \boxed{T_C = \frac{2\pi\hbar^2}{mk_B}\left[\frac{1}{\zeta(3/2)}\frac{N}{V}\right]^{\frac{2}{3}}} \tag{47}$$

It says that the thermal length is of the order of the average separation of particles.

The total energy, specific heat, pressure ($z = 1$) are:

$$E = \frac{3}{2}k_BT\frac{V}{\lambda^3}\zeta(5/2) = \frac{3}{2}Nk_B\frac{T^{5/2}}{T_c^{3/2}}\frac{\zeta(5/2)}{\zeta(3/2)} \tag{48}$$

$$c = \frac{1}{N}\frac{\partial E}{\partial T}\Big|_{V,N} = k_B\,\frac{15}{4}\frac{\zeta(5/2)}{\zeta(3/2)}\left(\frac{T}{T_c}\right)^{3/2} \tag{49}$$

$$p = -\frac{\Omega}{V} = \frac{2}{3}\frac{E}{V} = k_BT\frac{\zeta(5/2)}{\lambda^3(T)} \tag{50}$$

In pT diagram, isothermals are lines of constant pressure. The pressure vanishes at $T = 0$, with all particle condensed in $k = 0$.
At $T = T_c$ the pressure reaches the value

$$p_c = \frac{2\pi\hbar^2}{m}\frac{\zeta(5/2)}{\zeta(3/2)^{5/3}}\left(\frac{N}{V}\right)^{\frac{5}{3}}$$

B. Near the transition

For T just above T_c, the ratio n_0/N is zero in the thermodynamic limit.

$$\lambda(T) \approx \lambda(T_c)\left[1 - \frac{1}{2}\frac{T - T_c}{T_c} + ...\right]$$

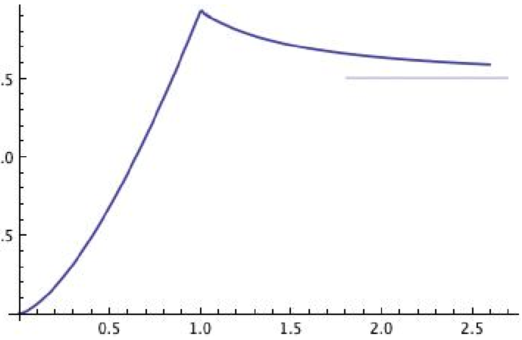

FIG. 1: The specific heat per particle in units k_B as a function of T/T_c. For $T/T_c \gg 1$ it is 3/2 (Mathematica).

Eq.(45) gives

$$n_0 \approx \frac{16\pi}{9\zeta(3/2)^2}\left(\frac{T - T_c}{T_c}\right)^{-2} + \dots \tag{51}$$

$z = 1 - 1/n_0$ follows from it. The energy per particle is Taylor-expanded in $z = 1$:

$$\frac{E}{N} = \frac{3}{2}k_BT\,\frac{V}{N\lambda^3}\left[\zeta(5/2) + (z-1)\zeta(3/2) + \dots\right]$$
$$= \frac{3}{2}k_BT_c\left[1 + \frac{5}{2}x + \frac{15}{8}x^2 + ...\right]\left[\frac{\zeta(\frac{5}{2})}{\zeta(\frac{3}{2})} - \frac{9\zeta(\frac{3}{2})^2}{16\pi}x^2 + ...\right]$$

with $x = \frac{T-T_c}{T_c}$. The leading term is the energy per particle in the condensed phase. The correction is valid for $T \approx T_c^+$. The specific heat per particle is:

$$c_V = \frac{15}{4}k_B\frac{\zeta(5/2)}{\zeta(3/2)}\begin{cases} 1 - \frac{3}{2}\frac{T_c - T}{T_c} & \text{if } T \lesssim T_c, \\ 1 - \frac{3}{2}(\gamma - 1)\,\frac{T-T_c}{T_c} & \text{if } T_c \gtrsim T \end{cases}$$

where $\gamma = \frac{3}{10\pi}\zeta(\frac{3}{2})^3/\zeta(\frac{5}{2})$. The specific heat is *continuous* across the transition, but discontinuous in its derivative.

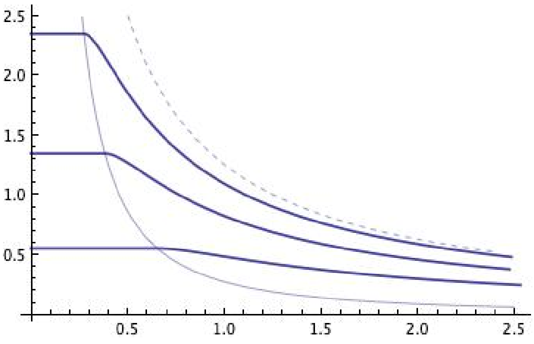

FIG. 2: Isothermal in (V, p) diagram (T decreases from above). In the BEC phase isothermals are constant pressure. The dashed line is the classical isothermal for the higher shown value of T. The light line is $p_c(V)$ (Mathematica).

For ^{4}He the critical temperature is 2.18K, and the specific heat is discontinuous. For a free boson with the Helium mass $T_c = 3.13$K.

C. Classical regime

Inversion of $N(z)$ in the small z regime gives:

$$z = \frac{N}{V}\lambda^3\left[1 - \frac{1}{2\sqrt{2}}\frac{N}{V}\lambda^3 + \dots\right] \tag{52}$$

The equation of state of the Bose gas is:

$$pV = Nk_BT\left[1 - \frac{1}{4\sqrt{2}}\frac{N}{V}\lambda^3 + \dots\right] \tag{53}$$

The quantum correction lowers the pressure (this term is opposite of the Fermi correction, up to the spin factor $2s+1$).

Exercise IV.2 *Evaluate the chemical potential near* T_c

Exercise IV.3 *Show that for the 2D ideal Bose gas there is no B.E. transition at a finite* T.

Exercise IV.4 *Many bosons are trapped in a isotropic 3D harmonic well. Show that* $N - n_0 = \zeta(3)(\beta\hbar\omega)^{-3}$. *The "critical temperature" is* $k_BT_c = \hbar\omega(N/\zeta(3))^{1/3}$. *What length does the thermal length compare with?*

V. PEIERL'S TRICK

For independent particles, the gran-canonical potential can be evaluated from the simpler canonical partition function. Write them as integrals in the density of states:

$$Z_c(\beta) = \int_0^\infty d\epsilon\, \rho(\epsilon) e^{-\beta\epsilon}$$
$$\Omega = \pm\frac{1}{\beta}\int_0^\infty d\epsilon \rho(\epsilon)\log(1 \mp e^{-\beta(\epsilon-\mu)})$$

Integrate by parts, with $\rho = \frac{dN}{d\epsilon}$. Boundary terms vanish:

$$Z_c(\beta) = \beta\int_0^\infty d\epsilon\, N(\epsilon)e^{-\beta\epsilon} \tag{54}$$
$$\Omega = -\int_0^\infty d\epsilon N(\epsilon)n(\epsilon) \tag{55}$$

where $n(\epsilon)$ is the BE or FD occupation number. Note that Z_c is a Laplace integral, which can be inverted.
For fermions at $T=0$ a further integration by parts is useful. Set $N(\epsilon) = d\zeta(\epsilon)/d\epsilon$. Then:

$$Z_c(\beta) = \beta^2\int_0^\infty d\epsilon\, \zeta(\epsilon)e^{-\beta\epsilon} \tag{56}$$
$$\Omega = \int_0^\infty d\epsilon\zeta(\epsilon)n'(\epsilon) \tag{57}$$

The inversion formula of the Laplace integral gives

$$\zeta(\epsilon) = \int_{c-i\infty}^{c+i\infty}\frac{d\beta}{2\pi i}\frac{Z(\beta)}{\beta^2}e^{\beta\epsilon} \tag{58}$$

At $T=0$: $n(\epsilon) = \theta(\epsilon_F - \epsilon)$. Then $\Omega(T=0) = -\zeta(\epsilon_F)$.

Example. Boltzmann's partition function for the ideal electron gas is

$$Z_c(\beta) = 2\sum\nolimits_{\mathbf{k}} e^{-\beta\frac{\hbar^2k^2}{2m}} = 2V\left(\frac{m}{2\pi\hbar^2\beta}\right)^{3/2}$$

The auxiliary function is evaluated:

$$\zeta(E) = 2V\left(\frac{m}{2\pi\hbar^2}\right)^{3/2}\int_{c-i\infty}^{c+i\infty}\frac{d\beta}{2\pi i}e^{\beta E}\beta^{-7/2}$$

The integral on Re $\beta = c$ coincides with the integral on the path σ around the cut, shown in Fig. (3). The latter is Hankel's representation of the Gamma function:

$$\frac{1}{\Gamma(z)} = \int_\sigma \frac{ds}{2\pi i}e^s s^{-z} \tag{59}$$

The potential Ω at $T=0$ is:

$$\Omega_0 = -V\frac{16}{15\sqrt{\pi}}\left(\frac{m}{2\pi\hbar^2}\right)^{3/2}\epsilon_F^{5/2} \tag{60}$$

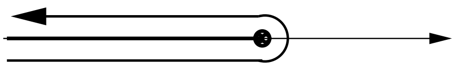

FIG. 3: The path σ around the cut.

A beautiful application of Peierl's trick is the evaluation of the diamagnetic response and the de Haas - van Alphen oscillations of the electron gas in a weak magnetic field^6 (respectively cut and poles contributions to the complex integral $\zeta(\epsilon)$).

VI. APPENDIX

Values of Riemann's Zeta function:
$\zeta(2) = \frac{\pi^2}{6}$, $\zeta(4) = \frac{\pi^4}{90}$, $\zeta(\frac{3}{2}) = 2.612$, $\zeta(\frac{5}{2}) = 1.342$.

Fermi integrals: small z

$$\int_0^\infty dx\frac{x^{\alpha-1}}{\frac{1}{z}e^x \mp 1} = \int_0^\infty dx\, x^{\alpha-1}\frac{ze^{-x}}{1 \mp ze^{-x}}$$
$$= \sum_{k=0}^\infty(\pm 1)^k z^{k+1}\int_0^\infty dx\, x^{\alpha-1}e^{-(k+1)x}$$
$$= \Gamma(\alpha)\sum_{k=1}^\infty(\pm 1)^{k+1}\frac{z^k}{k^\alpha}$$

Large-z (Sommerfeld) ($\nu = \log z$):

$$\int_0^\infty dx \frac{x^{\alpha-1}}{e^{x-\nu}+1} = \int_{-\nu}^\infty dx \frac{(\nu+x)^{\alpha-1}}{e^x+1}$$
$$= \int_\nu^\infty dx \frac{(\nu+x)^{\alpha-1}}{e^x+1}$$
$$+ \int_0^\nu dx \frac{(\nu+x)^{\alpha-1}}{e^x+1} + \int_0^\nu dx \frac{(\nu-x)^{\alpha-1}}{e^{-x}+1}$$

The first of the three integrals is of order $e^{-\nu}$ and is neglected for large ν. Write $(e^{-x}+1)^{-1} = 1-(e^x+1)^{-1}$:

$$= \frac{\nu^\alpha}{\alpha} + \int_0^\nu dx \frac{(\nu+x)^{\alpha-1} - (\nu-x)^{\alpha-1}}{e^x+1}$$
$$= \frac{\nu^\alpha}{\alpha} + \nu^{\alpha-1}\int_0^\nu dx \frac{(1+x/\nu)^{\alpha-1} - (1-x/\nu)^{\alpha-1}}{e^x+1}$$

Expand the binomials for small x/ν and replace the integration interval $[0,\nu]$ with $[0,\infty]$, with exponentially small error:

$$= \frac{\nu^\alpha}{\alpha} + 2(\alpha-1)\nu^{\alpha-1}\int_0^\infty \frac{dx}{e^x+1}\left[\frac{x}{\nu} + \frac{(\alpha-2)(\alpha-3)}{3!}\frac{x^3}{\nu^3} + \dots\right]$$
$$= \frac{\nu^\alpha}{\alpha}\left[1 + 2\alpha(\alpha-1)\frac{f_2(1)}{\nu^2} + 2\alpha(\alpha-1)(\alpha-2)(\alpha-3)\frac{f_4(1)}{\nu^4} + \dots\right]$$
$$= \frac{\nu^\alpha}{\alpha}\left[1 + \frac{\pi^2}{6}\frac{\alpha(\alpha-1)}{\nu^2} + \frac{7\pi^4}{360}\frac{\alpha(\alpha-1)(\alpha-2)(\alpha-3)}{\nu^4} + \dots\right]$$

Bose integrals.
The following holds (see NIST eq. 25.12.12), where $g_\alpha(z) = \mathrm{Li}_\alpha(z)$ (polylogarithm):

$$g_\alpha(z) = \Gamma(1-\alpha)(-\log z)^{s-1} + \sum_{k=0}^\infty \frac{\zeta(\alpha-k)}{k!}(\log z)^k$$

For $\alpha = 3/2$ and $z = 1-\eta$ it is:

$$\begin{aligned} g_{3/2}(1-\eta) - \zeta(\tfrac{3}{2}) =& \Gamma(-\tfrac{1}{2})\sqrt{\eta} - \zeta(\tfrac{1}{2})\eta + \mathcal{O}(\eta^2) \\ =& -2\sqrt{\pi\eta} - \zeta(\tfrac{1}{2})\eta + \mathcal{O}(\eta^2) \end{aligned} \tag{61}$$

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[7] Nov 2016, revised Nov 2023.

[8] The derivative of an operator at the exponent is done through the Lie-Trotter formula, which is needed when O and $dO/d\lambda$ do not commute:

$$\frac{d}{d\lambda}e^{\hat{O}(\lambda)} = \int_0^1 dt e^{t\hat{O}(\lambda)}\frac{d}{d\lambda}\hat{O}(\lambda)e^{(1-t)\hat{O}(\lambda)}$$

If the trace is taken, by the cyclic property:

$$\frac{d}{d\lambda}\mathrm{tr}[e^{\hat{O}(\lambda)}] = \mathrm{tr}\,[e^{\hat{O}(\lambda)}\frac{d}{d\lambda}\hat{O}(\lambda)]$$

[9] For fixed T, V, the equation $pV = -\Omega(T,V,\mu)$ gives a function $p(\mu)$. Then:

$$-\frac{\partial^2\Omega}{\partial\mu^2} = \frac{\partial N}{\partial\mu}\Big|_{T,V} = \frac{\partial N}{\partial p}\frac{\partial p}{\partial\mu} = \left[-\frac{\partial}{\partial\mu}\frac{\Omega}{V}\right]\frac{\partial N}{\partial p} = \frac{N}{V}\frac{\partial N}{\partial p}$$

At fixed density, $dN = \frac{N}{V}dV$ then: $\frac{\partial N}{\partial p} = \frac{N}{V}\frac{\partial V}{\partial p} = -NB_T$.

[10] for free particles $\alpha = d/2$