ELECTRODYNAMICS IN QUANTUM MECHANICS: GAUGE TRANSFORMATIONS

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.61.

A *gauge transformation* in classical electrodynamics is possible if we replace the scalar potential φ and the vector potential $\mathbf{A}$ by

$$\varphi' = \varphi - \frac{\partial\Lambda}{\partial t} \tag{1}$$

$$\mathbf{A}' = \mathbf{A} + \nabla\Lambda \tag{2}$$

where Λ is any function of position and time. These transformations (provided both are made at the same time) leave the fields $\mathbf{E}$ and $\mathbf{B}$ unchanged, as we can see by direct substitution.

Using the modified potentials we get

$$\mathbf{E} = -\nabla\varphi' - \frac{\partial\mathbf{A}'}{\partial t} \tag{3}$$

$$= -\nabla\varphi + \frac{\partial\nabla\Lambda}{\partial t} - \frac{\partial(\mathbf{A}+\nabla\Lambda)}{\partial t} \tag{4}$$

$$= -\nabla\varphi - \frac{\partial\mathbf{A}}{\partial t} \tag{5}$$

$$\mathbf{B} = \nabla\times\mathbf{A}' \tag{6}$$

$$= \nabla\times\mathbf{A} + \nabla\times\nabla\Lambda \tag{7}$$

$$= \nabla\times\mathbf{A} \tag{8}$$

where in the last line we used $\nabla\times\nabla\Lambda = 0$ for any function Λ. Test stuff.

In quantum mechanics, we would like to know if a gauge transformation leaves solutions of the Schrödinger equation unchanged. If so, then quantum theory is gauge invariant with respect to electrodynamics. In fact, it turns out that under a gauge transformation, the wave function for a particle of charge q changes from Ψ to

$$\Psi' = e^{iq\Lambda/\hbar}\Psi \tag{9}$$

To prove this, we can start with the Schrödinger equation from the post on the electromagnetic force law and use the same notation for derivatives and vector components as in the last part of that post (we will indicate a vector component by a subscript x,y or z and a derivative by a superscript. Thus $A_y^{xz}=\partial^2 A_y/dxdz$ and so on) we wish to show that if Ψ satisfies the equation

$$i\hbar\frac{\partial\Psi}{\partial t}=\frac{1}{2m}\left(-\hbar^2\nabla^2\Psi+\frac{\hbar q}{-i}(2\mathbf{A}\cdot\nabla\Psi+\Psi\nabla\cdot\mathbf{A})+q^2|\mathbf{A}|^2\Psi\right)+q\varphi\Psi \tag{10}$$

then replacing Ψ by $\Psi'=e^{iq\Lambda/\hbar}\Psi$ satisifes the same equation with the gauge transformed potentials. That is:

$$i\hbar\frac{\partial\Psi'}{\partial t}=\frac{1}{2m}\left(-\hbar^2\nabla^2\Psi'+i\hbar q(2\mathbf{A}'\cdot\nabla\Psi'+\Psi'\nabla\cdot\mathbf{A}')+q^2|\mathbf{A}'|^2\Psi'\right)+q\varphi'\Psi' \tag{11}$$

The left hand side is

$$i\hbar\frac{\partial\Psi'}{\partial t}=i\hbar\frac{\partial}{\partial t}(e^{iq\Lambda/\hbar}\Psi)=i\hbar\Psi^t e^{iq\Lambda/\hbar}-q\Lambda^t\Psi e^{iq\Lambda/\hbar} \tag{12}$$

To work out the right hand side, we note that each term inside the largest set of parentheses has the form of a sum of three terms, with the first of these three terms consisting of factors involving the x components of a vector or x derivatives of functions, the second term involving y and the third involving z. All three of these terms have the same form, so we will consider the x component in detail. We will first calculate the two derivatives of Ψ'

$$\Psi'=e^{iq\Lambda/\hbar}\Psi \tag{13}$$

$$(\Psi')^x=\left(\frac{iq}{\hbar}\Lambda^x\Psi+\Psi^x\right)e^{iq\Lambda/\hbar} \tag{14}$$

$$(\Psi')^{xx}=\left(\frac{iq}{\hbar}\Lambda^{xx}\Psi+\frac{iq}{\hbar}\Lambda^x\Psi^x+\Psi^{xx}\right)e^{iq\Lambda/\hbar}+\left(\frac{iq}{\hbar}\Lambda^x\Psi+\Psi^x\right)\frac{iq}{\hbar}\Lambda^x e^{iq\Lambda/\hbar} \tag{15}$$

Since every term in 11 is linear in either Ψ' or one of its derivatives, there will be a common factor of $e^{iq\Lambda/\hbar}$ which we can cancel off, so we will omit this term from now on to simplify the calculation. Now we consider each term in the large parentheses in 11 in turn.

$$-\hbar^2\nabla^2\Psi' = -iq\hbar\Lambda^{xx}\Psi - 2iq\hbar\Lambda^x\Psi^x + q^2(\Lambda^x)^2\Psi + \text{terms in } y \text{and } z \tag{16}$$

$$2i\hbar q\mathbf{A}'\cdot\nabla\Psi' = 2i\hbar q(A_x+\Lambda^x)(iq\Lambda^x\Psi/\hbar+\Psi^x) + \text{terms in } y \text{and } z \tag{17}$$

$$= -2q^2A_x\Lambda^x\Psi + 2i\hbar qA_x\Psi^x - 2q^2(\Lambda^x)^2\Psi + 2i\hbar q\Lambda^x\Psi^x + \text{terms in } y \text{and } z \tag{18}$$

$$i\hbar q\Psi'\nabla\cdot\mathbf{A}' = i\hbar q\Lambda^{xx}\Psi + i\hbar qA_x^x\Psi + \text{terms in } y \text{and } z \tag{19}$$

$$q^2|\mathbf{A}'|^2\Psi' = q^2\Psi A_x^2 + 2q^2\Psi A_x\Lambda^x + q^2\Psi(\Lambda^x)^2 + \text{terms in } y \text{and } z \tag{20}$$

Adding up all these terms, we find that all terms involving Λ and its derivatives cancel out, and we are left with

$$-\hbar^2\Psi^{xx} + 2i\hbar qA_x\Psi^x + i\hbar qA_x^x\Psi + q^2\Psi A_x^2 + \text{terms in } y \text{and } z \tag{21}$$

which is just the terms from the original equation before the gauge transformation.

Finally, we note that the last term in 11 is

$$q\varphi'\Psi' = q\varphi\Psi e^{iq\Lambda/\hbar} - q\Lambda^t\Psi e^{iq\Lambda/\hbar} \tag{22}$$

and the last term cancels the last term in 12, so all references to Λ cancel out of 11 and the original Schrodinger equation is recovered.