Ideal Quantum Gases I: Fermions [tsc15]

This module is structured in a way that highlights the mathematicl similarities and physical differences between ideal Fermi-Dirac (FD) and Bose-Einstein (BE) gases and their common Maxwell-Boltzmann limit.

Equation of state:

The thermodynamic equation of state of an ideal gas is a relation between pressure, volume per particle (or mole), and temperature.

For the classical ideal gas it reads[1] $pV = \mathcal{N} k_B T$.

For the ideal fermions gas we use (from [tsc13]) two sums over 1-particle states,

$$pV = -\Omega = k_B T \sum_{k=1}^{\infty} \ln\left(1 + z e^{-\beta\epsilon_k}\right), \quad \mathcal{N} = \sum_{k=1}^{\infty} \frac{1}{z^{-1} e^{\beta\epsilon_k} + 1},$$

and the density 1-particle states, $D(\epsilon) = \dfrac{gV}{\Gamma(\mathcal{D}/2)} \left(\dfrac{2\pi m}{h^2}\right)^{\mathcal{D}/2} \epsilon^{\mathcal{D}/2-1}$.

The factor g is included to account for any level degeneracy due to spin.

This allows us to convert the sums into integrals [tex113]:

$$\frac{pV}{k_B T} = \int_0^\infty d\epsilon\, D(\epsilon) \ln\left(1 + z e^{-\beta\epsilon}\right) = \frac{gV}{\lambda_T^{\mathcal{D}}} f_{\mathcal{D}/2+1}(z),$$

$$\mathcal{N} = \int_0^\infty d\epsilon\, \frac{D(\epsilon)}{z^{-1} e^{\beta\epsilon} + 1} = \frac{gV}{\lambda_T^{\mathcal{D}}} f_{\mathcal{D}/2}(z),$$

where we have introduced the polylogarithmic Fermi-Dirac functions,

$$f_n(z) = -\mathrm{Li}_n(-z) \doteq \frac{1}{\Gamma(n)} \int_0^\infty \frac{dx\; x^{n-1}}{z^{-1} e^x + 1}, \quad z \geq 0,$$

whose properties are elucidated in [tsl42].

Note that for fermions he range of fugacity has no upper limit: $0 \leq z \leq \infty$. The chemical potential μ is unrestricted.

Parametric representation of the thermodynamic equation of state:

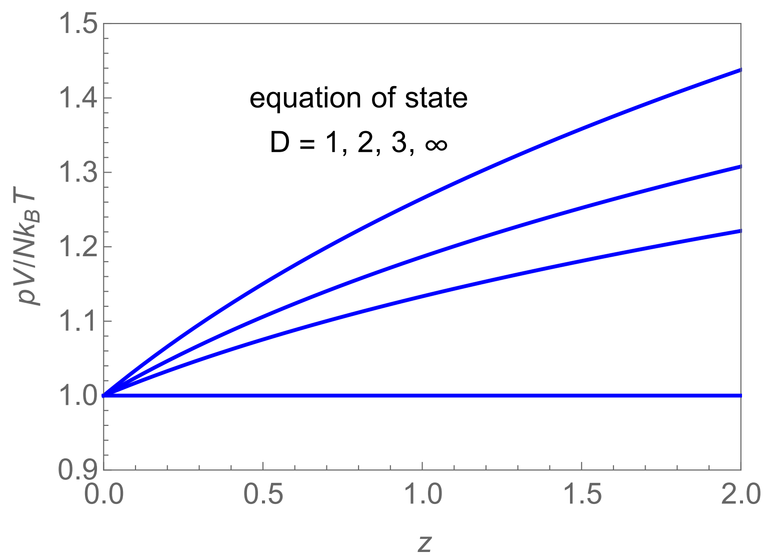
$$\frac{pV}{\mathcal{N} k_B T} = \frac{f_{\mathcal{D}/2+1}(z)}{f_{\mathcal{D}/2}(z)}, \quad 0 \leq z \leq 1.$$

[1] In the grandcanonical ensemble, $\mathcal{N}$ is the average number of particles in an open system, controlled by the chemical potential μ or the fugacity $z = e^{\beta\mu}$.

Low fugacity, $z \ll 1$, means high temperature and/or low density. Here the fermion equation of state deviates little from that of the MB gas.

At lower temperature and/or higher density, the pressure of fermions exceeds that of classical particles. The deviations are stronger in low dimensions.

The horizontal line indicates that the fermion gas in $\mathcal{D} = \infty$ dimensions behaves like a classical ideal gas.



Additional insight into the equation of state is gained by a look at isochores, isotherms, and isobars.

Here we again switch to the canonical ensemble. We keep the number of particles fixed ($N =$ const) and treat the fugacity (now a dependent thermodynamic variable) as a convenient parameter.

Chemical potential:

The chemical potential is a more prominent thermodynamic variable in the analysis of fermions than it is for bosons, particularly at low temperature.

Fermi energy/temperature: $\lim_{T\to 0} \mu = \epsilon_F = k_B T_F$.

Fugacity z from $\dfrac{\lambda_T^{\mathcal{D}}}{v} = f_{\mathcal{D}/2}(z)$, $\quad v \doteq \dfrac{gV}{\mathcal{N}}$, $\quad \lambda_T = \sqrt{\dfrac{h^2}{2\pi m k_B T}}$.

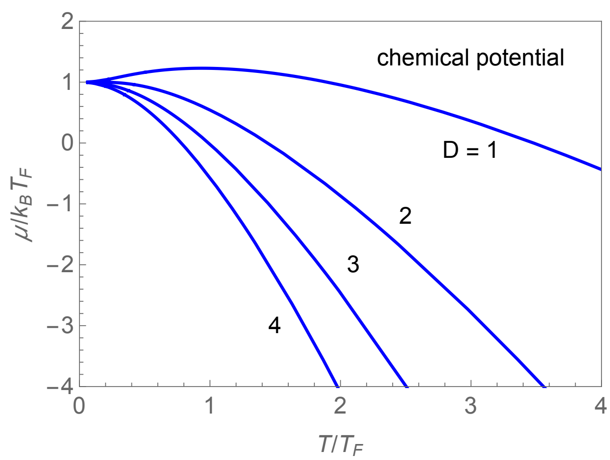
Scaled temperature (from [tsc14]): $\dfrac{T}{T_v} = [f_{\mathcal{D}/2}(z)]^{-2/\mathcal{D}}$.

Reference temperature (from [tsc14]): $k_B T_v = \frac{\Lambda}{v^{2/\mathcal{D}}}, \quad \Lambda \doteq \frac{h^2}{2\pi m}.$

Chemical potential: $\frac{\mu}{k_B T_v} = \frac{T}{T_v} \ln z.$

The Fermi temperature T_F is a more commonly used reference temperature than T_v is for fermions. The ratio is worked out in [tex117]:

$$\frac{T_F}{T_v} = [\Gamma(\mathcal{D}/2+1)]^{2/\mathcal{D}} \overset{\mathcal{D}\gg 1}{\rightsquigarrow} \frac{\mathcal{D}}{2e}.$$



The general trend is that the chemical potential decreases with increasing temperature. Only in $\mathcal{D} = 1$ does it increase initially, as shown in [tex118].

Level occupancies:

FD statistics limits one-particle states to single occupancy. The average occupancy of the level at energy ϵ as derived in [tsc13] is

$$\langle n_\epsilon \rangle = \frac{1}{e^{\beta(\epsilon-\mu)}+1}.$$

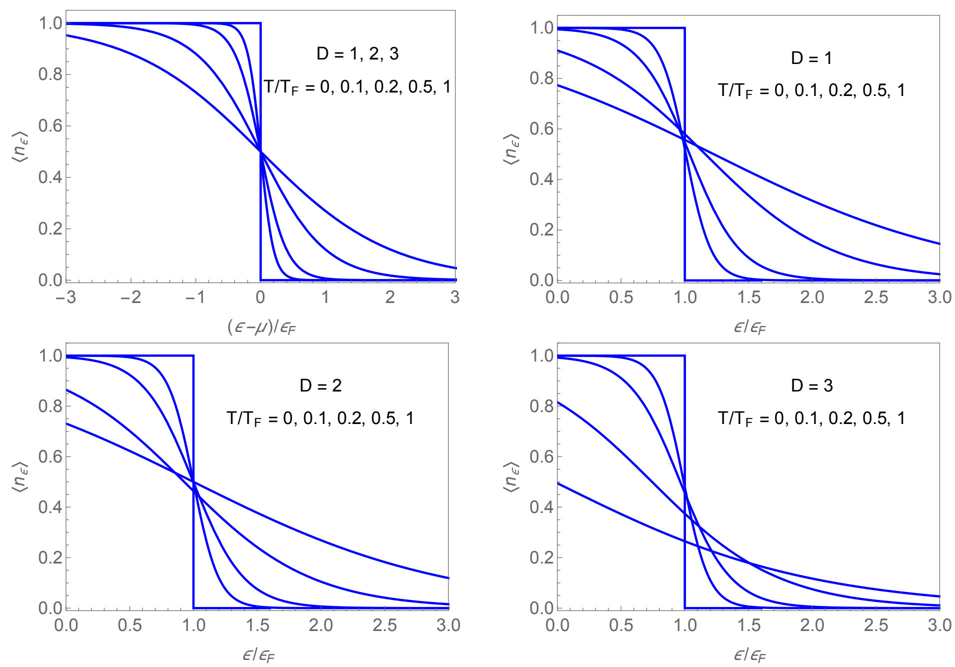
In an open system, the chemical potential μ controls the average number $\mathcal{N}$ of particles in the system. It is then custom to plot $\langle n_\epsilon \rangle$ versus $(\epsilon-\mu)/\epsilon_F$, using Fermi energy ϵ_F for scale (see first panel).

In this representation, the curves do not depend on the dimensionality $\mathcal{D}$ of the space. The dependence on $\mathcal{D}$ of the average particle number $\mathcal{N}$ is hidden in the density of energy levels $D(\epsilon)$.

In a closed system, the chemical potential is controlled by the (fixed) number N of particles and becomes a function $\mu(T)$, which also depends on $\mathcal{D}$.

In consequence, the level occupancies, plotted as $\langle n_\epsilon \rangle$ versus ϵ/ϵ_F, yield curves that depend on T and $\mathcal{D}$ (see remaining panels).

In both representations, the distribution of occupancies becomes a step function with the step at the Fermi energy $\epsilon = \epsilon_F$.



Isochores:

Universal isochore inferred from expressions for pV/k_BT and $\mathcal{N}$ [tex119]:

$$\frac{p}{p_F} = \frac{T}{T_F}\frac{f_{\mathcal{D}/2+1}(z)}{f_{\mathcal{D}/2}(z)}, \qquad \frac{T}{T_F} = \left[\Gamma\left(\frac{\mathcal{D}}{2}+1\right) f_{\mathcal{D}/2}(z)\right]^{-2/\mathcal{D}}.$$

Statistical interaction pressure (low-T limit) [tex119]:

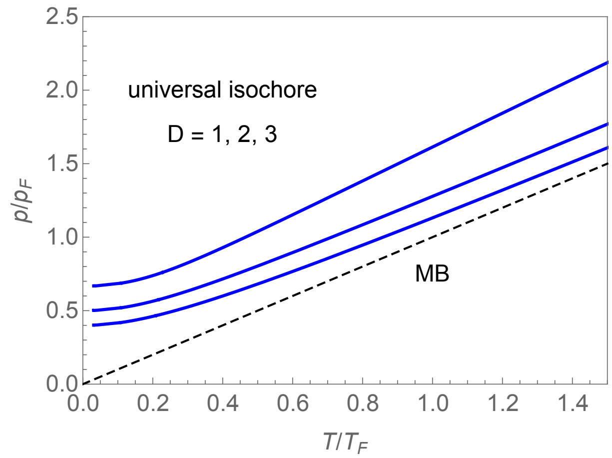
$$\lim_{T\to 0}\frac{p}{p_F} = \left(\frac{\mathcal{D}}{2}+1\right)^{-1}.$$

High-temperature asymptotic regime [tex119]:

$$\frac{pV}{\mathcal{N}k_BT_F} \sim \frac{T}{T_F}\left[1+\left[2^{\mathcal{D}/2+1}\Gamma\left(\frac{\mathcal{D}}{2}+1\right)\right]^{-1}\left(\frac{T_F}{T}\right)^{\mathcal{D}/2}\right].$$

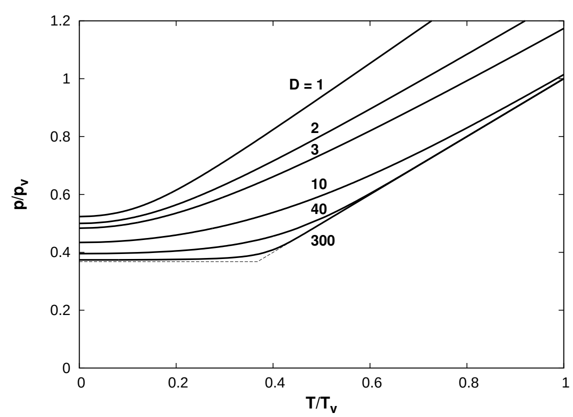
FD isochores are above the MB line, whereas BE isochores were below it.

Recall the distinction between kinematic pressure and interaction pressure from [tsc9]. In the MB gas there is only kinematic pressure. In the FD gas (BE gas) there is also positive (negative) statistical interaction pressure.



With $\mathcal{D}$ increasing, the FD isochores approach the MB line gradually and reach it in the limit $\mathcal{D} \to \infty$. There is a subtlety to that limit, which comes into view when we switch the scales from p_F, T_F to p_v, T_v:

$$\frac{p}{p_v} = \frac{f_{\mathcal{D}/2+1}(z)}{[f_{\mathcal{D}/2}(z)]^{1+2/\mathcal{D}}}, \quad \frac{T}{T_v} = \left[f_{\mathcal{D}/2}(z)\right]^{-2/\mathcal{D}}.$$



The FD isochores now approach a limiting line consisting of two straight segments, one horizontal and the other part of the MB isochore.

Phase transition:

Mapping out the limiting FD isochore requires that we take two non-commuting limits: $z \to \infty$ and $\mathcal{D} \to \infty$.

▷ $z < \infty, \ \mathcal{D} \to \infty$:

$$\frac{p}{p_v} = \frac{T}{T_v}\frac{f_{\mathcal{D}/2+1}(z)}{f_{\mathcal{D}/2}(z)} \overset{\mathcal{D}\to\infty}{\longrightarrow} \frac{T}{T_v} \qquad \text{(ideal MB gas).}$$

▷ $\mathcal{D} \to \infty, \ z \to \infty$ with $\mathcal{D}/2 = r \ln z, \ r \geq 0$:

$$\frac{p}{p_v} = \frac{f_{\mathcal{D}/2+1}(z)}{[f_{\mathcal{D}/2}(z)]^{1+2/\mathcal{D}}} \overset{\mathcal{D}\gg 1}{\rightsquigarrow} \frac{e^{-1}}{1+2/\mathcal{D}} \overset{\mathcal{D}\to\infty}{\longrightarrow} \frac{1}{e} \simeq 0.367\ldots,$$

$$\frac{T}{T_v} = \left[f_{\mathcal{D}/2}(z)\right]^{-2/\mathcal{D}} \overset{\mathcal{D}\gg 1}{\rightsquigarrow} \frac{\mathcal{D}}{2}\frac{e^{-1}}{\ln z} = \frac{r}{e} \qquad \text{(pure Fermi sea).}$$

Along the limiting FD isochore, the gas remains fully degenerate for $0 \leq T < T_v$ and then explodes into an MB gas.

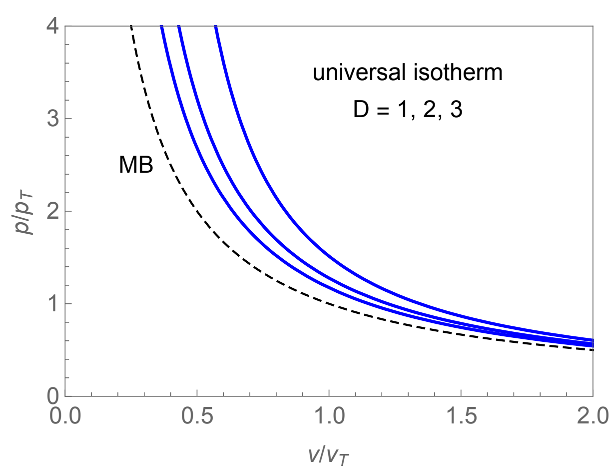
For large $\mathcal{D}$, nearly all occupied energy levels of the degenerate macrostates are at the Fermi surface. Here the density of states is very steep.

As T reaches T_v from below, almost all fermions spill into a super-abundance of empty states nearby.

Isotherms:

Universal isotherm inferred from expressions for pV/k_BT and $\mathcal{N}$ [tex120]:

$$\frac{p}{p_T} = f_{\mathcal{D}/2+1}(z), \qquad \frac{v}{v_T} = [f_{\mathcal{D}/2}(z)]^{-1}.$$



Isotherm at low density approaches Boyle's law [tex120]:

$$pv = \text{const}, \qquad v \gg v_T.$$

Isotherm at high density approaches adiabate [tex120]:

$$pv^{(\mathcal{D}+2)/\mathcal{D}} = \text{const}, \qquad v \ll v_T.$$

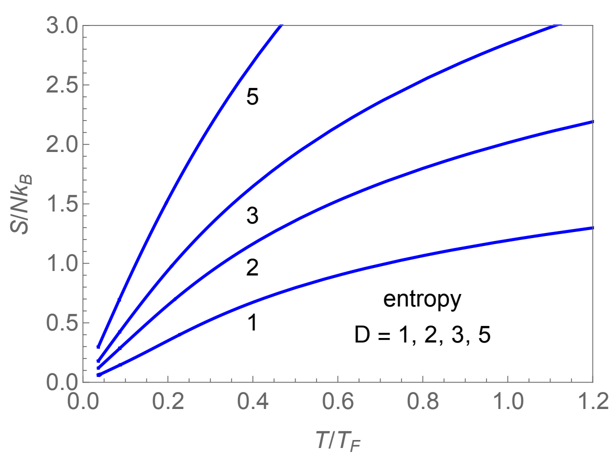
Entropy:

For the derivation of the entropy we recall the expression for the grand potential stated at the beginning of this module and its relation to the entropy:

$$\Omega = -\frac{gVk_BT}{\lambda_T^{\mathcal{D}}} f_{\mathcal{D}/2+1}(z), \quad S = -\left(\frac{\partial \Omega}{\partial T}\right)_{V,\mu}.$$

The result in parametric form for N particles confined to a rigid box reads:

$$\frac{S}{Nk_B} = \left(\frac{\mathcal{D}}{2}+1\right)\frac{f_{\mathcal{D}/2+1}(z)}{f_{\mathcal{D}/2}(z)} - \ln z, \quad \frac{T}{T_F} = \left[\Gamma\left(\frac{\mathcal{D}}{2}+1\right) f_{\mathcal{D}/2}(z)\right]^{-2/\mathcal{D}}.$$



– At high temperature, all curve rise logarithmically – an attribute shared with the MB gas.

– In the low-temperature limit all curves approach zero linearly – an attribute not shared with the MB gas.

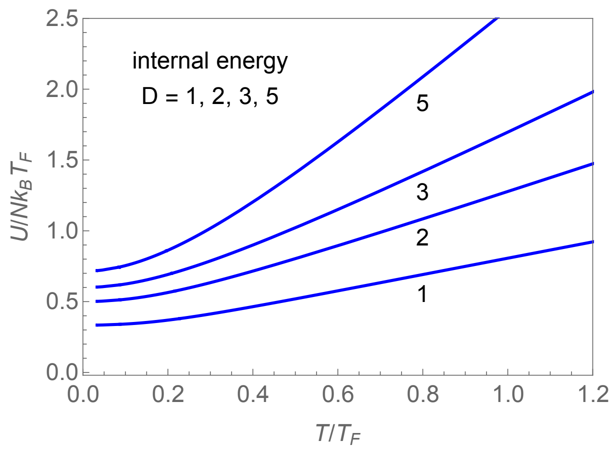
Internal energy:

Given the explicit expressions for Ω, S, N derived earlier, we can calculate the internal energy from the relation,

$$U = \Omega + TS + \mu N.$$

The result in parametric form for N particles confined to a rigid box reads:

$$\frac{U}{Nk_BT_F} = \frac{\mathcal{D}}{2}\frac{f_{\mathcal{D}/2+1}(z)}{f_{\mathcal{D}/2}(z)}\frac{T}{T_F}, \quad \frac{T}{T_F} = \left[\Gamma\left(\frac{\mathcal{D}}{2}+1\right) f_{\mathcal{D}/2}(z)\right]^{-2/\mathcal{D}}.$$



- At high temperature, all curve rise linearly – an attribute shared with the MB gas.
- In the low-temperature limit all curves approach a nonzero value – an attribute not shared with the MB gas.
- The scaled ground-state energy is [tex102]

$$\lim_{T\to 0}\frac{U}{Nk_BT_F} = \frac{U_0}{\epsilon_F} = \frac{\mathcal{D}}{\mathcal{D}+2}.$$

- An alternative and frequently used rendition of the ground-state energy is the following [tex102]:

$$\frac{U_0}{gV} \propto \epsilon_F^{\mathcal{D}/2+1}, \qquad \frac{\mathcal{N}}{gV} \propto \epsilon_F^{\mathcal{D}/2} \quad \Rightarrow \frac{U_0}{gV} \propto \left(\frac{\mathcal{N}}{gV}\right)^{(\mathcal{D}+2)/\mathcal{D}}.$$

Heat capacity:

Given the explicit expressions for U and S derived earlier, we can calculate the heat capacity from either result as follows:

$$C_v = \left(\frac{\partial U}{\partial T}\right)_{V,N} = T\left(\frac{\partial S}{\partial T}\right)_{V,N}.$$

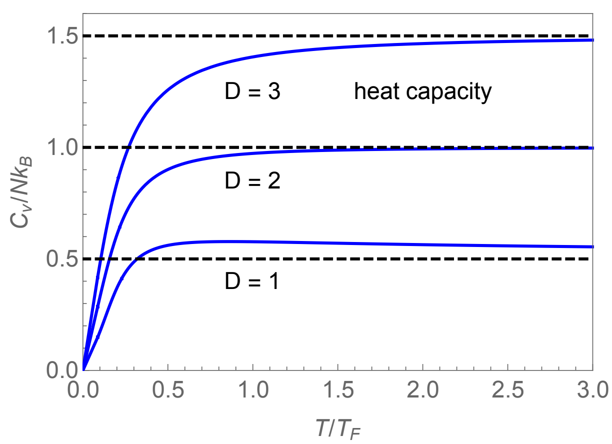
The derivatives carried out for $T \geq T_c$ yield the expression [tex100],

$$\frac{C_V}{\mathcal{N}k_B} = \left(\frac{\mathcal{D}}{2} + \frac{\mathcal{D}^2}{4}\right)\frac{f_{\mathcal{D}/2+1}(z)}{f_{\mathcal{D}/2}(z)} - \frac{\mathcal{D}^2}{4}\frac{f_{\mathcal{D}/2}(z)}{f_{\mathcal{D}/2-1}(z)}.$$

High-temperature asymptotics [tex100]:

$$\frac{C_V}{\mathcal{N}k_B} \sim \frac{\mathcal{D}}{2}\left[1 - \frac{\mathcal{D}/2-1}{2^{\mathcal{D}/2-1}\Gamma(\mathcal{D}/2)}\left(\frac{T_F}{T}\right)^{\mathcal{D}/2}\right].$$

Low-temperature asymptotics [tex101]: $\dfrac{C_V}{\mathcal{N}k_B} \sim \mathcal{D}\,\dfrac{\pi^2}{6}\,\dfrac{T}{T_F}.$



– All BE curves approach the MB result (dashed lines) in the high-T limit. The switch of side is reflected in the high-T asymptotics.

– All BE curves are approach zero in the low-T limit as required by the third law of thermodynamics. The approach is linear as reflected in the low-T asymptotics.

Exercises:

- ▷ Chemical potential I [tex117]
- ▷ Chemical potential II [tex118]
- ▷ Statistical interaction pressure [tex119]
- ▷ Isotherm and adiabate [tex120]
- ▷ Ground-state energy [tex102]
- ▷ Heat capacity at high temperature [tex100]
- ▷ Heat capacity at low temperature [tex101]
- ▷ Stable white dwarf star [tex121]
- ▷ Unstable white dwarf star [tex122]