



PHY 711 Classical Mechanics and Mathematical Methods

10-10:50 AM MWF in Olin 103

Notes on Lecture 14 -- Chap. 6 (F & W) Extensions of Hamiltonian formalism

- 1. Virial theorem**
- 2. Canonical transformations**
- 3. Hamilton-Jacobi formalism**

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment	Due
1	Mon, 8/22/2022		Introduction	#1	8/26/2022
2	Wed, 8/24/2022	Chap. 1	Scattering theory		
3	Fri, 8/26/2022	Chap. 1	Scattering theory	#2	8/29/2022
4	Mon, 8/29/2022	Chap. 1	Scattering theory	#3	8/31/2022
5	Wed, 8/31/2022	Chap. 1	Summary of scattering theory	#4	9/02/2022
6	Fri, 9/02/2022	Chap. 2	Non-inertial coordinate systems	#5	9/05/2022
7	Mon, 9/05/2022	Chap. 3	Calculus of Variation	#6	9/7/2022
8	Wed, 9/07/2022	Chap. 3	Calculus of Variation	#7	9/9/2022
9	Fri, 9/09/2022	Chap. 3 & 6	Lagrangian Mechanics		
10	Mon, 9/12/2022	Chap. 3 & 6	Lagrangian Mechanics	#8	9/14/2022
11	Wed, 9/14/2022	Chap. 3 & 6	Constants of the motion	#9	9/16/2022
12	Fri, 9/16/2022	Chap. 3 & 6	Hamiltonian equations of motion		
13	Mon, 9/19/2022	Chap. 3 & 6	Liouville theorem	#10	9/21/2022
14	Wed, 9/21/2022	Chap. 3 & 6	Canonical transformations	#11	9/23/2022
15	Fri, 9/23/2022	Chap. 4	Small oscillations about equilibrium		
16	Mon, 9/26/2022	Chap. 4	Normal modes of vibration		
17	Wed, 9/28/2022	Chap. 4	Normal modes of more complicated systems		



PHY 711 -- Assignment #11

Sept. 21, 2022

Finish reading Chapters 3 and 6 in **Fetter & Walecka**.

1. Consider the example of the mass m initially at height h falling from rest with constant acceleration g to verify the analysis of the action S at time $t > 0$ discussed in the lecture notes.

-- Thursday's Colloquium --

Opportunities for Physics Research Part III

Experimental & Theoretical/Computational Condensed Matter Physics

Featuring the laboratories/groups of Oana Jurchescu,
Stephen Winter, Timo Thonhauser, and Natalie Holzwarth



WAKE FOREST
UNIVERSITY

September 22, 2022 at 4 PM in Olin 101

Virial theorem (Rudolf Clausius ~ 1870)

$$2\langle T \rangle = - \left\langle \sum_{\sigma} \mathbf{F}_{\sigma} \cdot \mathbf{r}_{\sigma} \right\rangle$$

Proof:

Define: $A \equiv \sum_{\sigma} \mathbf{p}_{\sigma} \cdot \mathbf{r}_{\sigma}$

$$\frac{dA}{dt} = \sum_{\sigma} (\dot{\mathbf{p}}_{\sigma} \cdot \mathbf{r}_{\sigma} + \mathbf{p}_{\sigma} \cdot \dot{\mathbf{r}}_{\sigma}) = \sum_{\sigma} \mathbf{F}_{\sigma} \cdot \mathbf{r}_{\sigma} + 2T$$

Because $\dot{\mathbf{p}}_{\sigma} = \mathbf{F}_{\sigma}$

$$\left\langle \frac{dA}{dt} \right\rangle = \left\langle \sum_{\sigma} \mathbf{F}_{\sigma} \cdot \mathbf{r} \right\rangle + 2\langle T \rangle$$

$$\left\langle \frac{dA}{dt} \right\rangle = \frac{1}{\tau} \int_0^{\tau} \frac{dA(t)}{dt} dt = \frac{A(\tau) - A(0)}{\tau} \Rightarrow 0$$

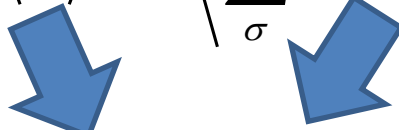
Note that this implies that the motion is periodic or bounded (not for all systems).

When it is true -- $\Rightarrow \left\langle \sum_{\sigma} \mathbf{F}_{\sigma} \cdot \mathbf{r} \right\rangle + 2\langle T \rangle = 0$

Examples of the Virial Theorem

Harmonic oscillator:

$$\mathbf{F} = -kx\hat{\mathbf{x}} \quad T = \frac{1}{2}m\dot{x}^2$$

$$2\langle T \rangle = -\left\langle \sum_{\sigma} \mathbf{F}_{\sigma} \cdot \mathbf{r}_{\sigma} \right\rangle$$

$$\langle m\dot{x}^2 \rangle = \langle kx^2 \rangle$$

Check: for $x(t) = X \sin\left(\sqrt{\frac{k}{m}}t + \alpha\right)$

$$\langle 2T \rangle = \langle m\dot{x}^2 \rangle = kX^2 \left\langle \cos^2\left(\sqrt{\frac{k}{m}}t + \alpha\right) \right\rangle = \frac{1}{2}kX^2$$

$$-\left\langle \sum_{\sigma} \mathbf{F}_{\sigma} \cdot \mathbf{r}_{\sigma} \right\rangle = \langle kx^2 \rangle = kX^2 \left\langle \sin^2\left(\sqrt{\frac{k}{m}}t + \alpha\right) \right\rangle = \frac{1}{2}kX^2$$

Premise true because of periodicity.



Examples of the Virial Theorem

$$2\langle T \rangle = - \left\langle \sum_{\sigma} \mathbf{F}_{\sigma} \cdot \mathbf{r}_{\sigma} \right\rangle$$

Circular orbit due to gravitational field
of massive object:

$$\mathbf{F} = -\frac{GMm}{r^2} \hat{\mathbf{r}} \quad T = \frac{1}{2}mv^2$$

$$\langle mv^2 \rangle = \left\langle \frac{GMm}{r} \right\rangle$$

Check: for $\frac{v^2}{r} = \frac{GM}{r^2}$

$$\Rightarrow \langle mv^2 \rangle = \left\langle \frac{GMm}{r} \right\rangle$$

centripetal
acceleration

gravitational
force

Premise true because of periodicity.



Hamiltonian formalism and the canonical equations of motion:

$$H = H(\{q_\sigma(t)\}, \{p_\sigma(t)\}, t)$$

Canonical equations of motion

$$\frac{dq_\sigma}{dt} = \frac{\partial H}{\partial p_\sigma}$$

$$\frac{dp_\sigma}{dt} = -\frac{\partial H}{\partial q_\sigma}$$

In the next slides we will consider finding different coordinates and momenta that can also describe the system. Why?

- a. Because we can
- b. Because it might be useful



Notion of “Canonical” generalized coordinate transformations

$$q_\sigma = q_\sigma(\{Q_1 \cdots Q_n\}, \{P_1 \cdots P_n\}, t) \quad \text{for each } \sigma$$

$$p_\sigma = p_\sigma(\{Q_1 \cdots Q_n\}, \{P_1 \cdots P_n\}, t) \quad \text{for each } \sigma$$

For some \tilde{H} and F , using Legendre transformations

Note that because of the way we set up the problem we can always add such a term.



$$\sum_\sigma p_\sigma \dot{q}_\sigma - H(\{q_\sigma\}, \{p_\sigma\}, t) = \sum_\sigma P_\sigma \dot{Q}_\sigma - \tilde{H}(\{Q_\sigma\}, \{P_\sigma\}, t) + \frac{d}{dt} F(\{q_\sigma\}, \{Q_\sigma\}, t)$$

Apply Hamilton's principle:

$$\delta \int_{t_i}^{t_f} \left[\sum_\sigma P_\sigma \dot{Q}_\sigma - \tilde{H}(\{Q_\sigma\}, \{P_\sigma\}, t) + \frac{d}{dt} F(\{q_\sigma\}, \{Q_\sigma\}, t) \right] dt = 0$$

$$\delta \int_{t_i}^{t_f} \left[\frac{d}{dt} F(\{q_\sigma\}, \{Q_\sigma\}, t) \right] dt = \int_{t_i}^{t_f} \left[\frac{d}{dt} \delta F(\{q_\sigma\}, \{Q_\sigma\}, t) \right] dt$$

$$= \delta F(t_f) - \delta F(t_i) = 0 \quad \text{and} \quad \dot{Q}_\sigma = \frac{\partial \tilde{H}}{\partial P_\sigma} \quad \dot{P}_\sigma = -\frac{\partial \tilde{H}}{\partial Q_\sigma}$$

Some details --

$$q_\sigma = q_\sigma(\{Q_1 \cdots Q_n\}, \{P_1 \cdots P_n\}, t) \quad \text{for each } \sigma$$

$$p_\sigma = p_\sigma(\{Q_1 \cdots Q_n\}, \{P_1 \cdots P_n\}, t) \quad \text{for each } \sigma$$

For some \tilde{H} and F , using Legendre transformations

$$\sum_\sigma p_\sigma \dot{q}_\sigma - H(\{q_\sigma\}, \{p_\sigma\}, t) = \sum_\sigma P_\sigma \dot{Q}_\sigma - \tilde{H}(\{Q_\sigma\}, \{P_\sigma\}, t) + \frac{d}{dt} F(\{q_\sigma\}, \{Q_\sigma\}, t)$$

Action integral:

$$S = \int_{t_i}^{t_f} dt \left(\sum_\sigma p_\sigma \dot{q}_\sigma - H(\{q_\sigma\}, \{p_\sigma\}, t) \right)$$

$$\delta S = \int_{t_i}^{t_f} dt \left(\sum_\sigma (\delta p_\sigma \dot{q}_\sigma + p_\sigma \delta \dot{q}_\sigma) - \delta H(\{q_\sigma\}, \{p_\sigma\}, t) \right)$$

Note that
$$\delta \int_{t_i}^{t_f} dt \left(\frac{dF(t)}{dt} \right) = \int_{t_i}^{t_f} dt \left(\frac{d\delta F(t)}{dt} \right) = 0$$

Some relations between old and new variables:


$$\sum_{\sigma} p_{\sigma} \dot{q}_{\sigma} - H(\{q_{\sigma}\}, \{p_{\sigma}\}, t) =$$

$$\sum_{\sigma} P_{\sigma} \dot{Q}_{\sigma} - \tilde{H}(\{Q_{\sigma}\}, \{P_{\sigma}\}, t) + \frac{d}{dt} F(\{q_{\sigma}\}, \{Q_{\sigma}\}, t)$$

$$\frac{d}{dt} F(\{q_{\sigma}\}, \{Q_{\sigma}\}, t) = \sum_{\sigma} \left(\left(\frac{\partial F}{\partial q_{\sigma}} \right) \dot{q}_{\sigma} + \left(\frac{\partial F}{\partial Q_{\sigma}} \right) \dot{Q}_{\sigma} \right) + \frac{\partial F}{\partial t}$$

$$\Rightarrow \sum_{\sigma} \left(p_{\sigma} - \left(\frac{\partial F}{\partial q_{\sigma}} \right) \right) \dot{q}_{\sigma} - H(\{q_{\sigma}\}, \{p_{\sigma}\}, t) =$$

$$\sum_{\sigma} \left(P_{\sigma} + \left(\frac{\partial F}{\partial Q_{\sigma}} \right) \right) \dot{Q}_{\sigma} - \tilde{H}(\{Q_{\sigma}\}, \{P_{\sigma}\}, t) + \frac{\partial F}{\partial t}$$


$$\sum_{\sigma} \left(p_{\sigma} - \left(\frac{\partial F}{\partial q_{\sigma}} \right) \right) \dot{q}_{\sigma} - H(\{q_{\sigma}\}, \{p_{\sigma}\}, t) =$$

$$\sum_{\sigma} \left(P_{\sigma} + \left(\frac{\partial F}{\partial Q_{\sigma}} \right) \right) \dot{Q}_{\sigma} - \tilde{H}(\{Q_{\sigma}\}, \{P_{\sigma}\}, t) + \frac{\partial F}{\partial t}$$

$$\Rightarrow p_{\sigma} = \left(\frac{\partial F}{\partial q_{\sigma}} \right) \quad P_{\sigma} = - \left(\frac{\partial F}{\partial Q_{\sigma}} \right)$$

$$\Rightarrow \tilde{H}(\{Q_{\sigma}\}, \{P_{\sigma}\}, t) = H(\{q_{\sigma}\}, \{p_{\sigma}\}, t) + \frac{\partial F}{\partial t}$$

Note that it is conceivable that if we were extraordinarily clever, we could find all of the constants of the motion!


$$\dot{Q}_\sigma = \frac{\partial \tilde{H}}{\partial P_\sigma} \quad \dot{P}_\sigma = -\frac{\partial \tilde{H}}{\partial Q_\sigma}$$

$$\text{Suppose: } \dot{Q}_\sigma = \frac{\partial \tilde{H}}{\partial P_\sigma} = 0 \quad \text{and} \quad \dot{P}_\sigma = -\frac{\partial \tilde{H}}{\partial Q_\sigma} = 0$$

$\Rightarrow Q_\sigma, P_\sigma$ are constants of the motion

Possible solution – Hamilton-Jacobi theory:

$$\text{Suppose: } F(\{q_\sigma\}, \{Q_\sigma\}, t) \Rightarrow -\sum_\sigma P_\sigma Q_\sigma + S(\{q_\sigma\}, \{P_\sigma\}, t)$$



$$\begin{aligned}
 \sum_{\sigma} p_{\sigma} \dot{q}_{\sigma} - H(\{q_{\sigma}\}, \{p_{\sigma}\}, t) &= \\
 \sum_{\sigma} P_{\sigma} \dot{Q}_{\sigma} - \tilde{H}(\{Q_{\sigma}\}, \{P_{\sigma}\}, t) + \frac{d}{dt} \left(- \sum_{\sigma} P_{\sigma} Q_{\sigma} + S(\{q_{\sigma}\}, \{P_{\sigma}\}, t) \right) & \\
 = -\tilde{H}(\{Q_{\sigma}\}, \{P_{\sigma}\}, t) - \sum_{\sigma} \dot{P}_{\sigma} Q_{\sigma} + \sum_{\sigma} \left(\frac{\partial S}{\partial q_{\sigma}} \dot{q}_{\sigma} + \frac{\partial S}{\partial P_{\sigma}} \dot{P}_{\sigma} \right) + \frac{\partial S}{\partial t} &
 \end{aligned}$$

Solution :

$$p_{\sigma} = \frac{\partial S}{\partial q_{\sigma}} \qquad Q_{\sigma} = \frac{\partial S}{\partial P_{\sigma}}$$

$$\tilde{H}(\{Q_{\sigma}\}, \{P_{\sigma}\}, t) = H(\{q_{\sigma}\}, \{p_{\sigma}\}, t) + \frac{\partial S}{\partial t}$$



When the dust clears :

Assume $\{Q_\sigma\}, \{P_\sigma\}, \tilde{H}$ are constants; choose $\tilde{H} = 0$

Need to find $S(\{q_\sigma\}, \{P_\sigma\}, t)$


$$p_\sigma = \frac{\partial S}{\partial q_\sigma} \quad Q_\sigma = \frac{\partial S}{\partial P_\sigma}$$

$$\Rightarrow H\left(\{q_\sigma\}, \left\{\frac{\partial S}{\partial q_\sigma}\right\}, t\right) + \frac{\partial S}{\partial t} = 0$$

Note: S is the "action":

$$\sum_{\sigma} p_{\sigma} \dot{q}_{\sigma} - H(\{q_{\sigma}\}, \{p_{\sigma}\}, t) =$$

$$\sum_{\sigma} P_{\sigma} \dot{Q}_{\sigma} - \tilde{H}(\{Q_{\sigma}\}, \{P_{\sigma}\}, t) + \frac{d}{dt} \left(- \sum_{\sigma} P_{\sigma} Q_{\sigma} + S(\{q_{\sigma}\}, \{P_{\sigma}\}, t) \right)$$


$$\sum_{\sigma} p_{\sigma} \dot{q}_{\sigma} - H(\{q_{\sigma}\}, \{p_{\sigma}\}, t) =$$

$$\sum_{\sigma} P_{\sigma} \dot{Q}_{\sigma} - \tilde{H}(\{Q_{\sigma}\}, \{P_{\sigma}\}, t) + \frac{d}{dt} \left(- \sum_{\sigma} P_{\sigma} Q_{\sigma} + S(\{q_{\sigma}\}, \{P_{\sigma}\}, t) \right)$$

$$\int_{t_i}^{t_f} \left(\sum_{\sigma} p_{\sigma} \dot{q}_{\sigma} - H(\{q_{\sigma}\}, \{p_{\sigma}\}, t) \right) dt = \int_{t_i}^{t_f} \left(\frac{d}{dt} (S(\{q_{\sigma}\}, \{P_{\sigma}\}, t)) \right) dt$$
$$= S(\{q_{\sigma}\}, \{P_{\sigma}\}, t) \Big|_{t_i}^{t_f}$$

Differential equation for **S**:

$$H\left(\{q_\sigma\}, \left\{\frac{\partial S}{\partial q_\sigma}\right\}, t\right) + \frac{\partial S}{\partial t} = 0$$

Example: $H(\{q\}, \{p\}, t) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2$

Hamilton - Jacobi Eq: $H\left(\{q\}, \left\{\frac{\partial S}{\partial q}\right\}, t\right) + \frac{\partial S}{\partial t} = 0$

$$\frac{1}{2m} \left(\frac{\partial S}{\partial q}\right)^2 + \frac{1}{2}m\omega^2 q^2 + \frac{\partial S}{\partial t} = 0$$

Does this look familiar?

Assume: $S(q, t) \equiv W(q) - Et$ (E constant)

Continued:

$$\frac{1}{2m} \left(\frac{\partial S}{\partial q} \right)^2 + \frac{1}{2} m \omega^2 q^2 + \frac{\partial S}{\partial t} = 0$$

Assume: $S(q, t) \equiv W(q) - Et$ (E constant)

$$\frac{1}{2m} \left(\frac{dW}{dq} \right)^2 + \frac{1}{2} m \omega^2 q^2 = E$$

$$\frac{dW}{dq} = \sqrt{2mE - (m\omega)^2 q^2}$$

$$W(q) = \int \sqrt{2mE - (m\omega)^2 q^2} dq$$

Continued:

$$W(q) = \int \sqrt{2mE - (m\omega)^2 q^2} dq$$

$$= \frac{1}{2} q \sqrt{2mE - (m\omega)^2 q^2} + \frac{E}{\omega} \sin^{-1} \left(\frac{m\omega q}{\sqrt{2mE}} \right) + C$$

$$S(q, E, t) = \frac{1}{2} q \sqrt{2mE - (m\omega)^2 q^2} + \frac{E}{\omega} \sin^{-1} \left(\frac{m\omega q}{\sqrt{2mE}} \right) - Et$$

$$\frac{\partial S}{\partial E} = Q = \frac{1}{\omega} \sin^{-1} \left(\frac{m\omega q}{\sqrt{2mE}} \right) - t$$

$$\Rightarrow q(t) = \frac{\sqrt{2mE}}{m\omega} \sin(\omega(t + Q))$$

Another example of Hamilton Jacobi equations

Example:
$$H(\{y\}, \{p\}, t) = \frac{p^2}{2m} + mgy$$

Assume $y(0) = h; \quad p(0) = 0$

Hamilton-Jacobi Eq:
$$H\left(\{y\}, \left\{\frac{\partial S}{\partial y}\right\}, t\right) + \frac{\partial S}{\partial t} = 0$$

$$\frac{1}{2m} \left(\frac{\partial S}{\partial y}\right)^2 + mgy + \frac{\partial S}{\partial t} = 0$$

Assume: $S(y, t) \equiv W(y) - Et \quad (E \text{ constant})$



Example:
$$H(\{y\}, \{p\}, t) = \frac{p^2}{2m} + mgy$$

Assume $y(0) = h; \quad p(0) = 0$

$$\frac{1}{2m} \left(\frac{dW}{dy} \right)^2 + mgy = E \equiv mgh$$

$$W(y) = m \int_y^h \sqrt{2g(h-y')} dy' = \frac{2}{3} m \sqrt{2g} (h-y)^{3/2}$$

$$S(y, t) = W(y) - Et = \frac{2}{3} m \sqrt{2g} (h-y)^{3/2} - mght$$



Check action:

For this case: $y(t) = h - \frac{1}{2}gt^2$

$$S = \int_0^t \left(\frac{1}{2}m\dot{y}^2 - mgy \right) dt' = \frac{1}{3}mg^2t^3 - mght$$

$$S(y, t) = W(y) - Et = \frac{2}{3}m\sqrt{2g}(h - y)^{3/2} - mght$$

Agrees with Hamilton-Jacobi analysis.

Alternatively, keeping E notation:

$$W(y) = \int_y^h \sqrt{2mE - 2m^2gy'} dy'$$

$$= \sqrt{\frac{2}{m}} \frac{1}{g} (E - mgy)^{3/2}$$

$$S(y, t) = W(y) - Et = \sqrt{\frac{2}{m}} \frac{2}{3g} (E - mgy)^{3/2} - Et$$

$$\frac{\partial S}{\partial E} = Q = \sqrt{\frac{2}{m}} \frac{1}{g} (E - mgy)^{1/2} - t$$

$$\Rightarrow y(t) = \frac{E}{mg} - \frac{1}{2} g (t + Q)^2$$

In our case, $Q = 0$

$$E = mgh$$

What do you think of Hamilton-Jacobi method

- a. Historically important
- b. Hysterical
- c. Painful
- d. Might be useful

The next 3 slides contain important equations that you will hopefully remember for this material contained in Chapters 3 & 6 of Fetter and Walecka. On Friday we will start with Chapter 4 and discuss one of the many applications of these ideas – the case of small oscillations near equilibrium.



Recap --

Lagrangian picture

For independent generalized coordinates $q_\sigma(t)$:

$$L = L(\{q_\sigma(t)\}, \{\dot{q}_\sigma(t)\}, t)$$

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{q}_\sigma} - \frac{\partial L}{\partial q_\sigma} = 0$$

\Rightarrow Second order differential equations for $q_\sigma(t)$

Hamiltonian picture

$$H = H(\{q_\sigma(t)\}, \{p_\sigma(t)\}, t)$$

$$\frac{dq_\sigma}{dt} = \frac{\partial H}{\partial p_\sigma} \quad \frac{dp_\sigma}{dt} = -\frac{\partial H}{\partial q_\sigma}$$

\Rightarrow Coupled first order differential equations for

$$q_\sigma(t) \quad \text{and} \quad p_\sigma(t)$$



General treatment of particle of mass m and charge q moving in 3 dimensions in an potential $U(\mathbf{r})$ as well as electromagnetic scalar and vector potentials $\Phi(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$:

Lagrangian:
$$L(\mathbf{r}, \dot{\mathbf{r}}, t) = \frac{1}{2} m \dot{\mathbf{r}}^2 - U(\mathbf{r}) - q\Phi(\mathbf{r}, t) + \frac{q}{c} \dot{\mathbf{r}} \cdot \mathbf{A}(\mathbf{r}, t)$$

Hamiltonian:
$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{r}}} = m\dot{\mathbf{r}} + \frac{q}{c} \mathbf{A}(\mathbf{r}, t)$$

$$\begin{aligned} H(\mathbf{r}, \mathbf{p}, t) &= \mathbf{p} \cdot \dot{\mathbf{r}} - L(\mathbf{r}, \dot{\mathbf{r}}, t) \\ &= \frac{1}{2m} \left(\mathbf{p} - \frac{q}{c} \mathbf{A}(\mathbf{r}, t) \right)^2 + U(\mathbf{r}) + q\Phi(\mathbf{r}, t) \end{aligned}$$

Recipe for constructing the Hamiltonian and analyzing the equations of motion

1. Construct Lagrangian function : $L = L(\{q_\sigma(t)\}, \{\dot{q}_\sigma(t)\}, t)$
2. Compute generalized momenta : $p_\sigma \equiv \frac{\partial L}{\partial \dot{q}_\sigma}$
3. Construct Hamiltonian expression : $H = \sum_\sigma \dot{q}_\sigma p_\sigma - L$
4. Form Hamiltonian function : $H = H(\{q_\sigma(t)\}, \{p_\sigma(t)\}, t)$
5. Analyze canonical equations of motion :

$$\frac{dq_\sigma}{dt} = \frac{\partial H}{\partial p_\sigma} \quad \frac{dp_\sigma}{dt} = -\frac{\partial H}{\partial q_\sigma}$$