Microcanonical Ensemble

Okay... but where did this canonical ensemble come from?! A more natural starting point for stat mech:

Suppose you are given Hamiltonian $H(\{\phi_n\})$ and energy E

Microcanonical ensemble: All states with energy E are equally likely!

ensure energy is E

$$p(\{\phi_n\}) = \frac{\delta(E - H(\{\phi_n\}))}{\int d\{\phi_n\} \; \delta(E - H(\{\phi_n\}))}$$

to normalize count up # of states with energy E

Density of states $N(E)$!!

Ideal gas in ME : N free particles in box of volume V

$$H = \frac{1}{2m}\sum_{i=1}^{N} p_i^2 = \frac{1}{2m}\sum\left(p_{xi}^2 + p_{yi}^2 + p_{zi}^2\right)$$

$$N(E) = V^N \int d^3p_1 \int d^3p_2 \ldots \int d^3p_N \, \delta\left(E - \frac{p_1^2}{2m} - \ldots - \frac{p_N^2}{2m}\right)$$

integral $\int dx_i\, dy_i\, dz_i$

2D $\int dx\,dy \to 2\pi \int r\,dr$

3D $\int dx\,dy\,dz \to 4\pi \int r^2\,dr$

answer depends on length of 3N dimensional vector

(high d analog of spherical coordinates)

$$N(E) = V^N \Omega_{3N} \int dp\, p^{3N-1}\, \delta(E - p^2/2m)$$

this is 4π in $d=3$

$$2m\,\delta(2mE - p^2)$$

$$2m\,\delta\left((\sqrt{2mE} - p)(\sqrt{2mE} + p)\right)$$

$$= V^N \Omega_{3N}\, 2m\, (2mE)^{(3N-1)/2} \frac{1}{2\sqrt{2mE}}$$

What the heck is Ω_{3N} ?!

$$\int d^D x\, e^{-x^2} = \pi^{D/2}$$

$$\Omega_D \int_0^\infty x^{D-1} e^{-x^2}\, dx \qquad x^2 = t \qquad 2x\,dx = dt$$

$$\frac{1}{2}\Omega_D \int_0^\infty dt\, t^{D/2-1} e^{-t} = \frac{1}{2}\Omega_D \Gamma(D/2)$$

gamma function

so $\Omega_D = 2\pi^{D/2} / \Gamma(D/2)$

$\Gamma(z) \equiv \int_0^\infty dt\, t^{z-1} e^{-t}$

$\Gamma(z+1) = \int_0^\infty t^z \underbrace{e^{-t}\, dt}_{du}$

$= -t^z e^{-t}\Big|_0^\infty + \int_0^\infty z t^{z-1} e^{-t} dt$

$\Gamma(z+1) = z\,\Gamma(z)$

generalization of factorial function to noninteger z.

Check formula for Ω_D in $D = 2, 3$

$\Omega_2 = 2\pi^{2/2} / \Gamma(1) = 2\pi$

$\Gamma(1) = \int_0^\infty dt\, e^{-t} = 1$

$\Omega_3 = 2\pi^{3/2} / \Gamma(3/2) = 2\pi^{3/2} / \pi^{1/2}/2 = 4\pi$ ✓✓

$dt = 2r\,dr$

$t = r^2$

$\Gamma(3/2) = \int_0^\infty dt\, t^{1/2} e^{-t}$

$= \int_0^\infty 2r\,dr\, r\, e^{-r^2} = 2\int_0^\infty r^2 dr\, e^{-r^2}$

$= 2\,\frac{1}{2}\;\frac{1}{2}\sqrt{\pi} = \sqrt{\pi}/2$

ME4

Thus, finally,

$$N(E) = V^N (2\pi m)^{3N/2} E^{3N/2-1}/\Gamma(3N/2).$$

Much of this nonsense is contained in a Mathematical Appendix to your text.

Let's be math studlies for a minute and compute $N(E)$ another way, the "Laplace transform method". It will turn out that this approach has close connections with the "canonical ensemble" as some of you will recognize from the notation. Define

problem #2

$$Z(\beta) = \int d\Gamma e^{-\beta H}.$$

Since $N(E) = \int d\Gamma \delta(E - H)$, this quantity $Z(\beta)$ is just the Laplace transform of $N(E)$

$$Z(\beta) = \int_0^\infty dE e^{-\beta E} N(E)$$

$$N(E) = 1/(2\pi i) \int_{0^+ - i\infty}^{0^+ + i\infty} d\beta Z(\beta) e^{+\beta E}.$$

review this inverse Laplace transform formula ?

But $Z(\beta)$ is trivial to compute. (This is why working in the canonical ensemble is usually simpler than the microcanonical ensemble).

$$Z(\beta) = V^N (2\pi m/\beta)^{3N/2}$$

So we compute $N(E)$ to be (draw a picture of contour of integration, closing the contour off to the left where β has negative real part)

pole of order $3N/2$

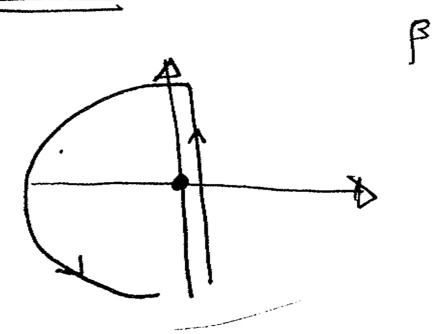
$$\begin{aligned} N(E) &= 1/(2\pi i) V^N (2\pi m)^{3N/2} \int_{0^+ - i\infty}^{0^+ + i\infty} d\beta \beta^{-3N/2} e^{+\beta E} \\ &= 1/(2\pi i) V^N (2\pi m)^{3N/2} 1/(3N/2-1)!(d/d\beta)^{3N/2-1} e^{\beta E}|_{\beta=0} \\ &= V^N (2\pi m)^{3N/2} E^{3N/2-1}/\Gamma(3N/2). \end{aligned}$$

go real slow !

as before! Whew!

One crucial feature is the rapid growth of $N(E)$ with E. We will see that this is central to ideas concerning how to systems come into equilibrium with each other.

~~Good~~ problem # 4 in HW!



Laplace Transform Review

$$f(s) = \int_0^\infty e^{-st} F(t)\,dt$$

$$F(t) = 1$$

$$f(s) = \int_0^\infty e^{-st}\,dt = 1/s$$

$$F(t) = e^{\omega t}$$

$$f(s) = \int_0^\infty e^{-st} e^{\omega t}\,dt = 1/(s-\omega)$$

$$F(t) = \cos\omega t = \tfrac{1}{2}\left(e^{i\omega t} + e^{-i\omega t}\right)$$

$\sin\omega t \leftrightarrow \dfrac{\omega}{s^2+\omega^2}$

$$f(s) = \frac{1}{2}\left[\frac{1}{s-i\omega} + \frac{1}{s+i\omega}\right] = \frac{s}{s^2+\omega^2}$$

derivatives $\displaystyle \int_0^\infty \underbrace{e^{-st}}_{u} \underbrace{F'(t)\,dt}_{dv} = e^{-st}F(t)\Big|_0^\infty - \int -s e^{-st} F(t)\,dt$

$$= -F(0) + s\,f(s)$$

similarly $\displaystyle \int_0^\infty e^{-st} F''(t)\,dt = s^2 f(s) - sF(0) - F'(0)$

L2

Solving $\quad m x''(t) = -kx$

$\boxed{?}$ $\quad x(t) = x(0)\cos\omega t + \frac{v(0)}{\omega}\sin\omega t \qquad \omega^2 = \frac{k}{m}$

$$s^2 X(s) - s X(0) - v(0) = -\underbrace{\frac{k}{m}}_{\omega^2} X(s)$$

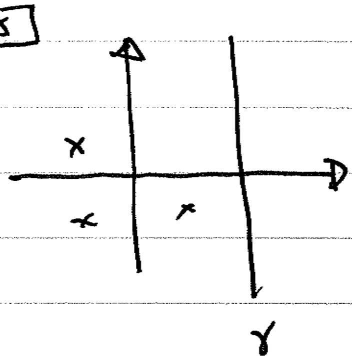
$$(s^2+\omega^2)\, X(s) = s\, X(0) + v(0)$$

$$X(s) = X(0) \underbrace{\frac{s}{s^2+\omega^2}} + \frac{v(0)}{\omega} \frac{\omega}{s^2+\omega^2}$$

$$x(t) = x(0)\cos\omega t + \frac{v(0)}{\omega}\sin\omega t .$$

Inverting $\quad F(t) = \frac{1}{2\pi i}\int_{\gamma - i\infty}^{\gamma + i\infty} e^{st} f(s)\, ds$

$\boxed{5}$



γ is a value such that all singularities of $f(s)$ are to left

$$f(s) = 1/s$$

$$F(t) = \frac{1}{2\pi i}\int_{\gamma - i\infty}^{\gamma + i\infty} \underbrace{e^{st}\frac{1}{s}}_{\text{pole at } s=0} ds \qquad \frac{e^{st}}{s} = \frac{1 + st + \frac{s^2t^2}{2}}{s}$$

$$\frac{1}{2\pi i}\, 2\pi i \text{ Residue} = 1$$

$$F(t) = 1$$

L3.

$f(s) = 1/s-\omega$ pole at $s = \omega$ $\qquad \gamma > \omega$

$$\frac{1}{2\pi i}\int_{\gamma - i\infty}^{\gamma + i\infty} e^{st}\,\frac{1}{s-\omega}\,ds$$

$$e^{\omega t}\, e^{(s-\omega)t}\,\frac{1}{s-\omega}$$

$$e^{\omega t}\,\frac{1 + (s-\omega)t + \frac{1}{2}(s-\omega)^2 t^2 + \cdots}{s-\omega}$$

Residue $= e^{\omega t}$

$f(t) = e^{\omega t}$ ✓✓