

Molecular quantum dynamics: Exercise series 11

Problem 1: Canonical momentum and Hamiltonian of a particle in an electromagnetic field

As I mentioned in the lecture, the Hamiltonian for a particle of mass m and charge e in an electromagnetic field is

$$H(\mathbf{x}, \mathbf{p}) = \frac{1}{2m} (\mathbf{p} - e\mathbf{A}(\mathbf{x}, t))^2 + e\varphi(\mathbf{x}, t), \quad (1)$$

where \mathbf{A} is the vector potential and φ is the scalar potential, from which the electric and magnetic fields are obtained as

$$\begin{aligned} \mathbf{B} &= \nabla \times \mathbf{A}, \\ \mathbf{E} &= -\nabla\varphi - \frac{\partial \mathbf{A}}{\partial t}. \end{aligned}$$

You can assume that \mathbf{x} are 3-dimensional Cartesian coordinates, so ∇ is the gradient in Cartesian coordinates. The main goal of this exercise is to derive this Hamiltonian from the Lagrangian that I derived in the lecture from symmetry of space-time.

Starting from the Lagrangian

$$L(\mathbf{x}, \mathbf{v}) = \frac{1}{2}mv^2 + e\mathbf{v} \cdot \mathbf{A}(\mathbf{x}, t) - e\varphi(\mathbf{x}, t), \quad (2)$$

use the Hamiltonian formalism in order to:

- Derive an expression for the canonical momentum \mathbf{p} .
- Derive the Hamiltonian (1).
- Derive Hamilton's equation of motion for $\dot{\mathbf{x}}$.
- Derive Hamilton's equation of motion for $\dot{\mathbf{p}}$. It can be simplified a little, but not too much. Instead, show that it is equivalent to Newton's equation using the Lorentz force:

$$m \frac{d^2}{dt^2} \mathbf{x} = e(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

Hint: You may use various identities of vector calculus (see the Wikipedia article “Vector calculus identities”). Alternatively, write the vectors in components. This problem is classical, so you do not need to think of \mathbf{x} and \mathbf{p} as operators. However, the resulting Hamiltonian (1) can be used as a quantum-mechanical operator.