Thermodynamics of Plasma

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CFRJS

Introduction

- Gas of ions and electrons without and with interaction
- Distribution functions
- Interaction term and its divergences
- Debye screening
- Pressure of the plasma
- Degree of ionization of the plasma
- Saha equation and its consequences
- Saha Equation: ionization via fast electron

Our discussion is based on the books:

V. A. Trubnikov: Teorija plasmy

L. D. Landau and E. M. Lifshitz: Statistical Physics I

Ideal gas of ions and electrons

- Ideal (i.e. non-interacting !!) gas of ions and electrons at temperature T contained inside the volume V:

$$E_{id} = \frac{3}{2}kT(N_e + N_i) \; ; \; p_{id} = (n_e + n_i)kT = \frac{N_e + N_i}{V}kT \qquad (1)$$

$N_{e,i}$ – number of electrons, ions and $n_{e,i} = N_{e,i}/V$ – their density.

- Quasi-neutrality condition:

$$e_e n_e + e_i n_i = 0 \quad \text{or} \quad n_e = Z n_i \; (e_i = Ze) \qquad (2)$$

- How do the above relations change when we turn on the interaction between particles?

.... and with interaction

Let's start from the Gibs distribution describing probability of some state:

$$dW = Ce^{-H(p,q)/(kT)} d\Gamma \quad ; \quad d\Gamma \equiv \prod_{e,i} \frac{d\mathbf{p}d\mathbf{q}}{(2\pi\hbar)^3} \tag{3}$$

$\int dW = 1 \Rightarrow C$ and

$$H(p,q) = \sum_{e,i} \frac{p^2}{2m} + U_{int} \; ; \; U_{int} = \sum_{j<k} \frac{e_i e_j}{r_{jk}} \; ; \; r_{jk} = | \mathbf{r}_j - \mathbf{r}_k | \tag{4}$$

In plasma interactions among charged particles need to be included:

$$E = \langle H \rangle = \int H dW = \frac{3}{2} kT(N_e + N_i) + \langle U_{int} \rangle \tag{5}$$

where

$$\langle U_{int} \rangle = \sum_{j<k} \int \frac{e_j e_k}{r_{jk}} dW \tag{6}$$

- First term in (5) corresponds to energy of ideal gas, second term accounts for the interaction.
- Integration in (6) is taken over all particles.

Distribution functions

Introducing distribution function of all particles forming the system:

$$dW_N \;=\; f_{1,2,3,\ldots,N} d\Gamma_1 d\Gamma_2 d\Gamma_3 \ldots d\Gamma_N \tag{7}$$

and integrating it over all particles except of n one obtains n-particle distribution function:

$$\begin{aligned} dW_n \;&=\; d\Gamma_1 d\Gamma_2 d \ldots d\Gamma_n \int f_{1,2,3,\ldots,N} d\Gamma_{n+1} d\Gamma_{n+2} \ldots d\Gamma_N \\ &=\; f_{1,2,3,\ldots,n} d\Gamma_1 d\Gamma_2 \ldots d\Gamma_n \end{aligned} \tag{8}$$

- one-particle function $dW_1 = f_1 d\Gamma_1$
- two-particle function $dW_{12} = f_{12} d\Gamma_1 d\Gamma_2$
- ...particle function $dW_{12\ldots} = f_{12\ldots} d\Gamma_1 \Gamma_2 \ldots$
- all they are normalized to one:

$$\int f_1 d\Gamma_1 = 1 \;;\; \int\int f_{12} d\Gamma_1 d\Gamma_2 = 1 \;;\; \ldots \tag{9}$$

Two-particle distribution function

For homogeneous classical plasma the one-particle function is given by the Maxwell distribution:

$$dW = f_1^0 d\Gamma_1 = e^{-p^2/(2mkT)} \frac{d\mathbf{p}}{(2\pi mkT)^{3/2}} \frac{dV}{V} \tag{10}$$

and two-particle by:

$$dW_{12} = f_{12} d\Gamma_1 d\Gamma_2 = w(r_{12}) f_1^0 f_2^0 d\Gamma_1 d\Gamma_2 \tag{11}$$

Integrating last expression over particle momenta

$$dQ_{12} = w(r_{12}) \frac{dV_1}{V} \frac{dV_2}{V} \tag{12}$$

we obtain two-particle probability distribution in configuration space
Particle 1 occupies volume dV_1, particle 2 volume dV_2.
$w(r_{12})$ is probability density of their relative distance distribution.

- Using (12) we can rewrite (6) as:

$$\langle U_{int}\rangle = \frac{N_e(N_e-1)}{2}e_e^2\int\frac{dQ_{ee}}{r_{12}} + \frac{N_i(N_i-1)}{2}e_i^2\int\frac{dQ_{ii}}{r_{12}} + N_eN_ie_ee_i\int\frac{dQ_{ei}}{r_{12}} \quad (13)$$

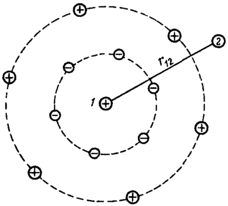
$$= V\left[\frac{(e_en_e)^2}{2}\int\frac{w_{ee}}{r}dV + \frac{(e_in_i)^2}{2}\int\frac{w_{ii}}{r}dV + e_en_ee_in_i\int\frac{w_{ei}}{r}dV\right]$$

- The 'only' unknown function here is $w(r_{12})$.
- N.B. $w(r_{12}) = 1$ corresponds to an ideal gas case.
- In terms of $$v_{12}(r) \equiv 1 - w_{12}(r)\ ;\ r = |\mathbf{r}_1 - \mathbf{r}_2| \quad (14)$$

  we have: $\langle U_{int}\rangle =$

$$\frac{1}{2}Ve^2n_e^2\int\frac{v_{ee}+v_{ii}-2v_{ei}}{r}dV = 2\pi Ve^2n_e^2\int_0^\infty(v_{ee}+v_{ii}-2v_{ei})rdr \quad (15)$$

- $\int_0^\infty v_{\alpha\beta}(r)rdr < \infty \;\Leftrightarrow\; v_{\alpha\beta}(r) \sim r^{-(2+\delta)}\ ;\ \delta > 0$
- In Gibbs distribution (3) two-particle interaction is included via Boltzmann factor:
$$w^*_{12} = exp(-\frac{e_1 e_2}{rkT}) \approx 1 - \frac{e_1 e_2}{rkT} \quad \Rightarrow v_{12}(r) \sim \frac{1}{r} \qquad (16)$$
(assuming interaction to be weak enough so that the exponential can be expanded). For this case integral (15) diverges!
- N.B. (16) does not include influence of remaining N-2 particles forming the medium into which particles 1 and 2 are submerged. $\Rightarrow$ Its validity is limited only to very small distances $r_{12} < n^{-1/3}$ when influence of other particles can be neglected.
- In reality particle 1 will polarize the surrounding medium by attracting particles of opposite charge and repelling same charge particles. This polarization will decrease Coulombic field of particle 1.



- Effective field due to particle 1 is:

$$\Delta\phi = \frac{1}{r}\frac{\partial^2}{\partial r^2}(r\phi) = -4\pi\rho_{el} = -4\pi(e_e\tilde{n}_e + e_i\tilde{n}_i) \tag{17}$$

- $\tilde{n}_e$, $\tilde{n}_i$ – particle density of electrons, ions where perturbation due to field ϕ of particle 1 is included via Boltzmann factor:

$$\tilde{n}_\alpha = n_\alpha e^{-\frac{U}{kT}} = n_\alpha e^{-\frac{e_\alpha\phi}{kT}} \approx n_\alpha(1 - \tfrac{e_\alpha\phi}{kT}) \; ; \qquad \alpha = e, i \tag{18}$$

- n_e and n_i are average densities fulfilling: $e_e n_e + e_i n_i = 0$.
- (17) & (18) $\Rightarrow$ $\Delta\phi = \left[\frac{4\pi}{kT}(n_e e_e^2 + n_i e_i^2)\right]\phi$ or $(r\phi)'' = \frac{1}{d^2}r\phi$ (19)

with Debye-Hückel radius

$$d = \sqrt{\frac{kT}{4\pi(n_e e_e^2 + n_i e_i^2)}} \tag{20}$$

- Solving (19) $\Rightarrow$ $\phi = C\cdot\frac{e^{-\frac{r}{d}}}{r}$, $C = e_1 \Leftarrow \lim_{r\to 0}\phi = \frac{e_1}{r}$ (21)

Debye Screening

- $\Rightarrow$ Polarization of the medium modifies the potential energy of two charged particles submerged into the plasma:

$$U_{12}^{eff} = e_2\phi_1 = \frac{e_1 e_2}{r} e^{-r/d} = U_{12}^{coul} e^{-r/d} \quad , \tag{22}$$

- as well as their relative distance probability distribution:

$$w_{12} = e^{\frac{-U_{12}^{eff}}{kT}} \approx 1 - \frac{U_{12}^{eff}}{kT} \tag{23}$$

- and hence $$v_{12} = -\frac{U_{12}^{eff}}{kT} = -\frac{e_1 e_2}{kTr} e^{-r/d} \tag{24}$$

- (15) & assuming only ions with charge Z in the plasma $\Rightarrow$

$$\langle U_{int} \rangle = 2\pi V e^2 n_e^2 \int_0^\infty (v_{ee} + v_{ii} - 2v_{ei}) r dr = \tag{25}$$

$$2\pi V \frac{e^2 n_e^2}{kT} \int_0^\infty (-e_e^2 - e_i^2 + 2e_i e_e) e^{-r/d} dr = \frac{VkT}{8\pi d^3} \tag{26}$$

Debye radius

- and finaly:

$$E = \langle E_{kin} \rangle + \langle U_{int} \rangle = \frac{3}{2} kT(N_e + N_i) - \sqrt{\frac{\pi}{VkT}} (N_e e_e^2 + N_i e_i^2)^{3/2} \tag{27}$$

- Basic parameter of the plasma:

$$\xi \equiv \frac{\langle U_{int} \rangle}{\langle E_{kin} \rangle} = \frac{1}{12\pi(n_e + n_i)d^3} \sim \frac{1}{N_d} \ll 1 \tag{28}$$

- $N_d \sim nd^3$ corresponds to the number of particles contained inside the Debay sphere.
- For $n \approx 10^{15} cm^{-3}$ and $kT \approx 1keV$: $d \approx 10^{-3} cm$
  $\Rightarrow N_d \approx 10^5 \gg 1$ and $\xi \approx 10^{-7} \ll 1$.

- Free energy $F(T,V,N) = E - TS$ can be used to calculate pressure of plasma $p = -\left(\frac{\partial F}{\partial V}\right)_{T,N}$:

$$dF = -SdT - pdV + \mu dN \tag{29}$$

- using (27) and integrating equation $F = E + T\left(\frac{\partial F}{\partial T}\right)_{N,V}$ we have:

$$F(T,V,N) - T\int \frac{dT}{T^2}E(T) = F_{id} - \frac{2}{3}\sqrt{\frac{\pi}{VkT}}(N_e e_e^2 + N_i e_i^2)^{3/2} \tag{30}$$

(the integration constant was determined from the condition $\lim_{T\to\infty} F = F_{id}$

- (30) $\Rightarrow$: $p = -\left(\frac{\partial F}{\partial V}\right)_{T,N} = (n_e + n_i)kT - \frac{1}{3}\sqrt{\frac{\pi}{kT}}(n_e e_e^2 + n_i e_i^2)$ (31)

$$p = p_{id} - \frac{kT}{24\pi d^3} = p_{id} - \frac{(4\pi\sum_\alpha n_\alpha e_\alpha^2)^{3/2}}{24\pi\sqrt{kT}} \tag{32}$$

Degree of Ionization of the Plasma

- Rough estimate: $$N_e^{free}/N_e^{bound} \sim e^{-\frac{I}{kT}} \tag{33}$$

  $I-$ ionization energy (for hydrogen $I = (1/2)me^4/\hbar^2 = 13.5eV$) $\Rightarrow$ ionization is important at $kT \approx I$ i.e. at $T \approx 10^6 K$
- In reality the ionization occurs already at $T \approx 10^3 K$ ... something is missing?
- The missing factor is the ratio of statistical weights corresponding to number of effectively possible states of free and bound electron, i.e.:

$$\gamma \equiv \frac{\Delta\Gamma_{free}}{\Delta\Gamma_{bound}} = \left(\frac{d\mathbf{p}dV}{(2\pi\hbar)^3}\right)_{eff} / N_i = \frac{(d\mathbf{p})_{eff}}{n_i(2\pi\hbar)^3} \tag{34}$$

  here $d\mathbf{p}$ is effective volume of the momentum space defined as:

$$(d\mathbf{p})_{eff} = \int e^{p^2/2mkT} d\mathbf{p} = (2\pi mkT)^{3/2} \tag{35}$$

Degree of Ionization of the Plasma

- Using electron de Broglie wavelength $\lambda_e = \hbar/\sqrt{2m_e kT}$ we get:

$$\gamma = \frac{(2\pi mkT)^{3/2}}{n_i(2\pi\hbar)^3} = \frac{1}{8\pi^{3/2}}\frac{1}{n_i\lambda_e^3} \gg 1 \quad (36)$$

  i.e. in typical circumstances the quantum wavelength is much smaller than inter-particle distances $\lambda_e^3 \ll n_i^{-1/3}$ i.e. $n_i\lambda_e^3 \ll 1$

- So now the right form of (33) reads:

$$N_e^{free}/N_e^{bound} = \gamma e^{-\frac{I}{kT}} = \frac{e^{-\frac{I}{kT}}}{8\pi^{3/2} n_i \lambda_e^3} \quad (37)$$

- Assume that **both** p and T of the gas are fixed $\Rightarrow$ total number of particles per unit volume:

$$n_{tot} = n_e + n_i + n_a = p/kT \;\; n_e = n_i \;,\;\; n_a = N_e^{bound}/V \quad (38)$$

  is also fixed. (We assume that plasma consists of electrons, ions and neutral atoms with densities n_e, n_i, n_a).

- (38) $\Rightarrow$ $$n_e = n_i = \frac{\alpha}{1+\alpha} n_{tot} \; ; \; n_a = \frac{1-\alpha}{1+\alpha} n_{tot} \tag{39}$$

  where α is degree of ionization of the plasma:

  $$\alpha = \frac{N_e^{free}}{N_e^{free} + N_e^{bound}} \tag{40}$$

  (We consider only single–ionized atoms - see(34)).

- (37) $\rightarrow$ $$N_e^{free}/N_e^{bound} = \frac{n_e}{n_a} = \gamma e^{-I/kT} = \frac{1+\alpha}{\alpha} \frac{1}{K(p,T)} \tag{41}$$

  where $K(p,T)$ is constant of ionization equilibrium:

$$K(p,T) = (8\pi^{3/2} n_{tot} \lambda_e^3) e^{I/kT} = \frac{p}{kT} \left(\frac{2\pi\hbar^2}{mkT} \right)^{3/2} e^{I/kT}$$

$$= 1.4 \cdot 10^{57} \frac{n_{tot}[cm^{-3}]}{kT[eV]} e^{I/kT} \tag{42}$$

Saha Equation and its Consequences

- (41) $\Rightarrow$ Saha equation $K = 1 - \alpha^{-2}\ ,\ \alpha = \dfrac{1}{\sqrt{1+K}}$ (43)

- For big K: $\alpha \simeq K^{-1/2} = (8\pi^{3/4} n_{tot} \lambda_e^3)^{-1/2} e^{-I/2kT} \ll 1$ (44)

- For small K and $\alpha \approx 1$: $1 - \alpha \simeq \dfrac{K}{2} = 4\pi^{3/2} n_{tot} \lambda_e^3 e^{I/kT} \ll 1$ (45)

- **Example**: **Air** (density $n = 3 \cdot 10^{19}$)
  - At $\mathbf{T = 1300K}$ $kT \approx 0.1eV$ hydrogen ($I = 13.5eV$) will be ionized to $\alpha \approx 10^{-10}$ i.e. $K \approx 0.5 \cdot 10^{22} \gg 1$.
  - However, already at $\mathbf{T = 11000K}$ $kT \approx 1eV$ the degree of ionization of the plasma will be $1 - \alpha \lesssim 10^{-30}$ i.e. $K \approx 10^{-30} \ll 1$
    $\Rightarrow$ hydrogen will be fully ionized!!
  - Between $10^3 - 10^4$ $^\circ$ C constant of ionization equilibrium K changes by 50 orders of magnitude!!!

Saha Equation: Ionization via Fast Electron

- Saha eqs. (43) assumes thermodynamical equilibrium between matter and radiation: $\hbar\omega + a \leftrightarrows e + i$ i.e. atom ionization and electron–ion recombination proceed with the same speed. In finite systems this is not fulfilled since photon can leave the system.
- (43) is valid $\Leftrightarrow$ electron mean free path is negligible compared to the size of the system: $\ell \ll L$.
- In the opposite case $\ell \gg L$
  (true for Sun corona or in thermonuclear environment)
  the recombination will be compensated not via $\hbar\omega + a \rightarrow e + i$
  but by the ionization due to fast electrons
  $e + i \rightarrow a + \hbar\omega$, $e + a \rightarrow e + e + i$.
  It this case the number of electrons will change as:

$$dn_e/dt = -\kappa_{rec} n_e n_i + \kappa_{ion} n_e n_a \tag{46}$$

  where κ_{rec}, κ_{ion} are (temperature–dependent) recombination and ionization coefficients.

Saha Equation: Ionization via Fast Electron

- For the stationary case $dn_e/dt = 0$ (39) $\rightarrow$

$$\frac{n_i}{n_e} = \frac{\alpha}{1-\alpha} = \frac{\kappa_{ion}}{\kappa_{rec}} = K(T) \quad ; \quad \alpha = \frac{K(T)}{1+K(T)} \tag{47}$$

where κ_{rec} and κ_{ion} are related to corresponding cross sections σ_{rec} and σ_{ion}

$$\kappa_{rec}(T) = \langle \sigma_{rec} \cdot v \rangle \quad \text{and} \quad \kappa_{ion}(T) = \langle \sigma_{ion} \cdot v \rangle \tag{48}$$

with averaging over Maxwell velocity distribution function $f(v)$.

- For temperatures close to the ionization energy $kT \simeq I$ the cross section is close to geometric dimensions of the atom $\sigma_{ion} \simeq 10^{-16} cm^2$ but $\sigma_{rec} \simeq 10^{-22} cm^2$. At the same time $K(T) \gg 1$ and ionization is close to 100%

$$\alpha \approx 1 - \frac{1}{K(T)} = 1 - \frac{\kappa_{rec}}{\kappa_{ion}} \tag{49}$$