VJEŽBE 7
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Ekviparticija energije

Kad god je energija kvadratična funkcija neke varijable, možemo lako odrediti doprinos odgovarajućeg stupnja slobode unutarnjoj energiji.

Općenito, neka je $-\infty < s < \infty$ bilo koja varijabla o kojoj energija ovisi kvadratično:

$$E = as^2 + (\text{doprinosi neovisni o } s)$$

→ možemo izračunati koliki je doprinos unutarnjoj (očekivanoj) energiji koji daje varijabla s:

$$\langle E \rangle = \mathcal{E}(s) + (\text{ostatak})$$

Po definiciji očekivane vrijednosti:

$$\mathcal{E}(s) = \frac{\int as^2 e^{-\beta a s^2} ds}{\int e^{-\beta a s^2} ds} = -\frac{\partial}{\partial \beta} \ln \Big(\underbrace{\int e^{-\beta a s^2} ds}_{I = \pi \sqrt{\beta a}} \Big)$$

$$\mathcal{E}(s) = -\frac{\partial}{\partial \beta} \ln \left(\frac{1}{\sqrt{\beta}} \right) = \frac{1}{2\beta}$$

$$\mathcal{E}(s) = \frac{1}{2} kT$$ EKVIPARTICIONI TEOREM

[Svaka varijabla o kojoj energija ovisi kvadratično, daje doprinos $kT/2$ unutarnjoj energiji.]

Slobodni jednoatomni plin:

$U = \frac{3}{2} NkT$ → $c_V = 3R$ po molu (Dulong-Petitovo pravilo)

Dvoatomni plin: $U = \frac{7}{2} NkT$ 3 kvadratična doprinosa translacija
2 rotacija
2 vibracija

GAMA FUNKCIJA (Bronštejn str. 463)

$$\Gamma(x) = \int_0^\infty e^{-t} t^{x-1} dt \qquad (x>0)$$

$$\Gamma(x) = \lim_{n\to\infty} \frac{n^x \cdot n!}{x(x+1)(x+2)\dots(x+n)}$$

Svojstva gama funkcije: tablica gama funkcija: Bronštejn str. 1055

$$\Gamma(x+1) = x\Gamma(x)$$

$$\Gamma(n+1) = n!$$

$$\Gamma\left(\tfrac{1}{2}\right) = 2\int_0^\infty e^{-t^2} dt = \sqrt{\pi}$$

KANONSKA RASPODJELA NA KLASIČNI MODEL IDEALNOG PLINA

1 stupanj slobode: $e^{-\beta E}$

$$e^{-\frac{mv^2}{2kT}} = e^{-\frac{p^2}{2mkT}}$$

$$P(q_1,\dots,q_N,p_1,\dots,p_N) \longrightarrow$$

$$\int e^{-\frac{1}{2m}\frac{(p_x^2+p_y^2+p_z^2)}{kT}} \underbrace{dp_x\,dp_y\,dp_z}_{p^2 4\pi\, dp} \rightarrow \text{prelazak u sferni sustav}$$

$$dx\,dy\,dz \rightarrow \int_0^R r^2 \underbrace{4\pi}_{\underbrace{\sin\theta d\theta}_{2}\, \underbrace{d\varphi}_{2\pi}} dr \rightarrow \frac{4\pi}{3}R^3$$

Onda imamo funkciju raspodjele po brzinama:

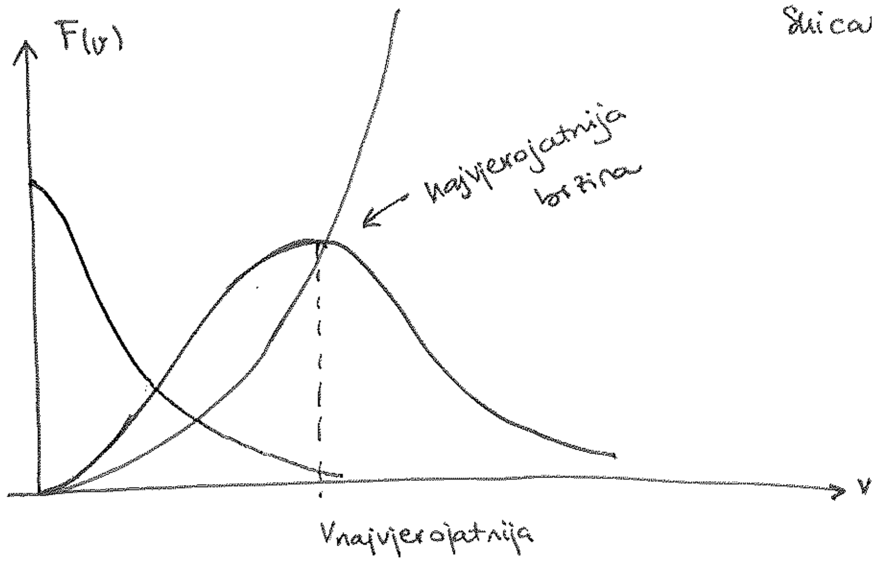
$$F(v) \sim v^2 e^{-\frac{mv^2}{2kT}} dv$$

Moramo se pobrinuti da je normalizirana!

$$\int_0^\infty F(v)\,dv = N \rightarrow \text{broj molekula}$$

$$\boxed{F(v) = \underbrace{4\pi \frac{N}{V}\left(\frac{m}{2\pi kT}\right)^{3/2}}_{\substack{\text{normalizacija} \\ A}} v^2 e^{-\frac{mv^2}{2kT}} dV}$$

Skica $F(v)$



Najvjerojatnija brzina → tražimo ekstrem raspodjele $F(v)$, moramo derivirati

$$\frac{\partial F(v)}{\partial v} = 0$$

$$F(v) = Av^2 e^{-bv^2} \qquad b = \frac{m}{2kT} \qquad A = 4\pi \frac{N}{V}\left(\frac{m}{2\pi kT}\right)^{3/2}$$

$$\frac{\partial F(v)}{\partial v} = 2Ave^{-bv^2} - 2Av^2 bve^{-bv^2} = 0$$

$$2e^{-bv^2} vA(1-bv^2) = 0$$

$v_1 = 0$ → to je minimum rasp.

$1 - bv_2^2 = 0$ → najvjerojatnija brzina

$$v_{najv} = \sqrt{\frac{1}{b}}$$

$$\boxed{v_{najv.} = \sqrt{\frac{2kT}{m}}}$$

→ Srednja brzina (iznos)

$$\langle v \rangle = \frac{1}{N} \int_0^\infty F(v)\, v\, dv$$

Str 1050

→ tablični int. Bronštejn 24.

$$4\pi \left(\frac{m}{2\pi kT}\right)^{3/2} \int_0^\infty e^{-\alpha v^2} v^3 dv \qquad \alpha = \frac{m}{2kT} \qquad \int_0^\infty e^{-\alpha v^2} v^3 dv = \frac{1}{2\alpha^2}$$

$$\langle v \rangle = 4\pi \left(\frac{m}{2\pi kT}\right)^{3/2} \cdot \frac{1}{2} \left(\frac{m}{2kT}\right)^{-2}$$

$$\underbrace{\langle v \rangle = \sqrt{\frac{8\pi kT}{m}}}$$

$$\langle v \rangle \cdot \left\langle \frac{1}{v} \right\rangle = \dots = \frac{4}{\pi}$$

Npr...

$$\left\langle \frac{1}{v} \right\rangle = \int_0^\infty F(v) \frac{1}{v} dv \Rightarrow \int_0^\infty e^{-\alpha v^2} v\, dv \quad \dots \quad \left\langle \frac{1}{v} \right\rangle = \sqrt{\frac{2m}{\pi kT}}$$

$$\left\langle \frac{1}{v^2} \right\rangle = \int_0^\infty F(v) \frac{1}{v^2} dv = \int_0^\infty e^{-\alpha v^2} dv \dots$$

$$\left\langle \frac{1}{v^3} \right\rangle = \int_0^\infty F(v) \frac{1}{v^3} dv = \int_0^\infty e^{-\alpha v^2} \frac{1}{v} dv \quad \rightarrow \text{DIVERGIRA!}$$

$$v_{RMS} = \sqrt{\langle v^2 \rangle}$$

$$\langle v^2 \rangle = \frac{1}{N}\int_0^\infty F(v)\,v^2 dv = 4\pi \left(\frac{m}{2\pi kT}\right)^{3/2}\int_0^\infty e^{-\alpha v^2} v^4 dv$$

$$\left\{ \int_0^\infty x^n e^{-\alpha x^2} dx = \frac{\Gamma\left(\frac{n+1}{2}\right)}{2\alpha^{\left(\frac{n+1}{2}\right)}} \quad \begin{matrix} a>0 \\ n>-1 \end{matrix} \right\} \quad \begin{matrix} n=4 \\ \alpha = \frac{m}{2kT} \end{matrix}$$

$$\langle v^2 \rangle = \overset{2}{\cancel{4}}\pi \left(\frac{m}{2\pi kT}\right)^{3/2} \frac{1}{\cancel{2}}\left(\frac{2kT}{m}\right)^{5/2} \Gamma\left(\frac{5}{2}\right)$$

$$= \frac{4kT}{m}\frac{1}{\sqrt{\pi}}\Gamma\left(\frac{5}{2}\right)$$

$$\Gamma\left(\frac{5}{2}\right) = \underbrace{\left(\frac{5}{2}-1\right)}_{3/2}\underbrace{\Gamma\left(\frac{3}{2}\right)}_{\underbrace{\left(\frac{3}{2}-1\right)}_{1/2}\underbrace{\Gamma\left(1/2\right)}_{\sqrt{\pi}}}$$

$$\Gamma\left(\frac{5}{2}\right) = \frac{3}{4}\sqrt{\pi}$$

$$\langle v^2 \rangle = \frac{\cancel{4}kT}{m}\frac{1}{\cancel{\sqrt{\pi}}}\frac{3}{\cancel{4}}\cancel{\sqrt{\pi}} \longrightarrow \langle v^2 \rangle = \frac{3kT}{m}$$

$$\boxed{v_{RMS} = \sqrt{\langle v^2 \rangle} = \sqrt{\frac{3kT}{m}}}$$