Formal Expressions for the Electromagnetic Potentials in Any Gauge

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(February 25, 2015; updated July 26, 2019)

1 Problem

Deduce expressions for the electromagnetic vector potential $\mathbf{A}$ in an arbitrary gauge, where the scalar potential $V(\mathbf{x}, t)$ has a specified form, via a gauge transformation from the potentials in the Lorenz gauge [1].[1]

2 Solution

In the Hamiltonian dynamics of a charged particle, the Hamiltonian (and Lagrangian) $H = U_{\text{mech}} + qV$, where U_{mech} is the "mechanical" energy of the particle, q is its electric charge, and V is the "external" electromagnetic scalar potential in some gauge. Yet, the equations of motion deduced from this Hamiltonian do not depend on the choice of gauge,[2] so we are free to use whatever gauge is convenient.

2.1 Gauge Transformations

We first review the notion of gauge transformations in classical electrodynamics.[3] We consider microscopic electrodynamics, and work in Gaussian units.

In electrostatics, Coulomb's law can be written as,

$$\mathbf{E}(\mathbf{x}) = \int \frac{\rho(\mathbf{x}')\,\mathbf{r}}{r^3}\, d\text{Vol}' = -\boldsymbol{\nabla} V, \qquad \text{where} \qquad V = \int \frac{\rho(\mathbf{x}')}{r}\, d\text{Vol}' \tag{1}$$

ρ is the volume density of electric charge, and $\mathbf{r} = \mathbf{x} - \mathbf{x}'$.

Faraday discovered (as later interpreted by Maxwell) that,[4]

$$\boldsymbol{\nabla} \times \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{B}}{\partial t}\,, \tag{2}$$

[1] For an illustration of such expressions for a Hertzian (point) oscillating dipole, see [2].

[2] See, for example, sec. 2.1 of [3].

[3] For historical surveys, see [4] and Appendix A of [5].

[4] Faraday's law, eq. (2), implies that the condition $\boldsymbol{\nabla} \times \mathbf{E} = 0$ of electrostatics (where $\mathbf{E}$ is independent of time) requires that the magnetic field $\mathbf{B}$ also be independent of time. That is, electrostatics and magnetostatics are equivalent (as reinforced by the 4^{th} Maxwell equation (9)).

where c is the speed of light in vacuum, which implies that time-dependent magnetic fields $\mathbf{B}$ are associated with additional electric fields beyond those deducible from the scalar potential V. The nonexistence (so far as we know) of magnetic charges (Gilbertian monopoles) implies that,

$$\boldsymbol{\nabla} \cdot \mathbf{B} = 0, \tag{3}$$

and hence that the magnetic field can be related to a vector potential $\mathbf{A}$ by,

$$\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}. \tag{4}$$

Using eq. (4) in (2), we can write,

$$\boldsymbol{\nabla} \times \left(\mathbf{E} + \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} \right) = 0, \tag{5}$$

which implies that $\mathbf{E} + (1/c)\partial\mathbf{A}/\partial t$ can be related to a scalar potential V as $-\boldsymbol{\nabla} V$, *i.e.*,

$$\mathbf{E} = -\boldsymbol{\nabla} V - \frac{1}{c} \frac{\partial \mathbf{A}}{\partial t}\,. \tag{6}$$

Then, using eq. (6) in the Maxwell equation,

$$\boldsymbol{\nabla} \cdot \mathbf{E} = 4\pi\rho \tag{7}$$

leads to,

$$\nabla^2 V + \frac{1}{c} \frac{\partial}{\partial t} \boldsymbol{\nabla} \cdot \mathbf{A} = -4\pi\rho. \tag{8}$$

Similarly, using eqs. (4) and (6) in the Maxwell equation,

$$\boldsymbol{\nabla} \times \mathbf{B} = \frac{4\pi}{c} \mathbf{J} + \frac{1}{c} \frac{\partial \mathbf{E}}{\partial t}\,, \tag{9}$$

where $\mathbf{J}$ is the volume density of electrical current, leads to,

$$\nabla^2 \mathbf{A} - \frac{1}{c^2} \frac{\partial^2 \mathbf{A}}{\partial t^2} = -\frac{4\pi}{c} \mathbf{J} + \boldsymbol{\nabla} \left(\boldsymbol{\nabla} \cdot \mathbf{A} + \frac{1}{c} \frac{\partial V}{\partial t} \right). \tag{10}$$

The differential equations (8) and (10) do not uniquely determine the potentials V and $\mathbf{A}$. As perhaps first clearly noted by Lorentz [6, 7],[5] if V_0, $\mathbf{A}_0$ are valid electromagnetic potentials, then so are,

$$V = V_0 - \frac{1}{c} \frac{\partial \chi}{\partial t}\,, \qquad \mathbf{A} = \mathbf{A}_0 + \boldsymbol{\nabla} \chi, \tag{11}$$

where χ is an arbitrary scalar function, now called the gauge-transformation function. That is, eqs. (4) and (6) give the same values for the electromagnetic fields $\mathbf{B}$ and $\mathbf{E}$ for either the potentials V, $\mathbf{A}$ or V_0, $\mathbf{A}_0$.

[5] A transformation $\mathbf{A}' = \mathbf{A} + \boldsymbol{\nabla}\chi$ of the vector potential was discussed by W. Thomson (1850) in sec. 82 of [8], without consideration of the electric field/potential. In sec. 98 of [9], Maxwell noted that if potentials V_0, $\mathbf{A_0}$ do not obey $\boldsymbol{\nabla} \cdot \mathbf{A}_0 = 0$, then the potentials V and $\mathbf{A}$ of eq. (11) [Maxwell's eqs. (74) and(77)] obey $\boldsymbol{\nabla} \cdot \mathbf{A} = 0$ (Coulomb gauge) if $\nabla^2\chi = \boldsymbol{\nabla} \cdot \mathbf{A}_0$, which he thereafter considered to be the proper type of potentials.

2.2 From Lorenz-Gauge Potentials to Those in Any Other Gauge

As deduced by Lorenz in 1867 [1],

$$V^{(\mathrm{L})}(\mathbf{r},t) = \int \frac{\rho(\mathbf{r}',t'=t-|\mathbf{r}-\mathbf{r}'|/c)}{|\mathbf{r}-\mathbf{r}'|}\,d\mathrm{Vol}' \qquad \text{(Lorenz)}, \tag{12}$$

$$\mathbf{A}^{(\mathrm{L})}(\mathbf{r},t) = \int \frac{\mathbf{J}(\mathbf{r}',t'=t-|\mathbf{r}-\mathbf{r}'|/c)}{c\,|\mathbf{r}-\mathbf{r}'|}\,d\mathrm{Vol}' \qquad \text{(Lorenz)}, \tag{13}$$

are formal expressions for the (retarded) potentials in what is now called the Lorenz gauge, for which the so-called gauge condition is,

$$\boldsymbol{\nabla}\cdot\mathbf{A}^{(\mathrm{L})} = -\frac{1}{c}\frac{\partial V^{(\mathrm{L})}}{\partial t} \qquad \text{(Lorenz)}. \tag{14}$$

Another set of potentials can be defined by the gauge condition that the scalar potential $V(\mathbf{x},t)$ is a specified, but arbitrary scalar function.[6] Then, we can formally integrate the first of eq. (11) for $V_0 = V^{(\mathrm{L})}$ to write the gauge-transformation function as,[7,8]

$$\chi(\mathbf{x},t) = c\int_{-\infty}^{t}\left\{V^{(\mathrm{L})}(\mathbf{x},t') - V(\mathbf{x},t')\right\}\,dt'. \tag{15}$$

Hence, a formal expression for the vector potential in the new gauge follows from the second of eq. (11),[9]

$$\begin{aligned}
\mathbf{A}(\mathbf{r},t) &= \mathbf{A}^{(\mathrm{L})} + \boldsymbol{\nabla}\chi = \mathbf{A}^{(\mathrm{L})}(\mathbf{r},t) + c\boldsymbol{\nabla}\int_{-\infty}^{t}\left\{V^{(\mathrm{L})}(\mathbf{r},t') - V(\mathbf{r},t')\right\}\,dt' \\
&= \mathbf{A}^{(\mathrm{L})}(\mathbf{r},t) - c\int_{-\infty}^{t}\left\{\frac{1}{c}\frac{\partial\mathbf{A}^{(\mathrm{L})}}{\partial t} - \frac{1}{c}\frac{\partial\mathbf{A}^{(\mathrm{L})}}{\partial t} - \boldsymbol{\nabla}V^{(\mathrm{L})}(\mathbf{r},t') + \boldsymbol{\nabla}V(\mathbf{r},t')\right\}\,dt' \\
&= \mathbf{A}^{(\mathrm{L})}(\mathbf{r},-\infty) - c\int_{-\infty}^{t}\left\{\mathbf{E}(\mathbf{r},t') + \boldsymbol{\nabla}V(\mathbf{r},t')\right\}\,dt'.
\end{aligned} \tag{16}$$

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[6] The potentials associated with given $\mathbf{E}$ and $\mathbf{B}$ fields, and subject to a particular gauge condition, are not unique. For example, one can add constant terms to V and $\mathbf{A}$ with no change to $\mathbf{E}$ or $\mathbf{B}$, and the gauge remains the same (except for the Gibbs gauge, sec. 23.3 below, in which $V = 0$ always). In case of potentials in the Lorenz gauge, if the (restricted) gauge-transformation function $\chi(\mathbf{x},t)$ obeys the wave equation $\nabla^2\chi = \partial^2\chi/\partial(ct)^2$, then the new potentials $\mathbf{A}'^{(\mathrm{L})} = \mathbf{A}^{(\mathrm{L})} + \boldsymbol{\nabla}\chi$ and $V'^{(\mathrm{L})} = V^{(\mathrm{L})} - \partial\chi/\partial(ct)$ obey $\boldsymbol{\nabla}\cdot\mathbf{A}'^{(\mathrm{L})} = \boldsymbol{\nabla}\cdot\mathbf{A}^{(\mathrm{L})} + \nabla^2\chi = -\partial V^{(\mathrm{L})}/\partial(ct) - \partial/\partial(ct)[-\partial\chi/\partial(ct)] = -\partial V'^{(\mathrm{L})}/\partial(ct)$, and so are also in the Lorenz gauge.

Thus, the specification of a gauge condition is not, in general, sufficient to determine the potentials uniquely. For the latter, one could also specify boundary conditions, such as the vector potential being normal, or tangential, to some bounding surface, as discussed, for example, in [11]. It is noteworthy that the retarded vector potential (13) will not generally satisfy such boundary conditions, so one may be led to Lorenz-gauge potentials which are not the retarded potentials. See, for example, sec. 2.2.3 of [12].

[7] Equation (15) is a slight generalization of the procedure given in sec. IIIA of [13]. The arguments there depend in part on eq. (2.10), which relations are more obvious if it is understood that eq. (2.9) is applied to Lorenz-gauge potentials, and that the function Ψ also serves as the gauge-transformation function from the Coulomb gauge to the Lorenz gauge.

[8] May 28, 2024. Additional discussion of eq. (15) is given in [14].

[9] May 17, 2024. A different derivation of eq. (16) is given in Sec. 2 of [15].

2.2.1 Propagation of the Fields and Potentials

The Lorenz-gauge potentials (12)-(13) can be said to propagate with speed c,[10] with the consequence that the fields $\mathbf{B}$ and $\mathbf{E}$ derived from them via eqs. (4) and (6) can also be said to propagate with speed c (as expected from Maxwell's electrodynamics [10]).[11]

When using eq. (16) to compute the magnetic field from the vector potential in an arbitrary gauge, we have that $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A} = \boldsymbol{\nabla} \times \mathbf{A}^{(\mathrm{L})}$. Similarly, the electric field, as computed from the potentials V and $\mathbf{A}$ in an arbitrary gauge, is,

$$\mathbf{E} = -\boldsymbol{\nabla} V - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} = -\boldsymbol{\nabla} V - \frac{1}{c}\frac{\partial \mathbf{A}^{(\mathrm{L})}}{\partial t} - \boldsymbol{\nabla} V^{(\mathrm{L})} + \boldsymbol{\nabla} V = -\boldsymbol{\nabla} V^{(\mathrm{L})} - \frac{1}{c}\frac{\partial \mathbf{A}^{(\mathrm{L})}}{\partial t}\,. \tag{17}$$

which reaffirms that $\mathbf{B}$ and $\mathbf{E}$ propagate with speed c. While the general scalar potential V can propagate arbitrarily, when considering the electric field $\mathbf{E}$ according to eq. (6), this arbitrary behavior is canceled by that of the time derivative of the third term in (the first line of) eq. (16) for the general vector potential $\mathbf{A}$.[12]

2.3 Examples

While the expression (16) applies for "any" gauge, to use it we must first know the scalar potential V in that gauge, which is not obvious in general. That is, the prescription (16) is a "solution looking for a problem".

The present general result (16) can be contrasted with prescriptions for transformations from the Lorenz-gauge potentials to those in several other gauges as given in [13].

2.3.1 Velocity Gauge

One application of eq. (16) is to the so-called velocity gauge in which the scalar potential is assumed to propagate with arbitrary speed v rather than c.[13,14] The velocity-gauge condition is,

$$\boldsymbol{\nabla} \cdot \mathbf{A}^{(\mathrm{v})} = -\frac{c}{v^2}\frac{\partial V^{(\mathrm{v})}}{\partial t} \qquad \text{(velocity gauge).} \tag{18}$$

With this, eqs. (8) and (10) become,

$$\nabla^2 V^{(\mathrm{v})} - \frac{1}{v^2}\frac{\partial^2 V^{(\mathrm{v})}}{\partial t^2} = -4\pi\rho, \tag{19}$$

[10]Strictly, this claim holds only for plane, cylindrical and spherical waves, while superpositions of such waves can propagate at any speed. See, for example, [16].

[11]General expressions for $\mathbf{B}$ and $\mathbf{E}$ deduced from the Lorenz-gauge potentials in terms of retarded quantities that propagate with speed c are given in eqs. (14-34) and (14-42) of [17]. See also [18], where it is shown in the Appendix that the general expressions for $\mathbf{B}$ and $\mathbf{E}$ can also be deduced from Maxwell's equations without use of potentials.

[12]Such a cancelation for the Coulomb-gauge potentials has been noted in [19, 20, 21, 22].

[13]The velocity gauge was initially called the α-Lorentz gauge in [23, 24]. See also [25].

In essence, the velocity gauge was used in 1870 by Helmholtz, eq. (3^a), p. 80 of [26], while he considered other vector potentials in eq. (1^a), p. 76. See also [27, 28].

[14]Nonphysical waves of the gravitational potential with arbitrary velocity were called gauge waves by Feynman on p. 52 of [29].

$$\nabla^2 \mathbf{A}^{(\mathrm{v})} - \frac{1}{c^2}\frac{\partial^2 \mathbf{A}^{(\mathrm{v})}}{\partial t^2} = -\frac{4\pi}{c}\left[\mathbf{J} + \frac{1}{4\pi}\left(\frac{c^2}{v^2} - 1\right)\boldsymbol{\nabla}\frac{\partial V^{(\mathrm{v})}}{\partial t}\right]. \tag{20}$$

and a formal solution of the scalar potential in the velocity gauge is,

$$V^{(\mathrm{v})}(\mathbf{r},t) = \int \frac{\rho(\mathbf{r}', t' = t - |\mathbf{r} - \mathbf{r}'|/v)}{|\mathbf{r} - \mathbf{r}'|}\, d\mathrm{Vol}', \tag{21}$$

If the scalar potential $V^{(\mathrm{v})}$ and the vector potential $\mathbf{A}^{(\mathrm{L})}$ are known, then eq. (16) can be used to deduce the vector potential $\mathbf{A}^{(\mathrm{v})}$, rather than by solving eq. (20).

The velocity-gauge potentials are not unique (for a given set of charges and currents), in that use of a *restricted* gauge-transformation function $\chi(\mathbf{x}, t)$ which obeys $\nabla^2\chi = \partial^2\chi/\partial(vt)^2$ leads to new potentials that also satisfy the condition (18). See sec. IIIC of [25].

2.3.2 Coulomb Gauge

A special case of a velocity gauge is the famous Coulomb gauge, in which,

$$\boldsymbol{\nabla}\cdot\mathbf{A}^{(\mathrm{C})} = 0 \qquad \text{(Coulomb)}, \tag{22}$$

corresponding to $v = \infty$ in eq. (21),[15]

$$V^{(\mathrm{C})}(\mathbf{r},t) = \int \frac{\rho(\mathbf{r}', t)}{|\mathbf{r} - \mathbf{r}'|}\, d\mathrm{Vol}' \qquad \text{(Coulomb)}. \tag{23}$$

The use of eq. (16) to compute the vector potential in the Coulomb gauge can be simpler than the classic prescription,[16]

$$\mathbf{A}^{(\mathrm{C})}(\mathbf{r},t) = \int \frac{[\mathbf{J}_t]}{c\,|\mathbf{r} - \mathbf{r}'|}\, d\mathrm{Vol}', \tag{24}$$

where the transverse current density is given by,

$$\mathbf{J}_t(\mathbf{r},t) = \frac{1}{4\pi}\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\int \frac{\mathbf{J}(\mathbf{r}', t)}{c\,|\mathbf{r} - \mathbf{r}'|}\, d\mathrm{Vol}' = \mathbf{J}(\mathbf{r},t) - \frac{1}{4\pi}\boldsymbol{\nabla}\frac{\partial V^{(\mathrm{C})}(\mathbf{r},t)}{\partial t}, \tag{25}$$

where the second form follows from eq. (20).

The Coulomb-gauge potentials are not unique for a given set of charges and currents, as use of a *restricted* gauge function χ which obeys $\nabla^2\chi = 0$ everywhere leads to alternative potentials $\mathbf{A}'^{(\mathrm{C})} = \mathbf{A}^{(\mathrm{C})} + \boldsymbol{\nabla}\chi$ and $V'^{(\mathrm{L})} = V^{(\mathrm{L})} - \partial\chi/\partial(ct)$ that obey $\boldsymbol{\nabla}\cdot\mathbf{A}'^{(\mathrm{c})} = \boldsymbol{\nabla}\cdot\mathbf{A}^{(\mathrm{C})} + \nabla^2\chi = 0$, and so are also in the Coulomb gauge.

See [31] for examples of several Coulomb-gauge potentials of a infinite, static solenoid.

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[15] The potentials used by Maxwell were always in the Coulomb gauge, as in sec. 617 of [10].

In eq. (68), p. 498 of [9], Maxwell nearly discovered the Lorenz gauge, which reads $kJ + 4\pi\mu\, d\Psi/dt = 0$ in the notation there. Instead, he argued after eq. (79) that J $(= \boldsymbol{\nabla}\cdot\mathbf{A})$ is either zero or constant for wave propagation. He was not bothered by the implication of eq. (79) that in this case the scalar potential φ "propagates" instantaneously, perhaps because of the great success that his assumptions about the potentials lead to propagation of the electric and magnetic fields at lightspeed $\sqrt{k/4\pi\mu}$.

[16] See, for example, sec. 6.3 of [30].

For an example of the vector potential in the Coulomb gauge obtained by transforming the vector potential from the Lorenz gauge via eq. (16), see sec. 2.4 of [2]. For the case of a uniformly moving charge, see [32, 33]. The case of a charge that is rapidly accelerated from rest to uniform motion is discussed in [34]. For an interesting dynamic example where it is simpler to use the Coulomb gauge than the Lorenz gauge, see [35].

2.3.3 Gibbs Gauge

Another case where the prescription (16) readily applies is the gauge where the scalar potential is defined to be zero, $V^{(\mathrm{G})} = 0$, such that $\mathbf{E} = -(1/c)\partial \mathbf{A}^{(\mathrm{G})}/\partial t$, as first proposed by Gibbs [36, 37].[17,18,19]

Since the Gibbs-gauge vector potential is an integral of the electric field, $\mathbf{A}^{(\mathrm{G})}(t) = -c\int_{t_0}^{t} \mathbf{E}(t')\, dt'$, this potential propagates at speed c. However, it differs from the Lorenz-gauge vector potential. Since $\boldsymbol{\nabla}\cdot\mathbf{E} = 4\pi\rho = -(1/c)\partial \boldsymbol{\nabla}\cdot\mathbf{A}^{(\mathrm{G})}/\partial t$, the Gibbs-gauge vector potential obeys $\boldsymbol{\nabla}\cdot\mathbf{A}^{(\mathrm{G})} = 0$ away from charged particles (whereas the Coulomb-gauge vector potential obeys $\boldsymbol{\nabla}\cdot\mathbf{A}^{(\mathrm{C})} = 0$ everywhere).[20]

According to eq. (16), the vector potential in the Gibbs gauge is,

$$\mathbf{A}^{(\mathrm{G})}(\mathbf{r},t) = \mathbf{A}^{(\mathrm{L})}(\mathbf{r},t) + c\boldsymbol{\nabla}\int_{-\infty}^{t} V^{(\mathrm{L})}(\mathbf{r},t')\, dt', \tag{26}$$

so that the vector potential in any other gauge, where the scalar potential is V, can be written as,

$$\mathbf{A}(\mathbf{r},t) = \mathbf{A}^{(\mathrm{G})} - c\boldsymbol{\nabla}\int_{-\infty}^{t} V(\mathbf{r},t')\, dt'. \tag{27}$$

That is, if the vector potential in Gibbs gauge in known, this provides an even simpler prescription than eq. (16) for the vector potential in another gauge.

For an example of the vector potential in the Gibbs gauge, which can also be obtained by transforming the vector potential from the Lorenz gauge via eq. (16), see sec. 2.5 of [2].

2.3.4 Static-Voltage Gauge

A variant of the Gibbs gauge is that the scalar potential is not zero, but rather is the instantaneous Coulomb potential at some arbitrary time t_0,

$$V^{(\mathrm{SV})}(\mathbf{r},t) = V^{(\mathrm{C})}(\mathbf{r},t_0) = \int \frac{\rho(\mathbf{r}',t_0)}{|\mathbf{r}-\mathbf{r}'|}\, d\mathrm{Vol}'. \tag{28}$$

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[17] Apparently the Gibbs gauge is also called the Hamiltonian, or temporal, or Weyl, gauge, as mentioned in sec. VIII of [13]. That is, the Gibbs gauge is handy in examples where the electric field is known, and the vector potential is needed for use in the Hamiltonian of the system, expressed in terms of canonical momenta of charges q as $\mathbf{p}_{\mathrm{canonical}} = \mathbf{p}_{\mathrm{mech}} + q\mathbf{A}/c$.

[18] The Gibbs gauge, where $V = 0$, was considered, but not so named, in [38]. See also [39], where if one takes the "mechanical" potential energy U of electric charge q to be qV, then the condition that $V = -U/q$ requires that $V = 0$.

[19] If the gauge-transformation function $\chi(\mathbf{x},t)$ obeys $\partial^2\chi/\partial t^2 = 0$, then potentials in the Gibbs gauge transform to others in this gauge.

[20] The distinction between $\boldsymbol{\nabla}\cdot\mathbf{A}$ in the Coulomb and Gibbs gauges is often slight, which may be why Gibbs thought that his new gauge was the Coulomb gauge used by Maxwell. See also [40].

This is the static-voltage gauge [41], called the Coulomb-static gauge in [42].

From eq. (27), we see that the vector potential in the static-voltage gauge differs only slightly from that in the Gibbs gauge,

$$\mathbf{A}^{(\mathrm{SV})}(\mathbf{r},t)=\mathbf{A}^{(\mathrm{G})}(\mathbf{r},t)-ct\boldsymbol{\nabla}V^{(\mathrm{C})}(\mathbf{r},t_0) \tag{29}$$

2.3.5 Kirchhoff Gauge

The earliest statement of a gauge condition appears to have been made by Kirchhoff in 1857 [43, 44], when he specified that,

$$\boldsymbol{\nabla}\cdot\mathbf{A}^{(\mathrm{K})}=\frac{1}{c}\frac{\partial V^{(\mathrm{K})}}{\partial t}\qquad\text{(Kirchhoff)}. \tag{30}$$

Using this gauge condition in the general wave equation (8) for the scalar potential, we have,

$$\boldsymbol{\nabla}^2V^{(\mathrm{K})}+\frac{1}{c^2}\frac{\partial^2V^{(\mathrm{K})}}{\partial t^2}=-4\pi\rho, \tag{31}$$

such that the Kirchhoff-gauge scalar potential can be said to propagate with imaginary speed, $v_K=ic$. In this sense, the Kirchhoff gauge is a special case of the velocity gauge of sec. 2.3.1.

The scalar potential in the Kirchhoff gauge can be written as a “retarded” potential which speed of propagation ic. Recalling eq. (12), we have,

$$V^{(\mathrm{K})}(\mathbf{r},t)\ =\ \int\frac{\rho(\mathbf{r}',t'=t-|\mathbf{r}-\mathbf{r}'|/ic)}{|\mathbf{r}-\mathbf{r}'|}\,d\mathrm{Vol}'\qquad\text{(Kirchhoff)}, \tag{32}$$

For further discussion of the Kirchhoff gauge, see [45].

2.3.6 Poincaré Gauge

In cases where the fields $\mathbf{E}$ and $\mathbf{B}$ are known, we can compute the potentials in the so-called Poincaré gauge (see sec. 9A of [13] and [46, 47, 48]),[21,22]

$$V^{(\mathrm{P})}(\mathbf{r},t)=-\mathbf{r}\cdot\int_0^1du\,\mathbf{E}(u\mathbf{r},t),\qquad\mathbf{A}^{(\mathrm{P})}(\mathbf{r},t)=-\mathbf{r}\times\int_0^1u\,du\,\mathbf{B}(u\mathbf{r},t)\qquad\text{(Poincaré)}. \tag{33}$$

These forms are remarkable in that they depend on the instantaneous value of the fields only along a line between the origin and the point of observation.[23,24]

[21]The Poincaré gauge is also called the multipolar gauge [49, 50].

[22]For a point charge q at rest at the origin, $\mathbf{E}=q\,\hat{\mathbf{r}}/r^2$, $\mathbf{B}=0$, $V^{(\mathrm{P})}=-\mathbf{r}\cdot\int_0^1du\,q\hat{\mathbf{r}}/u^2r^2=q/r-\infty$, and $\mathbf{A}^{(\mathrm{P})}=0$. Here, the Poincaré scalar potential $V^{(\mathrm{P})}$ is equivalent to the Coulomb potential $V^{(\mathrm{C})}=q/r$, but with an infinite offset. Of course, $q/r+C$ is also a Coulomb potential of the charge q for any constant C.

[23]The potentials in the Poincaré gauge depend on the choice of origin. If the origin is inside the region of electromagnetic fields, then the Poincaré potentials are nonzero throughout all space. If the origin is to one side of the region of electromagnetic fields, then the Poincaré potentials are nonzero only inside that region, and in the region on the “other side” from the origin.

[24]We transcribe Appendices C and D of [50] to verify that $\mathbf{E}$ and $\mathbf{B}$ indeed follow from the Poincaré potentials (33).

$$-\boldsymbol{\nabla}V^{(\mathrm{P})}\ -\ \frac{1}{c}\frac{\partial\mathbf{A}^{(\mathrm{P})}}{\partial t}=\int_0^1du\left\{\boldsymbol{\nabla}[\mathbf{r}\cdot\mathbf{E}(u\mathbf{r},t)]+\mathbf{r}\times\frac{u}{c}\frac{\partial\mathbf{B}(u\mathbf{r},t)}{\partial t}\right\}$$

The Poincaré-gauge condition can be stated as,[25]

$$\mathbf{r} \cdot \mathbf{A}^{(\mathrm{P})} = 0 \qquad \text{(Poincaré)}. \tag{36}$$

If the scalar potential in the Poincaré gauge can be computed, it may then be simpler to deduce the vector potential in this gauge via eq. (16) than via eq. (33).

See [53] for an application of the spirit of the Poincaré potentials to a relation between a physical charge and current densities ρ *and* $\mathbf{J}$ *and effective polarization and magnetization densities* $\mathbf{P}$ *and* $\mathbf{M}$*, such that* $\rho = -\boldsymbol{\nabla} \cdot \mathbf{P}$ *and* $\mathbf{J} = c\boldsymbol{\nabla} \times \mathbf{M} + \partial \mathbf{P}/\partial t$.

See [54] for examples of potentials of an infinite solenoid, and of a toroidal magnet, in the Poincaré gauge.

2.3.7 Length (Electric-Dipole) Gauge

We now focus on an example of particular interest in quantum analysis: a hydrogen atom interacting with a plane electromagnetic wave of optical frequency, or lower.[26] Then, the wavelength of the electromagnetic wave is large compared to the size of the atom, and it is a good approximation to think of the atom as an electric dipole whose moment has magnitude $d = er$, where r is the distance of the electron from the proton.

The rate of classical radiation by an oscillating electric dipole $\mathbf{d}$ scales as $d^2\omega^2$, as first deduced by Hertz [56]. Since the quantum rate goes as the square of a matrix element of a relevant operator, we might expect that the quantum description of the interaction of an electron with an electromagnetic wave would involve a term in the Hamiltonian of the form $-\mathbf{d} \cdot \mathbf{E}_{\mathrm{wave}}$, this being the interaction energy of an electric dipole $\mathbf{d}$ in an external wave field. However, the Hamiltonian (50) of Appendix A does not obviously contain such a term,

$$\mathsf{H} \;=\; \frac{p_{\mathrm{mech}}^2}{2m} + eV = \frac{1}{2m}\left(\mathbf{p} - \frac{e\mathbf{A}}{c}\right)^2 + eV = \frac{\mathbf{p}^2}{2m} + eV - \frac{e}{2mc}(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}) + \frac{e^2\mathbf{A}^2}{2mc^2}$$

$$\begin{aligned}
&= \int_0^1 du\, \{\boldsymbol{\nabla}[\mathbf{r} \cdot \mathbf{E}(u\mathbf{r}, t)] - \mathbf{r} \times [\boldsymbol{\nabla} \times \mathbf{E}(u\mathbf{r}, t)]\} \\
&= \int_0^1 du\, \{(\mathbf{r} \cdot \boldsymbol{\nabla})\mathbf{E}(u\mathbf{r}, t) + [\mathbf{E}(u\mathbf{r}, t) \cdot \boldsymbol{\nabla}]\mathbf{r} + \mathbf{E}(u\mathbf{r}, t) \times (\boldsymbol{\nabla} \times \mathbf{r})\} \\
&= \int_0^1 du\, \left\{u \frac{d(ux_i)}{du} \frac{\partial \mathbf{E}(u\mathbf{r}, t)}{\partial(ux_i)} + \mathbf{E}(u\mathbf{r}, t)\right\} = \int_0^1 du\, \frac{d}{du} u\mathbf{E}(u\mathbf{r}, t) = \mathbf{E}(\mathbf{r}, t),
\end{aligned} \tag{34}$$

$$\begin{aligned}
\boldsymbol{\nabla} \times \mathbf{A}^{(\mathrm{P})} &= -\int_0^1 u\, du\, \boldsymbol{\nabla} \times [\mathbf{r} \times \mathbf{B}(u\mathbf{r}, t)] \\
&= -\int_0^1 u\, du\, \{\mathbf{r}[\boldsymbol{\nabla} \cdot \mathbf{B}(u\mathbf{r}, t)] - \mathbf{B}(u\mathbf{r}, t)[\boldsymbol{\nabla} \cdot \mathbf{r}] + [\mathbf{B}(u\mathbf{r}, t) \cdot \boldsymbol{\nabla}]\mathbf{r} - (\mathbf{r} \cdot \boldsymbol{\nabla})\mathbf{B}(u\mathbf{r}, t)\} \\
&= \int_0^1 u\, du\, \left\{2\mathbf{B}(u\mathbf{r}, t) + ux_i \frac{\partial \mathbf{B}(u\mathbf{r}, t)}{\partial(ux_i)}\right\} = \int_0^1 u\, du\, \left\{\frac{1}{u}\frac{d}{du} u^2\mathbf{B}(u\mathbf{r}, t)\right\} = \mathbf{B}(\mathbf{r}, t).
\end{aligned} \tag{35}$$

[25] If we write $\mathbf{A}^{(\mathrm{P})}(\mathbf{r}) = \int \mathbf{A}_{\mathbf{k}}^{(\mathrm{P})}\, e^{i\mathbf{k}\cdot\mathbf{r}}\, d^3\mathbf{k}/(2\pi)^3$, then $\boldsymbol{\nabla}_{\mathbf{k}} \cdot \mathbf{A}_{\mathbf{k}}^{(\mathrm{P})} = \int \boldsymbol{\nabla}_{\mathbf{k}} \cdot \mathbf{A}^{(\mathrm{P})}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{r}}\, d^3\mathbf{k}$ $= -i \int \mathbf{r} \cdot \mathbf{A}^{(\mathrm{P})}(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{r}}\, d^3\mathbf{k} = 0$. That is, the Poincaré gauge is the Coulomb gauge in (reciprocal) **k**-space.
The relativistic version of the Poincaré gauge, with $x_\mu A^\mu = 0$, is called the Fock [51] or Schwinger [52] gauge, and is the Lorenz gauge in **k**-space.

[26] These remarks follow sec. $\mathrm{A_{XIII}}$ of [55].

$$= \frac{\mathbf{p}^2}{2m} + eV - \frac{e}{mc}\mathbf{A}\cdot\mathbf{p} - \frac{ie\hbar}{2mc}(\boldsymbol{\nabla}\cdot\mathbf{A}) + \frac{e^2\mathbf{A}^2}{2mc^2}\,, \tag{37}$$

where we now consider the Hamiltonian to be a quantum operator, with the canonical momentum $\mathbf{p}$ replaced by $-i\hbar\boldsymbol{\nabla}$.

We could, of course, simply proceed with the Hamiltonian (37), after choosing a gauge. For this, it would seem obvious to use a gauge in which the static electric field of the proton is related to the scalar potential $V_0 = e/r$ (with the corresponding vector potential $\mathbf{A}_0 = 0$), and write the quantum Hamiltonian (37) as,

$$\mathsf{H} = \mathsf{H}_0 + \mathsf{H}_{\rm int}, \tag{38}$$

with "unperturbed" Hamiltonian,

$$\mathsf{H}_0 = \frac{\mathbf{p}^2}{2m} + eV_0, \tag{39}$$

and the interaction Hamiltonian,

$$\mathsf{H}_{\rm int} = eV_{\rm wave} - \frac{e}{mc}\mathbf{A}_{\rm wave}\cdot\mathbf{p} - \frac{ie\hbar}{2mc}(\boldsymbol{\nabla}\cdot\mathbf{A}_{\rm wave}) + \frac{e^2\mathbf{A}_{\rm wave}^2}{2mc^2}\,, \tag{40}$$

that is to be regarded as a perturbation associated with the plane electromagnetic wave, say,

$$\mathbf{E}_{\rm wave} = E_0\,\cos(kz - \omega t)\,\hat{\mathbf{x}}, \tag{41}$$

As previously remarked, the scalar potential $V_0 = e/r$ is consistent with any velocity gauge (sec. 2.3.1). Thus, we might use the Lorenz gauge for the interaction Hamiltonian, noting that the plane wave (41) can be related to potentials in the Lorenz gauge,

$$V_{\rm wave}^{\rm (L)} = 0, \qquad \mathbf{A}_{\rm wave}^{\rm (L)} = \frac{E_0}{k}\,\sin(kz - \omega t)\,\hat{\mathbf{x}}. \tag{42}$$

The vector potential (42) obeys $\boldsymbol{\nabla}^{\rm (L)}\cdot\mathbf{A}_{\rm wave} = 0$,[27] such that if the field strength is not too large,[28] the interaction Hamiltonian in the Lorenz gauge simplifies to,

$$\mathsf{H}_{\rm int}^{\rm (L)} \approx -\frac{e}{mc}\mathbf{A}_{\rm wave}^{\rm (L)}\cdot\mathbf{p}. \tag{43}$$

Matrix elements for the interaction Hamiltonian (43) can then be computed with the usual wavefunctions of an unperturbed hydrogen-atom (based on the scalar potential V_0).

However, we might prefer to use a different gauge, in which the interaction Hamiltonian has the form $-\mathbf{d}\cdot\mathbf{E}_{\rm wave}$. For this, we make a gauge transformation from the Lorenz gauge to the length gauge, using the transformation function,

$$\chi^{\rm (L\to l)} = \frac{xE_0}{k}\sin\omega t. \tag{44}$$

[27] We could also say that the potentials (42) are in the Coulomb gauge (and also in the Gibbs gauge), although the vector potential propagates at speed c, whereas a time-dependent vector potential in the Coulomb gauge typically has a term that propagates instantaneously.

[28] By "not too large", we mean that the last term in eq. (40) is small compared to mc^2, *i.e.*, $eA^{\rm (L)}/mc^2 = eE/m\omega c \ll 1$. This is the now-standard criterion for a "weak" laser field.

The potentials of the wave in the length gauge are, according to eq. (11),

$$V^{(\mathrm{l})}_{\mathrm{wave}} = V^{(\mathrm{L})}_{\mathrm{wave}} - \frac{1}{c}\frac{\partial \chi^{(\mathrm{L}\to\mathrm{l})}}{\partial t} = -xE_0 \cos\omega t \qquad \text{(length gauge)}, \tag{45}$$

$$\mathbf{A}^{(\mathrm{l})}_{\mathrm{wave}} = \mathbf{A}^{(\mathrm{L})}_{\mathrm{wave}} + \boldsymbol{\nabla}\chi^{(\mathrm{L}\to\mathrm{l})} = \frac{xE_0}{k}[\sin(kz-\omega t) + \sin\omega t]\,\hat{\mathbf{x}} \qquad \text{(length gauge)}. \tag{46}$$

For long wavelengths, $kz \ll 1$ for the atomic electron, so we obtain the approximate potentials in the length gauge,[29]

$$V^{(\mathrm{l})}_{\mathrm{wave}} \approx -xE_0\cos(kz-\omega t) = -\mathbf{r}\cdot\mathbf{E}_{\mathrm{wave}}, \qquad \mathbf{A}^{(\mathrm{l})}_{\mathrm{wave}} \approx \frac{xE_0}{k}[\sin(-\omega t) + \sin\omega t]\,\hat{\mathbf{x}} = 0. \tag{47}$$

and the interaction Hamiltonian (40) in the length gauge is (for weak wave fields),

$$\mathsf{H}^{(\mathrm{l})}_{\mathrm{int}} \approx eV_{\mathrm{wave}} = -e\mathbf{r}\cdot\mathbf{E}_{\mathrm{wave}} = -\mathbf{d}\cdot\mathbf{E}_{\mathrm{wave}} \qquad (kr \ll 1), \tag{48}$$

as desired by those who feel that the interaction Hamiltonian should be based on the classical energy $-\mathbf{d}\cdot\mathbf{E}$ of an electric dipole $\mathbf{d}$ in an external electric field $\mathbf{E}$.[30]

Matrix element of operators in the length gauge should not be taken using the unperturbed wavefunctions in the Lorenz gauge. Rather, we must first transform those wavefunctions into the length gauge according to eq. (59),

$$\psi^{(\mathrm{l})} = e^{-ie\chi^{(\mathrm{L}\to\mathrm{l})}/\hbar c}\,\psi^{(\mathrm{L})} = e^{-iexE_0\sin(\omega t)/\hbar\omega}\,\psi^{(\mathrm{L})}. \tag{49}$$

However, the interaction-Hamiltonian operator (48) in the length gauge does not involve any derivatives, so its matrix elements are the same whether one uses wavefunctions in the length gauge or (nominally incorrectly) the usual hydrogen-atom wavefunctions (in the Lorenz gauge).

There seems to have been some controversy about the choice of gauge for quantum analyses of atom-wave interactions, particularly after Lamb's work [58] on the eponymous shift. Insufficient care led to some results differing when computed in different gauges, and specious claims that one gauge is more "correct" than another. Some of this history can be traced in [23, 49, 59, 60, 61, 62, 63, 64, 65, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76].

Appendix A: Gauge Invariance and Quantum Mechanics

Quantum mechanics can be considered as an extension of Hamiltonian dynamics, starting with Planck's introduction of h as the quantum of action $S = \int \mathcal{L}\,dt$ in eq. 41 of [77].[31]

[29] The approximate forms (47) for the potentials do not hold in general, but only for a long-wavelength plane wave. For example, the potential of a point charge q at the origin is $q/r = \mathbf{r}\cdot\mathbf{E}$ (and not $-\mathbf{r}\cdot\mathbf{E}$) if the corresponding vector potential is zero. That is, the length-gauge potentials (47) cannot be used to describe the interaction with the proton in the unperturbed Hamiltonian (39).

Also, the approximation that $\mathbf{A}^{(\mathrm{l})}_{\mathrm{wave}} = 0$ means that the analysis ignores possible effects of the magnetic field of the wave, such as its interaction with the magnetic moment of the electron. If the latter is of interest, the length-gauge approximation should not be used.

[30] The above argument (although not the name length gauge) may have originated with Göppert-Mayer in her doctoral thesis [57].

[31] Planck's relation that $U = nh\nu$ for the energy of a quantum harmonic oscillator came a year later [78].

The Hamiltonian function H played little role in the early development of quantum theory. The classical, nonrelativistic Hamiltonian for a spinless electric charge e with mass m in an electromagnetic field described by potentials V and $\mathbf{A}$ seems to have been first stated by Schwarzschild [79] (as recounted in sec. IID of [4]),

$$\mathsf{H} = \frac{p_{\rm mech}^2}{2m} + eV = \frac{1}{2m}\left(\mathbf{p} - \frac{e\mathbf{A}}{c}\right)^2 + eV, \tag{50}$$

where $\mathbf{p}$ is the canonical momentum (and the mechanical momentum is $\mathbf{p}_{\rm mech} = m\mathbf{v} = \mathbf{p} - e\mathbf{A}/c$).[32] Schwarzschild did not mention gauge invariance (a term invented by Weyl in 1928 [81]; in English on p. 330 of [82]), but he did show that the equations of motion deduced from his Lagrangian/Hamiltonian have the form $m\mathbf{a} = e(\mathbf{E} = \mathbf{v}/c \times \mathbf{B})$, which is gauge invariant.[33]

In 1916, Epstein [83] and Schwarzschild [84] gave analyses of the Stark effect starting from the Hamilton-Jacobi equation [86, 87, 88, 89],

$$\mathsf{H}\left(q_i, \frac{\partial S}{\partial q_i}\right) = \mathsf{H}(q_i, p_i) = -\frac{\partial S}{\partial t} \to E \qquad \text{when} \qquad S(q_i, t) = \sum_i p_i q_i - Et, \tag{51}$$

where the relation $\mathsf{H} = E$ (energy) holds when the Hamiltonian is independent of time t.

In 1926, Schrödinger argued that a quantum version of the (nonrelativistic) Hamilton-Jacobi equation can by obtained the substitutions,

$$S \to -i\hbar \ln\psi, \qquad \Rightarrow \qquad p_i = \frac{\partial S}{\partial q_i} = \frac{-i\hbar}{\psi}\frac{\partial \psi}{\partial q_i}, \qquad p_i\psi \to -i\hbar\frac{\partial}{\partial q_i}\psi, \qquad \mathbf{p} \to -i\hbar\boldsymbol{\nabla}. \tag{52}$$

where ψ is a scalar wavefunction and p_i is the canonical momentum $\partial\mathcal{L}/\partial\dot{q}_i$ associated with coordinate q_i. For a particle of mass m and electric charge e in a static electric field $\mathbf{E} = -\boldsymbol{\nabla}V$, its classical Hamiltonian H is,

$$\mathsf{H} = \frac{p^2}{2m} + eV, \tag{53}$$

and we arrive at Schrödinger's equation via eq. (52),

$$\frac{-\hbar^2}{2m}\nabla^2 + eV = \frac{i\hbar}{\psi}\frac{\partial\psi}{\partial t} = E\,, \qquad \left(\frac{-\hbar^2}{2m}\nabla^2 + eV\right)\psi = i\hbar\frac{\partial\psi}{\partial t} = E\psi, \tag{54}$$

where the terms in energy E apply only if the system has a definite total energy.[34]

[32]Strictly, Schwarzschild discussed the interaction Lagrangian, $\mathcal{L}_{\rm int} = eV - e\mathbf{v}\cdot\mathbf{A}/c$, which together with the free-particle Lagrangian, $\mathcal{L}_{\rm free} = mv^2/2$, leads to the Hamiltonian (50), as shown in sec. 16 of [80].

[33]Apparently, the first explicit discussion of the fact that while the Hamiltonian/Lagrangian of an electric charge in an electromagnetic field is gauge dependent, its equation of motion is gauge invariant, was given by Landau in sec. 16 of the 1941 edition of [80] (sec. 18 of later editions).

[34]While the term in $\partial\psi/\partial t$ is implicit in Schrödinger's first quantum paper [90], he omitted it. And in his fifth paper of 1926 [91] he seemed unsure of the sign of this term.

The sign appears correctly in eq. (2) of Dirac's first paper to use Schödinger's formalism [92].

It no doubt seemed obvious in early 1926 to regard the (static) scalar potential V as the Coulomb potential e/r of a proton in case of a hydrogen atom, but this choice implicitly assumes use of a velocity gauge (sec. 2.3.1 above), such as the Coulomb or Lorenz gauges.

The first consideration of the quantum dynamics of an electric charge in a general, time-dependent electromagnetic field seems to have been by Schrödinger in sec. 6 of [91], where he considered a relativistic wave equation for a (spinless) electron whose Hamiltonian involves both a scalar potential V,[35] and a vector potential $\mathbf{A}$, tacitly in the Coulomb gauge.[36] Here, we content ourselves with a nonrelativistic version, using the Hamiltonian (50). and follow Schrödinger's prescription (52) to find,

$$\begin{aligned} i\hbar\frac{\partial\psi}{\partial t} &= \left[\frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} - \frac{e\mathbf{A}}{c}\right)^2 + eV\right]\psi \\ &= -\frac{\hbar^2}{2m}\nabla^2\psi + \frac{ie\hbar}{2mc}[\boldsymbol{\nabla}\cdot(\mathbf{A}\psi) + \mathbf{A}\cdot\boldsymbol{\nabla}\psi] + \frac{e^2A^2}{2mc^2}\psi + eV\psi \\ &= -\frac{\hbar^2}{2m}\nabla^2\psi + \frac{ie\hbar}{mc}\mathbf{A}\cdot\boldsymbol{\nabla}\psi + \frac{ie\hbar}{2mc}(\boldsymbol{\nabla}\cdot\mathbf{A})\psi + \frac{e^2A^2}{2mc^2}\psi + eV\psi. \end{aligned} \tag{55}$$

In principle, we should be able to use any gauge for the potentials $\mathbf{A}$ and V in eq. (55), and the physical predictions of the quantum analysis should be the same.

A first step towards demonstrating the gauge invariance of quantum analyses was made by Fock (1926) [94]. See also [95] and p. 206 of [96]. In somewhat more contemporary notation, Fock noted that eq. (55) for an electric charge e of mass m in electromagnetic fields described by potentials $A_\mu = (V, \mathbf{A})$ can be written as,[37]

$$\frac{(-i\hbar\mathbf{D})^2}{2m}\psi = i\hbar D_0\,\psi, \tag{56}$$

using the "altered" (covariant) derivative,

$$D_\mu = \partial_\mu - \frac{ieA_\mu}{\hbar c}, \qquad \partial_\mu = \left(\frac{\partial}{\partial t}, \boldsymbol{\nabla}\right). \tag{57}$$

Then, the form of eq. (56) is gauge invariant only if a gauge transformation of the potentials,

$$A_\mu(x_\nu) \to A_\mu + \partial_\mu\chi, \tag{58}$$

is accompanied by a phase change of the wavefunction,

$$\psi(x_\nu) \to e^{-ie\chi/\hbar c}\,\psi, \tag{59}$$

where the scalar gauge-transformation function χ is "arbitrary" (but differentiable).[38]

The further demonstration that quantum expectation values for wavefunctions which obey eq. (56) are also gauge invariant can be found in sec. $\mathrm{H_{III}}$ of [55] (which may the only demonstration of this in a "textbook").

[35]Klein published slightly earlier [93] a relativistic wave equation for an electron interacting with only a scalar potential.

[36]In eq. (36) of [91], the term in $\boldsymbol{\nabla}\cdot\mathbf{A}$ in the last line of our eq. (55) had been set to zero.

[37]Fock actually discussed the relativistic case, referencing Klein [93], but not Schrödinger [91].

[38]On pp. 330-331 of [82], Weyl inverted Fock's argument (without referencing him), concluding that for

Appendix B: Hydrogen-Atom Wavefunctions in a Gauge where the Hamiltonian is Time Dependent

In [72, 75] it is argued that gauges are "unphysical" if the Hamiltonian for a system in that gauge is time dependent, while it has no time dependence is some other gauge.[39] This view goes against the notion of gauge invariance, so we illustrate here how one can use a gauge in which the Hamiltonian is time dependent to find the quantum wavefunctions of a hydrogen atom.

First, we recall that in a velocity gauge, including the Coulomb and Lorenz gauges, the classical Hamiltonian H of a nonrelativistic electron of charge e and mass m and a proton of charge $q = -e$, that is approximated to be at rest at the origin, can be written as,

$$H = \frac{\mathbf{p}_{\rm mech}}{2m} + eV = \frac{(\mathbf{p} - e\mathbf{A}/c)^2}{2m} + eV, \tag{60}$$

where the electromagnetic potentials of the proton are,

$$\mathbf{A}^{(\rm v)} = 0, \qquad V^{(\rm v)} = \frac{q}{r}\,. \tag{61}$$

This Hamiltonian is independent of time, and equals the total energy E of the electron.[40] The eigenstates $\psi_n^{(\rm v)}$ of the quantum version $\mathsf{H}^{(\rm v)} = \mathsf{E}^{(\rm v)}$ of this Hamiltonian were found by Schrödinger [90] (who was not aware that he was working in a velocity gauge).

In the Gibbs gauge (sec. 2.3.3 above), the potentials are,

$$\mathbf{A}^{(\rm G)} = -\frac{cqt}{r^2}\,\hat{\mathbf{r}}, \qquad V^{(\rm G)} = 0, \tag{62}$$

so the time-dependent, quantum Hamiltonian $\mathsf{H}^{(\rm G)}$ obtained from eq. (60) equals only the kinetic energy (operator) $\mathbf{p}_{\rm mech}^2/2m$.

It is interesting to consider an "oddball" gauge in which the scalar potential is,

$$V^{(\rm odd)} = k\frac{q}{r}\,, \tag{63}$$

for some real value of k. Then, according to sec. 2.2 above, we can make a gauge transformation from the Lorenz (velocity) gauge to the "oddball" gauge using a gauge-transformation

physics be invariant under a local phase change as in eq. (59), there must exist a 4-vector potential that obeys eq. (58), and *If our view is correct, then the electromagnetic field is a necessary accompaniment of the matter-wave field.*

The argument that local phase invariance of the quantum wavefunction requires a gauge theory was applied by Yang and Mills [97] to a (nonviable) theory of pions interactions, by Weinberg [98] and Salam [99] to the Standard Model (electroweak theory), and by Gross and Wilczek [100] and Politzer [101] to quantum chromodynamics. It remains that gravity is not described by a gauge theory, since in such theories antimatter has gauge anticharge, but antimatter does not have negative mass (see, for example, [102]).

[39] The electromagnetic potentials are not measurable in any gauge, so many people (including the authors) regard the potentials as "unphysical" in any gauge.

[40] That this Hamiltonian equals the energy is not an illustration of Noether's theorem [103], which formally applies only for field theories. For example, a Hamiltonian that is independent of time can be given for a damped harmonic oscillator, which does not have a conserved energy. See sec. 2.6 of [104], and also [105, 106].

function,

$$\chi(\mathbf{x},t) = c\int_{-\infty}^{t} \left\{V^{(\mathrm{L})}(\mathbf{x},t') - V^{(\mathrm{odd})}(\mathbf{x},t')\right\}\, dt' = (1-k)\frac{cqt}{r}\,, \tag{64}$$

and the vector potential is,

$$\mathbf{A}^{(\mathrm{odd})} = \mathbf{A}^{(\mathrm{L})} + \boldsymbol{\nabla}\chi = \boldsymbol{\nabla}\chi = -\chi\frac{\hat{\mathbf{r}}}{r} = -(1-k)\frac{cgt}{r^2}\,\hat{\mathbf{r}}. \tag{65}$$

While it is perhaps not straightforward to solve Schrödinger's equation using the Hamiltonian (60) in the "oddball" gauge, we know from the general argument of Fock [94] (our eq. (59)), that the energy eigenfunctions $\psi_n^{(\mathrm{odd})}$ in this gauge are related to the well-known wavefunctions $\psi_n^{(\mathrm{v})}$ in a velocity gauge by,

$$\psi_n^{(\mathrm{odd})} = e^{-ie\chi/\hbar c}\,\psi_n^{(\mathrm{v})} = e^{-(1-k)eqt/\hbar cr}\,\psi_n^{(\mathrm{v})}. \tag{66}$$

For completeness, we display the energy operator $\mathsf{E}^{(\mathrm{odd})}$ such that,

$$\mathsf{E}^{(\mathrm{odd})}\,\psi_n^{(\mathrm{odd})} = E_n\,\psi_n^{(\mathrm{odd})}, \tag{67}$$

where E_n is the energy eigenvalue of wavefunction $\psi_n^{(\mathrm{v})}$, *i.e.*, $\mathsf{E}^{(\mathrm{v})}\,\psi_n^{(\mathrm{v})} = E_n\,\psi_n^{(\mathrm{v})}$ in a velocity gauge, where $\mathsf{E}^{(\mathrm{v})} = \mathbf{p}^2/2m + eq/r$. For this, we note that the classical energy E of our system is, in the "oddball" gauge,

$$\begin{aligned} E &= \frac{\left(\mathbf{p}_{\mathrm{mech}}^{(\mathrm{odd})}\right)^2}{2m} + \frac{eq}{r} = \frac{\left(\mathbf{p} - e\mathbf{A}^{(\mathrm{odd})}/c\right)^2}{2m} + eV^{(\mathrm{odd})} + (1-k)\frac{eq}{r} = H^{(\mathrm{odd})} + (1-k)\frac{eq}{r} \\ &= \frac{\left(\mathbf{p} - e\mathbf{A}^{(\mathrm{odd})}/c\right)^2}{2m} + \frac{eq}{r}\,. \end{aligned} \tag{68}$$

Then, the energy operator $\mathsf{E}^{(\mathrm{odd})}$ in the "oddball" gauge is the quantum version of eq. (68), obtained by taking $\mathbf{p} = -i\hbar\boldsymbol{\nabla}$, *i.e.*, $\mathsf{E}^{(\mathrm{odd})} = \left(\mathbf{p}_{\mathrm{mech}}^{(\mathrm{odd})}\right)^2/2m + eq/r$.

Now, in the quantum analysis,

$$\begin{aligned} \mathbf{p}_{\mathrm{mech}}^{(\mathrm{odd})}\,\psi^{(\mathrm{odd})} &= \left(\mathbf{p} - e\mathbf{A}\psi_n^{(\mathrm{odd})}/c\right)\,\psi^{(\mathrm{odd})} = \left(-i\hbar\boldsymbol{\nabla} - e\mathbf{A}^{(\mathrm{odd})}/c\right)e^{-ie\chi/\hbar c}\,\psi^{(\mathrm{v})} \\ &= -i\hbar\psi^{(\mathrm{v})}\,\boldsymbol{\nabla}e^{-ie\chi/\hbar c} + e^{-ie\chi/\hbar c}\left(-i\hbar\boldsymbol{\nabla} - e\mathbf{A}^{(\mathrm{odd})}/c\right)\psi^{(\mathrm{v})} \\ &= \frac{e}{c}\,e^{-ie\chi/\hbar c}\,\psi^{(\mathrm{v})}\boldsymbol{\nabla}\chi + e^{-ie\chi/\hbar c}\left(-i\hbar\boldsymbol{\nabla} - e\mathbf{A}^{(\mathrm{odd})}/c\right)\psi^{(\mathrm{v})} \\ &= e^{-ie\chi/\hbar c}\left(e\mathbf{A}^{(\mathrm{odd})}\psi^{(\mathrm{v})}/c\right) + e^{-ie\chi/\hbar c}\left(-i\hbar\boldsymbol{\nabla} - e\mathbf{A}^{(\mathrm{odd})}/c\right)\psi^{(\mathrm{v})} \\ &= e^{-ie\chi/\hbar c}\,(-i\hbar\boldsymbol{\nabla})\psi^{(\mathrm{v})} = e^{-ie\chi/\hbar c}\,\mathbf{p}\,\psi^{(\mathrm{v})} = e^{-ie\chi/\hbar c}\,\mathbf{p}_{\mathrm{mech}}^{(\mathrm{v})}\,\psi^{(\mathrm{v})}, \end{aligned} \tag{69}$$

and so,

$$\left(\psi^{(\mathrm{odd})}\right)^*\,\mathbf{p}_{\mathrm{mech}}^{(\mathrm{odd})}\,\psi^{(\mathrm{odd})} = \left(\psi^{(\mathrm{v})}\right)^*\,e^{ie\chi/\hbar c}\,e^{-ie\chi/\hbar c}\,\mathbf{p}_{\mathrm{mech}}^{(\mathrm{v})}\,\psi^{(\mathrm{v})} = \left(\psi^{(\mathrm{v})}\right)^*\,\mathbf{p}_{\mathrm{mech}}^{(\mathrm{v})}\,\psi^{(\mathrm{v})}. \tag{70}$$

This illustrates that the expectation value of a physical operator, such as the mechanical momentum $\mathbf{p}_{\rm mech}$, is gauge invariant.[41]

Furthermore, $\mathbf{p}_{\rm mech}^2$ is a physical operator, with the implication that,

$$\left(\mathbf{p}_{\rm mech}^{(\rm odd)}\right)^2 \psi^{(\rm odd)} = \left(\mathbf{p} - e\mathbf{A}\psi_n^{(\rm odd)}/c\right)^2 \psi^{(\rm odd)} = e^{-ie\chi/\hbar c} \left(\mathbf{p}_{\rm mech}^{(\rm v)}\right)^2 \psi^{(\rm v)} = e^{-ie\chi/\hbar c}\, \mathbf{p}^2\, \psi^{(\rm v)}. \tag{71}$$

Then,

$$\begin{aligned} \mathsf{E}^{(\rm odd)}\psi_n^{(\rm odd)} &= \frac{\left(\mathbf{p}_{\rm mech}^{(\rm odd)}\right)^2}{2m}\psi_n^{(\rm odd)} + \frac{eq}{r}\,\psi_n^{(\rm odd)} = e^{-ie\chi/\hbar c}\left(\frac{\mathbf{p}^2}{2m} + \frac{eq}{r}\right)\psi_n^{(\rm v)} \\ &= e^{-ie\chi/\hbar c}\,\mathsf{E}^{(\rm v)}\,\psi_n^{(\rm v)} = e^{-ie\chi/\hbar c}\,E_n\,\psi_n^{(\rm v)} = E_n\,\psi_n^{(\rm odd)}, \end{aligned} \tag{72}$$

which confirms that the $\psi_n^{(\rm odd)}$ are indeed the energy eigenstates in the "oddball" gauge.

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