Harmonic oscillator expanded

$L = \frac{1}{2} m\dot{x}^2 - \frac{1}{2} m\omega^2 x^2$ $\qquad p = \frac{\partial L}{\partial \dot{x}} = m\dot{x} \rightarrow \dot{x} = p/m$

$\Rightarrow H = \frac{p^2}{m} - \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$

$\Rightarrow \frac{\partial H}{\partial p} = \frac{p}{m} = \dot{x} \Rightarrow p = m\dot{x}$ (cf. above)

$\frac{\partial H}{\partial x} = m\omega^2 x = -\dot{p} \Rightarrow m\ddot{x} = -m\omega^2 x \Rightarrow \ddot{x} + \omega^2 \omega = 0$

$x(t) = x_0 \cos(\omega t + \phi_x)$

$\Rightarrow p(t) = -m\omega x_0 \sin(\omega t + \phi_x)$

~~$= p_0 \cos(\omega t + \phi_p)$~~

$\downarrow$

$\ddot{p} = -m\omega^2 \dot{x} = -\omega^2 p \Rightarrow \ddot{p} + \omega^2 p = 0 \Rightarrow p(t) = p_0 \cos(\omega t + \phi_p)$

$\rightarrow x(t) = -\frac{p_0 \cancel{\omega}}{m\omega^{\cancel{2}}} \sin(\omega t + \phi_p)$

We also know $\frac{\partial H}{\partial t} = 0 \Rightarrow H = \text{const} \underset{\uparrow}{=} E$

here ... not in general!

$\Rightarrow 1 = \frac{H}{E} = \frac{p^2}{2mE} + \frac{q^2}{2E/m\omega^2}$ ellipse in phase space

~~Ex. (1) Harmonic Oscillator~~

~~$L = \frac{1}{2} m \dot{x}^2 - \frac{1}{2} m \omega^2 x^2$ $\qquad p = \frac{\partial L}{\partial \dot{x}}$~~ new version below.

~~$H = \frac{p^2}{m} - \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2 = \frac{p^2}{2m} + \frac{1}{2} m \omega^2 x^2$~~

~~(Interesting side note: introduce~~ ~~$x_0 = \sqrt{\frac{1}{m\omega}}$, H~~

~~$\frac{H}{\omega} = \frac{p^2}{2m\omega} + \frac{1}{2} m \omega x^2 \qquad x_0 = \sqrt{\frac{1}{m\omega}}, \quad p_0 = \sqrt{m\omega}$~~

~~$= \frac{1}{2} \frac{p^2}{p_0^2} + \frac{1}{2} \frac{x^2}{x_0^2}$)~~

The Virial Theorem

Mean value of a function $f(t)$:

$$\langle f \rangle = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^{\tau} f(t)\, dt$$

specifically for periodic functions:

$$\langle f \rangle = \frac{1}{T} \int_0^T f(t)\, dt \qquad \left(\leftrightarrow \langle \sin^2 x \rangle = \frac{1}{2\pi} \int_0^{2\pi} \sin^2 x'\, dx' = 1/2 \right)$$

Now consider a mechanical system with (q_j, p_j), $j = 1, \dots, n$; with Hamiltonian $H(q_j, p_j, t)$. Define the virial

~~$\mathcal{V} = \sum_i q_i \frac{\partial H}{\partial q_i}$~~ $\qquad \mathcal{V} \equiv \sum_j q_j \dot{p}_j = - \sum_j q_j \frac{\partial H}{\partial q_j}$

~~[illegible]~~

In certain cases, $\mathcal{V}$ can be related to dynamical quantities:

Virial Theorem If $q_j(t)$, $p_j(t)$ are bounded and if

$$\left\langle \sum_i q_i \frac{\partial H}{\partial q_i} \right\rangle, \quad \left\langle \sum_j p_j \frac{\partial H}{\partial p_j} \right\rangle$$

exist separately, they must be equal

$$\left\langle \sum_j q_j \frac{\partial H}{\partial q_j} \right\rangle = \left\langle \sum_j p_j \frac{\partial H}{\partial p_j} \right\rangle$$

Proof

$$G(t) \equiv \sum_j p_j(t) q_j(t)$$ **bounded** since q, p bounded

$$\Rightarrow \frac{dG}{dt} = \sum_i p_i \dot{q}_i + \sum_i \dot{p}_i q_i = \sum_j p_j \frac{\partial H}{\partial p_j} - \sum_i q_j \frac{\partial H}{\partial q_j}$$

$$\rightsquigarrow \left\langle \frac{dG}{dt} \right\rangle = \left\langle \sum_j p_j \frac{\partial H}{\partial p_j} - \sum_j q_j \frac{\partial H}{\partial q_j} \right\rangle$$

$$\left\langle \frac{dG}{dt} \right\rangle = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau \frac{dG}{dt} dt = \lim_{\tau \to \infty} \frac{G(\tau) - G(0)}{\tau} = 0$$

$$\Rightarrow \left\langle \sum_j p_j \frac{\partial H}{\partial p_j} - \sum_j q_j \frac{\partial H}{\partial q_j} \right\rangle = 0$$

If mean values exist separately

$$\left\langle \sum_j p_j \frac{\partial H}{\partial p_j} \right\rangle - \left\langle \sum_j q_j \frac{\partial H}{\partial q_j} \right\rangle = 0$$ ★

Applications:

Central Force, **bounded** orbit:

$$H = T + V = \frac{p^2}{2m} + V(r)$$

$$\rightsquigarrow \left\langle \vec{p} \cdot \frac{\vec{p}}{m} \right\rangle = \langle \vec{r} \cdot \nabla V(r) \rangle = \left\langle \vec{r} \cdot \left(\frac{\partial V}{\partial r} \frac{\vec{r}}{r} \right) \right\rangle = \left\langle r \frac{dV}{dr} \right\rangle$$

For $V(r) = \frac{A}{r^n}$, this equation becomes

$$2\langle T \rangle = -n \left\langle r \frac{A}{r^{n+1}} \right\rangle = -n \langle V \rangle$$

$$\Rightarrow \langle T \rangle = -\frac{n}{2} \langle V \rangle$$

For $n=1$, i.e., Kepler or Coulomb

$$\langle T \rangle = -\frac{1}{2} \langle V \rangle, \quad \langle E \rangle = \langle T \rangle + \langle V \rangle$$

$$= -\frac{1}{2}\langle V \rangle + \langle V \rangle = \frac{\langle V \rangle}{2}$$

$$= -\langle T \rangle$$ bound states have *negative* energy since $T > 0$

Oscillator: $n = -2$

$$\langle T \rangle = \langle V \rangle$$

$$\Rightarrow \langle E \rangle = 2\langle T \rangle = 2\langle V \rangle$$

bound states have positive energy.

Equation of State of an Ideal Gas

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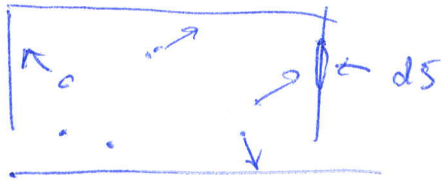

Gas molecules experience forces when they hit the wall:

$$d\vec{F} = -\underset{\substack{\uparrow\\\text{pressure}}}{P}\,\underset{\substack{\uparrow\\\text{surface normal}}}{\hat{n}}\,dS \leftarrow \text{surface}$$

$$\Rightarrow \quad 2\langle T\rangle = -\Big\langle \sum_i \vec{r}_i\cdot\vec{F}_i\Big\rangle \rightarrow -\oint_S \vec{r}\,d\vec{F} = \oint_S P\,\vec{r}\cdot\hat{n}\,dS$$

continuum limit &
P = const.
(takes care of time int.)

But Gauss' law/divergence theorem

$$\oint_S \vec{r}\cdot\hat{n}\,dS = \int_V \nabla\cdot\vec{r}\,dV = \int_V \underbrace{\left(\frac{\partial x}{\partial x}+\frac{\partial y}{\partial y}+\frac{\partial z}{\partial z}\right)}_{=3} dV = 3V$$

$$\Rightarrow 2\langle T\rangle = 3PV$$

Equipartition principle: energy per molecule with three d.o.f. is $\frac{3}{2}k_B T$ with Boltzmann const. k_B and temperature T, so

$$2\cdot\tfrac{3}{2}k_B\cdot T\cdot N = 3PV$$

$$\Rightarrow N k_B T = PV$$

Hamilton's Equs. from the Variational principle

$$\delta S = \delta \int_{t_1}^{t_2} L(q_j, \dot q_j, t)\, dt = 0$$

path variations are now in phase space, δq_j, δp_j are independent

$$\rightarrow \quad \delta S = \delta \int_{t_1}^{t_2} \Big(\sum_k p_k \dot q_k - H(q_j, p_j, t) \Big) dt = 0$$

$$\Rightarrow \quad \delta S = \int_{t_1}^{t_2} \sum_k \Big(p_k \delta \dot q_k + \dot q_k \delta p_k - \frac{\partial H}{\partial q_k} \delta q_k - \frac{\partial H}{\partial p_k} \delta p_k \Big) dt = 0$$

(Recall: no time variation for δ)

integrate by parts:

$$\int_{t_1}^{t_2} p_k \delta \dot q_k \, dt = \underbrace{p_k \delta q_k \Big|_{t_1}^{t_2}}_{=0} - \int_{t_1}^{t_2} \dot p_k \delta q_k \, dt$$

$(\delta q(t_2) = \delta q(t_1) = 0)$ But note that we do not need $\delta p(t_1) = \delta p(t_2) = 0$ here!!

$$\Rightarrow \quad \delta S = \int_{t_1}^{t_2} \sum_k \Big(-\Big(+ \dot p_k + \frac{\partial H}{\partial q_k} \Big) \delta q_k + \Big(\dot q_k - \frac{\partial H}{\partial p_k} \Big) \delta p_k \Big) = 0$$

$\rightarrow$ independent variations $\Rightarrow$

$$\dot p_k + \frac{\partial H}{\partial q_k} = 0 \quad , \quad \dot q_k - \frac{\partial H}{\partial p_k} = 0$$

$$\hookrightarrow \quad f(q_j, p_j, \dot q_j, \dot p_j, t) \equiv \sum_{k=1}^{n} p_k \dot q_k - H(q_j, p_j, t)$$

$$\Rightarrow \quad \frac{d}{dt} \frac{\partial f}{\partial \dot q_i} - \frac{\partial f}{\partial q_i} = 0 \Rightarrow \dot p_i + \frac{\partial H}{\partial q_i} = 0$$

only first term depends on $\dot q$, only second term on q

$$\frac{d}{dt} \underbrace{\frac{\partial f}{\partial \dot p_i}}_{=0} - \frac{\partial f}{\partial p_i} = 0 \Rightarrow -\dot q_i + \frac{\partial H}{\partial p_i} = 0$$

From variational principle, it is clear that $f' = f + \frac{dF}{dt}$ will yield the same Hamilton equs.