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

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

Solve the Eulero-Lagrange equation

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

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

$$\text{(Remember the definition of a conservative force)}$$

$$= \mathbf{F}_i$$

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

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

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

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

Reminder of Statistical Mechanics

The Hidden Math

From the Lagrangian…

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

…to the Hamiltonian

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

… via Legendre transform

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

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

$$\mathcal{H}(\mathbf{r}_i,\mathbf{p}_i) = \mathcal{L}(\mathbf{r}_i,\mathbf{p}_i) - \sum_i \mathbf{p}_i\dot{\mathbf{r}}_i$$

$$= \mathcal{L}(\mathbf{r}_i,\mathbf{p}_i) - \sum_i \frac{\mathbf{p}_i^2}{m_i} \quad \text{as} \quad \dot{\mathbf{r}}_i = \mathbf{v}_i = \frac{\mathbf{p}_i}{m_i}$$

$$= \frac{1}{2}\sum_i m_i \left(\frac{\mathbf{p}}{m_i}\right)^2 - U(\mathbf{r}_i) - \sum_i \frac{\mathbf{p}_i^2}{m_i}$$

$$= -\sum_i \frac{\mathbf{p}_i^2}{2m_i} - U(\mathbf{r}_i)$$

$$\mathcal{L} = -\mathcal{H}$$

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

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

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

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

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

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 $|\psi(t)\rangle = e^{-\frac{i}{\hbar}\hat{\mathcal{H}}t}|\psi(0)\rangle$

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:

$$\frac{\partial}{\partial t}\hat{\rho} = \frac{\partial}{\partial t}|\psi\rangle\langle\psi|$$

$$= \frac{\partial}{\partial t}\left(e^{-\frac{i\mathcal{H}t}{\hbar}}|\psi_0\rangle \cdot \langle\psi_0|e^{\frac{i\mathcal{H}t}{\hbar}}\right)$$

$$= -\frac{i\mathcal{H}}{\hbar}e^{-\frac{i\mathcal{H}t}{\hbar}}|\psi_0\rangle \cdot \langle\psi_0|e^{\frac{i\mathcal{H}t}{\hbar}} + e^{-\frac{i\mathcal{H}t}{\hbar}}|\psi_0\rangle\langle\psi_0|\frac{i\mathcal{H}}{\hbar}e^{\frac{i\mathcal{H}t}{\hbar}}$$

$$= -\frac{i\mathcal{H}}{\hbar}|\psi_0\rangle\langle\psi_0| + \frac{i}{\hbar}|\psi_0\rangle\langle\psi_0|\mathcal{H}$$

$$= \frac{i}{\hbar}(\hat{\rho}\mathcal{H} - \mathcal{H}\hat{\rho}) = \frac{i}{\hbar}[\hat{\rho}, \mathcal{H}] = \frac{1}{i\hbar}[\mathcal{H}, \hat{\rho}]$$

$$\rightarrow \frac{\partial}{\partial t}\hat{\rho} = \frac{1}{i\hbar}[\mathcal{H}, \hat{\rho}]$$