Magnetic Fields in Quantum Mechanics and the Classical Hamiltonian Formalism

Andreas Wacker[1]
Mathematical Physics, Lund University
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The interaction of matter with electromagnetic fields is central for many physical processes. Thus its quantum treatment is of high relevance. However, this topic is difficult for many students, in particular, if they are unaware of the basic foundations for the Hamilton operator in classical mechanics. In these notes, the key results will be given in Sec. 1, which are required to operate in practical situations. Sec. 2 provides a very brief introduction to the ideas behind the classical Hamilton function and the concept of canonical variables, which are central for the quantization performed in Sec. 4. The particular classical form for the Hamiltonian is derived in Sec. 3 and its proper quantization provides the results given in Sec. 1.

1 Key results for quantum mechanics with magnetic field

The electric field $\mathbf{E}(\mathbf{r},t)$ and the magnetic field $\mathbf{B}(\mathbf{r},t)$ are conveniently described by the scalar potential $\phi(\mathbf{r},t)$ and vector potential $\mathbf{A}(\mathbf{r},t)$ according to

$$\mathbf{E}(\mathbf{r},t) = -\nabla\phi(\mathbf{r},t) - \frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t} \quad \text{and} \quad \mathbf{B}(\mathbf{r},t) = \nabla\times\mathbf{A}(\mathbf{r},t)\,. \tag{1}$$

This is equivalent to the homogeneous Maxwell equations $\nabla\cdot\mathbf{B}=0$ and $\nabla\times\mathbf{E} = -\partial\mathbf{B}/\partial t$, as explained in any textbook on electrodynamics.[1]

As motivated from classical analytical mechanics in the subsequent sections, the Hamilton operator for a particle with mass m and charge q reads

$$\hat{H} = \frac{(\hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{r}},t))^2}{2m} + q\phi(\hat{\mathbf{r}},t) \tag{2}$$

where the operators $\hat{\mathbf{p}}$ and $\hat{\mathbf{r}}$ satisfy the canonical commutation relations

$$[\hat{p}_j,\hat{r}_k] = \frac{\hbar}{\mathrm{i}}\delta_{ij} \qquad [\hat{p}_j,\hat{p}_k]=0 \qquad [\hat{r}_j,\hat{r}_k]=0 \quad \text{for } j,k\in x,y,z \tag{3}$$

Using wave functions $\Psi(\mathbf{r},t)$, the momentum operator $\hat{\mathbf{p}}$ becomes $\frac{\hbar}{\mathrm{i}}\nabla$ as usual. Note that the average velocity is given by

$$\langle\mathbf{v}\rangle = \frac{\langle\hat{\mathbf{p}}^{\text{kinetic}}\rangle}{m} \quad \text{with the kinetic momentum} \quad \hat{\mathbf{p}}^{\text{kinetic}} = \hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{r}},t) \tag{4}$$

A straightforward calculation shows that the commutation relation

$$[\hat{p}_j^{\text{kinetic}},\hat{p}_k^{\text{kinetic}}] = \mathrm{i}\hbar q\sum_l \epsilon_{jkl}B_l$$

[1] Andreas.Wacker@fysik.lu.se

differs form the canonical relations (3). Here the Levi-Civita tensor ϵ_{jkl} has the values $\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = 1$, $\epsilon_{321} = \epsilon_{213} = \epsilon_{132} = -1$, while it is zero if two indices are equal.

The operator of angular momentum is usually taken as $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$ and corresponds to the canonical angular momentum of classical mechanics. Straightforward calculation provides the commutation relations

$$[\hat{L}_j, \hat{L}_k] = \mathrm{i}\hbar \sum_l \epsilon_{jkl} \hat{L}_l$$

while these do not hold for the operator of the kinetic angular momentum $\hat{\mathbf{L}}^{\text{kinetic}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}^{\text{kinetic}}$, which seems hardly to be used.

For stationary systems with a homogeneous magnetic field $\mathbf{B}$, we may choose the vector potential $\mathbf{A}(\mathbf{r}, t) = \frac{1}{2}\mathbf{B} \times \mathbf{r}$. Then we obtain after some algebra

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{q}{2m}\hat{\mathbf{L}} \cdot \mathbf{B} + \frac{q^2}{8m}\hat{\mathbf{r}}_\perp^2 \mathbf{B}^2 + q\phi(\hat{\mathbf{r}}) \tag{5}$$

where $\mathbf{r}_\perp$ is the part of $\mathbf{r}$, which is perpendicular to the magnetic field $\mathbf{B}$. This is frequently used for the electrons (with $q = -e$) in atoms or solids, where $\phi(\hat{\mathbf{r}})$ is the electrostatic potential resulting from the nuclei or ionic cores.

2 Main results from analytical mechanics

Analytical mechanics provides a general formalism to obtain equations of motion for arbitrary mechanical systems, where the motion may be restricted by external conditions. In this case one uses a set of generalized coordinates q_i with $i = 1, 2, \ldots f$, where f is the number of degrees of freedom. Here a short overview is given. Details can be found in Ref. [2].

> `Example I:` A free particle of mass m affected by the force $\mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r})$ has the coordinates $q_1 = x$, $q_2 = y$, $q_3 = z$. There are $f = 3$ degrees of freedom

> `Example II:` A planar pendulum of length l, where $q_1 = \varphi$ is the angle describing the elongation from the position at rest in earths gravitational field.

Then the equations of motion are given by the *Lagrange equations*

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathcal{L}(q_1, \ldots q_f, \dot{q}_1, \ldots \dot{q}_f, t)}{\partial \dot{q}_j}\right) = \frac{\partial \mathcal{L}(q_1, \ldots q_f, \dot{q}_1, \ldots \dot{q}_f, t)}{\partial q_j} \qquad \text{for } j = 1, 2, \ldots f \tag{6}$$

where the *Lagrange function* $\mathcal{L}(q_1, \ldots q_f, \dot{q}_1, \ldots \dot{q}_f, t)$ is a function of the generalized coordinates and their derivatives in time. For mechanical systems, $\mathcal{L} = T - V$, where T is the kinetic and V the potential energy, both expressed in terms of the generalized coordinates.

> `Example I:` $\mathcal{L}(\mathbf{r}, \dot{\mathbf{r}}, t) = \frac{m}{2}\dot{\mathbf{r}}^2 - V(\mathbf{r})$ and we find
>
> $$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathcal{L}(\mathbf{r}, \dot{\mathbf{r}}, t)}{\partial \dot{x}}\right) = m\ddot{x} \quad \text{and} \quad \frac{\partial \mathcal{L}(\mathbf{r}, \dot{\mathbf{r}}, t)}{\partial x} = -\frac{\partial V}{\partial x} \quad \Rightarrow \quad m\ddot{x} = -\frac{\partial V}{\partial x}$$

> `Example II:` $T = \frac{m}{2} l^2 \dot{\varphi}^2$, $V = mgz = -mgl\cos\varphi$ and thus
>
> $$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathcal{L}(\varphi, \dot{\varphi}, t)}{\partial \dot{\varphi}}\right) = ml^2\ddot{\varphi} \quad \text{and} \quad \frac{\partial \mathcal{L}(\varphi, \dot{\varphi}, t)}{\partial \varphi} = -mgl\sin\varphi \quad \Rightarrow \quad l\ddot{\varphi} = -g\sin\varphi$$

We define the *canonical momentum* as

$$p_i = \frac{\partial \mathcal{L}(q_1 \dots q_f, \dot{q}_1, \dots \dot{q}_f, t)}{\partial \dot{q}_i} \quad \text{for} \quad i = 1, \dots f$$

which is not necessarily identical with the standard expression $m\dot{\mathbf{r}}$.

`Example I:` $p_1 = m\dot{x}$ or $\mathbf{p} = m\dot{\mathbf{r}}$ which agrees with the kinetic momentum $\mathbf{p}^{\text{kinetic}} = m\mathbf{v}$

`Example II:` $p_\varphi = ml^2\dot{\varphi}$. This is actually the angular momentum in the direction perpendicular the plane of motion.

We define the *Hamilton function* as

$$\mathcal{H}(p_1 \dots p_f, q_1 \dots q_f, t) = \sum_{i=1}^{f} \dot{q}_i p_i - \mathcal{L}\,, \tag{7}$$

where one has to express the generalized velocities by functions of coordinates and generalized momenta, $\dot{q}_i = g_i(q_1, \dots q_f, p_1, \dots p_f, t)$.

In this way one obtains a set of first-order differential equations, the *Hamilton equations*

$$\dot{q}_i = \frac{\partial \mathcal{H}(p_1, \dots p_f, q_1, \dots q_f, t)}{\partial p_i} \tag{8}$$

$$\dot{p}_i = -\frac{\partial \mathcal{H}(p_1, \dots p_f, q_1, \dots q_f, t)}{\partial q_i} \tag{9}$$

which determine the dynamics of the system in the $2f$-dimensional phase space of the variables $(p_1 \dots p_f, q_1 \dots q_f)$.

`Example I:` $\mathcal{H}(\mathbf{p}, \mathbf{r}, t) = \frac{1}{2m}\mathbf{p}^2 + V(\mathbf{r})$

$$\dot{x} = \frac{\partial \mathcal{H}(\mathbf{p}, \mathbf{r}, t)}{\partial p_x} = \frac{1}{m}p_x \quad \text{and} \quad \dot{p_x} = -\frac{\partial \mathcal{H}(\mathbf{p}, \mathbf{r}, t)}{\partial x} = -\frac{\partial V(\mathbf{r})}{\partial x}$$

`Example II:` $\mathcal{H}(p_\varphi, \varphi, t) = \frac{1}{2ml^2}p_\varphi^2 + mgl\cos\varphi$

$$\dot{\varphi} = \frac{\partial \mathcal{H}(p_\varphi, \varphi, t)}{\partial p_\varphi} = \frac{1}{ml^2}p_\varphi \quad \text{and} \quad \dot{p}_\varphi = -\frac{\partial \mathcal{H}(p_\varphi, \varphi, t)}{\partial \varphi} = -mgl\sin\varphi$$

Finally note, that the Hamilton function is constant in time under the evolution of the system according to Eqs. (8,9) unless it has an explicit time-dependence. This reflects the energy conservation in classical system.

3 Electromagnetic fields

We consider a free particle with mass m and charge q moving in an electromagnetic field. The force is given by

$$m\ddot{\mathbf{r}} = \mathbf{F}_{\text{Lorentz}} = q\big(\mathbf{v} \times \mathbf{B}(\mathbf{r}, t) + \mathbf{E}(\mathbf{r}, t)\big) \tag{10}$$

Inserting the electromagnetic potentials (1) and treating $\mathbf{v} = \dot{\mathbf{r}}$ and $\mathbf{r}$ as independent variables, we find

$$m\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v} = \underbrace{q\mathbf{v}\times\left(\frac{\partial}{\partial\mathbf{r}}\times\mathbf{A}\right)}_{=q\frac{\partial}{\partial\mathbf{r}}(\mathbf{v}\cdot\mathbf{A})-q\left(\mathbf{v}\cdot\frac{\partial}{\partial\mathbf{r}}\right)\mathbf{A}} - q\frac{\partial\mathbf{A}}{\partial t} - q\frac{\partial\phi}{\partial\mathbf{r}} = q\frac{\partial}{\partial\mathbf{r}}(\mathbf{v}\cdot\mathbf{A}) - q\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{A}(\mathbf{r}(t),t) - q\frac{\partial\phi}{\partial\mathbf{r}}$$

and thus

$$\frac{\mathrm{d}}{dt}(m\mathbf{v}+q\mathbf{A}) = \frac{\partial}{\partial\mathbf{r}}(q\mathbf{v}\cdot\mathbf{A}-q\phi)$$

Now the left-hand side can be interpreted as $\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial\mathcal{L}}{\partial\mathbf{v}}$ and the right-hand side as $\frac{\partial\mathcal{L}}{\partial\mathbf{r}}$ in the spirit of the Lagrange equations (6) if we define the *Lagrange function of a free particle in the electromagnetic field*

$$\mathcal{L}(\mathbf{r},\mathbf{v},t) = \frac{m\mathbf{v}^2}{2} + q\mathbf{v}\cdot\mathbf{A}(\mathbf{r},t) - q\phi(\mathbf{r},t) \tag{11}$$

Then we obtain the generalized momentum, usually called *canonical momentum*

$$\mathbf{p} = \frac{\partial\mathcal{L}(\mathbf{r},\mathbf{v},t)}{\partial\mathbf{v}} = m\mathbf{v}+q\mathbf{A} \tag{12}$$

which differs from the conventional *kinetic momentum* $\mathbf{p}^{\mathrm{kinetic}} = m\mathbf{v}$ and the Hamilton function

$$\mathcal{H}(\mathbf{p},\mathbf{r},t) = \frac{1}{2m}\left[\mathbf{p}-q\mathbf{A}(\mathbf{r},t)\right]^2 + q\phi(\mathbf{r},t) \tag{13}$$

Similarly to the canonical and kinetic momentum, two different angular momenta exist, see, e.g. pages 404,405 of [2]

$$\mathbf{L}^{\mathrm{kinetic}} = \mathbf{r}\times\mathbf{p}^{\mathrm{kinetic}} \quad \text{and} \quad \mathbf{L}^{\mathrm{canonical}} = \mathbf{r}\times\mathbf{p} = \mathbf{L}^{\mathrm{kinetic}} + q\mathbf{r}\times\mathbf{A} \tag{14}$$

Considering the force $\mathbf{F}$ on the particle we find the common relations

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{p}^{\mathrm{kinetic}} = \mathbf{F} \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{L}^{\mathrm{kinetic}} = \mathbf{r}\times\mathbf{F}$$

while an effective force $\mathbf{F}' = \mathbf{F} + q\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t}$ enters the corresponding equations for $\mathbf{p}^{\mathrm{canonical}}$ and $\mathbf{L}^{\mathrm{canonical}}$.

On the other hand, the Lagrange equations (6) show that $\frac{d}{\mathrm{d}t}p_i^{\mathrm{canonical}} = 0$, if the Lagrange function does not depend on r_i. Regarding the angular momentum we consider the Lagrange function (11) in cylindrical coordinates:

$$\mathcal{L}(\rho,\varphi,z,\dot\rho,\dot\varphi,\dot z,t) = \frac{m}{2}\left(\dot\rho^2+\rho^2\dot\varphi^2+\dot z^2\right) + q\left(\dot\rho A_r + \rho\dot\varphi A_\varphi + \dot z A_z\right) - q\phi(\rho,\varphi,z,t)$$

Here we can identify

$$\begin{aligned}\frac{\partial\mathcal{L}(\rho,\varphi,z,\dot\rho,\dot\varphi,\dot z,t)}{\partial\dot\varphi} =& m\rho^2\dot\varphi + \rho q A_\varphi \\ =& \mathbf{e}_z\cdot\left[(\rho\mathbf{e}_\rho + z\mathbf{e}_z)\times(m\dot\rho\mathbf{e}_\rho + m\rho\dot\varphi\mathbf{e}_\varphi + \dot z\mathbf{e}_z + qA_\rho\mathbf{e}_\rho + qA_\varphi\mathbf{e}_\varphi + qA_z\mathbf{e}_z)\right] \\ =& L_z^{\mathrm{canonical}}\end{aligned}$$

Thus the Lagrange equations (6) provide $\frac{d}{\mathrm{d}t}L_z^{\mathrm{canonical}} = 0$, if the potentials $\mathbf{A}$ and ϕ do not depend on φ.

The conservation of $\mathbf{p}^{\mathrm{canonical}}$ and $\mathbf{L}^{\mathrm{canonical}}$ is related to the symmetry of the system with respect to translations and rotations.

Thus $\mathbf{p}^{\mathrm{canonical}}$ and $\mathbf{L}^{\mathrm{canonical}}$ should be considered as the primary quantities even if their time derivatives do not agree with the physical force and torque, respectively.

4 Transition to quantum mechanics

Quantum mechanical equations can be obtained by replacing the canonical variables q_i, p_i with operators $\hat{q}_i, \hat{p}_i$, satisfying the commutation relations

$$[\hat{p}_i, \hat{q}_j] = \frac{\hbar}{\mathrm{i}}\delta_{i,j}\,, \quad [\hat{p}_i, \hat{p}_j] = 0\,, \quad \text{and} \quad [\hat{q}_i, \hat{q}_j] = 0 \tag{15}$$

and the Schrödinger equations $\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\Psi\rangle = \hat{H}|\Psi\rangle$ with the *Hamilton operator*

$$\hat{H} = \mathcal{H}(\hat{p}_1, \ldots \hat{p}_f, \hat{q}_1, \ldots \hat{q}_f, t) \tag{16}$$

obtained from the Hamilton function (7) of the classical system. If we represent the state $|\Psi\rangle$ by a wave function $\Psi(q_1, \ldots q_f, t)$, the operators $\hat{p}_i$ become the partial derivatives $\frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial q_i}$. In this way the Hamilton operator (2) is obtained from the classical expression (13).

References

[1] J. D. Jackson, *Classical Electrodynamics*, 3 ed. (John Wiley & Sons, New York, 1998).

[2] H. Goldstein, C. P. Poole, and J. L. Safko, *Classical Mechanics* (Addison Wesley, San Francisco, 2001).