Quantum Mechanical Hamiltonian for a Charged Particle in an Electromagnetic Field

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Equations from Electromagnetics

Consider a particle of charge q and mass m in an external electromagnetic field and a static potential well $V(\vec{r})$ of some sort (could be from electrostatic sources). By external electromagnetic field we mean that we are not considering the electromagnetic fields produced by the charged particle under consideration. The fields are in general the function of spatial coordinates $\vec{r}$ and time t. According to the Lorentz force equation, the rate of change in momentum $\vec{p}$ is given as follows.

$$\frac{d\vec{p}}{dt} = q\left(\vec{E} + \vec{v} \times \vec{B}\right) - \nabla V. \qquad (1)$$

Here $\vec{v} = \frac{d}{dt}\vec{r}$. In non-relativistic approximation,

$$\vec{p} = m\vec{v}. \qquad (2)$$

The electromagnetic fields are given in terms of scalar and vector potentials,

$$\vec{E} = -\nabla\phi - \frac{\partial}{\partial t}\vec{A}, \qquad (3a)$$

$$\vec{B} = \nabla \times \vec{A}. \qquad (3b)$$

Note the gauge invariance:

$$\vec{A} \rightarrow \vec{A} - \nabla\Lambda, \qquad (4a)$$

$$\phi \rightarrow \phi + \frac{\partial}{\partial t}\Lambda. \qquad (4b)$$

Note that, explicitly stating, $\vec{E}$ is $\vec{E}\left(\vec{r}, t\right)$, $\vec{B}$ is $\vec{B}\left(\vec{r}, t\right)$, $\vec{A}$ is $\vec{A}\left(\vec{r}, t\right)$, ϕ is $\phi\left(\vec{r}, t\right)$, and Λ is $\Lambda\left(\vec{r}, t\right)$. Only the static potential V is $V\left(\vec{r}\right)$.

Also note that $\nabla.\vec{E} = 0$ implies that

$$\nabla^2\phi = -\frac{\partial}{\partial t}\left(\nabla.\vec{A}\right). \qquad (5)$$

Lagrangian

Let us show that the following lagrangian yields the correct equation of motion given in Eq. (1).

$$\mathcal{L}(\vec{r}, \vec{v}, t) = \frac{1}{2}mv^2 + q\left(\vec{v}.\vec{A} - \phi\right) - V + \frac{d}{dt}\Omega. \qquad (6a)$$

$$\mathcal{L}(\vec{r}, \vec{v}, t) = \frac{1}{2}mv^2 + q\left(\vec{v}.\vec{A} - \phi\right) - V + \frac{\partial}{\partial t}\Omega + \vec{v}.\nabla\Omega. \qquad (6b)$$

Here we have included an arbitrary function $\Omega\left(\vec{r}, t\right)$. Consider the generalized momentum.

$$\vec{P} \equiv \frac{\partial}{\partial \vec{v}}\mathcal{L}(\vec{r}, \vec{v}, t) = m\vec{v} + q\vec{A} + \nabla\Omega. \quad (7)$$

From the principle of least action, the lagrangian satisfies the Euler-Lagrange equation:

$$\frac{d}{dt}\left(\vec{P}\right) - \frac{\partial}{\partial \vec{r}}\mathcal{L}(\vec{r}, \vec{v}, t) = 0. \qquad (8)$$

If Eq. (8) yields (1) then the Lagrangian given in Eq. (6) is right. Let's see that. We use Einstein's notation of repeating coordinates where $i = 1, 2, 3$ correspond to the three spatial cartesian coordinates.

$$\frac{d}{dt}\left(P_i\right) = \frac{d}{dt}\left(mv_i + qA_i + \partial_i\Omega\right).$$

$$\frac{\partial}{\partial r_i}\mathcal{L}(\vec{r}, \vec{v}, t) \equiv \partial_i\mathcal{L}(\vec{r}, \vec{v}, t) = qv_j\partial_iA_j - q\partial_i\phi - \partial_iV + \partial_i\left(\frac{d}{dt}\Omega\right).$$

Substituting the last two in Eq. (8)

$$\frac{d}{dt}\left(mv_i + qA_i + \partial_i\Omega\right) - qv_j\partial_iA_j + q\partial_i\phi + \partial_iV - \partial_i\left(\frac{d}{dt}\Omega\right) = 0.$$

$$\frac{d}{dt}\left(mv_i\right) + q\frac{\partial}{\partial t}A_i + qv_j\partial_jA_i + \frac{d}{dt}\left(\partial_i\Omega\right) - qv_j\partial_iA_j + q\partial_i\phi + \partial_iV - \partial_i\left(\frac{d}{dt}\Omega\right) = 0.$$

$$\frac{d}{dt}\left(mv_i\right) + q\frac{\partial}{\partial t}A_i + q\partial_i\phi + qv_j\left(\partial_jA_i - \partial_iA_j\right) + \partial_iV = 0.$$

$$\frac{d}{dt}\left(mv_i\right) - qE_i + qv_j\left(\partial_jA_i - \partial_iA_j\right) + \partial_iV = 0.$$

Now, instead of using the difficult to track symbol ϵ_{ijk}, consider $i = 1$.

$$\frac{d}{dt}\left(mv_1\right) - qE_1 + qv_1\left(\partial_1A_1 - \partial_1A_1\right) + qv_2\left(\partial_2A_1 - \partial_1A_2\right) + qv_3\left(\partial_3A_1 - \partial_1A_3\right) + \partial_1V = 0.$$

$$\frac{d}{dt}\left(mv_1\right) - qE_1 - qv_2B_3 + qv_3B_2 + \partial_1V = 0.$$

$$\frac{d}{dt}\left(mv_1\right) - qE_1 - q\left(\vec{v} \times \vec{B}\right)_1 + \partial_1V = 0.$$

Generalizing again,

$$\frac{d}{dt}\left(m\vec{v}\right) - q\vec{E} - q\left(\vec{v} \times \vec{B}\right) + \nabla V = 0.$$

Thus Eq. (1) is the Euler-Lagrange equation corresponding to the Lagrangian in Eq. (5). Note that we are free to choose $\Omega\left(\vec{r}, t\right)$ just like we are free to choose $\Lambda\left(\vec{r}, t\right)$.

Hamiltonian

Let us obtain the Hamiltonian by Legendre Transformation.

$$\mathcal{H}(\vec{r},\vec{P},t) = \vec{v}.\vec{P} - \mathcal{L}, \qquad (9)$$

$$\mathcal{H}(\vec{r},\vec{P},t) = mv^2 + q\vec{v}.\vec{A} + \vec{v}.\nabla\Omega - \frac{1}{2}mv^2 - q\left(\vec{v}.\vec{A} - \phi\right) + V - \frac{\partial}{\partial t}\Omega - \vec{v}.\nabla\Omega,$$

$$\mathcal{H}(\vec{r},\vec{P}) = \frac{1}{2}m\left(\vec{v}\right)^2 + q\phi + V - \frac{\partial}{\partial t}\Omega.$$

Substituting $\vec{v}$ from Eq. (7).

$$\mathcal{H}(\vec{r},\vec{P},t) = \frac{1}{2m}\left(\vec{P} - q\vec{A} - \nabla\Omega\right)^2 + V + q\phi - \frac{\partial}{\partial t}\Omega. \qquad (10)$$

Let us confirm Hamilton's equations of motion explicitly (just to check our math so far).

$$\frac{\partial}{\partial\vec{P}}\mathcal{H}(\vec{r},\vec{P},t) = \frac{1}{m}\left(\vec{P} - q\vec{A} - \nabla\Omega\right) = \vec{v},$$

$$\frac{d}{dt}\vec{r} = \frac{\partial}{\partial\vec{P}}\mathcal{H}(\vec{r},\vec{P},t). \qquad (11a)$$

$$\partial_i\mathcal{H}(\vec{r},\vec{P},t) = \frac{1}{m}\left(\vec{P} - q\vec{A} - \nabla\Omega\right).\partial_i\left(\vec{P} - q\vec{A} - \nabla\Omega\right) + q\partial_i\phi + \partial_i V - \partial_i\frac{\partial}{\partial t}\Omega,$$

$$\partial_i\mathcal{H}(\vec{r},\vec{P},t) = \vec{v}.\partial_i\left(-q\vec{A} - \nabla\Omega\right) + q\partial_i\phi + \partial_i V - \partial_i\frac{\partial}{\partial t}\Omega,$$

$$\partial_i\mathcal{H}(\vec{r},\vec{P},t) =- qv_j\partial_i A_j - v_j\partial_i\left(\partial_j\Omega\right) + q\partial_i\phi + \partial_i V - \partial_i\frac{\partial}{\partial t}\Omega,$$

$$\partial_i\mathcal{H}(\vec{r},\vec{P},t) = - qv_j\partial_i A_j + q\partial_i\phi + \partial_i V - v_j\partial_j\left(\partial_i\Omega\right) - \frac{\partial}{\partial t}\left(\partial_i\Omega\right),$$

$$\partial_i\mathcal{H}(\vec{r},\vec{P},t) =- qv_j\partial_i A_j + q\partial_i\phi + \partial_i V - \frac{d}{dt}\left(\partial_i\Omega\right),$$

$$\partial_i\mathcal{H}(\vec{r},\vec{P},t) =- qv_j\partial_i A_j + q\partial_i\phi + \partial_i V - \partial_i\frac{d}{dt}(\Omega)$$

$$\partial_i\mathcal{H}(\vec{r},\vec{P},t) =- \partial_i\mathcal{L}(\vec{r},\vec{v},t) =- \frac{dP_i}{dt}$$

$$\frac{d}{dt}\vec{P} =- \frac{\partial}{\partial\vec{r}}\mathcal{H}(\vec{r},\vec{P},t). \qquad (11b)$$

Length Gauge Formulation ($\vec{E}.\vec{d}$ Interaction)

Here, we do two things:

1. Choose $\Omega =- \vec{d}.\vec{A}$, where $\vec{d} = q\vec{r}$ is called the dipole term.
2. Assume ϕ and $\vec{A}$ are fairly constant over the spatial range of interest. Hence spatial derivatives of ϕ and $\vec{A}$ vanish.

Thus,

$$\partial_i\Omega =- q\partial_i r_j A_j \approx- qA_j\partial_i r_j =- qA_j\delta_{ij} =- qA_i,$$

$$\nabla\Omega \approx- q\vec{A}. \qquad (12)$$

$$\vec{E} =- \nabla\phi - \frac{\partial}{\partial t}\vec{A} \approx- \frac{\partial}{\partial t}\vec{A}. \qquad (13)$$

$$\frac{\partial}{\partial t}\Omega = -q\vec{r}.\frac{\partial}{\partial t}\vec{A} = q\vec{r}.\vec{E} = \vec{E}.\vec{d}. \qquad (14)$$

Also, from Eq. (5)

$$\nabla^2\phi = 0 \Rightarrow \phi = 0. \qquad (15)$$

Substituting Eq. (12, 14, 15) in Eq. (10).

$$\mathcal{H}(\vec{r},\vec{P},t) = \frac{1}{2m}P^2 + V(\vec{r}) - \vec{E}(t).\vec{d}. \qquad (16)$$

Now we promote the position, conjugate momentum, and hamiltonian to quantum mechanical operators. In position basis.

$$\vec{r} \rightarrow \hat{r}$$

$$\vec{P} \rightarrow -i\hbar\nabla$$

$$V(\vec{r}) \rightarrow V(\hat{r})$$

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\nabla^2 + V(\hat{r}) - q\hat{E}(t).\hat{r}. \qquad (17)$$

Thus, in this so called length gauge formulation, hamiltonian consists of following two terms:

- Time independent hamiltonian: $\hat{\mathcal{H}}_0 = -\frac{\hbar^2}{2m}\nabla^2 + V(\hat{r})$.
- Time dependent hamiltonian: $\hat{\mathcal{H}}_{int}(t) = -\hat{E}(t).\hat{d}$.

The interaction hamiltonian represented as $\hat{E}(t).\hat{d}$ is also called direct coupling term.

Velocity Gauge Formulation ($\vec{A}.\vec{p}$ Interaction)

In this case we do the following:

1. We use gauge freedom to choose
   $$\nabla.\vec{A} = 0. \ (18)$$
   Note that this is different from assuming that all spatial derivatives vanish. We are exploiting gauge freedom here and not making any assumption, at least so far. From (5), Eq. (15) still holds.
2. We choose Ω to be zero.
   $$\Omega = 0. \ (19)$$
3. We neglect the term of order A^2 assuming weak interaction.

In this case, using Eq. (15) and (19) in Eq. (10), we get.

$$\mathcal{H}(\vec{r},\vec{P},t) = \frac{1}{2m}\left(\vec{P} - q\vec{A}(\vec{r},t)\right)^2 + V(\vec{r}). \qquad (20)$$

Promoting to quantum mechanical operators in the position basis.

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(-i\hbar\nabla - q\hat{A}(\hat{r},t)\right)^2 + V(\hat{r}).$$

$$\hat{\mathcal{H}} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{i\hbar q}{2m}\left(\nabla.\hat{A}(\hat{r},t) + \hat{A}(\hat{r},t).\nabla\right) + \frac{q^2}{2m}\hat{A}^2(\hat{r},t) + V(\hat{r}). \qquad (21)$$

Consider the following operator. Imagining it acting on a wavefunction in position basis might help.

$$\nabla.\hat{A}\left(\hat{r},t\right) = \nabla.\vec{A}\left(\hat{r},t\right) + \hat{A}\left(\hat{r},t\right).\nabla = \hat{A}\left(\hat{r},t\right).\nabla. \qquad (22)$$

Substituting Eq. (22) in (21),

$$\hat{\mathcal{H}} =- \frac{\hbar^2}{2m}\nabla^2 + \frac{i\hbar q}{m}\vec{A}\left(\hat{r},t\right).\nabla + \frac{q^2}{2m}\hat{A}^2\left(\hat{r},t\right) + V\left(\hat{r}\right). \qquad (23)$$

Finally, neglecting the term of order A^2 in Eq. (23), we get,

$$\hat{\mathcal{H}} =- \frac{\hbar^2}{2m}\nabla^2 + V\left(\hat{r}\right) + \frac{i\hbar q}{m}\hat{A}\left(\hat{r},t\right).\nabla. \qquad (24a)$$

$$\hat{\mathcal{H}} =- \frac{\hbar^2}{2m}\nabla^2 + V\left(\hat{r}\right) - \frac{q}{m}\hat{A}\left(\hat{r},t\right).\hat{P}. \qquad (24n)$$

Thus, in this velocity gauge formulation the hamiltonian consists of the following time dependent term besides the time independent hamiltonian: $\hat{\mathcal{H}}_0 =- \frac{\hbar^2}{2m}\nabla^2 + V\left(\hat{r}\right)$.

- Time dependent hamiltonian: $\hat{\mathcal{H}}_{int}(t) =- \frac{q}{m}\hat{A}\left(\hat{r},t\right).\hat{P}$.

The interaction hamiltonian represented as $\hat{A}.\hat{P}$ is also called minimal coupling term.

The following paper discusses the equivalence of the length gauge and velocity gauge formulations:

K. Rzazewski and R. W. Boyd, "Equivalence of interaction Hamiltonians in the electric dipole approximation," Journal of Modern Optics, vol. 51, no. 8, 1137–1147, May 2004