Onsager's Relation and Other Results for Relativistic Electrons in Magnetic Fields

A. Holas and S. Olszewski
Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw, Poland

D. Pfirsch
Max-Planck-Institut für Plasmaphysik, EURATOM Association, D-8046 Garching, F.R. Germany

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Onsager's result concerning the quantization of the magnetic flux enclosed by the orbit of an electron moving in a static uniform magnetic field is shown to hold also in the relativistic case, and not to be restricted to the regime considered by Onsager in which the correspondence principle can be applied. The results obtained via the correspondence principle and via expectation values differ, however, in the deails. It is shown also that the eigenenergies and eigenfunctions of Dirac's relativistic equation for an electron in a static non-uniform and arbitrarily strong magnetic field may be obtained directly from the solutions of Schrödinger's non-relativistic equation. In this case the expectation value of an observable depending on coordinates only equals the one calculated directly with the non-relativistic eigenfunctions.

Key words: Electron, Relativistic, Orbit, Magnetic Field.

1. Introduction

More than 35 years ago Onsager [1] found that during the motion of an electron in a static uniform magnetic field "the cross-section of the helical orbit is determined by the condition that the enclosed magnetic flux equals $(n+\Theta)$ 'force lines'". This relation happened to be very useful in the context of the de Haas–van Alphen effect in metals. The motion considered by Onsager was obviously of non-relativistic character. The aim of the present paper is to examine the same problem in the relativistic case. The derivations are, on the one hand, based on the correspondence principle used by Onsager (Sect. 4) and, on the other hand, on expectation values (Section 5).

2. Reduction of Dirac's Equation for Static Non-uniform Magnetic Fields to a Schrödinger-Type Equation

In order to account for both the quantum and the relativistic character of the electron motion, Dirac's equation containing an electromagnetic field (see e.g. [2]) must be solved:

$$i\hbar\frac{\partial}{\partial t}\psi=\left[c\left(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A}\right)\cdot\boldsymbol{\alpha}+m c^2\beta-e\Phi\right]\psi, \tag{2.1}$$

Reprint requests to Prof. Dr. S. Olszewski, Institute of Physical Chemsistry, Kasprzaka 44/52, 01-224 Warsaw, Poland.

where Φ and $\boldsymbol{A}$ are the scalar and vector potential of the electromagnetic field, β and $\boldsymbol{\alpha}$ are standard Dirac matrices. The electron charge is $-e$, where e denotes the elementary charge. The four-component wave function ψ may be represented as a column of two spinors ϕ and χ

$$\psi=\begin{pmatrix}\phi\\ \chi\end{pmatrix}. \tag{2.2}$$

For time independent fields, stationary solutions $\psi\propto\exp(i\,E\,t/\hbar)$ are possible and, under the additional assumption $\Phi=0$, (2.1) can be written as

$$\begin{aligned}(E-m c^2)\,\phi&=c\,\boldsymbol{\sigma}\cdot\left(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A}\right)\chi,\\ (E+m c^2)\,\chi&=c\,\boldsymbol{\sigma}\cdot\left(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A}\right)\phi.\end{aligned} \tag{2.3}$$

Here $\boldsymbol{\sigma}$ represents three Pauli's matrices. The second of these equations yields χ in terms of ϕ:

$$\chi=\frac{c}{E+m c^2}\,\boldsymbol{\sigma}\cdot\left(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A}\right)\phi. \tag{2.4}$$

When this is used in the first of the Eqs. (2.3), the following equation for ϕ alone results:

$$(E-m c^2)\,\phi=\frac{c^2}{E+m c^2}\left[\boldsymbol{\sigma}\cdot\left(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A}\right)\right]^2\phi. \tag{2.5}$$

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With the identity obeyed by Pauli's matrices

$$\left[\boldsymbol{\sigma}\cdot\left(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A}\right)\right]^2=\left(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A}\right)^2+\frac{e\hbar}{c}\boldsymbol{\sigma}\cdot\boldsymbol{H}, \tag{2.6}$$

where $\boldsymbol{H}=\operatorname{curl}\boldsymbol{A}$ is the magnetic field, (2.5) can be written in the form (comp. [3])

$$\mathscr{H}\phi=\left[\frac{1}{2m}\left(\boldsymbol{p}+\frac{e}{c}\boldsymbol{A}\right)^2+\frac{e\hbar}{2mc}\boldsymbol{\sigma}\cdot\boldsymbol{H}\right]\phi=\tilde{E}\,\phi, \tag{2.7}$$

where

$$\tilde{E}=\frac{E^2-m^2c^4}{2mc^2}. \tag{2.8}$$

This is formally a Schrödinger equation for a non-relativistic particle in a static non-uniform magnetic field, with $\tilde{E}$ and ϕ playing the roles of the eigenenergy and the eigenfunction, respectively.

For a solution $\tilde{E}_q$, ϕ_q of (2.7), where q stands for a set of quantum numbers, the relativistic energy E_q is given by

$$E_q=(m^2c^4+2mc^2\tilde{E}_q)^{1/2}=mc^2\left[1+\frac{2\tilde{E}_q}{mc^2}\right]^{1/2} \tag{2.9}$$

and the density by

$$\psi_q^*\psi_q=\phi_q^*\phi_q+\chi_q^*\chi_q=\left[1+\frac{2m\tilde{E}_qc^2}{(E_q+mc^2)^2}\right]\phi_q^*\phi_q$$
$$=\left[1+\frac{E_q-mc^2}{E_q+mc^2}\right]\phi_q^*(\boldsymbol{r})\,\phi_q(\boldsymbol{r}). \tag{2.10}$$

This differs from its non-relativistic counterpart only by a factor independent of $\boldsymbol{r}$. This factor must be taken into account when the normalized ψ_q is calculated from the normalized ϕ_q.

3. Solution of Dirac's Equation in the Case of a Static Uniform Magnetic Field

Landau [4] found the solutions of the Schrödinger equation for a particle in a static uniform magnetic field $\boldsymbol{H}=(0,0,H)$ for two different gauges, $\boldsymbol{A}=(-Hy,0,0)$ and

$$\boldsymbol{A}=-\tfrac{1}{2}\boldsymbol{r}\times\boldsymbol{H}=(-\tfrac{1}{2}Hy,\tfrac{1}{2}Hx,0), \tag{3.1}$$

where it was convenient to introduce cylindrical coordinates ϱ, ϑ, z with

$$x=\varrho\cos\vartheta,\quad y=\varrho\sin\vartheta. \tag{3.2}$$

The second gauge is the appropriate one for the present purpose. In this case Landau obtained for the energy eigenvalues

$$\tilde{E}_{nlsp_z}=\left[n+\frac{1}{2}(1+s+l+|l|)\right]\hbar\,\omega_H+\frac{1}{2m}p_z^2, \tag{3.3}$$

where

$$\omega_H=(eH)/(mc) \tag{3.4}$$

is the cyclotron frequency in the field H. Three quantum numbers – the radial mode number n, the z component l of the angular momentum, and the spin s – are discrete:

$$n=0,1,2,\ldots;\quad l=0,\pm1,\pm2,\ldots;\quad s=-1,+1, \tag{3.5}$$

while the fourth number, p_z, is a continuous variable. The corresponding non-normalized wave function is

$$\phi_{nlsp_z}(\varrho,\vartheta,z)$$
$$=\exp i(l\vartheta+p_z z/\hbar)\exp(-\xi/2)\,\xi^{|l|/2}L_n^{|l|}(\xi)\,|s\rangle, \tag{3.6}$$

where

$$\xi=\varrho^2/(2a_H^2);\quad a_H^2=\hbar/(m\,\omega_H). \tag{3.7}$$

The functions $L_n^\alpha(x)$ are Laguerre polynomials, and the spinor $|s\rangle$ is $|1\rangle=\begin{pmatrix}1\\0\end{pmatrix}$ and $|-1\rangle=\begin{pmatrix}0\\1\end{pmatrix}$. We note that the electron density corresponding to (3.6) does not depend on the coordinates ϑ and z and the quantum numbers s and p_z:

$$\phi_{nlsp_z}^*\phi_{nlsp_z}=e^{-\xi}\xi^{|l|}[L_n^{|l|}(\xi)]^2. \tag{3.8}$$

Having $\tilde{E}_{nlsp_z}$, (3.3), and ϕ_{nlsp_z}, (3.6), we find the corresponding solution of Dirac's equation by applying (2.9) and (2.2) with (2.4).

4. Derivation of Onsager's Relation by Means of the Correspondence Principle

Onsager's relation concerns the helical orbit of an electron, which is primarily a classical concept. Therefore, Onsager applied the correspondence principle for his derivation. In this section, we do the same for the relativistic theory. An exact quantum mechanical treatment is presented in the next section.

In classical relativistic mechanics the gyroradius of an electron is given by (see e.g. [5])

$$R=v_\perp/\omega, \tag{4.1}$$

where

$$\omega=(ecH)/E \tag{4.2}$$

is the frequency of the gyromotion and

$$E=mc^2\left[1-\frac{v^2}{c^2}\right]^{-1/2} \tag{4.3}$$

is the energy of an electron with velocity $\boldsymbol{v}$. $\boldsymbol{v}_\perp$ is the component of this velocity perpendicular to $\boldsymbol{H}$. $v_\perp$ and v are both constant.

In the following we choose a frame of reference in which $p_z=0$ and therefore

$$v_\perp = v. \tag{4.4}$$

The energy E occurring in (4.2) and (4.3) is the kinetic energy of the electron. It should therefore be given by the eigenenergy E_{nls0} with s set equal to zero. Of course, in fact only values $s=\pm 1$ are allowed, but with these values of s, E_{nls0} also contains contributions stemming from the magnetic moment and the magnetic field. According to (4.2) and (2.9) this leads to

$$\omega = \omega_H \left[1 + \frac{2\tilde{E}_{nls=00}}{m c^2}\right]^{-1/2}. \tag{4.5}$$

This quasi-classical frequency depends on the quantum numbers n and l, while in the limit $c\to\infty$ it is simply ω_H, i.e. independent of n and l.

Essentially the same result can be obtained by Bohr-Sommerfeld's old quantum theory (see e.g. [6]) applied by Onsager. It leads to

$$E = \{m^2 c^4 + 2 m c^2 \hbar\, \omega_H [n + \Theta + \tfrac{1}{2}(l + |l|)]\}^{1/2}. \tag{4.6}$$

This Bohr-Sommerfeld expression for the energy is equal to that given by (2.9) and (3.3) for Θ – which has to be of order 1 – equal to $\frac{1}{2}(1+s)$, with $s=0$. The well known Bohr-Sommerfeld rule yields the frequency of the orbital motion as

$$\omega = \frac{\partial E}{\hbar\,\partial n} = \frac{\omega_H}{\left[1 + \dfrac{2\hbar\,\omega_H [n + \Theta + (l+|l|)/2]}{m c^2}\right]^{1/2}}, \tag{4.7}$$

which agrees with the expression (4.5).

From (4.3), (2.9) and (3.3), we obtain

$$v = \left\{\frac{2\tilde{E}_{nl00}}{m}\left[1 + \frac{2\tilde{E}_{nl00}}{m c^2}\right]^{-1}\right\}^{1/2}. \tag{4.8}$$

This expression differs from the non-relativistic one by the factor appearing in the square brackets. The gyroradius R resulting from (4.1) is then

$$R = \frac{\left\{\dfrac{2\tilde{E}_{nl00}}{m}\left[1 + \dfrac{2\tilde{E}_{nl00}}{m c^2}\right]^{-1}\right\}^{1/2}}{\omega_H \left[1 + \dfrac{2\tilde{E}_{nl00}}{m c^2}\right]^{-1/2}} = \left[\frac{2\tilde{E}_{nl00}}{m}\right]^{1/2} \frac{1}{\omega_H}. \tag{4.9}$$

An important feature of this expression is that the relativistic corrections have cancelled exactly: the radius of a relativistic orbit is given by the same expression as in the non-relativistic case. The corresponding flux of the magnetic field enclosed by the electron orbit,

$$H \pi R^2 = \left[n + \frac{1}{2}(1 + l + |l|)\right]\frac{h c}{e}, \tag{4.10}$$

is therefore also the same, relativistically as well as non-relativistically, and hence identical with Onsager's relation quoted in the Introduction. The shift Θ occuring in Onsager's formula should be of order 1, as mentioned before. In the present derivation it was obtained to be 1/2. Our integer combination $n+\frac{1}{2}(l+|l|)$ corresponds to Onsager's n.

5. Derivation of Onsager's Relation by Means of Exact Quantum-Mechanical Expectation Values

The conclusion of the previous section, that the magnetic flux enclosed by an electron orbit is described relativistically and non-relativistically by the same formula, was obtained for a regime in which the correspondence principle is valid. In this section we generalize the result to arbitrary regimes. The method is to treat this quantity in terms of the expectation value for the flux $H\pi\varrho^2$, where $\varrho^2 = x^2 + y^2$ (see (3.2)).

According to (2.10), the expectation value of any function $\Omega(\boldsymbol{r})$ for a stationary relativistic state, having the quantum number q, is given by

$$\begin{aligned}\langle\Omega\rangle_q &= \langle\psi_q|\Omega\,\psi_q\rangle \\ &= \{\textstyle\int d^3 r\, \psi_q^*(\boldsymbol{r})\,\psi_q(\boldsymbol{r})\,\Omega(\boldsymbol{r})\}/\{\int d^3 r\, \psi_q^*(\boldsymbol{r})\,\psi_q(\boldsymbol{r})\} \\ &= \{\textstyle\int d^3 r\, \phi_q^*(\boldsymbol{r})\,\phi_q(\boldsymbol{r})\,\Omega(\boldsymbol{r})\}/\{\int d^3 r\, \phi_q^*(\boldsymbol{r})\,\phi_q(\boldsymbol{r})\} \\ &= \langle\phi_q|\Omega\,\phi_q\rangle,\end{aligned} \tag{5.1}$$

so it is the same as for a non-relativistic state having the same quantum number q. These states correspond to the electron motion in a static non-uniform magnetic field. Based on this relation, we present here two ways of obtaining an expression for $\langle\varrho^2\rangle$.

The first one makes use of the eigenfunctions (3.6) (see also (3.8)):

$$\langle\varrho^2\rangle = 2 a_H^2 \int_0^\infty d\xi\, e^{-\xi}\,\xi^{|l|+1}\,[L_n^{|l|}(\xi)]^2 \Big/ \int_0^\infty d\xi\, e^{-\xi}\,\xi^{|l|}\,[L_n^{|l|}(\xi)]^2. \tag{5.2}$$

Applying the properties of the Laguerre polynomials [7], namely

$$\int_0^\infty \mathrm{d}\xi\, e^{-\xi}\, \xi^\alpha\, L_n^\alpha(\xi)\, L_{n'}^\alpha(\xi) = \frac{(\alpha+n)!}{n!}\,\delta_{nn'} \tag{5.3}$$

and

$$L_n^\alpha(\xi) = L_n^{\alpha+1}(\xi) - L_{n-1}^{\alpha+1}(\xi);\quad L_0^\alpha = 1;\quad L_{-1}^\alpha = 0, \tag{5.4}$$

we obtain

$$\langle \varrho^2 \rangle = 2\, a_H^2\, (2n + |l| + 1) \tag{5.5}$$

and therefore, with (3.7)

$$H\,\pi\,\langle \varrho^2 \rangle = (2n + |l| + 1)\,\frac{h\,c}{e}. \tag{5.6}$$

This version of Onsager's relation is, according to (5.1), valid relativistically and non-relativistically. The combination $(2n+|l|+1)$ may be any positive integer number. We note, however, that the relations (5.6) and (4.10) are different; this concerns especially the minimum flux obtained for $n=l=0$. Of course, relation (4.10) is not expected to be valid for these values of n and l.

The second way to obtain an expression for $\langle \varrho^2 \rangle$ does not make use of an explicit knowledge of the wave function. We evaluate it for the same states as before, defined by n, l, s, $p_z=0$. The eigenenergy (3.3) of the Schrödinger equation (2.7) may be written as

$$\langle \mathscr{H} \rangle = \frac{1}{2m}\left\langle \left(\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\right)^2 \right\rangle + \frac{e\hbar}{2mc}\langle \boldsymbol{\sigma}\cdot\boldsymbol{H} \rangle$$

$$= \tilde{E}_{nls0} = \hbar\,\omega_H \left[n + \frac{1}{2}(1 + s + l + |l|) \right]. \tag{5.7}$$

With the potential $\boldsymbol{A}$ given by (3.1), one has

$$\frac{1}{2m}\left\langle \left(\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\right)^2 \right\rangle$$

$$= \frac{1}{2m}\langle p_x^2 + p_y^2 \rangle + \frac{e^2 H^2}{8mc^2}\langle x^2 + y^2 \rangle$$

$$+ \frac{eH}{2mc}\langle p_y\, x - p_x\, y \rangle. \tag{5.8}$$

Since the operators $\boldsymbol{\sigma}\cdot\boldsymbol{H}$ and $p_x\, x - p_y\, y$ appearing in (5.7) and (5.8) commute with the Hamiltonian, the quantum numbers l and s correspond to the expectation values

$$\langle p_y\, x - p_x\, y \rangle = l\,\hbar \tag{5.9}$$

and

$$\frac{e\hbar}{2mc}\langle \boldsymbol{\sigma}\cdot\boldsymbol{H} \rangle = \hbar\,\omega_H\,\frac{1}{2}\,s. \tag{5.10}$$

Therefore, (5.7) reduces to

$$\frac{1}{2m}\langle p_x^2 + p_y^2 \rangle + \frac{e^2 H^2}{8mc^2}\langle x^2 + y^2 \rangle$$

$$= \hbar\,\omega_H \left[n + \frac{1}{2}(1 + |l|) \right]. \tag{5.11}$$

Then, owing to the virial theorem, the expectation value of the operator

$$\frac{\mathrm{d}}{\mathrm{d}t}(x\,p_x + y\,p_y) = \frac{i}{\hbar}[\mathscr{H}, x\,p_x + y\,p_y]$$

$$= 2\left[\frac{1}{2m}(p_x^2 + p_y^2) - \frac{e^2 H^2}{8mc^2}(x^2 + y^2) \right] \tag{5.12}$$

vanishes. After inserting this result in (5.11) we obtain

$$\frac{e^2 H^2}{4mc^2}\langle x^2 + y^2 \rangle = \hbar\,\omega_H \left[n + \frac{1}{2}(1 + |l|) \right], \tag{5.13}$$

or, with the definitions (3.4) and (3.7),

$$\langle \varrho^2 \rangle = 2\, a_H^2\, (2n + 1 + |l|) \tag{5.14}$$

which is again the result (5.5).

[1] L. Onsager, Phil. Mag. **43,** 1006 (1952).

[2] V. B. Berestetzkii, E. M. Lifshitz, and L. P. Pitaevskii, Relativistic Quantum Theory, Vol. 4 of Course of Theoretical Physics, Nauka, Moscow 1962 (in Russian), or Quantum Electrodynamics, Vol. 4 of Course of Theoretical Physics, Pergamon Press, Oxford 1982.

[3] L. I. Schiff, Quantum Mechanics, MacGraw-Hill Book Company Inc., New York 1955, p. 329, Eq. (43.25).

[4] L. D. Landau and E. M. Lifshitz, Quantum Mechanics (Non-relativistic Theory), Vol. 3 of Course of Theoretical Physics, Nauka, Moscow 1974 (in Russian), or Pergamon Press, Oxford 1965.

[5] L. D. Landau and E. M. Lifshitz, Course of Theoretical Physics, Vol. 2: The Classical Theory of Fields, Pergamon Press, Oxford 1975.

[6] A. Sommerfeld, Atombau und Spektrallinien, Vol. 1 5th ed., Vieweg, Braunschweig 1931.

[7] Higher Transcendental Functions, Vol. 2, Editor: A. Erdélyi, MacGraw-Hill, New York 1953.