

Reminder of Statistical Mechanics

The Hidden Math

Derivation of Newton's equations of motion via the Eulero-Lagrange equation

$$\mathcal{L}(\mathbf{r}_1, \dots, \mathbf{r}_N, \dot{\mathbf{r}}_1, \dots, \dot{\mathbf{r}}_N) = K(\dot{\mathbf{r}}_1, \dots, \dot{\mathbf{r}}_N) - U(\mathbf{r}_1, \dots, \mathbf{r}_N)$$

Solve the Eulero-Lagrange equation

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}_i} \right) - \frac{\partial \mathcal{L}}{\partial \mathbf{r}_i} = 0$$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{r}_i} = \frac{\partial}{\partial \mathbf{r}_i} (K(\dot{\mathbf{r}}_i) - U(\mathbf{r}_i)) = -\frac{\partial}{\partial \mathbf{r}_i} U(\mathbf{r}_i) = -\nabla U(\mathbf{r}_i)$$

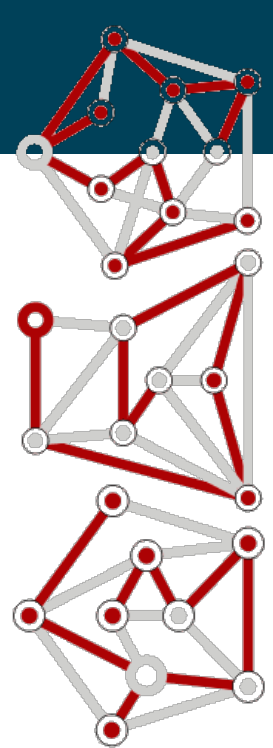
(Remember the definition of a conservative force)
 $= \mathbf{F}_i$

$$\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}_i} = \frac{\partial}{\partial \dot{\mathbf{r}}_i} (K(\dot{\mathbf{r}}_i) - U(\mathbf{r}_i)) = \frac{\partial}{\partial \dot{\mathbf{r}}_i} K(\dot{\mathbf{r}}_i) = \frac{\partial}{\partial \dot{\mathbf{r}}_i} \frac{1}{2} m_i \dot{\mathbf{r}}_i^2 = m_i \dot{\mathbf{r}}_i$$

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}_i} = \frac{d}{dt} (m_i \dot{\mathbf{r}}_i) = m_i \ddot{\mathbf{r}}_i = m_i \mathbf{a}_i$$

$$\frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}_i} = \frac{\partial \mathcal{L}}{\partial \mathbf{r}_i}$$

$$\mathbf{F}_i = m_i \mathbf{a}_i$$



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From the Lagrangian...

$$\mathcal{L}(\mathbf{r}_1, \dots, \mathbf{r}_N, \dot{\mathbf{r}}_1, \dots, \dot{\mathbf{r}}_N) = K(\dot{\mathbf{r}}_1, \dots, \dot{\mathbf{r}}_N) - U(\mathbf{r}_1, \dots, \mathbf{r}_N)$$

...to the Hamiltonian

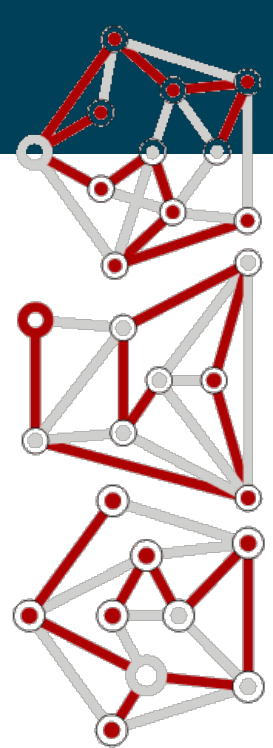
$$\mathcal{H}(\mathbf{r}_1, \dots, \mathbf{r}_N, \mathbf{p}_1, \dots, \mathbf{p}_N) = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m_i} + U(\mathbf{r}_1, \dots, \mathbf{r}_N)$$

... via Legendre transform

$$\tilde{f}(s) = f(x(s)) - sx(s), \quad s = f'(x)$$

$f = \mathcal{L}$, $\tilde{f} = \mathcal{H}$, $x = \dot{\mathbf{r}}_i$, $s = \mathbf{p}_i$, the positions \mathbf{r}_i stay as they are...

$$\begin{aligned}
 \mathcal{H}(\mathbf{r}_i, \mathbf{p}_i) &= \mathcal{L}(\mathbf{r}_i, \mathbf{p}_i) - \sum_i \mathbf{p}_i \dot{\mathbf{r}}_i \\
 &= \mathcal{L}(\mathbf{r}_i, \mathbf{p}_i) - \sum_i \frac{\mathbf{p}_i^2}{m_i} \text{ as } \dot{\mathbf{r}}_i = \mathbf{v}_i = \frac{\mathbf{p}_i}{m_i} \\
 &= \frac{1}{2} \sum_i m_i \left(\frac{\mathbf{p}_i}{m_i} \right)^2 - U(\mathbf{r}_i) - \sum_i \frac{\mathbf{p}_i^2}{m_i} \\
 &= - \sum_i \frac{\mathbf{p}_i^2}{2m_i} - U(\mathbf{r}_i) \\
 \mathcal{L} &= -\mathcal{H}
 \end{aligned}$$



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Proof of the zero divergence of an Hamiltonian field

$$\nabla \cdot v_H(v_{\mathbf{r}_i}, v_{\mathbf{p}_i}) = 0$$

$$\nabla \cdot v_H(v_{\mathbf{r}_i}, v_{\mathbf{p}_i}) = \sum_i \left(\frac{\partial}{\partial \mathbf{r}_i} v_{\mathbf{r}_i} + \frac{\partial}{\partial \mathbf{p}_i} v_{\mathbf{p}_i} \right)$$

However:

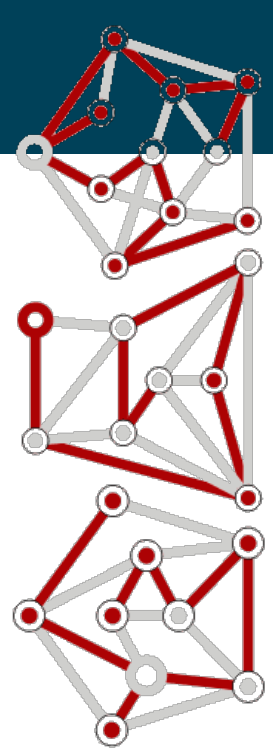
$$\frac{\partial \mathcal{H}}{\partial \mathbf{p}_i} = \frac{\partial}{\partial \mathbf{p}_i} \frac{\mathbf{p}_i^2}{2m_i} = v_{\mathbf{r}_i}$$

and

$$\frac{\partial \mathcal{H}}{\partial \mathbf{r}_i} = \frac{\partial}{\partial \mathbf{r}_i} U(\mathbf{r}_i) = -\mathbf{F}_i = -m_i \mathbf{a}_i = -\dot{\mathbf{p}}_i = -v_{\mathbf{p}_i}$$

so that

$$\nabla \cdot v_H(v_{\mathbf{r}_i}, v_{\mathbf{p}_i}) = \sum_i \left(\frac{\partial \mathcal{H}}{\partial \mathbf{r}_i \mathbf{p}_i} - \frac{\partial \mathcal{H}}{\partial \mathbf{p}_i \mathbf{r}_i} \right) = 0$$



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Quantum ensemble averages via the density matrix

$$\langle \hat{\mathcal{P}} \rangle = \frac{1}{\mathcal{Z}} \sum_{k,l} \rho_{lk} \langle \phi_k^{(\lambda)} | \hat{\mathcal{P}} | \phi_l^{(\lambda)} \rangle$$

$$\langle \hat{\mathcal{P}} \rangle = \frac{1}{\mathcal{Z}} \sum_{\lambda=1}^{\mathcal{Z}} \langle \psi^{(\lambda)} | \hat{\mathcal{P}} | \psi^{(\lambda)} \rangle$$

Expand the wave function on a basis - which basis vectors have norm=1

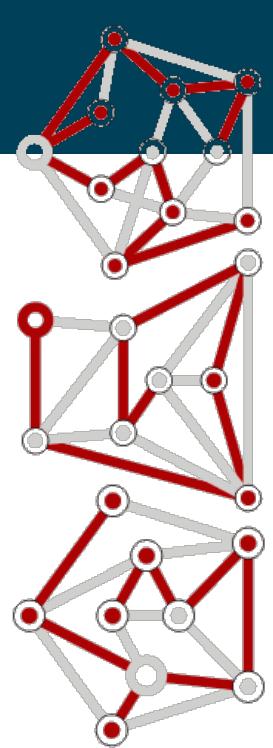
$$|\psi^{(\lambda)}\rangle = \sum_l C_l^{(\lambda)} |\phi_l^{(\lambda)}\rangle$$

$$|\psi^{(\lambda)}\rangle = \sum_k C_k^{(\lambda)} |\phi_k^{(\lambda)}\rangle \rightarrow \langle \psi^{(\lambda)} | = \sum_k C_k^{*,(\lambda)} \langle \phi_k^{(\lambda)} |$$

so that

$$\langle \hat{\mathcal{P}} \rangle = \frac{1}{\mathcal{Z}} \sum_{\lambda=1}^{\mathcal{Z}} \sum_{k,l} C_l^{(\lambda)} C_k^{*,(\lambda)} \langle \phi_k^{(\lambda)} | \hat{\mathcal{P}} | \phi_l^{(\lambda)} \rangle$$

$$\langle \hat{\mathcal{P}} \rangle = \frac{1}{\mathcal{Z}} \sum_{k,l} \rho_{lk} \langle \phi_k^{(\lambda)} | \hat{\mathcal{P}} | \phi_l^{(\lambda)} \rangle$$



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Derivation of the Liouville-Von Neumann equation

(I'll drop summations and indexes but for 0 and t (time 0 and time t))

Recall how we evolve the wave function in time $|\psi(t)\rangle = e^{-\frac{i}{\hbar}\mathcal{H}t}|\psi(0)\rangle$

Also recall the commutator $[\hat{\mathcal{H}}, \hat{\rho}] = \mathcal{H}\hat{\rho} - \hat{\rho}\mathcal{H}$

All we have to do is to take the time derivative of the density matrix:

$$\begin{aligned}\frac{\partial}{\partial t}\hat{\rho} &= \frac{\partial}{\partial t}|\psi\rangle\langle\psi| \\&= \frac{\partial}{\partial t}\left(e^{-\frac{i\mathcal{H}t}{\hbar}}|\psi_0\rangle \cdot \langle\psi_0|e^{\frac{i\mathcal{H}t}{\hbar}}\right) \\&= -\frac{i\mathcal{H}}{\hbar}e^{-\frac{i\mathcal{H}t}{\hbar}}|\psi_0\rangle \cdot \langle\psi_0|e^{\frac{i\mathcal{H}t}{\hbar}} + e^{-\frac{i\mathcal{H}t}{\hbar}}|\psi_0\rangle\langle\psi_0|\frac{i\mathcal{H}}{\hbar}e^{\frac{i\mathcal{H}t}{\hbar}} \\&= -\frac{i\mathcal{H}}{\hbar}|\psi_0\rangle\langle\psi_0| + \frac{i}{\hbar}|\psi_0\rangle\langle\psi_0|\mathcal{H} \\&= \frac{i}{\hbar}(\hat{\rho}\mathcal{H} - \mathcal{H}\hat{\rho}) = \frac{i}{\hbar}[\hat{\rho}, \mathcal{H}] = \frac{1}{i\hbar}[\mathcal{H}, \hat{\rho}] \\&\rightarrow \frac{\partial}{\partial t}\hat{\rho} = \frac{1}{i\hbar}[\mathcal{H}, \hat{\rho}]\end{aligned}$$