Week 8

Quantum Statistic and Fermi gas

Quantum statistics: Discussion

- **Non-relativistic gas: high temperature, low density limit**

$$P_\eta = n_\eta k_B T\left[1-\frac{\eta}{2^{5/2}}\left(\frac{n_\eta \lambda^3}{g}\right)+\left(\frac{1}{8}-\frac{2}{3^{5/2}}\right)\left(\frac{n_\eta \lambda^3}{g}\right)^2+\cdots\right] \qquad \beta P=\frac{N}{V}\left[1+B_2(T)\frac{N}{V}+B_3(T)\left(\frac{N}{V}\right)^2+\cdots\right].$$

Question_1: This is ideal gas, why we get non-zero B_2?

Quantum effect results in "interactions" in the ideal quantum gas!

Question_2: Under which condition, the quantum effect is strong?

The natural expansion parameter is $n_\eta \lambda^3/g$, and quantum mechanical effects become important when $\boldsymbol{n_\eta \lambda^3 \geq g}$; in the so-called ***quantum degenerate limit***.

Question_3: What is the difference of B_2 between Fermi and Bose gas?

"Repulsive" force for Fermi gas and "attractive" force for Bose gas. The behavior of Fermi and Bose gases is even more different at low temperatures and high densities, and the two cases will be discussed separately.

For **low-temperature limit**, and we have to discuss Fermi and Boson gas separately.

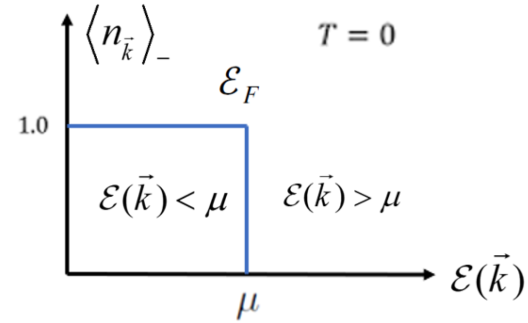
Fermi gas

- **The lowest temperature: $T = 0$, high density**

$$\langle n_{\vec{k}} \rangle_- = \frac{1}{z^{-1} e^{\beta \mathcal{E}(\vec{k})} + 1} \qquad z = \exp(\beta\mu)$$

✓ **Q:** At zero temperature, the *fermi occupation number*?

$$\langle n_{\vec{k}} \rangle_- = \frac{1}{z^{-1} e^{\beta \mathcal{E}(\vec{k})} + 1} = \begin{cases} 1, & \mathcal{E}(\vec{k}) < \mu \\ 0, & \text{otherwise} \end{cases}$$



✓ The limiting value of μ at zero temperature is called the *fermi energy ε_F*, and all one-particle states of energy less than ε_F are occupied, forming a *fermi sea*.

✓ For the ideal gas with $\varepsilon = \hbar^2 k^2/2m$, there is a corresponding *fermi wavenumber k_F*, determined by N/V, and can be calculated from

$$N = g \int \rho(\vec{k}) d^3\vec{k} \langle n_{\vec{k}} \rangle_- = g \int \frac{V d^3\vec{k}}{(2\pi)^3} \frac{1}{z^{-1}\exp(\beta\varepsilon) + 1} = gV \int^{k<k_F} \frac{d^3\vec{k}}{(2\pi)^3} = g \frac{V}{6\pi^2} k_F^3$$

In terms of density $n = N/V$, $\quad k_F = \left(\frac{6\pi^2 n}{g} \right)^{1/3}, \qquad \mathcal{E}_F(n) = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{6\pi^2 n}{g} \right)^{2/3}$

Fermi gas

- **Internal Energy and Zero-point Pressure: $T = 0$, high density**

$$\langle n_{\vec{k}} \rangle_- = \begin{cases} 1, & \mathcal{E}(\vec{k}) < \mu \\ 0, & \text{otherwise} \end{cases} \qquad N = g\frac{V}{6\pi^2}k_F^3 \qquad k_F = \left(\frac{6\pi^2 n}{g}\right)^{1/3}, \qquad \mathcal{E}_F(n) = \frac{\hbar^2 k_F^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{6\pi^2 n}{g}\right)^{2/3}$$

The ground state internal energy is?

$$E_0 = g\int \rho(\vec{k})\mathrm{d}^3\vec{k}\,\varepsilon_{\vec{k}}\langle n_{\vec{k}} \rangle_- = g\int \frac{V\mathrm{d}^3\vec{k}}{(2\pi)^3}\varepsilon_{\vec{k}}\langle n_{\vec{k}} \rangle_- = g\frac{V}{(2\pi)^3}\int_0^{k_F} 4\pi k^2 dk\,\frac{\hbar^2 k^2}{2m}$$

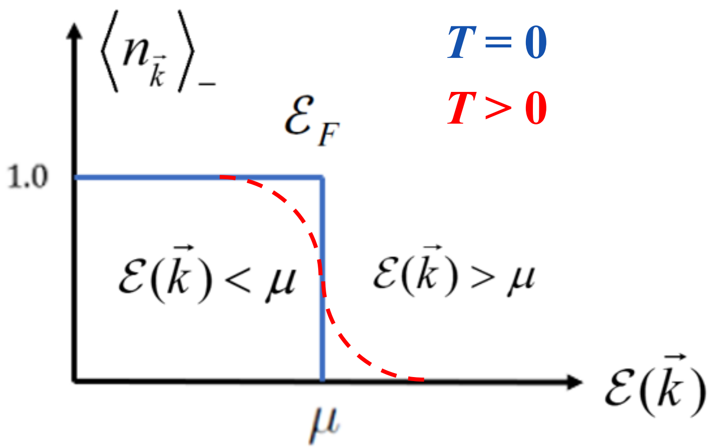
$$= \frac{g}{(2\pi)^3}\frac{4\pi V}{5}k_F^3\frac{\hbar^2 k_F^2}{2m} = \frac{3}{5}N\varepsilon_F = 3N\frac{\hbar^2}{10m}\left(\frac{6\pi^2 N}{gV}\right)^{2/3}$$

The zero-point pressure $P_0 = \frac{2}{3}\frac{E_0}{V} = \frac{2}{5}\frac{N}{V}\varepsilon_F = \frac{N}{V}\frac{\hbar^2}{5m}\left(\frac{6\pi^2 N}{gV}\right)^{2/3}$

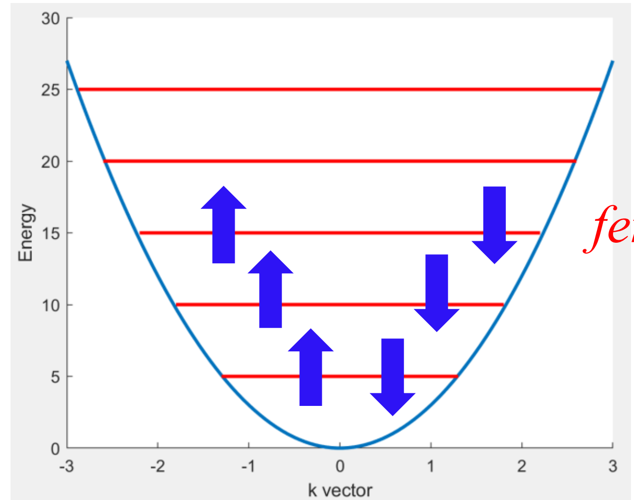
In contrast to the classical ideal gas, a Fermi gas *has finite zero-point pressure* which is again a consequence of the Pauli principle and is responsible for the stability of metals, neutron stars etc.

Fermi gas: Discussion

❑ **The lowest temperature: $T > 0$, high density**



$N = 6$



Questions:

[1] What is the configuration of energy diagram at $T = 0$? How do the fermions occupy the energy levels at $T = 0$? What is the entropy at $T = 0$?

✓ The quantum fermi gas has a unique ground state with $\Omega = 1$. Once the one-particle momenta are specified (all k for $k < k_F$), there is only one anti-symmetrized state. $S = 0$ at $T = 0$.

[2] How is the fermi sea modified at $T > 0$? How is the configuration is modified? What will happen to the occupation number?

Fermi gas

- **The degenerate fermi gas (low $T > 0$, high density)**

$$
\begin{cases}
\beta P_\eta = \dfrac{g}{\lambda^3} f_{5/2}^{\eta}(z) = \dfrac{g}{\lambda^3}\dfrac{4}{3\sqrt{\pi}}\displaystyle\int_0^\infty \dfrac{\mathrm{d}x x^{3/2}}{z^{-1}\mathrm{e}^x - \eta}, \\
n_\eta = \dfrac{g}{\lambda^3} f_{3/2}^{\eta}(z) = \dfrac{g}{\lambda^3}\dfrac{2}{\sqrt{\pi}}\displaystyle\int_0^\infty \dfrac{\mathrm{d}x x^{1/2}}{z^{-1}\mathrm{e}^x - \eta}, \\
\beta \varepsilon_\eta = \dfrac{3}{2}\beta P_\eta = \dfrac{g}{\lambda^3}\dfrac{2}{\sqrt{\pi}}\displaystyle\int_0^\infty \dfrac{\mathrm{d}x x^{3/2}}{z^{-1}\mathrm{e}^x - \eta}
\end{cases}
$$

$$
f_m^-(z) = \frac{1}{(m-1)!}\int_0^\infty \frac{\mathrm{d}x x^{m-1}}{z^{-1}\mathrm{e}^x + 1}
$$

$$
z = \exp(\beta\mu)
$$

At low T, $\mu \geq 0$, so z is very large.

✓ We need the behavior of $f_m^-(z)$ for large z (low T),

$$
\frac{x^{m-1}}{(m-1)!}\left(\frac{1}{z^{-1}\mathrm{e}^x + 1}\right)dx = d\left(\frac{x^m}{m!}\frac{1}{z^{-1}\mathrm{e}^x + 1}\right) - \frac{x^m}{m!}d\left(\frac{1}{z^{-1}\mathrm{e}^x + 1}\right)
$$

Integration by parts for $f_m^-(z)$

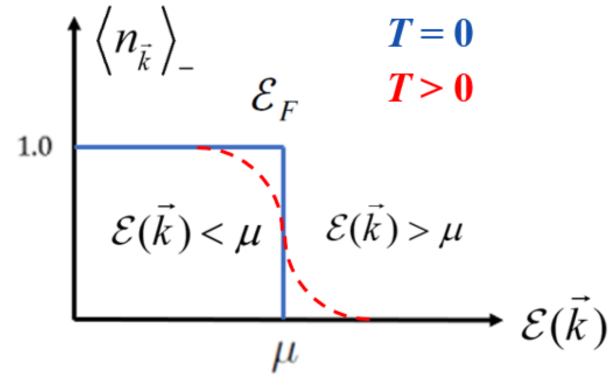
$$
f_m^-(z) = \int_0^\infty dx \frac{d}{dx}\left(\frac{1}{m!}\frac{x^m}{z^{-1}\mathrm{e}^x + 1}\right) - \frac{1}{m!}\int_0^\infty dx x^m \frac{d}{dx}\left(\frac{1}{z^{-1}\mathrm{e}^x + 1}\right) = 0 + \frac{1}{m!}\int_0^\infty dx x^m \frac{d}{dx}\left(\frac{-1}{z^{-1}\mathrm{e}^x + 1}\right)
$$

Fermi gas

❑ **The degenerate fermi gas (low T, high density)**

$$f_m^-(z) = \frac{1}{m!}\int_0^\infty dx x^m \frac{d}{dx}\left(\frac{-1}{z^{-1}e^x+1}\right) \qquad z=\exp(\beta\mu)$$

$$\langle n_{\vec{k}}\rangle_- \qquad x=\beta\varepsilon$$



The occupation number changes abruptly near μ, the above derivative is sharply peaked, and the largest contribution is near $\varepsilon \approx \mu$, where $(\varepsilon-\mu)$ is very small.

We can expand around this peak by setting $x = \ln z + t$, and extending the range of integration to $-\infty < t < +\infty$,

$$t=\beta(\varepsilon-\mu), \qquad z^{-1}e^x = e^t, \qquad x=\ln z + t$$

$$f_m^-(z) \approx \frac{1}{m!}\int_{-\infty}^{\infty} dt(\ln z + t)^m \frac{d}{dt}\left(\frac{-1}{e^t+1}\right)$$

$$= \frac{1}{m!}\int_{-\infty}^{\infty} dt \sum_{\alpha=0} \frac{m!}{\alpha!(m-\alpha)!} t^\alpha (\ln z)^{m-\alpha} \frac{d}{dt}\left(\frac{-1}{e^t+1}\right)$$

$$= \frac{(\ln z)^m}{m!}\sum_{\alpha=0} \frac{m!}{\alpha!(m-\alpha)!}(\ln z)^{-\alpha}\int_{-\infty}^{\infty} dt t^\alpha \frac{d}{dt}\left(\frac{-1}{e^t+1}\right)$$

Binominal formula

$$(x+y)^m = \sum_{\alpha=0}^{m} \frac{m!}{\alpha!(m-\alpha)!} x^\alpha y^{m-\alpha}$$

Fermi gas

❑ The degenerate fermi gas

$$f_m^-(z) = \frac{(\ln z)^m}{m!}\sum_{\alpha=0}\frac{m!(\ln z)^{-\alpha}}{(m-\alpha)!}\frac{1}{\alpha!}\int_{-\infty}^{\infty}\mathrm{d}t\,t^\alpha\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{-1}{\mathrm{e}^t+1}\right) \qquad f_m^-(z) = \frac{1}{(m-1)!}\int_0^\infty \frac{\mathrm{d}x\,x^{m-1}}{z^{-1}\mathrm{e}^x+1}$$

Use the anti-symmetry of the integrand under $t \to -t$, and do the integration by parts,

$$\frac{1}{\alpha!}\int_{-\infty}^{\infty}\mathrm{d}t\,t^\alpha\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{-1}{\mathrm{e}^t+1}\right) = \begin{cases} 0 & \text{, for } \alpha \text{ odd,} \\ \dfrac{2}{(\alpha-1)!}\displaystyle\int_0^\infty \mathrm{d}t\,\frac{t^{\alpha-1}}{\mathrm{e}^t+1} = 2f_\alpha^-(1) & \text{, for } \alpha \text{ even.} \end{cases}$$

Inserting the above into $f_m^-(z)$, and using tabulated values for the integrals $f_\alpha^-(1)$, leads to the *Sommerfeld expansion*,

$$f_m^-(z) = \frac{(\ln z)^m}{m!}\sum_{\alpha=0}^{\text{even}} 2f_\alpha^-(1)\frac{m!}{(m-\alpha)!}(\ln z)^{-\alpha} \qquad f_\alpha^-(1) = \frac{1}{(\alpha-1)!}\int_0^\infty \frac{x^{\alpha-1}}{\mathrm{e}^x+1}\mathrm{d}x$$

$$= \frac{(\ln z)^m}{m!}\left[1 + \frac{\pi^2}{6}\frac{m(m-1)}{(\ln z)^2} + \frac{7\pi^4}{360}\frac{m(m-1)(m-2)(m-3)}{(\ln z)^4} + \cdots\right]$$

$$f_{\alpha=0}^-(1) = \frac{1}{2}, \quad f_{\alpha=2}^-(1) = \frac{\pi^2}{12}, \quad f_{\alpha=4}^-(1) = \frac{7\pi^4}{720},$$

Fermi gas: Discussion

- **The degenerate fermi gas (low $T > 0$, high density)**

$$f_m^-(z) = \frac{(\ln z)^m}{m!}\left[1 + \frac{\pi^2}{6}\frac{m(m-1)}{(\ln z)^2} + \frac{7\pi^4}{360}\frac{m(m-1)(m-2)(m-3)}{(\ln z)^4} + \cdots\right]$$

In the degenerate limit, the density and chemical potential are related by

$$\frac{n\lambda^3}{g} = f_{3/2}^-(z) = \frac{(\ln z)^{3/2}}{(3/2)!}\left[1 + \frac{\pi^2}{6}\frac{3}{2}\frac{1}{2}(\ln z)^{-2} + \cdots\right]$$

Questions:

[1] Can you guess the results of the lowest order?

[2] For the lowest order, what is the Fermi energy? Total energy?

[3] For the lowest order, what is the pressure?

Fermi gas

❑ **The degenerate fermi gas (low $T > 0$, high density)**

$$f_m^-(z) = \frac{(\ln z)^m}{m!}\left[1 + \frac{\pi^2}{6}\frac{m(m-1)}{(\ln z)^2} + \frac{7\pi^4}{360}\frac{m(m-1)(m-2)(m-3)}{(\ln z)^4} + \cdots\right]$$

In the degenerate limit, the density and chemical potential are related by

$$\frac{n\lambda^3}{g} = f_{3/2}^-(z) = \frac{(\ln z)^{3/2}}{(3/2)!}\left[1 + \frac{\pi^2}{6}\frac{3}{2}\frac{1}{2}(\ln z)^{-2} + \cdots\right]$$

Let's look at the lowest-order result first: it reproduces the fermi energy at $T = 0$,

$$\lim_{T\to 0}\ln z = \left[(\frac{3}{2})!\frac{n\lambda^3}{g}\right]^{2/3} = \left[\frac{3}{4}\sqrt{\pi}\frac{n\lambda^3}{g}\right]^{2/3} = \frac{\beta\hbar^2}{2m}\left(\frac{6\pi^2 n}{g}\right)^{2/3} = \beta\mathcal{E}_F$$

$$(\frac{3}{2})! = \frac{3\sqrt{\pi}}{4} \qquad \lambda = \hbar\sqrt{\frac{2\pi}{mk_BT}} \qquad \mathcal{E}_F(n) = \frac{\hbar^2}{2m}\left(\frac{6\pi^2 n}{g}\right)^{2/3} \qquad \left[(\frac{3}{2})!\frac{n\lambda^3}{g}\right]^{2/3} = \beta\mathcal{E}_F$$

Fermi gas

❑ **The degenerate fermi gas (low $T > 0$, high density): chemical potential**

$$\frac{n\lambda^3}{g} = f^-_{3/2}(z) = \frac{(\ln z)^{3/2}}{(3/2)!}\left[1+\frac{\pi^2}{6}\frac{3}{2}\frac{1}{2}(\ln z)^{-2}+\cdots\right]$$

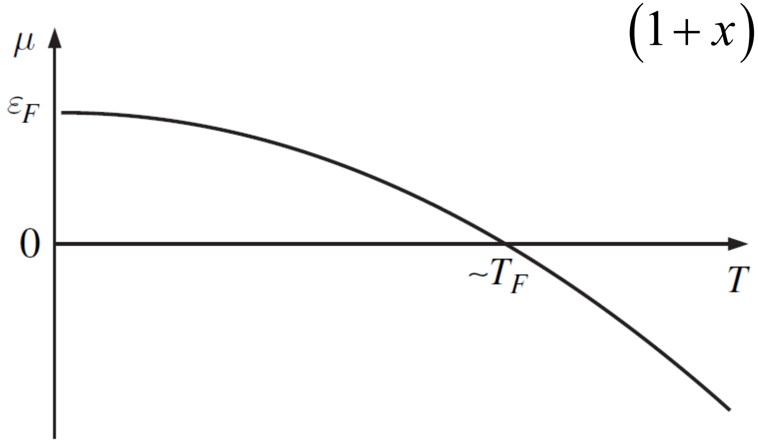
Lowest order:

$$\lim_{T\to 0}\ln z = \beta\mathcal{E}_F \qquad \left[\left(\frac{3}{2}\right)!\frac{n\lambda^3}{g}\right]^{2/3} = \beta\mathcal{E}_F$$

Now let's look at the first-order correction: Insert the lowest order result ln$z = \beta\varepsilon_F$ in the square bracket of the above equation, we get:

$$\beta\mu = \ln z = \beta\mathcal{E}_F\left[1+\frac{\pi^2}{8}\left(\frac{k_BT}{\mathcal{E}_F}\right)^2+\cdots\right]^{-2/3} \simeq \beta\mathcal{E}_F\left[1+\left(-\frac{2}{3}\right)\frac{\pi^2}{8}\left(\frac{k_BT}{\mathcal{E}_F}\right)^2+\cdots\right]$$

$$(1+x)^{-n} \approx 1-nx+\ldots$$



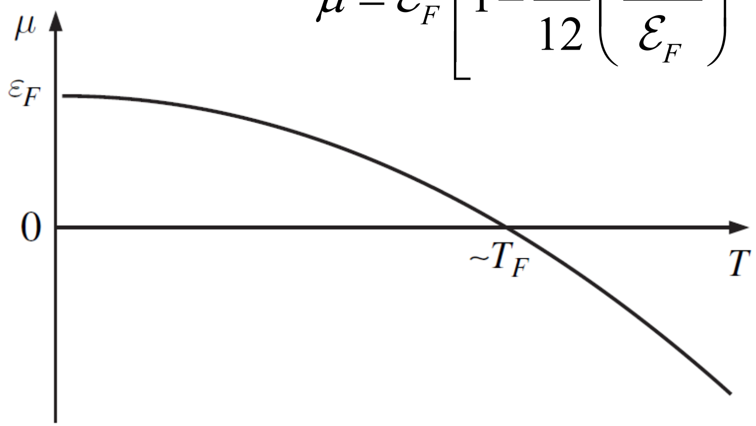
$$\mu = \mathcal{E}_F\left[1-\frac{\pi^2}{12}\left(\frac{k_BT}{\mathcal{E}_F}\right)^2+\cdots\right]$$

Note that the fermion chemical potential is positive at low temperatures, and negative at high temperatures. It changes sign at a temperature of the order of ε_F/k_B, set by the fermi energy.

Fermi gas: Discussion

- **The degenerate fermi gas (low $T > 0$, high density): chemical potential**

$$\mu = \varepsilon_F \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F} \right)^2 + \cdots \right]$$



high temperature, classical

$$dE = TdS - pdV + \mu dN$$

$$\mu = \left. \frac{\partial E}{\partial N} \right|_{S,V}$$

The S increases with increasing the N. To increase N keeping the V and S constant, we have to change the E by a negative amount. So, μ *must be negative* at high temperature.

Questions:

[1] Why is the fermion chemical potential positive at low temperatures?

[2] Why is the fermion chemical potential negative at high temperatures?

[3] What is the physical meaning of fermi temperature $T_F \sim \varepsilon_F / k_B$?

[4] For classical ideal gas, is the chemical potential negative or positive? Why?

Fermi gas

❑ **The degenerate fermi gas (low *T* > 0, high density): pressure**

$$f_m^-(z) = \frac{(\ln z)^m}{m!}\left[1 + \frac{\pi^2}{6}\frac{m(m-1)}{(\ln z)^2} + \frac{7\pi^4}{360}\frac{m(m-1)(m-2)(m-3)}{(\ln z)^4} + \cdots\right]$$

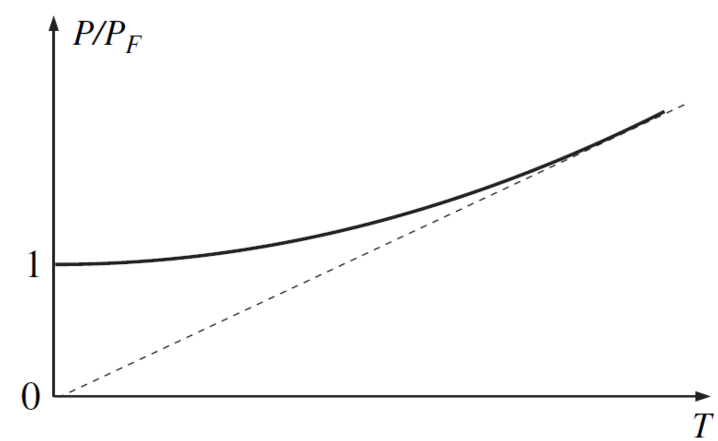
$$\beta P = \frac{g}{\lambda^3} f_{5/2}^-(z) = \frac{g}{\lambda^3}\frac{(\ln z)^{5/2}}{(5/2)!}\left[1 + \frac{\pi^2}{6}\frac{5}{2}\frac{3}{2}(\ln z)^{-2} + \cdots\right] \qquad \ln z = \beta\mathcal{E}_F\left[1 - \frac{\pi^2}{12}\left(\frac{k_B T}{\mathcal{E}_F}\right)^2 + \cdots\right]$$

$$= \left[\frac{g}{\lambda^3}\frac{8}{15\sqrt{\pi}}\right](\beta\mathcal{E}_F)^{5/2}\left[1 - \frac{5}{2}\frac{\pi^2}{12}\left(\frac{k_B T}{\mathcal{E}_F}\right)^2 + \cdots\right]\left[1 + \frac{5\pi^2}{8}\left(\frac{k_B T}{\mathcal{E}_F}\right)^2 + \cdots\right] \qquad \ln z = \beta\mathcal{E}_F$$

$$= \beta P_F\left[1 + \frac{5}{12}\pi^2\left(\frac{k_B T}{\mathcal{E}_F}\right)^2 + \cdots\right]$$

where $P_F = (2/5)n\varepsilon_F$ is the *fermi pressure* (your homework).

Unlike its classical counterpart, the fermi gas at zero temperature has finite pressure and internal energy.



Fermi gas: Discussion

- **The degenerate fermi gas: heat capacity**

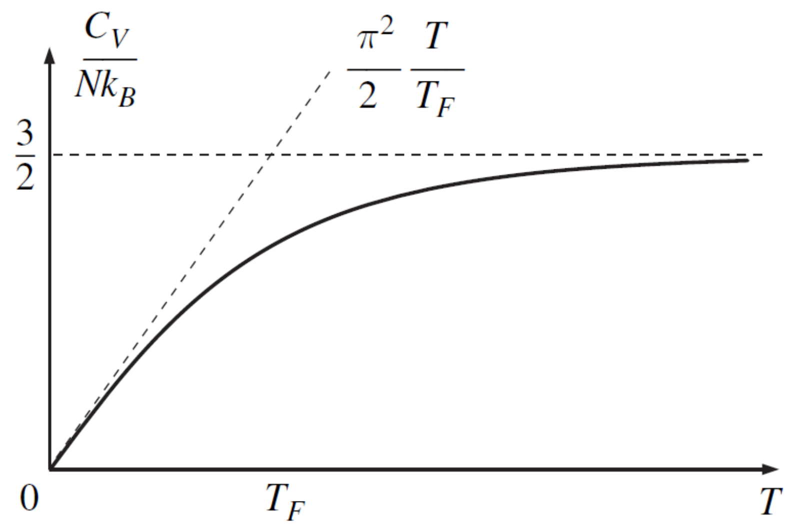
$$P = \frac{2}{5} n \varepsilon_F \left[1 + \frac{5}{12}\pi^2 \left(\frac{k_B T}{\varepsilon_F} \right)^2 + \cdots \right]$$

The low-temperature internal energy is

$$\frac{E}{V} = \frac{3}{2}P = \frac{3}{5} n k_B T_F \left[1 + \frac{5}{12}\pi^2 \left(\frac{T}{T_F} \right)^2 + \cdots \right]$$

introduced the *fermi temperature* $T_F = \varepsilon_F / k_B$.

$$C_V = \frac{\mathrm{d}E}{\mathrm{d}T} = \frac{\pi^2}{2} N k_B \left(\frac{T}{T_F} \right) + \mathcal{O}\left(\frac{T}{T_F} \right)^3$$



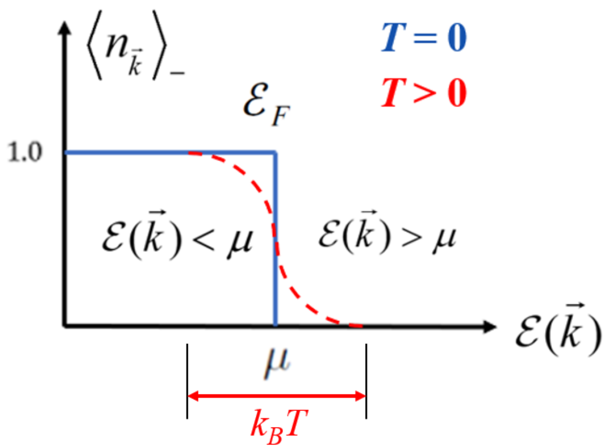
- The linear heat capacity as $T \rightarrow 0$ is a general feature of a fermi gas, valid in all dimensions.

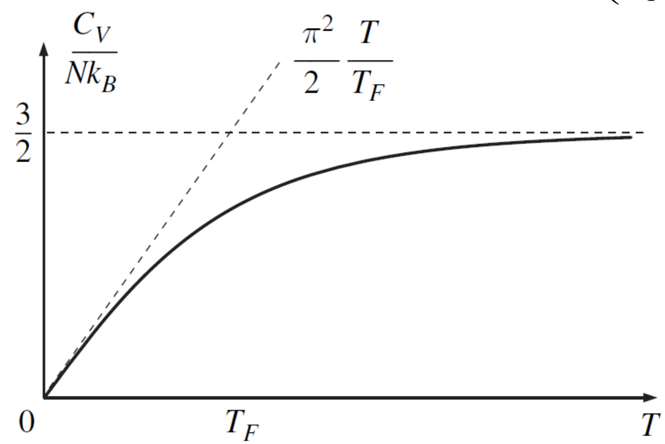
Question: Why the heat capacity decrease linearly with temperature, instead of T^3 like Debye solid?

Fermi gas

- **The degenerate fermi gas: heat capacity**

$$C_V = \frac{\pi^2}{2} N k_B \left(\frac{T}{T_F}\right) + \mathcal{O}\left(\frac{T}{T_F}\right)^3$$





The linear heat capacity as $T \to 0$ is a general feature of a fermi gas, valid in all dimensions.

Origin of linear heat capacity: Only particles within a distance of approximately $k_B T$ of the fermi energy ε_F can be thermally excited. This represents only a small fraction, T/T_F , of the total number of fermions.

Each excited particle gains an energy of the order of $k_B T$, leading to a change in the internal energy of approximately $k_B T N(T/T_F)$. Hence the heat capacity is given by $C_V = \mathrm{d}E/\mathrm{d}T \sim N k_B T/T_F$.

Qualifying exam problem

The conduction electrons in metals can be described by a model of non-interacting Fermi gas. You are given the number density n and the Fermi energy ε_F of the non-interacting Fermi gas at zero absolute temperature, ***T* = 0 K**. Find the isothermal compressibility

$$\kappa = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T,$$

where V is volume, p is pressure. We need to find $\kappa(n, \varepsilon_F)$.

Solutions:

At $T = 0$ K, $p = \frac{2E}{3V} = \frac{2}{3V} 2 \frac{V}{(2\pi)^3} \int_{k<k_F} d^3k \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 k_F^5}{15 m \pi^2}$

With $nV = N = 2\frac{V}{(2\pi)^3}\int_{k<k_F} d^3k$ We obtain $\frac{N}{V} = \frac{k_F^3}{3\pi^2} = n$, so $k_F = (\frac{N 3\pi^2}{V})^{1/3}$

Rewrite $p = \frac{\hbar^2}{15 m\pi^2}(\frac{N3\pi^2}{V})^{5/3}$, therefore $\kappa = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T = \frac{3}{5p} = \frac{3}{2n\varepsilon_F}$

Bose gas: Discussion

- **Bose Gas.** In terms of particle number N, there are two situations for Bosons:
  - ✓ Bosons which results as modes of harmonic oscillators (particle number not fixed), e.g. photons, phonons, etc. chemical potentiel $\mu = 0$.
  - ✓ a system with well-defined particle number, e.g. bosonic atoms, such as the ^{4}He; Let's look at this now. chemical potentiel $\mu =$?
- **Bosonic Atoms.** We consider Bosons without spin ($S = 0$) for which ^{4}He is a good example. Analogously to the Fermions we introduce functions of z to express the equation of state and the particle number. The bose occupation number

$$\langle n_{\vec{k}} \rangle_+ = \frac{1}{\exp[\beta(\varepsilon(\vec{k}) - \mu)] - 1}, \qquad \varepsilon = \hbar^2 k^2 / 2m$$

Questions:

[1] Any requirements on the the value of $\langle n_{\vec{k}} \rangle_+$ we must consider?

[2] Any requirements on the chemical potential we have to consider?
Positive/negative at high temperature? Positive/negative at low temperature?

[3] How does chemical potential change with decreasing temperature?

[4] How does $\langle n_{\vec{k}} \rangle_+$ change with decreasing temperature?