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Gauge invariance of the energy shift of a bound electron in an electromagnetic field

Donald H Kobe and Shahram M Golshan

Department of Physics, North Texas State University, Denton, TX 76203, USA

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Abstract. The shift in the energy of a bound electron due to an electromagnetic field is shown to be gauge invariant if eigenvalues of the energy operator, which is not in general the Hamiltonian, are used. Using eigenvalues of the energy operator, we show by a direct calculation that the energy shift in a zero electromagnetic field is zero, even if the potentials are not zero.

1. Introduction

For a bound electron in an external electromagnetic field, the energy levels are shifted. The energy shift should, of course, be the same regardless of what gauge is chosen for the vector and scalar potentials in terms of which the interaction is formulated. This paper proves that the energy shift is indeed gauge invariant if eigenvalues of the energy operator [1-3], not the Hamiltonian, are used. The eigenvalues of the Hamiltonian are shown to be gauge dependent, and so cannot in general be the energy eigenvalues. Since the energy operator used here has recently been criticised [4], it is important to show that even in static problems it is necessary to make the distinction between the Hamiltonian and the energy operator.

If the electromagnetic field is zero, the energy shift is zero because the zero electromagnetic field can be described by zero vector and scalar potentials. If non-zero vector and scalar potentials are chosen to describe the zero electromagnetic field [5], the energy shift should still be zero by gauge invariance. The explicit formula for the energy shift is not, however, obviously zero in this case. It has been conjectured that, if the potentials are not zero in a field-free region, an energy shift could be induced by these non-zero potentials [6]. If no magnetic flux pierces the electron's orbit this bound-state Aharonov-Bohm effect [7, 8] should be zero by gauge invariance. We show by a direct calculation that in this case the energy shift does vanish if the energy operator, not the Hamiltonian, is used.

The energy shift is calculated using the energy operator of the electron, which is not in general its Hamiltonian [1-3]. If the gauge function depends on the time (on which it can be chosen to depend even in static problems), the Hamiltonian and the energy operator are different. In this case, eigenvalues of the Hamiltonian are gauge dependent and so do not satisfy the requirement of gauge invariance which is required for an observable [9, 10]. The calculations of this paper vindicate the use of the energy operator over the Hamiltonian to determine the energy eigenstates of the system.

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In § 2 the general formula for the energy shift of an electron in an electromagnetic field is determined. When the electromagnetic field is zero, § 3 shows that the energy shift is indeed zero even if non-zero potentials are used. In § 4 the general expression for the energy shift is shown to be gauge invariant. The gauge dependence of the Hamiltonian and its eigenvalues is discussed in § 5. Finally, the conclusions are given in § 6.

2. Energy shift in an electromagnetic field

An electron of charge q and mass m is in a time-dependent electromagnetic field $\boldsymbol{E}(\boldsymbol{r}, t)$ and $\boldsymbol{B}(\boldsymbol{r}, t)$ characterised by the vector potential $\boldsymbol{A}(\boldsymbol{r}, t)$ and the scalar potential $\phi(\boldsymbol{r}, t)$, where

$$\boldsymbol{E} = -\nabla\phi - \partial\boldsymbol{A}/\partial tc \qquad \boldsymbol{B} = \nabla \times \boldsymbol{A}. \tag{2.1}$$

The Schrödinger equation for the wavefunction ψ of the electron is

$$H(\boldsymbol{A}, \phi)\psi = \mathrm{i}\hbar\partial\psi/\partial t. \tag{2.2}$$

The Hamiltonian in equation (2.2) is

$$H = H(\boldsymbol{A}, \phi) = (2m)^{-1}(\boldsymbol{p} - q\boldsymbol{A}/c)^2 + V(\boldsymbol{r}) + q\phi(\boldsymbol{r}, t) \tag{2.3}$$

where $\boldsymbol{p} = -\mathrm{i}\hbar\nabla$ is the canonical momentum operator. The (conservative) potential energy $V(\boldsymbol{r})$ of the electron can be of gravitational, nuclear or electrostatic origin. The scalar potential term $q\phi(\boldsymbol{r}, t)$ of the time-dependent electromagnetic field is not conservative.

The energy operator for the electron [1-3]

$$\mathscr{E} = \tfrac{1}{2}mv^2 + V(\boldsymbol{r}) \tag{2.4}$$

is the sum of the kinetic energy operator and the conservative potential energy $V(\boldsymbol{r})$. The velocity operator $\boldsymbol{v}$ times the mass m is the kinetic momentum

$$m\boldsymbol{v} = \boldsymbol{p} - q\boldsymbol{A}/c. \tag{2.5}$$

Using equations (2.4) and (2.5) we see that the energy operator $\mathscr{E}$ is related to the Hamiltonian H in equation (2.3) by

$$\mathscr{E} = H - q\phi \tag{2.6}$$

where $\phi = \phi(\boldsymbol{r}, t)$ is the scalar potential of the time-dependent electromagnetic field.

The eigenenergies of the electron with potential energy $V(\boldsymbol{r})$ in the electromagnetic field is found from the eigenvalue equation for the energy operator $\mathscr{E}$

$$\mathscr{E}\psi_n = \varepsilon_n\psi_n \tag{2.7}$$

where ε_n is the eigenenergy and ψ_n is the energy eigenstate. This eigenvalue problem may be difficult to solve in practice, and it may be necessary to use perturbation [11] or other approximation methods. An explicit expression can be obtained for the energy shift. The energy operator $\mathscr{E}$ in equation (2.4) may be written as

$$\mathscr{E} = H_0 + \mathscr{V}. \tag{2.8}$$

The perturbation $\mathscr{V}$ may be written as the sum of two terms

$$\mathscr{V} = \mathscr{V}^{(1)} + \mathscr{V}^{(2)} \tag{2.9}$$

where the first-order term in q is

$$\mathcal{V}^{(1)} = -(q/2mc)(\boldsymbol{A}\cdot\boldsymbol{p}+\boldsymbol{p}\cdot\boldsymbol{A}) \tag{2.10}$$

and the second-order term in q is

$$\mathcal{V}^{(2)} = (q^2/2mc^2)A^2. \tag{2.11}$$

Note that because of equation (2.6) the $q\phi$ term does not appear in equation (2.10). The unperturbed Hamiltonian H_0 in equation (2.8) is

$$H_0 = p^2/2m + V(\boldsymbol{r}) \tag{2.12}$$

where $\boldsymbol{p}$ is the canonical momentum. The eigenvalue problem for the unperturbed Hamiltonian is

$$H_0\phi_n = E_n\phi_n \tag{2.13}$$

where E_n is the unperturbed energy and ϕ_n is the unperturbed energy eigenstate.

The energy shift which results from the presence of the electromagnetic field can be calculated by substituting equation (2.8) into equation (2.7), and taking the inner product with ϕ_n in equation (2.13). We then obtain

$$\Delta\varepsilon_n = \varepsilon_n - E_n = \langle\phi_n|\mathcal{V}\psi_n\rangle/\langle\phi_n|\psi_n\rangle \tag{2.14}$$

where the interaction $\mathcal{V}$ is given in equation (2.9). The energy shift in equation (2.14) may now be calculated from perturbation theory or other approximation. As shown in § 4 the energy shift in equation (2.14) is gauge invariant.

3. Energy shift in zero electromagnetic field

In the special case that the electromagnetic field is zero, the energy shift can be calculated from equation (2.14). If zero potentials are used, the interaction $\mathcal{V}$ is zero and the corresponding energy shift is zero. However, non-zero potentials,

$$\boldsymbol{A} = -\nabla\Lambda \qquad \phi = \partial\Lambda/\partial tc \tag{3.1}$$

where $\Lambda = \Lambda(\boldsymbol{r}, t)$ is an arbitrary differentiable function, such that $\nabla\partial\Lambda/\partial t = \partial\nabla\Lambda/\partial t$, can be used to describe the zero electromagnetic field [4]. If equation (3.1) is used in equation (2.1) the result is $\boldsymbol{E} = 0$ and $\boldsymbol{B} = 0$.

The energy shift due to the zero electromagnetic field described by the non-zero potentials is

$$\Delta\varepsilon_n = \langle\phi_n|\mathcal{V}_0\psi_n\rangle/\langle\phi_n|\psi_n\rangle. \tag{3.2}$$

The 'pseudointeraction' [12] $\mathcal{V}_0$ due to the zero electromagnetic field described by the non-zero potentials in equation (3.1) is

$$\mathcal{V}_0 = \mathcal{V}_0^{(1)} + \mathcal{V}_0^{(2)} \tag{3.3}$$

where the first-order term in q is

$$\mathcal{V}_0^{(1)} = (q/2mc)(\nabla\Lambda\cdot\boldsymbol{p}+\boldsymbol{p}\cdot\nabla\Lambda) \tag{3.4}$$

from equation (2.10), and the second-order term in q is

$$\mathcal{V}_0^{(2)} = (q^2/2mc^2)(\nabla\Lambda)^2 \tag{3.5}$$

from equation (2.11). The eigenfunction ψ_n of the energy operator $\mathscr{E}$ in equation (2.4) with $\boldsymbol{A} = -\nabla\Lambda$ is

$$\psi_n = \exp(-iq\Lambda/\hbar c)\phi_n \tag{3.6}$$

where ϕ_n is the eigenstate of H_0 in equation (2.13). When equation (3.6) is substituted into equation (2.7), the eigenvalue problem reduces to equation (2.13) if $\varepsilon_n = E_n$. Therefore the energy shift $\Delta\varepsilon_n = \varepsilon_n - E_n = 0$ in this case.

On the other hand, the energy shift $\Delta\varepsilon_n$ is given by equation (3.2), which becomes

$$\Delta\varepsilon_n = \langle\phi_n|\mathscr{V}_0 \exp(-iq\Lambda/\hbar c)\phi_n\rangle / \langle\phi_n|\exp(-iq\Lambda/\hbar c)\phi_n\rangle \tag{3.7}$$

when equation (3.6) is used. This energy shift should, of course, be zero if the energy shift is gauge invariant. A direct calculation shows that equation (3.7) is indeed zero. The operator $\mathscr{V}_0 \exp(-iq\Lambda/\hbar c)$ can be written as

$$\mathscr{V}_0 \exp(-iq\Lambda/\hbar c) = \tfrac{1}{2}\{\mathscr{V}_0, \exp(-iq\Lambda/\hbar c)\} + \tfrac{1}{2}[\mathscr{V}_0, \exp(-iq\Lambda/\hbar c)] \tag{3.8}$$

where $\{,\}$ is the anticommutator and $[,]$ is the commutator. The commutator in equation (3.8) is

$$\begin{aligned}[\mathscr{V}_0, \exp(-iq\Lambda/\hbar c)] &= -(q^2/mc^2)(\nabla\Lambda)^2 \exp(-iq\Lambda/\hbar c) \\ &= -2\mathscr{V}_0^{(2)} \exp(-iq\Lambda/\hbar c)\end{aligned} \tag{3.9}$$

from equations (3.4) and (3.5). If equation (3.9) is substituted into equation (3.8), the result is

$$\mathscr{V}_0 \exp(-iq\Lambda/\hbar c) = \tfrac{1}{2}\{\mathscr{V}_0^{(1)}, \exp(-iq\Lambda/\hbar c)\} \tag{3.10}$$

when equation (3.3) is used. The numerator of the energy shift in equation (3.7) is therefore

$$\begin{aligned}&\langle\phi_n|\mathscr{V}_0 \exp(-iq\Lambda/\hbar c)\phi_n\rangle \\ &\quad = \mathrm{Re}\langle\phi_n|\cos(q\Lambda/\hbar c)\mathscr{V}_0^{(1)}\phi_n\rangle - i\,\mathrm{Re}\langle\phi_n|\sin(q\Lambda/\hbar c)\mathscr{V}_0^{(1)}\phi_n\rangle\end{aligned} \tag{3.11}$$

when equation (3.10) and the hermiticity of $\mathscr{V}_0^{(1)}$ are used.

The first term on the right-hand side of equation (3.11) can be written as

$$\begin{aligned}\mathrm{Re}\langle\phi_n|\cos(q\Lambda/\hbar c)\mathscr{V}_0^{(1)}\phi_n\rangle &= (\hbar/m)\,\mathrm{Re}\langle\phi_n|\nabla\sin(q\Lambda/\hbar c)\cdot\boldsymbol{p}\phi_n\rangle \\ &= \hbar\int \mathrm{d}^3r\,\nabla\sin(q\Lambda/\hbar c)\cdot\boldsymbol{J}_n(\boldsymbol{r}).\end{aligned} \tag{3.12}$$

The probability current density $\boldsymbol{J}_n$ in the state ϕ_n is

$$\boldsymbol{J}_n(\boldsymbol{r}) = m^{-1}\,\mathrm{Re}\,\phi_n^*\boldsymbol{p}\phi_n \tag{3.13}$$

which satisfies the equation of continuity [13]

$$\nabla\cdot\boldsymbol{J}_n = 0 \tag{3.14}$$

for the stationary state ϕ_n by equation (2.13). Using the vector identity for the divergence of a vector times a scalar and the divergence theorem, we can transform equation (3.12) into

$$\begin{aligned}&\mathrm{Re}\langle\phi_n|\cos(q\Lambda/\hbar c)\mathscr{V}_0^{(1)}\phi_n\rangle \\ &\quad = \hbar\oint_{S=\partial\infty} \mathrm{d}\mathscr{A}\cdot\boldsymbol{J}_n(\boldsymbol{r})\sin(q\Lambda/\hbar c) - \hbar\int \mathrm{d}^3r\sin(q\Lambda/\hbar c)\nabla\cdot\boldsymbol{J}_n(\boldsymbol{r}) \\ &\quad = 0.\end{aligned} \tag{3.15}$$

The second term on the right-hand side of equation (3.15) vanishes because of equation (3.14). The first term on the right-hand side vanishes because the probability current $d\mathscr{A} \cdot \boldsymbol{J}_n(\boldsymbol{r})$ vanishes for the surface S at infinity, $S = \partial\infty$.

In a similar manner it can be shown that the second term on the right-hand side of equation (3.11) is also zero,

$$\mathrm{Re}\langle\phi_n|\sin(q\Lambda/\hbar c)\mathscr{V}_0^{(1)}\phi_n\rangle$$

$$= -\hbar \oint_{S=\partial\infty} d\mathscr{A} \cdot \boldsymbol{J}_n(\boldsymbol{r}) \cos(q\Lambda/\hbar c) + \hbar \int d^3r \cos(q\Lambda/\hbar c)\nabla \cdot \boldsymbol{J}_n = 0 \quad (3.16)$$

where the right-hand side vanishes as in equation (3.15). Thus equation (3.11) vanishes because of equations (3.15) and (3.16). Since equation (3.11) is the numerator of the energy shift in equation (3.7), we have

$$\Delta\varepsilon_n = 0 \quad (3.17)$$

for a zero electromagnetic field. The direct calculation shows that for a zero electromagnetic field the energy shift is gauge invariant.

4. Gauge invariance of the energy shift

Even when the electromagnetic field is non-zero, the energy shift $\Delta\varepsilon_n$ in equation (2.14) is gauge invariant. If we make a transformation on the potentials to a new gauge

$$\boldsymbol{A}' = \boldsymbol{A} + \nabla\Lambda \qquad \phi' = \phi - \partial\Lambda/\partial tc \quad (4.1)$$

the wavefunctions ψ and ψ_n must also be transformed

$$\psi' = \exp(iq\Lambda/\hbar c)\psi \qquad \psi'_n = \exp(iq\Lambda/\hbar c)\psi_n. \quad (4.2)$$

The gauge transformed energy operator $\mathscr{E}'$ is [1-3]

$$\mathscr{E}' = (2m)^{-1}(\boldsymbol{p} - q\boldsymbol{A}'/c)^2 + V(\boldsymbol{r}) = \exp(iq\Lambda/\hbar c)\mathscr{E}\exp(-iq\Lambda/\hbar c) \quad (4.3)$$

which is a unitary transformation on equation (2.4). When equation (2.7) is multiplied by $\exp(iq\Lambda/\hbar c)$, the energy eigenvalue problem in equation (2.7) becomes

$$\mathscr{E}'\psi'_n = \varepsilon_n\psi'_n \quad (4.4)$$

with the same energy eigenvalue ε_n.

In the new gauge the energy shift in equation (2.14) becomes

$$\Delta\varepsilon'_n = \langle\phi_n|\mathscr{V}'\psi'_n\rangle/\langle\phi_n|\psi'_n\rangle. \quad (4.5)$$

The new interaction $\mathscr{V}'$ is the same as the old interaction $\mathscr{V}$ in equation (2.9) but with $\boldsymbol{A}$ replaced by $\boldsymbol{A}'$ in equations (2.10) and (2.11). The new interaction can be written as

$$\mathscr{V}' = \mathscr{E}' - H_0 \quad (4.6)$$

where the new energy operator $\mathscr{E}'$ is given in equation (4.3). Therefore the energy shift in equation (4.5) is

$$\Delta\varepsilon'_n = \langle\phi_n|(\mathscr{E}' - H_0)\psi'_n\rangle/\langle\phi_n|\psi'_n\rangle$$

$$= \varepsilon_n - E_n = \Delta\varepsilon_n \quad (4.7)$$

when equations (4.4), (2.13) and (2.14) are used. Thus when eigenvalues of the energy operator are used, the energy shift is gauge invariant.

In particular, the result of § 3 can be understood because a zero electromagnetic field can be described equally well by the potentials in equation (3.1) or by the new potentials $\boldsymbol{A}' = 0$, $\phi' = 0$ when equation (3.1) is used in equation (4.1). The energy shift in equation (4.5) in the new gauge is obviously $\Delta\varepsilon'_n = 0$ because the interaction $\mathscr{V}'_0 = 0$. This result agrees with $\Delta\varepsilon_n = 0$ in equation (3.17).

5. Gauge dependence of the Hamiltonian

In this section we show that the Hamiltonian is gauge dependent. The eigenvalue problem for the Hamiltonian gives gauge-dependent eigenvalues and eigenstates. Since the energy is an observable it is essential that energy differences be gauge invariant, which is guaranteed by using the energy operator. Since the Hamiltonian is gauge dependent, it is not in general an observable. Only in certain gauges does the Hamiltonian reduce to the energy operator.

Under the gauge transformation of equation (4.1) the Schrödinger equation in equation (2.2) becomes

$$H(\boldsymbol{A}', \phi')\psi' = \mathrm{i}\hbar\partial\psi'/\partial t \tag{5.1}$$

where the gauge transformed wavefunction ψ' is given in equation (4.2). The new gauge transformed Hamiltonian $H' = H(\boldsymbol{A}', \phi')$ is related to the old Hamiltonian $H = H(\boldsymbol{A}, \phi)$ by [1-3]

$$H(\boldsymbol{A}', \phi') = \exp(\mathrm{i}q\Lambda/\hbar c)H(\boldsymbol{A}, \phi)\exp(-\mathrm{i}q\Lambda/\hbar c) - q\partial\Lambda/\partial tc. \tag{5.2}$$

Because of the last term in equation (5.2) the expectation value of the Hamiltonian is not gauge invariant.

The eigenvalue problem for H is

$$H\chi_n = h_n\chi_n \tag{5.3}$$

where h_n is the eigenvalue and χ_n is the eigenstate. For the Hamiltonian H' in the new gauge the eigenvalue problem is

$$H'\chi'_n = h'_n\chi'_n. \tag{5.4}$$

The new eigenvalue $h'_n \neq h_n$, in general, and the new eigenstate χ'_n is not in general equal to $\exp(\mathrm{i}q\Lambda/\hbar c)\chi_n$. The reason for the gauge dependence of the eigenvalues is the last term in equation (5.2), which does not vanish for gauge functions Λ which depend on the time. For the eigenvalues of the Hamiltonian, the shift $h_n - E_n$ is not an energy shift. Because the eigenvalues are gauge dependent $h'_n - E_n \neq h_n - E_n$, in general.

In the special case that the temporal gauge $\phi' = 0$ is chosen, the Hamiltonian $H' = H(\boldsymbol{A}', 0)$ is equal to the energy operator $\mathscr{E}' = H' - q\phi' = H'$. In this gauge the eigenstates and eigenvalues of the Hamiltonian and energy operator coincide.

6. Conclusion

The energy shift of an electron due to an electromagnetic field is proved in this paper to be gauge invariant. Eigenvalues of the Hamiltonian are in general gauge dependent, since the Hamiltonian is a gauge-dependent operator with a gauge-dependent expectation value. It is essential when dealing with gauge functions Λ which depend on the

time to use the energy operator, which has a gauge-invariant expectation value and gauge-invariant eigenvalues. It is the energy operator, not in general the Hamiltonian, which is the proper quantum mechanical observable when the energy is measured. The distinction between the Hamiltonian and the energy operator resolves the problem stated by Kramers [14] that '... even the extremely important problem of the energy [has] not a gauge invariant meaning.'

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