G. VECTOR AND SCALAR POTENTIALS

Maxwell equations

The electromagnetic field is described by two vector fields: the electric field intensity $\boldsymbol{\mathcal{E}}$ and the magnetic field intensity $\boldsymbol{H}$, both depending on position in space (Cartesian coordinates x, y, z) and time t. The vectors $\boldsymbol{\mathcal{E}}$ and $\boldsymbol{H}$ are determined by the electric charges and their currents. The charges are defined by the *charge density* function $\rho(x, y, z, t)$ such that $\rho(x, y, z, t)\,\mathrm{d}V$ at time t represents the charge in the infinitesimal volume $\mathrm{d}V$ that contains the point (x, y, z). The velocity of the charge in position x, y, z measured at time t represents the vector field $\boldsymbol{v}(x, y, z, t)$, while the *current* at point x, y, z measured at t is equal to $\boldsymbol{i}(x, y, z, t) = \rho(x, y, z, t)\boldsymbol{v}(x, y, z, t)$.

charge density

current

It turns out (as shown by James Maxwell), that $\boldsymbol{H}$, $\boldsymbol{\mathcal{E}}$, ρ and $\boldsymbol{i}$ are interrelated by the Maxwell equations (c stands for the speed of light)

$$\nabla \times \boldsymbol{\mathcal{E}} + \frac{1}{c}\frac{\partial \boldsymbol{H}}{\partial t} = \boldsymbol{0}, \tag{G.1}$$

$$\nabla \times \boldsymbol{H} - \frac{1}{c}\frac{\partial \boldsymbol{\mathcal{E}}}{\partial t} = \frac{4\pi}{c}\boldsymbol{i}, \tag{G.2}$$

$$\nabla \cdot \boldsymbol{\mathcal{E}} = 4\pi\rho, \tag{G.3}$$

$$\nabla \cdot \boldsymbol{H} = 0. \tag{G.4}$$

The Maxwell equations have an alternative notation, which involves two new quantities: the *scalar potential* ϕ and the *vector potential* $\boldsymbol{A}$ that replace $\boldsymbol{\mathcal{E}}$ and $\boldsymbol{H}$:

$$\boldsymbol{\mathcal{E}} = -\nabla\phi - \frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t}, \tag{G.5}$$

$$\boldsymbol{H} = \nabla \times \boldsymbol{A}. \tag{G.6}$$

After inserting $\boldsymbol{\mathcal{E}}$ from eq. (G.5) into eq. (G.1), we obtain its automatic satisfaction:

$$\begin{aligned}\nabla \times \boldsymbol{\mathcal{E}} + \frac{1}{c}\frac{\partial \boldsymbol{H}}{\partial t} &= \nabla \times \left(-\nabla\phi - \frac{1}{c}\frac{\partial \boldsymbol{A}}{\partial t}\right) + \frac{1}{c}\frac{\partial \boldsymbol{H}}{\partial t} \\ &= -\nabla \times \nabla\phi - \frac{1}{c}\frac{\partial \nabla \times \boldsymbol{A}}{\partial t} + \frac{1}{c}\frac{\partial \boldsymbol{H}}{\partial t} = \boldsymbol{0},\end{aligned}$$

because

$$\nabla \times \nabla\phi = \left[\frac{\partial}{\partial y}\left(\frac{\partial\phi}{\partial z}\right) - \frac{\partial}{\partial z}\left(\frac{\partial\phi}{\partial y}\right), \frac{\partial}{\partial z}\left(\frac{\partial\phi}{\partial x}\right) - \frac{\partial}{\partial x}\left(\frac{\partial\phi}{\partial z}\right), \frac{\partial}{\partial x}\left(\frac{\partial\phi}{\partial y}\right) - \frac{\partial}{\partial y}\left(\frac{\partial\phi}{\partial x}\right)\right]$$
$$= [0, 0, 0] = \mathbf{0} \tag{G.7}$$

and $\nabla \times \boldsymbol{A} = \boldsymbol{H}$.

Eq. (G.4) gives also automatically

$$\nabla \cdot (\nabla \times \boldsymbol{A}) = \frac{\partial}{\partial x}\left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z}\right) + \frac{\partial}{\partial y}\left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}\right) + \frac{\partial}{\partial z}\left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y}\right) = 0.$$

Eqs. (G.2) and (G.3) transform into

$$\nabla \times (\nabla \times \boldsymbol{A}) + \frac{1}{c}\frac{\partial \nabla\phi}{\partial t} + \frac{1}{c^2}\frac{\partial^2 \boldsymbol{A}}{\partial t^2} = \frac{4\pi}{c}\boldsymbol{i},$$
$$-\nabla \cdot (\nabla\phi) - \frac{1}{c}\frac{\partial \nabla \cdot \boldsymbol{A}}{\partial t} = 4\pi\rho,$$

which in view of the identity $\nabla \times (\nabla \times \boldsymbol{A}) = \nabla(\nabla \cdot \boldsymbol{A}) - \Delta\boldsymbol{A}$ and $\nabla \cdot (\nabla\phi) = \Delta\phi$, gives two additional Maxwell equations (besides eqs. (G.5) and (G.6))

$$\boxed{\begin{aligned} \nabla\left(\nabla \cdot \boldsymbol{A} + \frac{1}{c}\frac{\partial\phi}{\partial t}\right) - \Delta\boldsymbol{A} + \frac{1}{c^2}\frac{\partial^2 \boldsymbol{A}}{\partial t^2} &= \frac{4\pi}{c}\boldsymbol{i}, &\text{(G.8)}\\ \Delta\phi + \frac{1}{c}\nabla \cdot \frac{\partial \boldsymbol{A}}{\partial t} &= -4\pi\rho. &\text{(G.9)} \end{aligned}}$$

To characterize the electromagnetic field we may use either $\boldsymbol{\mathcal{E}}$ and $\boldsymbol{H}$ or the two potentials, ϕ and $\boldsymbol{A}$.

Arbitrariness of the potentials ϕ and A

Potentials ϕ and $\boldsymbol{A}$ *are not defined uniquely, i.e. many different potentials lead to the same intensities of electric and magnetic fields*. If we made the following modifications in ϕ and $\boldsymbol{A}$:

$$\phi' = \phi - \frac{1}{c}\frac{\partial f}{\partial t}, \tag{G.10}$$
$$\boldsymbol{A}' = \boldsymbol{A} + \nabla f, \tag{G.11}$$

where f is an *arbitrary differentiable function* (of x, y, z, t), then ϕ' and $\boldsymbol{A}'$ lead to *the same* (see the footnote) $\boldsymbol{\mathcal{E}}$ and $\boldsymbol{H}$:

$$\boldsymbol{\mathcal{E}}' = -\nabla\phi' - \frac{1}{c}\frac{\partial \boldsymbol{A}'}{\partial t} = \left(-\nabla\phi + \frac{1}{c}\nabla\frac{\partial f}{\partial t}\right) - \frac{1}{c}\left(\frac{\partial \boldsymbol{A}}{\partial t} + \frac{\partial}{\partial t}(\nabla f)\right) = \boldsymbol{\mathcal{E}},$$
$$\boldsymbol{H}' = \nabla \times \boldsymbol{A}' = \nabla \times \boldsymbol{A} + \nabla \times \nabla f = \boldsymbol{H}.$$

Choice of potentials A and ϕ for a homogeneous magnetic field

From the second Maxwell equation (G.6), we see that, if the magnetic field $\boldsymbol{H}$ is time-independent, we get the time-independent $\boldsymbol{A}$. Profiting from the non-uniqueness of $\boldsymbol{A}$, we choose it in such a way as to satisfy (what is called the *Coulombic gauge*)[1]

Coulombic gauge

$$\nabla \cdot \boldsymbol{A} = 0, \tag{G.12}$$

which diminishes the arbitrariness, but does not remove it.

Let us take the example of an atom in a homogeneous magnetic field $\boldsymbol{H}$. Let us locate the origin of the coordinate system on the nucleus, the choice being quite natural for an atom, and let us construct the vector potential at position $\boldsymbol{r} = (x, y, z)$ as

$$\boldsymbol{A}(\boldsymbol{r}) = \frac{1}{2}[\boldsymbol{H} \times \boldsymbol{r}]. \tag{G.13}$$

As has been shown above, this is not a unique choice, there are an infinite number of them. All the choices are equivalent from the mathematical and physical point of view, they differ however by a peanut, the economy of computations. It appears that this choice of $\boldsymbol{A}$ is at least a logical one. The choice is also consistent with the Coulombic gauge (eq. (G.12)), because

$$\begin{aligned}
\nabla \cdot \boldsymbol{A} &= \frac{1}{2}\nabla \cdot [\boldsymbol{H} \times \boldsymbol{r}] = \frac{1}{2}\nabla \cdot [\boldsymbol{H} \times \boldsymbol{r}] \\
&= \frac{1}{2}\nabla \cdot [H_y z - yH_z, H_z x - zH_x, H_x y - xH_y] \\
&= \frac{1}{2}\left[\frac{\partial}{\partial x}(H_y z - yH_z) + \frac{\partial}{\partial y}(H_z x - zH_x) + \frac{\partial}{\partial z}(H_x y - xH_y)\right] = 0,
\end{aligned}$$

and also with the Maxwell equations (p. 962), because

$$\begin{aligned}
&\nabla \times \boldsymbol{A} \\
&= \frac{1}{2}\nabla \times [\boldsymbol{H} \times \boldsymbol{r}] = \frac{1}{2}\nabla \cdot [\boldsymbol{H} \times \boldsymbol{r}] \\
&= \frac{1}{2}\nabla \times [H_y z - yH_z, H_z x - zH_x, H_x y - xH_y] \\
&= \frac{1}{2}\left[\begin{array}{c} \frac{\partial}{\partial y}(H_x y - xH_y) - \frac{\partial}{\partial z}(H_z x - zH_x), \frac{\partial}{\partial z}(H_y z - yH_z) - \frac{\partial}{\partial x}(H_x y - xH_y), \\ \frac{\partial}{\partial x}(H_z x - zH_x) - \frac{\partial}{\partial y}(H_y z - yH_z) \end{array}\right] \\
&= \boldsymbol{H}.
\end{aligned}$$

Thus, this is the correct choice.

[1]The Coulombic gauge, even if only one of the possibilities, is almost exclusively used in molecular physics. The word "*gauge*" comes from the railway terminology referring to the different distances between the rails.

Practical importance of this choice

An example of possible choices of $\boldsymbol{A}$ is given in Fig. G.1.

If we shifted the vector potential origin far from the physical system under consideration (Fig. G.1.b), the values of $|\boldsymbol{A}|$ on all the particles of the system would be gigantic. $\boldsymbol{A}$ would be practically homogeneous *within* the atom or molecule. If we calculated $\nabla \times \boldsymbol{A} = \boldsymbol{H}$ on a particle of the system, then however horrifying it might look, we would obtain almost $\mathbf{0}$, because $\nabla \times \boldsymbol{A}$ means the differentiation of $\boldsymbol{A}$, and for a homogeneous field this yields zero. Thus we are going to study the system in a magnetic field, but the field disappeared! Very high accuracy would be needed to calculate $\nabla \times \boldsymbol{A}$ correctly as differences between two large numbers, which is always a risky business numerically due to the cancellation of accuracies. *It is therefore seen that the numerical results do depend critically on the choice of the origin of* $\boldsymbol{A}$ (arbitrary from the point of view of mathematics and physics). *It is always better to have the origin inside the system.*

Vector potential causes the wave function to change phase

The Schrödinger equation for a particle of mass m and charge q is

$$-\frac{\hbar^2}{2m}\Delta\Psi(\boldsymbol{r}) + V\Psi = E\Psi(\boldsymbol{r}),$$

where $V = q\phi$ with ϕ standing for the scalar electric potential.

The probability density of finding the particle at a given position depends on $|\Psi|$ rather than Ψ itself. This means that the wave function could be harmlessly multiplied by a phase factor $\Psi'(\boldsymbol{r}) = \Psi(\boldsymbol{r})\exp[-\frac{iq}{\hbar c}\chi(\boldsymbol{r})]$, where $\chi(\boldsymbol{r})$ could be any (smooth[2]) function of the particle's position $\boldsymbol{r}$. Then we have $|\Psi| = |\Psi'|$ at any $\boldsymbol{r}$. If $\Psi'(\boldsymbol{r})$ is as good as Ψ is, it would be nice if it kindly satisfied the Schrödinger equation like Ψ does, of course with the same eigenvalue

$$-\frac{\hbar^2}{2m}\Delta\Psi'(\boldsymbol{r}) + V\Psi'(\boldsymbol{r}) = E\Psi'(\boldsymbol{r}).$$

Let us see what profound consequences this has. The left-hand side of the last equation can be transformed as follows

$$\begin{aligned}
&-\frac{\hbar^2}{2m}\Delta\Psi'(\boldsymbol{r}) + V\Psi'(\boldsymbol{r}) \\
&= -\frac{\hbar^2}{2m}\left[\exp\left(-\frac{iq}{\hbar c}\chi\right)\Delta\Psi + \Psi\Delta\exp\left(-\frac{iq}{\hbar c}\chi\right) + 2(\nabla\Psi)\left(\nabla\exp\left(-\frac{iq}{\hbar c}\chi\right)\right)\right] \\
&\quad + V\exp\left(-\frac{iq}{\hbar c}\chi\right)\Psi \\
&= -\frac{\hbar^2}{2m}\left[\exp\left(-\frac{iq}{\hbar c}\chi\right)\Delta\Psi + \Psi\nabla\left[\left(-\frac{iq}{\hbar c}\right)\exp\left(-\frac{iq}{\hbar c}\chi\right)\nabla\chi\right]\right.
\end{aligned}$$

[2] See Fig. 2.5.

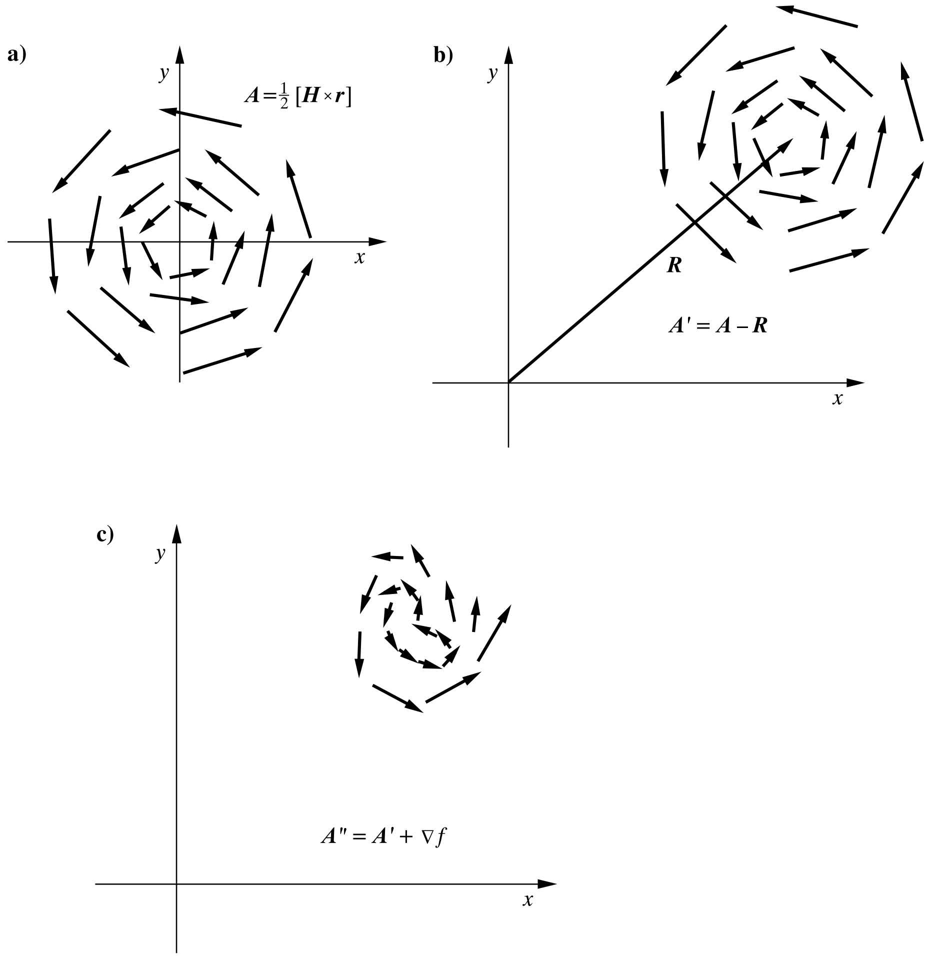

Fig. G.1. How do we understand the arbitrariness of the vector potential $\boldsymbol{A}$? Figs. (a), (b), (c) represent schematically three physically equivalent vector potentials $\boldsymbol{A}$. Fig. (a) shows a section in the plane $z = 0$ (axis z protrudes towards the reader from the xy plane) of the vector field $\boldsymbol{A} = \frac{1}{2}(\boldsymbol{H} \times \boldsymbol{r})$ with $\boldsymbol{H} = (0, 0, H)$ and $H > 0$. We see that vectors $\boldsymbol{A}$ become longer and longer, when we leave the origin (where $\boldsymbol{A} = \boldsymbol{0}$), they "rotate" counter-clockwise. Such $\boldsymbol{A}$ therefore determines $\boldsymbol{H}$ directed perpendicularly to the page and oriented towards the reader. By the way, note that any *shift* of the potential obtained should give the same magnetic field perpendicular to the drawing, Fig. (b). This is what we get (Fig. (b)) after adding, according to eq. (G.11), the gradient of function $f = ax + by + c$ to potential $\boldsymbol{A}$, because $\boldsymbol{A} + \nabla f = \boldsymbol{A} + (\boldsymbol{i}a + \boldsymbol{j}b) = \boldsymbol{A} - \boldsymbol{R} = \boldsymbol{A}'$, where $\boldsymbol{R} = -(\boldsymbol{i}a + \boldsymbol{j}b) = \text{const}$. The transformation is only one of the possibilities. If we took an arbitrary smooth function $f(x, y)$, e.g., with many maxima, minima and saddle points (as in the mountains), we would deform Fig. (b) by expanding or shrinking it like a pancake. In this way we might obtain the situation shown in Fig. (c). All these situations a,b,c are physically indistinguishable (on condition that the scalar potential ϕ is changed appropriately).

$$+2(\nabla\Psi)\left[\left(-\frac{iq}{\hbar c}\right)\exp\left(-\frac{iq}{\hbar c}\chi\right)\nabla\chi\right]\Bigg] + V\exp\left(-\frac{iq}{\hbar c}\chi\right)\Psi$$

$$= -\frac{\hbar^2}{2m}\left[\exp\left(-\frac{iq}{\hbar c}\chi\right)\Delta\Psi + \Psi\left(-\frac{iq}{\hbar c}\right)\left[\left(-\frac{iq}{\hbar c}\right)\exp\left(-\frac{iq}{\hbar c}\chi\right)(\nabla\chi)^2\right.\right.$$

$$\left.\left. + \exp\left(-\frac{iq}{\hbar c}\chi\right)\Delta\chi\right]\right] - \frac{\hbar^2}{2m}2(\nabla\Psi)\left[\left(-\frac{iq}{\hbar c}\right)\exp\left(-\frac{iq}{\hbar c}\chi\right)\nabla\chi\right]$$

$$+ V\exp\left(-\frac{iq}{\hbar c}\chi\right)\Psi.$$

Dividing the Schrödinger equation by $\exp(-\frac{iq}{\hbar c}\chi)$ we obtain

$$-\frac{\hbar^2}{2m}\left[\Delta\Psi + \Psi\left(-\frac{iq}{\hbar c}\right)\left[\left(-\frac{iq}{\hbar c}\right)(\nabla\chi)^2 + \Delta\chi\right] + 2(\nabla\Psi)\left[\left(-\frac{iq}{\hbar c}\right)\nabla\chi\right]\right] + V\Psi$$
$$= E\Psi(\boldsymbol{r}).$$

Let us define a vector field $\boldsymbol{A}(\boldsymbol{r})$ using function $\chi(\boldsymbol{r})$

$$\boldsymbol{A}(\boldsymbol{r}) = \nabla\chi(\boldsymbol{r}). \tag{G.14}$$

Hence, we have

$$-\frac{\hbar^2}{2m}\left[\Delta\Psi + \Psi\left(-\frac{iq}{\hbar c}\right)\left[\left(-\frac{iq}{\hbar c}\right)\boldsymbol{A}^2 + \nabla\boldsymbol{A}\right] + 2(\nabla\Psi)\left[\left(-\frac{iq}{\hbar c}\right)\boldsymbol{A}\right]\right] + V\Psi = E\Psi(\boldsymbol{r}),$$

and introducing the momentum operator $\hat{\boldsymbol{p}} = -i\hbar\nabla$ we obtain

$$\frac{1}{2m}\left[\hat{\boldsymbol{p}}^2\Psi + \Psi\left[\left(\frac{q}{c}\right)^2\boldsymbol{A}^2 - \left(\frac{q}{c}\right)\hat{\boldsymbol{p}A}\right] - 2(\hat{\boldsymbol{p}}\Psi)\left(\frac{q}{c}\right)\boldsymbol{A}\right] + V\Psi = E\Psi(\boldsymbol{r}),$$

or finally

$$\frac{1}{2m}\left(\hat{\boldsymbol{p}} - \frac{q}{c}\boldsymbol{A}\right)^2\Psi + V\Psi = E\Psi, \tag{G.15}$$

which is the equation corresponding to the particle moving in electromagnetic field with vector potential $\boldsymbol{A}$, see p. 654.

Indeed, the last equation can be transformed in the following way

$$\frac{1}{2m}\left[\hat{\boldsymbol{p}}^2\Psi + \left(\frac{q}{c}\right)^2\boldsymbol{A}^2\Psi - \frac{q}{c}\hat{\boldsymbol{p}}(\boldsymbol{A}\Psi) - \frac{q}{c}\boldsymbol{A}\hat{\boldsymbol{p}}\Psi\right] + V\Psi = E\Psi,$$

which after using the equality[3] $\hat{\boldsymbol{p}}(\boldsymbol{A}\Psi) = \Psi\hat{\boldsymbol{p}}\boldsymbol{A} + \boldsymbol{A}\hat{\boldsymbol{p}}\Psi$ gives the expected result [eq. (G.15)].

[3] Remember that $\hat{\boldsymbol{p}}$ is proportional to the first derivative operator.

In conclusion, if a particle moves in a vector potential field $\boldsymbol{A}$ from $\boldsymbol{r}_0$ to $\boldsymbol{r}$, then its wave function changes the phase by δ

$$\delta = -\frac{q}{\hbar c}\int_{\boldsymbol{r}_0}^{\boldsymbol{r}} \boldsymbol{A}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r},$$

or, putting it in a different way: if the wave function undergoes a phase change, it means that the particle moves in the vector potential of an electromagnetic field.

The incredible Aharonov–Bohm effect

In a small area (say, in the centre of the Grand Place in Brussels, where we like to locate the origin of the coordinate system) there is a magnetic field flux corresponding to field intensity $\boldsymbol{H}$ directed along the z axis (perpendicular to the market place surface). Now let us imagine a particle of electric charge q enclosed in a 3D box (say, a cube) of small dimensions located at a *very long distance* from the origin, and therefore from the magnetic flux, say, in Lisbon. Therefore, the *magnetic field in the box is equal to zero.* Now we decide to travel with the box: Lisbon, Cairo, Ankara, StPetersburg, Stockholm, Paris, and back to Lisbon. Did the wave function of the particle in the box change during the journey?

Let us see. The magnetic field $\boldsymbol{H}$ is related to the vector potential $\boldsymbol{A}$ through the relation $\nabla \times \boldsymbol{A} = \boldsymbol{H}$. This means that the particle was subject to a huge vector potential field (see Fig. G.1) all the time, although the magnetic field was practically zero. Since the box is back to Lisbon, the phase acquired by the particle in the box[4] is an integral over the closed trajectory (loop)

$$\delta = -\frac{q}{\hbar c}\oint \boldsymbol{A}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r}.$$

However, from the Stokes equation, we can replace the integral by an integral over a surface enclosed by the loop

$$\delta = -\frac{q}{\hbar c}\oint \boldsymbol{A}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} = -\frac{q}{\hbar c}\iint \nabla \times \boldsymbol{A}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{S}.$$

This may be written as

$$\delta = -\frac{q}{\hbar c}\iint \boldsymbol{H}\,\mathrm{d}\boldsymbol{S} = -\frac{q}{\hbar c}\Phi,$$

where Φ is the magnetic flux (of the magnetic field $\boldsymbol{H}$) intersecting the loop surface, which contains, in particular, the famous market place of Brussels. Thus, despite the fact that the particle could not feel the magnetic field $\boldsymbol{H}$ (because it was zero in the box), its wave function underwent a change of phase, which is detectable experimentally (in interference experiments).

Does the pair of potentials $\boldsymbol{A}$ and ϕ contain the same information as $\boldsymbol{\mathcal{E}}$ and $\boldsymbol{H}$? The Aharonov–Bohm effect (see also p. 780) suggests that $\boldsymbol{A}$ and ϕ are more important.

[4] A non-zero δ requires a more general $\boldsymbol{A}$ than that satisfying eq. (G.14).