Four Lectures in Particle Dynamics

Lecture 1: The Hamiltonian

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Summary

In this course we will learn how to transport a single particle and a group of particles under the effect of an electromagnetic potential.

- The first lecture introduces the Hamiltonian formalism that we will use in the other three lectures;
- the second lecture discusses the linear solutions of the Hamilton equations;
- the third lecture treats the non-linear solutions of the Hamilton equations;
- the fourth lecture is the treatment of symplectic integrators.

Newton Equation

We are familiar with the Newton equation. For a particle with coordinate vector $q(t) = (q_1(t), \ldots, q_n(t))$ moving in an external potential $V(q)$ the equations are:

$$m\ddot{q} = -\nabla V(q), \tag{1}$$

where ∇ is the gradient function. The above are second order differential equations in time t.

Hamilton Equations

It exists an alternative way to write the equations of Newton by splitting them into two first-order differential equations using the Hamiltonian function H and the equations of motion

$$\dot{q} = \frac{\partial H}{\partial p}; \quad \dot{p} = -\frac{\partial H}{\partial q}. \tag{2}$$

In this lectures I assume that the reader is familiar with the Least-Action principle, the Lagrangian and the rigorous definition of Hamiltonian and momentum as per [2] Chapter 8. For the purpose of this course the Hamiltonian will be the total energy of the particle

$$H = T + V. \tag{3}$$

Exercise: from Hamilton to Newton equations

Assuming that p and q are the canonical variables in one dimension, prove that if $T = \frac{p^2}{2m}$ and $V = V(q)$ the Eqs. (2) are equivalent to the Eq. (1) (the solution can be easily extended to the many variables case).

Exercise: the free particle

Calculate the trajectory of a free particle, i.e. $V = 0$ with the classical Hamiltonian

$$H = \frac{p^2}{2m} \tag{4}$$

and with the relativistic Hamiltonian

$$H = \sqrt{p^2c^2 + m^2c^4}. \tag{5}$$

Symplecticity

Symplecticity and Hamiltonian are tight connect and a proper treatment can be found in [1]. Here we will introduce it with a simple algebraic approach. The Hamilton equations are

$$
\begin{pmatrix} \dot{q}_1 \\ \vdots \\ \dot{q}_n \\ \dot{p}_1 \\ \vdots \\ \dot{p}_n \end{pmatrix}
=
\begin{pmatrix}
0 & \cdots & 0 & 1 & \cdots & 0 \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
0 & \cdots & 0 & 0 & \cdots & 1 \\
-1 & \cdots & 0 & 0 & \cdots & 0 \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
0 & \cdots & -1 & 0 & \cdots & 0
\end{pmatrix}
\begin{pmatrix} \partial H/\partial q_1 \\ \vdots \\ \partial H/\partial q_n \\ \partial H/\partial p_1 \\ \vdots \\ \partial H/\partial p_n \end{pmatrix}
\tag{6}
$$

Symplecticity

In a more compact form they are

$$\frac{dv}{dt} = S\nabla^T H \tag{7}$$

where $v = (q_1, \ldots, q_n, p_1, \ldots, p_n)$ is the vector for both coordinates and momenta; $\nabla^T H$ is the gradient of the Hamiltonian calculated with respect to the coordinates and momenta and it is transposed because the gradient is generally defined as a row vector; S is the matrix

$$\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

where I is the $n \times n$ identity matrix.

Symplecticity

Now we imagine that there exists an interval $[t_0, t_1] \subseteq \mathbb{R}$ such that for any v_0 in an open subset $U \subseteq \mathbb{R}^{2n}$ there exists a unique solution $M(t, v_0)$ in the whole interval $[t_0, t_1]$ of the Hamilton equations with initial condition $M(t_0, v_0) = v_0$. For any $t \in [t_0, t_1]$ define the map

$$M_t \colon U \to \mathbb{R}^{2n} \qquad v_0 \mapsto M(t, v_0).$$

Under opportune hypothesis on the Hamiltonian H the above unique solutions exist and the maps M_t are smooth for any t in the given interval.

Symplecticity

One says that M_t is symplectic at v_0 if its jacobian J at that point satisfies

$$J^T S J = S. \tag{8}$$

Recall that the jacobian matrix is given by

$$J = \begin{pmatrix} \frac{\partial M_{q_1}}{\partial q_1} & \dots & \frac{\partial M_{q_1}}{\partial q_n} & \frac{\partial M_{q_1}}{\partial p_1} & \dots & \frac{\partial M_{q_1}}{\partial p_n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial M_{q_n}}{\partial q_1} & \dots & \frac{\partial M_{q_n}}{\partial q_n} & \frac{\partial M_{q_n}}{\partial p_1} & \dots & \frac{\partial M_{q_n}}{\partial p_n} \\ \frac{\partial M_{p_1}}{\partial q_1} & \dots & \frac{\partial M_{p_1}}{\partial q_n} & \frac{\partial M_{p_1}}{\partial p_1} & \dots & \frac{\partial M_{p_1}}{\partial p_n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{\partial M_{p_n}}{\partial q_1} & \dots & \frac{\partial M_{p_n}}{\partial q_n} & \frac{\partial M_{p_n}}{\partial p_1} & \dots & \frac{\partial M_{p_n}}{\partial p_n} \end{pmatrix} \tag{9}$$

The map M_t is symplectic if it is symplectic at any point of U.

Every solution of Hamilton equations is Symplectic

To prove that for each solution of an Hamiltonian problem the condition (8) holds, we first note that J can be written as

$$J = M\nabla, \tag{10}$$

we can then calculate the total time derivative of J as

$$\dot{J} = \frac{d}{dt}(M)\,\nabla. \tag{11}$$

The time derivative of the n-th component of M, $M_{\{q,p\}_n}$, is

$$\frac{d}{dt}M_{\{q,p\}_n} = \frac{\partial M_{\{q,p\}_n}}{\partial q_1}\frac{dq_1}{dt} + \cdots + \frac{\partial M_{\{q,p\}_n}}{\partial p_n}\frac{dp_n}{dt} \tag{12}$$

then we have

$$\frac{d}{dt}J = J\dot{v}\nabla = JS\nabla^T H\nabla \tag{13}$$

where we used the Eq. 7 for $\dot{v}$.

Every solution of Hamilton equations is Symplectic

We calculate now

$$\begin{aligned}
\frac{d}{dt}\left(JSJ^T\right) &= \dot{J}SJ^T + JS\dot{J}^T \\
&= JS\nabla^T H\nabla SJ^T + JS\left(JS\nabla^T H\nabla\right)^T \\
&= JS\nabla^T H\nabla SJ^T + JS\nabla^T\nabla HS^T J^T \\
&= 0. \qquad (14)
\end{aligned}$$

Where we used $S^T = -S$ and $\nabla^T\nabla H = \nabla^T H\nabla$ bcecause the partial derivatives of the Hamiltonian commute. We just proved that JSJ^T is a constant that we can evaluate when $t = 0$ and $J = \mathbb{I}$ obtaining

$$JSJ^T = S. \qquad (15)$$

Every solution of Hamilton equations is Symplectic

The final step is obtained through simple algebra

$$
\begin{aligned}
JSJ^T &= S \\
SJ^T &= J^{-1}S \\
J^T &= S^{-1}J^{-1}S \\
J^TS &= S^{-1}J^{-1}SS \\
J^TSJ &= S^{-1}J^{-1}SSJ \\
J^TSJ &= S.
\end{aligned}
\tag{16}
$$

Where $S^{-1} = -S$ and $S^2 = -\mathbb{I}$.

Exercise: Determinant of Symplectic matrix

Prove that if J is symplectic, then

$$\det(J) = 1. \tag{17}$$

If this exercise is too complicate you can try to prove at least that $\det(J) = \pm 1$, this is much simpler.

Liouville's Theorem

A consequence of Eq. (17) is the Liouville's Theorem. It states that the volume of the phase space is preserved by the Hamiltonian equations of motion. Let say that M is the solution of the Hamiltonian, then M will send the coordinates and momenta (q, p) into a new set of coordinates and momenta $(Q, P) = M(q, p)$.

The infinitesimal volume element is the $2n$-form that transforms according to

$$\begin{aligned} V_{\text{final}} &= dQ_1 \wedge \cdots \wedge dQ_n \wedge dP_1 \wedge \cdots \wedge dP_n \\ &= \det(J) dq_1 \wedge \cdots \wedge dq_n \wedge dp_1 \wedge \cdots \wedge dp_n \\ &= \det(J) V_{\text{initial}} \\ &= V_{\text{initial.}} \end{aligned} \tag{18}$$

Physical interpretation of Liouville's Theorem

The Liouville's Theorem can be seen for one or multiple particles. If a particle moves around a periodic path, then the volume spanned in the phase space will be constant in time. We can see this for example in a pendulum: Single Particle Video.

The Theorem applies also for a group of particles. If we start from a configuration spanning a certain volume in the phase space, its evolution will preserve such a volume: Multy Particle Video.

Electromagnetic Hamiltonian

In the next lectures we will focus on a specific Hamiltonian, this is the Hamiltonian of an electrically charged particle that travels in an electromagnetic field. We assume that the electric field E and the magnetic field B are written in terms of potentials as

$$\begin{aligned} E &= \nabla\phi(q) && (19) \\ B &= \nabla \times A(q) && (20) \end{aligned}$$

then the Hamiltonian associated to a particle with a charge q_c interacting with the fields E and B is

$$H = \frac{(p - q_c A(q))^2}{2m} + q_c \phi(q). \tag{21}$$

Exercise: Lorentz Force

We can derive the Hamiltonian (21) in several ways, but none of them is a warranty that we are representing the correct physical behaviour. The only possibility is to verify the generated equations of motion experimentally.

We know, from experiments, that the Lorentz force is correct, so we can prove that the Hamiltonian is correct if we show that

$$H = \frac{(p - q_c A)^2}{2m} + q_c \phi \tag{22}$$

generates the Lorentz force

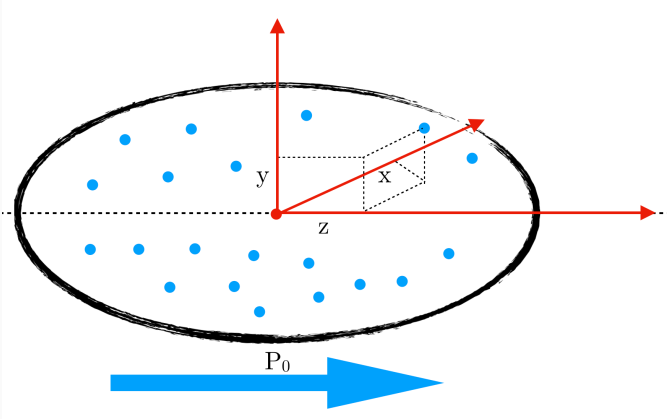
$$F = q_c(E + v \times B) \tag{23}$$

when the fields are expressed with the conditions

$$\begin{aligned} E &= \nabla \phi &(24)\\ B &= \nabla \times A. &(25) \end{aligned}$$

Charged Particles Hamiltonian

Finally we will not use exactly the Hamiltonian (21) but we will change the coordinates to a frame that is more suitable for a bunch of particles traveling in a particle accelerator as in figure.



x and y are simply the distances with respect to the reference particle and are unchanged compared to the laboratory frame. If s is the space traveled by the reference particle in a time t then the z coordinate of a particle is $z = \frac{s}{\beta_0} - ct$ where β_0 is the speed of the reference particle with respect to c. The transverse momenta are given by $p_x = \frac{\beta_x \gamma_x mc + q_c A_x}{p_0}$, $p_y = \frac{\beta_y \gamma_y mc + q_c A_y}{p_0}$, while the longitudinal momentum is simply the energy deviation from the reference partilce $\delta = \frac{E}{cp_0} - \frac{1}{\beta_0}$ where p_0 is the total momentum of the reference particle $p_0 = \beta_0 \gamma_0 mc$. The magnetic field is also scaled with the reference momentum such as $a = \frac{q_c}{p_0} A$.

Charged Particles Hamiltonian

With this new set of coordinates we can write the Hamiltonian of a charged particle that travels in a particle accelerator as

$$H = \frac{\delta}{\beta_0} - \sqrt{\left(\delta + \frac{1}{\beta_0} - \frac{q_c \phi}{c p_0}\right)^2 - (p_x - a_x)^2 - (p_y - a_y)^2 - \frac{1}{\beta_0^2 \gamma_0^2}} - a_z. \quad (26)$$

The full derivation of Eq. (26) it is not straightforward and it is well detailed in the Chapter 2 of [3].

Solutions to proposed exercises.

Solution: from Hamilton to Newton equations

Assuming that p and q are the canonical varialbes in one dimension, prove that if $T = \frac{p^2}{2m}$ and $V = V(q)$ the Eqs. (2) are equivalent to the Eq. (1) (the solution can be easily extended in many variables).

Solution: from Hamilton to Newton equations

$$H = \frac{p^2}{2m} + V(q) \tag{27}$$

the Hamilton equations are

$$\dot{q} \quad = \quad \frac{\partial}{\partial p}\left[\frac{p^2}{2m} + V(q)\right] = \frac{p}{m} \tag{28}$$

$$\dot{p} \quad = - \quad \frac{\partial}{\partial q}\left[\frac{p^2}{2m} + V(q)\right] = -\frac{\partial V(q)}{\partial q} \tag{29}$$

and deriving the Eq. (28) with respect to time we have the Newton equation in 1 dimension

$$m\ddot{q} = -\frac{\partial V(q)}{\partial q}. \tag{30}$$

Solution: the free particle

Calculate the trajectory of a free particle, i.e. $V = 0$ with the classical Hamiltonian

$$H = \frac{p^2}{2m} \tag{31}$$

and with the relativistic Hamiltonian

$$H = \sqrt{p^2c^2 + m^2c^4}. \tag{32}$$

Solution: the free particle

For the classical Hamiltonian we have

$$\dot{q} = \frac{\partial}{\partial p}\frac{p^2}{2m} = \frac{p}{m} \tag{33}$$

$$\dot{p} = -\frac{\partial}{\partial q}\frac{p^2}{2m} = 0 \tag{34}$$

whit the solutions

$$q(t) = \frac{p_0}{m}t + q_0 \tag{35}$$

$$p(t) = p_0 \tag{36}$$

with $q_0 = q(0)$ and $p_0 = p(0)$. This is the usual inertial motion with constant speed and no acceleration.

Solution: the free particle

For the relativistic Hamiltonian we have

$$\dot{q} = \frac{\partial}{\partial p}\sqrt{p^2c^2 + m^2c^4} = \frac{pc}{\sqrt{p^2 + m^2c^2}} \tag{37}$$

$$\dot{p} = -\frac{\partial}{\partial q}\sqrt{p^2c^2 + m^2c^4} = 0. \tag{38}$$

Recalling that the relativistic momentum $p = \gamma\beta mc$ and that $\gamma^2 - 1 = \gamma^2\beta^2$ we have

$$\dot{q} = \frac{p}{\gamma m} \tag{39}$$

$$\dot{p} = 0 \tag{40}$$

The relativistic particle has exactly the same equations of motion of the classic particle, the only difference is that its mass now is γm and depends on its velocity as predicted by the Einstein's theory.

Solution: Determinant of Symplectic matrix

Prove that if J is symplectic, then

$$\det(J) = 1. \tag{41}$$

Solution: Determinant of Symplectic matrix

It is easy to see that $\det(J) = \pm 1$ because from Eq. (8) we have

$$\det(J^T S J) = \det(S) \tag{42}$$

but $\det(S) = 1$ and $\det(J^T) = \det(J)$ so the equation is

$$\det(J)^2 = 1 \tag{43}$$

that means that the determinant can be ± 1.

To prove that the determinant is 1 is a bit more complicate. We start noticing that

$$\det(J^T J + I) > 1 \tag{44}$$

because $J^T J$ is symmetric and positive definite.

Solution: Determinant of Symplectic matrix

We then use the symplectic condition to calculate the inverse of J^T as $J^{T^{-1}} = SJS^{-1}$ to write

$$J^T J + I = J^T (J + SJS^{-1}). \tag{45}$$

Now we will search a factorization of the quantity $J + SJS^{-1}$. We write it in blocks of $N \times N$ matrices as

$$\begin{aligned} J + SJS^{-1} &= \begin{pmatrix} J_1 & J_2 \\ J_3 & J_4 \end{pmatrix} + \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \begin{pmatrix} J_1 & J_2 \\ J_3 & J_4 \end{pmatrix} \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix} \\ &= \begin{pmatrix} J_1 + J_4 & J_2 - J_3 \\ J_3 - J_2 & J_1 + J_4 \end{pmatrix} = \begin{pmatrix} J_{14} & J_{23} \\ -J_{23} & J_{14} \end{pmatrix} \end{aligned} \tag{46}$$

where $J_{14} = J_1 + J_4$ and $J_{23} = J_2 - J_3$.

Solution: Determinant of Symplectic matrix

We can now perform the complex factorization

$$J + SJS^{-1} = \begin{pmatrix} J_{14} & J_{23} \\ -J_{23} & J_{14} \end{pmatrix} = \tag{47}$$

$$\frac{1}{2}\begin{pmatrix} I & I \\ iI & -iI \end{pmatrix}\begin{pmatrix} J_{14}+iJ_{23} & 0 \\ 0 & J_{14}-iJ_{23} \end{pmatrix}\begin{pmatrix} I & -iI \\ I & iI \end{pmatrix}.$$

We return to the determinants

$$\begin{aligned} \det(J^T J + I) &= \det(J^T)\det(J + SJS^{-1}) \\ &= \det(J)|\det(J_{14} + iJ_{23})|^2 > 1 \end{aligned} \tag{48}$$

this means that $\det(J)$ has to be strictly positive and we already knew that it can be only $\det(J) = 1$.

Solution: Lorentz Force

We can derive the Hamiltonian (21) in several ways, but none of them is a warranty that we are representing the correct physical behaviour. The only possibility is to verify the generated equations of motion experimentally.

We know, from experiments, that the Lorentz force is correct, so we can prove that the Hamiltonian is correct if we show that

$$H = \frac{(p - q_c A)^2}{2m} + q_c \phi \tag{49}$$

generates the Lorentz force

$$F = q_c(E + v \times B) \tag{50}$$

when the fields are expressed with the conditions

$$\begin{aligned} E &= \nabla\phi && (51) \\ B &= \nabla \times A. && (52) \end{aligned}$$

Solution: Lorentz Force

We write H in cartesian coordinates

$$H = \frac{(p_x - q_c A_x)^2 + (p_y - q_c A_y)^2 + (p_z - q_c A_z)^2}{2m} + q_c \phi \qquad (53)$$

and we calculate the equations of Hamilton

$$\dot{x} = \frac{\partial H}{\partial p_x} = \frac{(p_x - q_c A_x)}{m} \qquad (54)$$

$$\dot{y} = \frac{\partial H}{\partial p_y} = \frac{(p_y - q_c A_y)}{m} \qquad (55)$$

$$\dot{z} = \frac{\partial H}{\partial p_z} = \frac{(p_z - q_c A_z)}{m} \qquad (56)$$

Solution: Lorentz Force

$$\dot{p}_x = -\frac{\partial H}{\partial x} = \frac{1}{m}\left[(p_x - q_c A_x) q_c \frac{\partial A_x}{\partial x} + (p_y - q_c A_y) q_c \frac{\partial A_y}{\partial x} + (p_z - q_c A_z) q_c \frac{\partial A_z}{\partial x}\right] - q_c \frac{\partial \phi}{\partial x} \tag{57}$$

$$\dot{p}_y = -\frac{\partial H}{\partial y} = \frac{1}{m}\left[(p_x - q_c A_x) q_c \frac{\partial A_x}{\partial y} + (p_y - q_c A_y) q_c \frac{\partial A_y}{\partial y} + (p_z - q_c A_z) q_c \frac{\partial A_z}{\partial y}\right] - q_c \frac{\partial \phi}{\partial y} \tag{58}$$

$$\dot{p}_z = -\frac{\partial H}{\partial z} = \frac{1}{m}\left[(p_x - q_c A_x) q_c \frac{\partial A_x}{\partial z} + (p_y - q_c A_y) q_c \frac{\partial A_y}{\partial z} + (p_z - q_c A_z) q_c \frac{\partial A_z}{\partial z}\right] - q_c \frac{\partial \phi}{\partial z} \tag{59}$$

substituting (54,55,56) we have

$$\dot{p}_x = q_c \dot{x} \frac{\partial A_x}{\partial x} + q_c \dot{y} \frac{\partial A_y}{\partial x} + q_c \dot{z} \frac{\partial A_z}{\partial x} - q_c \frac{\partial \phi}{\partial x} \tag{60}$$

$$\dot{p}_y = q_c \dot{x} \frac{\partial A_x}{\partial y} + q_c \dot{y} \frac{\partial A_y}{\partial y} + q_c \dot{z} \frac{\partial A_z}{\partial y} - q_c \frac{\partial \phi}{\partial y} \tag{61}$$

$$\dot{p}_z = q_c \dot{x} \frac{\partial A_x}{\partial z} + q_c \dot{y} \frac{\partial A_y}{\partial z} + q_c \dot{z} \frac{\partial A_z}{\partial z} - q_c \frac{\partial \phi}{\partial z} \tag{62}$$

Solution: Lorentz Force

we calculate finally the three components of the force deriving with respect to time the Eqs. (54,55,56)

$$m\ddot{x} = \dot{p}_x - q_c\dot{x}\frac{\partial A_x}{\partial x} - q_c\dot{y}\frac{\partial A_x}{\partial y} - q_c\dot{z}\frac{\partial A_x}{\partial z} \tag{63}$$

$$m\ddot{y} = \dot{p}_y - q_c\dot{x}\frac{\partial A_y}{\partial x} - q_c\dot{y}\frac{\partial A_y}{\partial y} - q_c\dot{z}\frac{\partial A_y}{\partial z} \tag{64}$$

$$m\ddot{z} = \dot{p}_z - q_c\dot{x}\frac{\partial A_z}{\partial x} - q_c\dot{y}\frac{\partial A_z}{\partial y} - q_c\dot{z}\frac{\partial A_z}{\partial z} \tag{65}$$

and substituting the Eqs. (60,61,62) we obtain the Lorentz force

Solution: Lorentz Force

$$m\ddot{x} = q_c\left[\dot{y}\left(\frac{\partial A_y}{\partial x}-\frac{\partial A_x}{\partial y}\right)+\dot{z}\left(\frac{\partial A_z}{\partial x}-\frac{\partial A_x}{\partial z}\right)-\frac{\partial \phi}{\partial x}\right] \quad (66)$$

$$m\ddot{y} = q_c\left[\dot{x}\left(\frac{\partial A_x}{\partial y}-\frac{\partial A_y}{\partial x}\right)+\dot{z}\left(\frac{\partial A_z}{\partial y}-\frac{\partial A_y}{\partial z}\right)-\frac{\partial \phi}{\partial y}\right] \quad (67)$$

$$m\ddot{z} = q_c\left[\dot{x}\left(\frac{\partial A_x}{\partial z}-\frac{\partial A_z}{\partial x}\right)+\dot{y}\left(\frac{\partial A_y}{\partial z}-\frac{\partial A_z}{\partial y}\right)-\frac{\partial \phi}{\partial z}\right] \quad (68)$$

in vectorial format

$$F = q_c\left(-\nabla\phi + v\times\nabla\times A\right) \quad (69)$$

$$F = q_c\left(E + v\times B\right). \quad (70)$$

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