Hamiltonian with z as the Independent Variable

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1 Problem

Deduce the form of the Hamiltonian when z rather than t is considered to be the independent variable. Illustrate this for the case of a particle of charge q and mass m in an external electromagnetic field.

2 Solution

This solution follows Appendix B of [1]. See also sec. 1.6 of [2].[1] For simplicity we consider only a single particle.

2.1 Use of t as the Independent Variable

We recall the usual Hamiltonian description of a particle of charge q and mass m in external electromagnetic fields $\mathbf{E}$ and $\mathbf{B}$, which can be deduced from scalar and vector potentials V and $\mathbf{A}$ (in some gauge) according to,

$$\mathbf{E} = -\boldsymbol{\nabla} V - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}, \qquad \mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}, \tag{1}$$

$$\begin{aligned} H_t(x, y, z, p_x, p_y, p_z) &= E_{\rm mech} + qV = c\sqrt{m^2c^2 + p_{{\rm mech},x}^2 + p_{{\rm mech},y}^2 + p_{{\rm mech},z}^2} + qV \\ &= c\sqrt{m^2c^2 + (p_x - qA_x/c)^2 + (p_y - qA_y/c)^2 + (p_z - qA_z/c)^2} + qV, \end{aligned} \tag{2}$$

in Gaussian units, where c is the speed of light in vacuum, and the components of $\mathbf{p} = \mathbf{p}_{\rm mech} + q\mathbf{A}/c$ are the canonical momenta associated with coordinates $\mathbf{x} = (x, y, z)$. The subscript on H_t indicates that time t is the independent variable in this Hamiltonian. Hamilton's equations of motion for this case are,

$$\frac{dx_i}{dt} = \frac{\partial H_t}{\partial p_i} = \frac{c^2 p_{{\rm mech},i}}{E_{\rm mech}} = v_i, \tag{3}$$

$$\begin{aligned} \frac{dp_i}{dt} &= -\frac{\partial H_t}{\partial x_i} = q\sum_j \frac{v_j}{c}\frac{\partial A_j}{\partial x_i} - q\frac{\partial V}{\partial x_i} \\ &= \frac{dp_{{\rm mech},i}}{dt} + \frac{q}{c}\frac{dA_i}{dt} = \frac{dp_{{\rm mech},i}}{dt} + \frac{q}{c}\frac{\partial A_i}{\partial t} + q\sum_j \frac{v_j}{c}\frac{\partial A_i}{\partial x_j}, \end{aligned} \tag{4}$$

[1]This topic is also discussed in Art. 431, p. 353 of [3], which refers to earlier French papers.

using the convective derivative $d\mathbf{A}/dt = \partial\mathbf{A}/\partial t + (\mathbf{v}\cdot\boldsymbol{\nabla})\mathbf{A}$ for the vector potential at the position of the moving particle. Hence,

$$\frac{dp_{\mathrm{mech},i}}{dt} = q\left[-\frac{\partial V}{\partial x_i} - \frac{1}{c}\frac{\partial A_i}{\partial t} + \sum_j \frac{v_j}{c}\left(\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j}\right)\right] = q\left(\mathbf{E} + \frac{\mathbf{v}}{c}\times\mathbf{B}\right)_i = F_{\mathrm{Lorentz},i}\,, \tag{5}$$

such that the equation of motion for the mechanical momentum $\mathbf{p}_{\mathrm{mech}}$ is gauge invariant, although the Hamiltonian (2) is not.

2.2 Use of z as the Independent Variable

In some applications, such as transport of particles in accelerators and storage rings, it is often preferable to consider a set of particles at fixed values of a spatial coordinate, say z, rather than at fixed time.[2] So, we seek a Hamiltonian formalism in which z is the independent variable, and t is the third q-coordinate, along with x and y. We must identify a canonical momentum p_t that is conjugate to coordinate t, and a Hamiltonian $H_z(x, y, t, p_x, p_y, p_t)$ such that the equations of motion can be deduced from this Hamiltonian in the usual way.

We anticipate that the (total) energy is conjugate to the time coordinate, so we tentatively identify,

$$p_t \stackrel{?}{=} E_{\mathrm{total}} = E_{\mathrm{mech}} + qV = H_t. \tag{6}$$

We might then guess that, by analogy, the desired Hamiltonian H_z equals the canonical momentum p_z,

$$\begin{aligned} H_z &\stackrel{?}{=} p_z = p_{\mathrm{mech},z} + \frac{qA_z}{c} = \sqrt{\frac{E_{\mathrm{mech}}^2}{c^2} - m^2c^2 - p_{\mathrm{mech},x}^2 - p_{\mathrm{mech},y}^2} + \frac{qA_z}{c} \\ &= \sqrt{\frac{(p_t - qV)^2}{c^2} - m^2c^2 - \left(p_x - \frac{qA_x}{c}\right)^2 - \left(p_x - \frac{qA_x}{c}\right)^2} + \frac{qA_z}{c}\,. \end{aligned} \tag{7}$$

The test is whether the equations of motion that follow from these identifications are consistent with those associated with H_t,

$$\frac{dx}{dz} \stackrel{?}{=} \frac{\partial H_z}{\partial p_x} = -\frac{p_{\mathrm{mech},x}}{p_{\mathrm{mech},}\,z} = -\frac{v_x}{v_z}\,. \tag{8}$$

The magnitude is correct, but the sign is wrong. This suggests that there should have been a minus sign in both eqs. (6) and (7),

$$p_t = -E_{\mathrm{total}} = -E_{\mathrm{mech}} - qV = -H_t, \tag{9}$$

[2]It is often desirable that the new independent variable be the path length s along a curved, central trajectory in, say, a ring. However, only in the linear approximation can the formalism of this section be applied to a curvilinear coordinate s.

$$
\begin{aligned}
H_z &= -p_z = -p_{\text{mech},z} - \frac{qA_z}{c} = -\sqrt{\frac{E_{\text{mech}}^2}{c^2} - m^2c^2 - p_{\text{mech},x}^2 - p_{\text{mech},y}^2} - \frac{qA_z}{c} \\
&= -\sqrt{\frac{(p_t + qV)^2}{c^2} - m^2c^2 - \left(p_x - \frac{qA_x}{c}\right)^2 - \left(p_x - \frac{qA_x}{c}\right)^2} - \frac{qA_z}{c}\,. \qquad (10)
\end{aligned}
$$

Now, as desired,

$$
\frac{dt}{dz} = \frac{\partial H_z}{\partial p_t} = -\frac{-E_{\text{mech}}}{c^2 p_{\text{mech}\,,\,z}} = \frac{1}{v_z}\,. \qquad (11)
$$

Also,

$$
\begin{aligned}
\frac{dp_x}{dz} &= -\frac{\partial H_z}{\partial x} = -\frac{q}{v_z}\frac{\partial V}{\partial x} + \frac{q}{v_z}\sum_j \frac{v_j}{c}\frac{\partial A_i}{\partial x_j} \\
&= \frac{dp_{\text{mech},x}}{dz} + \frac{q}{cv_z}\frac{dA_x}{dt} = \frac{dp_{\text{mech},x}}{dz} + \frac{q}{cv_z}\frac{\partial A_x}{\partial t} + \frac{q}{v_z}\sum_j \frac{v_j}{c}\frac{\partial A_x}{\partial x_j}\,, \qquad (12)
\end{aligned}
$$

and hence,

$$
\begin{aligned}
\frac{dp_{\text{mech},x}}{dz} &= \frac{q}{v_z}\left[-\frac{\partial V}{\partial x} - \frac{1}{c}\frac{\partial A_x}{\partial t} + q\sum_j \frac{v_j}{c}\left(\frac{\partial A_j}{\partial x} - \frac{\partial A_x}{\partial x_j}\right)\right] = \frac{q}{v_z}\left(\mathbf{E} + \frac{\mathbf{v}}{c}\times\mathbf{B}\right)_x \\
&= \frac{F_{\text{Lorentz},x}}{v_z}. \qquad (13)
\end{aligned}
$$

Finally,

$$
\begin{aligned}
\frac{dp_t}{dz} &= -\frac{\partial H_z}{\partial t} = -\frac{q}{v_z}\frac{\partial V}{\partial t} + \frac{q}{v_z}\frac{\mathbf{v}}{c}\cdot\frac{\partial \mathbf{A}}{\partial t} \\
&= -\frac{dE_{\text{mech}}}{dz} - \frac{q}{v_z}\frac{dV}{dt} = -\frac{dE_{\text{mech}}}{dz} - \frac{q}{v_z}\frac{\partial V}{\partial t} - \frac{q}{v_z}\mathbf{v}\cdot\boldsymbol{\nabla}V, \qquad (14)
\end{aligned}
$$

and hence,

$$
\frac{dE_{\text{mech}}}{dz} = \frac{q}{v_z}\mathbf{v}\cdot\left(-\boldsymbol{\nabla}V - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t}\right) = \frac{q}{v_z}\mathbf{v}\cdot\mathbf{E} = \frac{\mathbf{F}_{\text{Lorentz}}\cdot\mathbf{v}}{v_z}\,. \qquad (15)
$$

Thus, Hamilton's equations for H_z, eq. (10), are consistent with the usual equations of motion deduced from H_t, and it is valid to use either Hamiltonian as most convenient.

In practice, the importance of the Hamiltonian H_z is in assuring that Liouville's theorem holds for canonical coordinates (x, y, t, p_x, p_y, p_t). When considering the phase space of these coordinates, it is common to write $p_t = E_{\text{mech}} + qV$ (and $H_z = p_z$), which is not strictly correct, but causes no error unless one tries to deduce the equations of motion from this H_z.

3 Liouville's Theorem

Liouville's theorem [4, 5, 6] is that the (phase) volume $\Pi_i\, dq_i dp_i$ in canonical-coordinate space (q_i, p_i) is invariant under canonical transformations, if those transformations do not involve scale changes of the coordinates. A canonical transformation operates on one set of canonical coordinates (q_i, p_i), for which there exists a Hamiltonian $h(q_i, p_i; t)$ and for which the equations of motion are,

$$\frac{dq_i}{dt} = \frac{\partial h}{\partial p_i}, \qquad \frac{dp_i}{dt} = -\frac{\partial h}{\partial q_i}, \tag{16}$$

to arrive at another set of canonical coordinates (Q_i, P_i) with Hamiltonian $H(Q_i, P_i; t)$ for which the equations of motion are,

$$\frac{dQ_i}{dt} = \frac{\partial H}{\partial P_i}, \qquad \frac{dP_i}{dt} = -\frac{\partial H}{\partial Q_i}. \tag{17}$$

Liouville's theorem is often applied to a system of N particles, for which canonical-coordinate space has $6N$ dimensions. If interactions between these particles can be ignored, we can consider the N particles as being within some volume in the 6-dimensional phase space (q_i, p_i), $i = 1, 2, 3$, and Liouville's theorem for the latter phase space implies that the 6-dimensional phase volume of the set of particles is invariant under canonical transformations of the six coordinates (q_i, p_i).

Liouville's theorem has the corollaries that the 2-dimensions subvolumes $dq_i\, dp_i$ and the 4-dimensional subvolumes $dq_i\, dp_i\, dq_j\, dp_j$ have the invariants under scale-preserving canonical transformations,

$$\sum_i dq_i\, dp_i\,, \qquad \text{and} \qquad dq_i\, dp_i + dq_j\, dp_j\, dq_k\, dp_k, \tag{18}$$

for indices i, j and k all different.

Evolution in time, $(q_i(t_0), p_i(t_0)) \to (q_i(t), p_i(t))$, is an example of a canonical transformation, and Liouville's theorem is often stated in the more restricted sense that phase volume is invariant under this subset of canonical transformations.

An electromagnetic gauge transformation, $\mathbf{A} \to \mathbf{A} + \boldsymbol{\nabla} f$, $V \to V - \partial f/\partial ct$, where f is any differentiable scalar function, is also a canonical transformation. Hence, phase volume, along with Hamilton's equations of motion, are invariant under gauge transformations (although the Hamiltonian itself is not).[3]

The transformation $(x, y, z, p_x, p_y, p_z) \to (x, y, t, p_x, p_y, p_t)$ considered in sec. 2 is also a canonical transformation in a broader sense of this term.[4] This transformation changes the 2-dimensional phase volume $dz\, dp_z$ to,

$$|J|\; dt\, dp_t = \begin{vmatrix} \frac{\partial z}{\partial t} & \frac{\partial z}{\partial p_t} \\ \frac{\partial p_z}{\partial t} & \frac{\partial p_z}{\partial p_t} \end{vmatrix} dt\, dp_t = \begin{vmatrix} v_z & 0 \\ 0 & \frac{1}{v_z} \end{vmatrix} dt\, dp_t = dt\, dp_t \tag{19}$$

which confirms that Liouville's theorem holds for this canonical transformation.

[3]In practice, one considers a system in a particular gauge. Particularly convenient for Hamiltonian dynamics is the so-called Hamiltonian gauge (introduced by Gibbs in 1896 [7]; see, for example, sec. 8 of [8]) in which the scalar potential V is everywhere zero. For oscillatory electromagnetic fields with time dependence $e^{-i\omega t}$ and wave number $k = \omega/c$, the Hamiltonian-gauge vector potential is $\mathbf{A} = -i\mathbf{E}/k$; for static electric fields $\mathbf{A} = -c(t - t_0)\mathbf{E}$; and for static magnetic fields the vector potential is the same as that in the Coulomb gauge (and also in the Lorenz gauge).

[4]Canonical transformations that do not change the independent variable are sometimes called restricted canonical transformations.

4 Swann's Theorem

In one of the first applications of Liouville's theorem to a "beam" of particles, Swann [9] showed that the phase volume in coordinates (x, y, z, p_x, p_y, p_z), where the canonical momenta are those for a particle in an electromagnetic field, $\mathbf{p} = \mathbf{p}_{\rm mech} + q\mathbf{A}/c$, is the same as that for coordinates $(x, y, z, p_{{\rm mech},x}, p_{{\rm mech},y}, p_{{\rm mech},z})$. The proof is straightforward, in that the determinant of the Jacobian matrix of the (noncanonical) transformation, $(x, y, z, p_{{\rm mech},x}, p_{{\rm mech},y}, p_{{\rm mech},z}) \to (x, y, z, p_x, p_y, p_z)$, is unity,

$$|J| = \begin{vmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ \frac{q}{c}\frac{\partial A_x}{\partial x} & \frac{q}{c}\frac{\partial A_x}{\partial y} & \frac{q}{c}\frac{\partial A_x}{\partial z} & 1 & 0 & 0 \\ \frac{q}{c}\frac{\partial A_y}{\partial x} & \frac{q}{c}\frac{\partial A_y}{\partial y} & \frac{q}{c}\frac{\partial A_y}{\partial z} & 0 & 1 & 0 \\ \frac{q}{c}\frac{\partial A_z}{\partial x} & \frac{q}{c}\frac{\partial A_z}{\partial y} & \frac{q}{c}\frac{\partial A_z}{\partial z} & 0 & 0 & 1 \end{vmatrix} = 1. \qquad (20)$$

This argument clearly holds if only one or two of the canonical momenta are replaced by mechanical momenta. Likewise, the argument holds for any 2-dimensional or 4-dimensional subvolume in phase space. Furthermore, when using z as the independent variable, with t as a coordinate with canonical momentum $p_t = -E_{\rm mech} - qV$, Swann's argument holds when p_t is replaced by $-E_{\rm mech}$ (or $E_{\rm mech}$).

Appendix: Extended Phase Space

A particle with definite mass has three degrees of freedom, so it is natural to consider its phase space as having six dimensions. Yet, in the relativistic view of four-dimensional space-time, one is led to consider the eight-dimensional extended phase space $(x, p_x, y, p_y, z, p_z, t, p_t)$ where $p_t = -E$, as apparently first done by Sundman in 1912 [10]. "Textbook discussions are given in sec. 6.10 of [11] and sec. 5.5 of [12]. One use of extended phase space is in deducing Hamiltonians for systems with time-dependent forces, as discussed in [13].

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