Relativistic and radiative corrections to the dynamic Stark shift: Gauge invariance and transition currents in the velocity gauge

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We investigate the gauge invariance of the dynamic (ac) Stark shift under "hybrid" gauge transformations from the "length" ($\vec{E}\cdot\vec{r}$) to the "velocity" ($\vec{A}\cdot\vec{p}$) gauge. By a "hybrid" gauge transformation, we understand a transformation in which the scalar and vector potentials are modified, but the wave function remains unaltered. The gauge invariance of the leading term is well known, while we here show that gauge invariance under perturbations holds only if one takes into account an additional correction to the transition current, which persists only in the velocity gauge. We find a general expression for this current, and apply the formalism to radiative and relativistic corrections to the dynamic Stark effect, which is described by the sum of two polarizability matrix elements.

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I. INTRODUCTION

One might think that all conceivable questions regarding the gauge invariance of physical processes in quantum electrodynamics (QED) have already been addressed in the literature. That is not the case. The point is that strictly speaking, a transformation from the "length" ($\vec{E}\cdot\vec{r}$) to the "velocity" ($\vec{A}\cdot\vec{p}$) gauge requires a gauge transformation of the wave function, which is, however, inconvenient to implement in practice, and whose necessity is almost always ignored in practical calculations [1]. Indeed, a particularly interesting gauge transformation is the Power-Zienau transformation, which transforms the QED Hamiltonian from the $\vec{A}\cdot\vec{p}$ ("velocity") to the $\vec{E}\cdot\vec{r}$ ("length") form [2,3].

The question then is which gauge should be used in the analysis, e.g., of spectroscopic experiments as one models the excitation dynamics [1,4,5]. In a now famous remark on page 268 of Ref. [4], Lamb notices that the interpretation of the wave function is only preserved in the length gauge, and that this gauge should be used, therefore, in the description of his experiments. Specifically, this is because the momentum operator retains its physical interpretation only in the length gauge, without being modified by the presence of a nonvanishing vector potential, which otherwise makes it necessary to distinguish kinetic and canonical momenta [1].

Here, we would like to refer to a gauge transformation which ignores the phase of the wave function as a "hybrid" gauge transformation. Recently, it has been shown in Ref. [6] that, under "hybrid" gauge transformations, two-photon transition matrix elements are manifestly gauge "dependent" (not gauge invariant) off resonance (i.e., when one transforms from the length to the velocity gauge and ignores the gauge transformation of the wave function). Specifically, in two-photon transitions, the gauge invariance of transition matrix elements under the hybrid scheme holds only at exact resonance [6].

In contrast, it is well known [5,7–10] that a number of other processes which involve laser-atom interactions, such as the ac Stark shift, or radiative corrections to the real and imaginary part of the polarizability [9,10], are in fact gauge invariant under the "hybrid" transformations. The common picture here is that one could, in principle, formulate these effects in terms of an adiabatic switching of the interaction Hamiltonian with a factor $\exp(-\varepsilon|t|)$, where ε is infinitesimal and t is the time variable, invoke the Gell-Mann and Low theorem (Eq. (21) of Ref. [11]), and carry out the gauge transformation of the wave function at $t=\pm\infty$, where it amounts to the identity transformation (because the perturbing fields vanish). All processes which allow for such a description have been found to be gauge invariant under "hybrid" transformations [5,7–10].

We here investigate questions related to processes which are gauge invariant under "hybrid" gauge transformations. Let us suppose that the (Schrödinger) Hamiltonian H of the system is being perturbed by an additional Hamiltonian δH. This perturbation induces a change in the energy by $\delta E = \langle\phi|\delta H|\phi\rangle$, and the wave function perturbation is $|\delta\phi\rangle = [1/(E-H)']\delta H|\phi\rangle$, where $[1/(E-H)']$ is the reduced Green's function. The question we pose is as follows: Which perturbation to the interaction Hamiltonian (i.e., to the transition current) needs to be added in the velocity gauge, for general δH, in order to ensure gauge invariance of energy shifts, when we consider the transformation from the velocity to the length gauge?

We shall investigate this question, using the ac Stark shift as an example. Indeed, quite recently, the ac Stark shift has been investigated in strong laser fields [12,13], with an emphasis on the dressed-state formalism, and on the nontrivial additional QED corrections which influence the Mollow spectrum of the emitted radiation, beyond the trivial shift of the unperturbed atomic levels, due to QED effects. The relativistic and radiative corrections to the incoherent radiation spectrum emitted by the dressed states have been analyzed. By contrast, in a weak laser field, the atom-laser interaction can be treated perturbatively. The perturbative effect of a time-varying electric field is commonly referred to as the dynamic or ac ("alternating current") Stark shift [11,14].

We organize this paper as follows. After recalling fundamental aspects of a gauge transformations in Sec. II A, we present in Sec. II B a short orientation on the leading-order dynamic (ac) Stark shift. In Secs. III A and III B, we examine the question of how a perturbative potential modifies the dynamic polarizability and, hence, the ac Stark shift in the length and in the velocity gauges, respectively. A proof of the gauge invariance of the dynamic polarizability induced by a perturbative potential is presented in Sec. IV A. Two special cases of perturbative potentials are of phenomenological relevance (see Sec. IV B), namely, (i) an effective Lamb-shift potential which describes the leading radiative correction to the ac Stark shift, and (ii) the Hamiltonian describing the leading relativistic correction.

II. FOUNDATIONS

A. Gauge transformation

We recall that under an electromagnetic U(1) gauge transformation, a wave function $\phi(\vec{r},t)$ transforms as follows,

$$\phi(\vec{r},t) \to \phi'(\vec{r},t) = \exp\left(\frac{ie\Lambda(\vec{r},t)}{\hbar}\right)\phi(\vec{r},t), \qquad \text{(1a)}$$

and the scalar and vector potentials transform as

$$\vec{A}(\vec{r},t) \to \vec{A}'(\vec{r},t) = \vec{A}(\vec{r},t) + \vec{\Delta}\Lambda(\vec{r},t), \qquad \text{(1b)}$$

$$\Phi(\vec{r},t) \to \Phi'(\vec{r},t) = \Phi(\vec{r},t) - \frac{\partial}{\partial t}\Lambda(\vec{r},t), \qquad \text{(1c)}$$

where $\Lambda(\vec{r},t)$ is an arbitrary function of $\vec{r}$ and t, while $\vec{A}(\vec{r},t)$ and $\Phi(\vec{r},t)$ are, respectively, the vector and the scalar potentials. Under a full gauge transformation of the wave function and the potentials, transition matrix elements and energy shifts are invariant. However, it is sometimes computationally cumbersome to implement a gauge transformation of both the wave function and potentials, and one often resorts to a hybrid gauge transformation [1,6,15,16], where the wave function is left invariant, and only the (vector) potentials are transformed.

B. Leading (nonrelativistic) dynamic Stark shift

We assume an atom to be irradiated by a laser with polarization vector $\hat{\epsilon}_{\rm L}$. To good approximation, one may ignore the magnetic field which leads to a small perturbation of the interaction. We implicitly assume that the atom is in a standing-wave laser field at a point of maximum electric field intensity, where the magnetic field completely vanishes. This approximation was also made in Ref. [14]. Field-configuration dependent corrections are discussed in Sec. IV of Ref. [5] and in Sec. III of Ref. [17].

The dynamic Stark shift $\Delta E_{\rm ac}$ is given by

$$\Delta E_{\rm ac} = -\frac{e^2 I_L Q}{2c\epsilon_0\omega^2}, \qquad \text{(2a)}$$

$$Q = \omega^2\biggl(\langle\phi|(\vec{\epsilon}_{\rm L}\cdot\vec{x})\frac{1}{H-E+\omega}(\vec{\epsilon}_{\rm L}\cdot\vec{x})|\phi\rangle + \langle\phi|(\vec{\epsilon}_{\rm L}\cdot\vec{x})\frac{1}{H-E-\omega}(\vec{\epsilon}_{\rm L}\cdot\vec{x})|\phi\rangle\biggr). \qquad \text{(2b)}$$

Here ω is the angular laser frequency, and I_L is the laser intensity. Here and in the following, we will assume, without loss of generality, that the laser field is oriented along the z axis, i.e., $\vec{\epsilon}_{\rm L} = \hat{z}$. The corresponding canonically conjugate momentum will be denoted by $p^z = -i\partial/(\partial z)$. We can restrict the discussion to a z-polarized laser field with frequency ω because the only atomic states under investigation here are S states which are isotropic. In contrast, the dynamic Stark shift would depend on the magnetic quantum number of P states and states with higher orbital angular momenta.

III. PERTURBATIONS

A. Length-gauge perturbation

In the following, we use natural units with $\epsilon_0 = \hbar = c = 1$, as is customary in the treatment of relativistic corrections in atomic physics. Thus, for example, in our unit system, the Rydberg constant R_∞ is equal to $\alpha^2 m/2$. Our unit of length is the reduced electron Compton wavelength. We consider a perturbation to the dynamic Stark shift (2) due to some perturbation δH which is added to the Schrödinger Hamiltonian. Because both relativistic as well as the leading logarithmic radiative corrections can be expressed in terms of perturbative potentials, the formalism developed here allows for a unified treatment of the relativistic and radiative corrections to the dynamic polarizability, as discussed below in Sec. IV B.

In the length gauge, the dynamic Stark shift is proportional to the quantity Q [see Eq. (2)] which may be expressed as

$$Q = \omega^2\rho, \qquad \rho = \rho_1 + \rho_2, \qquad \text{(3)}$$

where in turn (the reference state is $|\phi\rangle$),

$$\rho_1 = \langle\phi|z\frac{m}{H-E+\omega}z|\phi\rangle, \qquad \text{(4a)}$$

$$\rho_2 = \langle\phi|z\frac{m}{H-E-\omega}z|\phi\rangle. \qquad \text{(4b)}$$

We now consider the first-order perturbation received by the quantity ρ via the action of a perturbative Hamiltonian δH which modifies the Schrödinger Hamiltonian H according to $H \to H + \delta H$. The perturbation δH leads to a perturbation of the energy of the bound state, of the wave function and, of course, δH also constitutes a correction to the Hamiltonian H in the propagator denominator. In general, we have the following first-order perturbations:

$$H \to H + \delta H, \qquad \text{(5a)}$$

$$E \to E + \delta E, \qquad \delta E = \langle\phi|\delta H|\phi\rangle, \qquad \text{(5b)}$$

$$|\phi\rangle \to |\phi\rangle + \left(\frac{1}{E-H}\right)'\delta H|\phi\rangle. \qquad \text{(5c)}$$

Here, the prime in the operator $1/(E-H)'$ indicates that the reference state is excluded from the spectral decomposition of the operator ("reduced Green's function"). The correction received by Q via the action of δH is then

$$\delta Q = \omega^2\delta\rho, \qquad \text{(6)}$$

where $\delta\rho$ is the sum of six terms,

$$\delta\rho = \sum_{j=1}^{6}\delta\rho_j. \qquad \text{(7)}$$

Here, $\delta\rho_1$ and $\delta\rho_2$ are perturbations to the Hamiltonian,

$$\delta\rho_1 = -\langle\phi|z\frac{m}{H-E+\omega}\delta H\frac{1}{H-E+\omega}z|\phi\rangle, \quad (8a)$$

$$\delta\rho_2 = -\langle\phi|z\frac{m}{H-E-\omega}\delta H\frac{1}{H-E-\omega}z|\phi\rangle. \quad (8b)$$

The quantities $\delta\rho_3$ and $\delta\rho_4$ are energy perturbations,

$$\delta\rho_3 = \langle\phi|z\left(\frac{m}{H-E+\omega}\right)^2 z|\phi\rangle\frac{\langle\phi|\delta H|\phi\rangle}{m}, \quad (8c)$$

$$\delta\rho_4 = \langle\phi|z\left(\frac{m}{H-E-\omega}\right)^2 z|\phi\rangle\frac{\langle\phi|\delta H|\phi\rangle}{m}. \quad (8d)$$

Finally, the terms $\delta\rho_{5,6}$ are perturbations to the wave function,

$$\delta\rho_5 = 2\langle\phi|z\frac{m}{H-E+\omega}z\left(\frac{1}{E-H}\right)'\delta H|\phi\rangle, \quad (8e)$$

$$\delta\rho_6 = 2\langle\phi|z\frac{m}{H-E-\omega}z\left(\frac{1}{E-H}\right)'\delta H|\phi\rangle. \quad (8f)$$

B. Velocity-gauge perturbation

The dynamic Stark shift, in the velocity gauge, is proportional to the quantity Q' which may be expressed as

$$Q' = \chi, \qquad \chi = \chi_1 + \chi_2 + \chi_3, \quad (9)$$

where

$$\chi_1 = \langle\phi|\frac{p^z}{m}\frac{m}{H-E+\omega}\frac{p^z}{m}|\phi\rangle, \quad (10a)$$

$$\chi_2 = \langle\phi|\frac{p^z}{m}\frac{m}{H-E-\omega}\frac{p^z}{m}|\phi\rangle, \quad (10b)$$

$$\chi_3 = -\langle\phi|\phi\rangle = -1. \quad (10c)$$

The seagull term is responsible for χ_3. The prime in Q' denotes the velocity-gauge form of the correction. It is instructive to observe that the large-ω asymptotic of Q' reads as follows,

$$\begin{aligned} Q' &= -1 - 2\frac{m}{\omega^2}\langle\phi|\frac{p^z}{m}(H-E)\frac{p^z}{m}|\phi\rangle \\ &= -1 - \frac{m}{\omega^2}\langle\phi|\frac{1}{3}\vec{\nabla}^2(V)|\phi\rangle \\ &= -1 - \frac{m}{\omega^2}\langle\phi|\frac{4}{3}\frac{\pi(Z\alpha)}{m^2}\delta^{(3)}(\vec{r})|\phi\rangle \\ &= -1 - \frac{4}{3}\frac{(Z\alpha)^4}{n^3}\frac{m^2}{\omega^2}\delta_{\ell 0}, \end{aligned} \quad (11)$$

where we assume a hydrogenic state with principal quantum number n that is nonvanishing at the origin only for S symmetry,

$$\langle\phi|\delta^{(3)}(\vec{r})|\phi\rangle = \frac{(Z\alpha m)^3}{\pi n^3}\delta_{\ell 0}. \quad (12)$$

The first-order correction to the dynamic polarizability, in the velocity gauge, is

$$\delta Q' = \delta\chi, \quad (13)$$

where again the prime denotes the velocity-gauge form of the correction. Eventually, we desire to show that $\delta Q = \delta Q'$.

Just like its length-gauge counterpart $\delta\rho$, the velocity-gauge correction $\delta\chi$ is the sum of various terms,

$$\delta\chi = \sum_{j=1}^{8}\delta\chi_j. \quad (14)$$

Here, $\delta\chi_1$ and $\delta\chi_2$ are perturbations of the Hamiltonian,

$$\delta\chi_1 = -\langle\phi|\frac{p^z}{m}\frac{m}{H-E+\omega}\delta H\frac{1}{H-E+\omega}\frac{p^z}{m}|\phi\rangle, \quad (15a)$$

$$\delta\chi_2 = -\langle\phi|\frac{p^z}{m}\frac{m}{H-E-\omega}\delta H\frac{1}{H-E-\omega}\frac{p^z}{m}|\phi\rangle. \quad (15b)$$

The quantities $\delta\chi_3$ and $\delta\chi_4$ are energy perturbations,

$$\delta\chi_3 = \langle\phi|\frac{p^z}{m}\left(\frac{m}{H-E+\omega}\right)^2\frac{p^z}{m}|\phi\rangle\frac{\langle\phi|\delta H|\phi\rangle}{m}, \quad (15c)$$

$$\delta\chi_4 = \langle\phi|\frac{p^z}{m}\left(\frac{m}{H-E-\omega}\right)^2\frac{p^z}{m}|\phi\rangle\frac{\langle\phi|\delta H|\phi\rangle}{m}. \quad (15d)$$

The terms $\delta\chi_{5,6}$ are perturbations to the wave function,

$$\delta\chi_5 = 2\langle\phi|\frac{p^z}{m}\frac{m}{H-E+\omega}\frac{p^z}{m}\left(\frac{1}{E-H}\right)'\delta H|\phi\rangle, \quad (15e)$$

$$\delta\chi_6 = 2\langle\phi|\frac{p^z}{m}\frac{m}{H-E-\omega}\frac{p^z}{m}\left(\frac{1}{E-H}\right)'\delta H|\phi\rangle. \quad (15f)$$

Quite surprisingly, in the velocity gauge, there are two more terms,

$$\delta\chi_7 = 2i\langle\phi|\frac{p^z}{m}\frac{m}{H-E+\omega}[\delta H,z]|\phi\rangle, \quad (15g)$$

$$\delta\chi_8 = 2i\langle\phi|\frac{p^z}{m}\frac{m}{H-E-\omega}[\delta H,z]|\phi\rangle. \quad (15h)$$

These corrections are due to a modification of the transition current in the velocity gauge,

$$\frac{p^i}{m} \to \frac{p^i}{m} + \delta j^i, \qquad \delta j^i = i[\delta H, x^i], \quad (16)$$

with the correction δj^i perturbing both transition currents in the polarizability matrix element.

For clarification, we should add that the correction to the wave function (5c) is orthogonal to the first-order wave function (conservation of the norm), and hence, the seagull-term contribution χ_3 receives no correction due to the perturbative potential [see Eq. (10c)].

IV. GAUGE INVARIANCE

A. Proof of gauge invariance

First, let us point out that the gauge invariance of the *leading-order* dynamic polarizability [Eq. (3) vs (9)] requires the relation

$$Q' = \chi = \omega^2\rho = Q. \quad (17)$$

We will skip the details of the derivation of this identity which may be found in [7] and on pages 357–359 of Ref. [18]. Indeed, the verification of the identity $Q' = Q$ is a rather easy, albeit somewhat tedious exercise involving the repeated application of the commutator relation

$$\frac{p^z}{m} = i[H,z] = i[H - E \pm \omega,z]. \tag{18}$$

The gauge invariance $Q = Q'$ of the leading-order dynamic Stark shift (17) raises pertinent questions concerning a potentially similar relation $\delta Q = \delta Q'$ for the first-order correction to this quantity. In detail, for the nonrelativistic case, the gauge-invariance relation is

$$Q = Q' \;\Leftrightarrow\; \omega^2\left(\sum_{i=1}^{2} \rho_i\right) = \sum_{i=1}^{3} \chi_i, \tag{19}$$

with two terms in the length gauge, but three terms in the velocity gauge. For the correction, the appropriate form is

$$\delta Q = \delta Q' \;\Leftrightarrow\; \omega^2\left(\sum_{i=1}^{6} \delta\rho_i\right) = \sum_{i=1}^{8} \delta\chi_i. \tag{20}$$

We now present the derivation of the formula (20) (gauge invariance of the correction to the dynamic polarizability mediated by a perturbative potential δH), by first investigating the velocity-gauge form of the correction, and then transforming into the length gauge. For $\delta\chi_1$ as defined in (15a), we have

$$\begin{aligned}
\delta\chi_1 &= -\langle\phi|\frac{p^z}{m}\frac{m}{H-E+\omega}\delta H\frac{1}{H-E+\omega}\frac{p^z}{m}|\phi\rangle \\
&= -\omega^2\langle\phi|z\frac{m}{H-E+\omega}\delta H\frac{1}{H-E+\omega}z|\phi\rangle \\
&\quad + 2\omega\langle\phi|z\frac{m}{H-E+\omega}\delta H z|\phi\rangle + \langle\phi|zm\delta H z|\phi\rangle \\
&= \omega^2\delta\rho_1 + 2\omega\langle\phi|z\frac{m}{H-E+\omega}\delta H z|\phi\rangle \\
&\quad + \langle\phi|zm\delta H z|\phi\rangle.
\end{aligned} \tag{21a}$$

An analogous relation, valid for $\delta\chi_2$, can be obtained by the replacement $\omega \to -\omega$ in Eq. (21a). We transform $\delta\chi_3$ as defined in (15c) according to

$$\begin{aligned}
\delta\chi_3 &= \langle\phi|\frac{p^z}{m}\left(\frac{m}{H-E+\omega}\right)^2\frac{p^z}{m}|\phi\rangle\frac{\langle\phi|\delta H|\phi\rangle}{m} \\
&= \omega^2\delta\rho_3 - 2\omega\langle\phi|z\frac{m}{H-E+\omega}z|\phi\rangle\langle\phi|\delta H|\phi\rangle \\
&\quad + \langle\phi|z^2|\phi\rangle\langle\phi|m\delta H|\phi\rangle.
\end{aligned} \tag{21b}$$

Again, an analogous relation, valid for $\delta\chi_4$, can be obtained by the replacement $\omega \to -\omega$ in Eq. (21b). For $\delta\chi_5$, the following relation is useful,

$$\begin{aligned}
\delta\chi_5 &= 2\langle\phi|\frac{p^z}{m}\frac{m}{H-E+\omega}\frac{p^z}{m}\left(\frac{1}{E-H}\right)'\delta H|\phi\rangle \\
&= \omega^2\delta\rho_5 - 2\omega\langle\phi|z\frac{m}{H-E+\omega}z\delta H|\phi\rangle \\
&\quad + 2\omega\langle\phi|z\frac{m}{H-E+\omega}z|\phi\rangle\langle\phi|\delta H|\phi\rangle \\
&\quad + \langle\phi|z^2 m\delta H|\phi\rangle - \langle\phi|z^2|\phi\rangle\langle\phi|m\delta H|\phi\rangle \\
&\quad + 2\omega\langle\phi|z^2\left(\frac{1}{E-H}\right)'m\delta H|\phi\rangle.
\end{aligned} \tag{21c}$$

Replacement of ω by $-\omega$ in Eq. (21c) yields $\delta\chi_6$. Using Eqs. (21a)–(21c), we finally obtain the simple and compact relation

$$\begin{aligned}
\omega^2\sum_{i=1}^{6}\delta\rho_i &= \sum_{i=1}^{6}\delta\chi_i - 2\omega\langle\phi|z\frac{m}{H-E+\omega}[\delta H,z]|\phi\rangle \\
&\quad + 2\omega\langle\phi|z\frac{m}{H-E-\omega}[\delta H,z]|\phi\rangle \\
&\quad - 2\langle\phi|zm[\delta H,z]|\phi\rangle.
\end{aligned} \tag{22}$$

We recall that the expression $\sum_{i=1}^{6}\delta\chi_i$ represents the sum of the wave-function correction, the correction to the Hamiltonian, and the correction due to the energy perturbation mediated by a perturbative potential δH.

What remains to be shown is that the sum of the additional terms $\delta\chi_7$ and $\delta\chi_8$, as defined in Eqs. (15g) and (15h), reproduces the remaining terms on the right-hand side of Eq. (22). This can be accomplished as follows,

$$\begin{aligned}
\sum_{i=7}^{8}\delta\chi_i &= 2i\left\{\langle\phi|\frac{p^z}{m}\frac{m}{H-E+\omega}[\delta H,z]|\phi\rangle\right. \\
&\quad \left. + \langle\phi|\frac{p^z}{m}\frac{m}{H-E-\omega}[\delta H,z]|\phi\rangle\right\} \\
&= -2\left\{\langle\phi|[H-E+\omega,z]\frac{m}{H-E+\omega}[\delta H,z]|\phi\rangle\right. \\
&\quad \left. + (\omega \to -\omega)\right\} \\
&= -2\omega\langle\phi|z\frac{m}{H-E+\omega}[\delta H,z]|\phi\rangle \\
&\quad + 2\omega\langle\phi|z\frac{m}{H-E-\omega}[\delta H,z]|\phi\rangle \\
&\quad - 2\langle\phi|zm[\delta H,z]|\phi\rangle.
\end{aligned} \tag{23}$$

We recognize, in the last line, the terms on the right-hand side of Eq. (22). This concludes the proof of Eq. (20).

B. Relativistic and radiative effects

1. Leading relativistic correction

A Foldy-Wouthuysen transformation of the Dirac-Coulomb Hamiltonian [19] gives us the following relativistic correction, (see, e.g., [20, page 19]):

$$\delta H = -\frac{\vec{p}^{\,4}}{8m^3} + \frac{\pi(Z\alpha)}{2m^2}\delta^{(3)}(\vec{r}) + \frac{Z\alpha}{4m^2r^3}\vec{L}\cdot\vec{S}. \tag{24}$$

For the relativistic correction to the current, we need the commutator

$$[\delta H,z] = -\frac{1}{8m^3}[\vec{p}^{\,4},z] = \frac{i}{2m^3}p^z\vec{p}^{\,2}. \tag{25}$$

The two additional terms, in this case [see Eqs. (15g) and (15h)], are

$$\delta\chi_{\delta H,7} = 2\langle\phi|\frac{p^z}{m}\frac{m}{H-E+\omega}\left(-\frac{1}{2m^3}p^z\vec{p}^{\,2}\right)|\phi\rangle, \tag{26}$$

$$\delta\chi_{\delta H,8} = 2\langle\phi|\frac{p^z}{m}\frac{m}{H-E-\omega}\left(-\frac{1}{2m^3}p^z\vec{p}^{\,2}\right)|\phi\rangle. \tag{27}$$

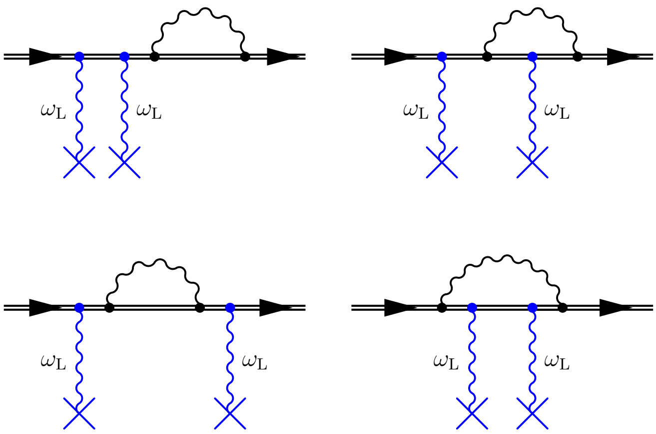

FIG. 1. Feynman diagrams for the self-energy radiative correction to the dynamic Stark shift. Interactions with the external laser field are labeled with $\omega_{\rm L}$.

We observe that these terms are exactly equal to the terms on the right-hand side of Eq. (22), which leads us immediately to the gauge-invariance relation

$$\omega^2 \sum_{i=1}^{6} \delta\rho_i(\delta H) = \sum_{j=1}^{8} \delta\chi_j(\delta H). \qquad (28)$$

The two additional terms $\delta\chi_7$ and $\delta\chi_8$ in the velocity gauge are definitely necessary in order to ensure gauge invariance; they are due to correction to the current which prevails only in the velocity, but not in the length gauge (see page 21 of Ref. [20]).

2. *Leading radiative correction*

Inspired by effective field theory, or nonrelativistic quantum electrodynamics [21], we here pursue an effective treatment in which the leading logarithmic QED correction due to radiative photons is described by an effective Lamb-shift potential (see also Fig. 1)

$$\delta H = \delta V_{\rm Lamb} = \frac{4}{3}\alpha(Z\alpha)\ln[(Z\alpha)^{-2}]\frac{\delta^{(3)}(\vec{r})}{m^2}. \qquad (29)$$

It is sometimes useful to consider a "standard" perturbative potential [22]

$$\delta V = \frac{\pi(Z\alpha)}{m^2}\delta^{(3)}(\vec{r}), \qquad (30)$$

which is related to $\delta V_{\rm Lamb}$ by a simple prefactor,

$$\delta V_{\rm Lamb} = \frac{4\alpha}{3\pi}[\pi(Z\alpha)]\ln[(Z\alpha)^{-2}]\frac{\delta^{(3)}(\vec{r})}{m^2} = \frac{4\alpha}{3\pi}\ln[(Z\alpha)^{-2}]\delta V. \qquad (31)$$

The standard potential (30) leads to a "normalized" energy shift with unit prefactors,

$$\delta E(\phi\ell_j) = \frac{(Z\alpha)^4 m}{n^3}\delta_{\ell 0}, \qquad (32)$$

for hydrogenic states with the principal quantum number n, orbital quantum number ℓ, and total angular momentum quantum number j. If a numerical evaluation is desired, then

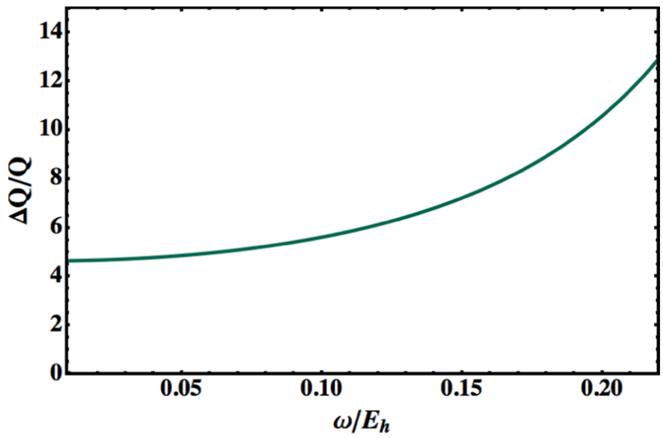

FIG. 2. Ratio of the first-order radiative correction of the dynamic polarizability to the unperturbed dynamic polarizability as a function of the laser photon energy ω (we set $\hbar = 1$), divided by the Hartree energy E_h. The data are obtained for the ground state of hydrogen. The quantity ΔQ is defined in Eq. (34).

the radiative corrections δQ can be read off from the sum of the various terms listed in Eq. (8). A generalization to the leading effect of vacuum polarization, replacing δV by the Uehling potential [23], is immediate.

In general, for a perturbative potential δV that fulfills $[\delta V, z] = 0$, the additional terms $\delta\chi_7$ and $\delta\chi_8$ are not necessary. In this case, the gauge-invariance statement can be summarized as follows,

$$[\delta V, z] = 0 \quad \Rightarrow \quad \omega^2 \sum_{i=1}^{6} \delta\rho_i(\delta V) = \sum_{j=1}^{6} \delta\chi_j(\delta V), \qquad (33)$$

leaving out $\delta\chi_7 = \delta\chi_8 = 0$.

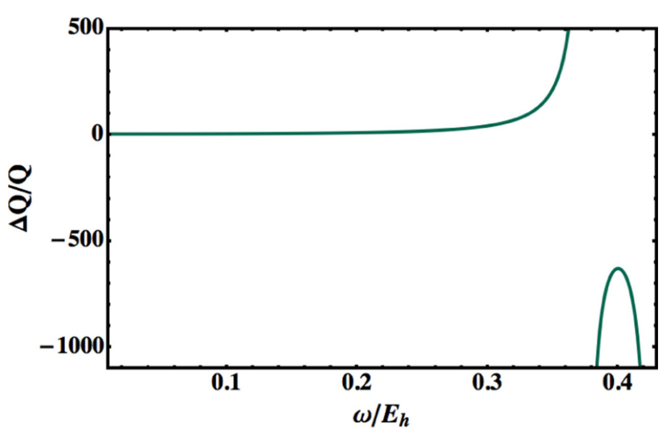

FIG. 3. Same as Fig. 2, but in a frequency range which covers the intermediate $2P$ state, where the laser frequency can excite the $1S$-$2P$ transition resonantly. The plot is included for reference. Of course, near resonance, the second-order perturbation treatment of the atom-laser interaction, which is the basis for Eq. (2), breaks down, and the dressed-state formalism has to be used (see Ref. [13]). The $2P$ resonance is responsible for the first peak in the radiative correction at $\omega = \frac{3}{8}E_h$, and the second pole is due to the zero of the unperturbed matrix element Q at $\omega = 0.429538 E_h$. All calculations are performed in the nonrecoil approximation. The figure illustrates the dramatic increase of the radiative correction as the resonance is approached.

In Figs. 2 and 3, we present numerical data for the frequency-dependent radiative correction (the "logarithmic coefficient")

$$\frac{\Delta Q}{Q} = \left(\frac{4\alpha^3}{3\pi}\ln(\alpha^{-2})\right)^{-1}\frac{\delta Q}{Q}, \tag{34}$$

where δQ is the leading logarithmic radiative correction due to the effective potential (31), evaluated for the ground state of hydrogen. The numerical calculations use techniques originally developed in self-energy calculations [24]. Large coefficients are obtained for the leading logarithmic correction.

V. CONCLUSIONS

We have investigated the gauge invariance of the dynamic (ac) Stark shift under the "hybrid" gauge transformation from the length to the velocity gauge. The length-gauge perturbations due to a perturbative Hamiltonian δH have been discussed in Sec. III A, while the velocity-gauge formulation is given in Sec. III B.

In the velocity gauge, six perturbations, two each to the Hamiltonian, to the energy, and to the wave function, have been given in Eq. (8), while the eight terms in the velocity gauge can be found in Eq. (15). Gauge invariance amounts to showing the identity (20). This is accomplished in Sec. IV A, where we also give a general form of the additional correction to the current, which is necessary to include in the velocity gauge [see Eq. (16)]. Indeed, the general form of the correction to the current, induced by the perturbative Hamiltonian δH,

$$\delta j^i = i[\delta H, x^i], \tag{35}$$

constitutes a main result of our investigations.

While all derivations discussed in the current paper have been given for one-electron atoms, the generalization to many-electron systems is straightforward: One simply sums over the electron coordinates. One should add that the derivation here is related to the one recently presented in Appendix A of [8] in the context of the gauge invariance of radiative corrections to the two-photon decay width, and to Refs. [9,10] for the gauge invariance of the imaginary part of the atomic polarizability.

In general, the length gauge is favorable for the formulation of relativistic corrections because the number of terms is smaller in this gauge, and the interactions are formulated in terms of gauge-invariant field strengths ($\vec{E}$ and $\vec{B}$) instead of gauge-dependent scalar and vector potentials (Φ and $\vec{A}$); see Refs. [1,6] for further discussions on this point.

A specific picture is emerging from the recent investigations on gauge invariance: For resonant processes which involve eigenstates of the same energy, of the combined atom + radiation field system, the "hybrid" gauge invariance holds. This is, e.g., the case for the two-photon decay width [8], where the initial $2S$ state has the same energy as the final state (atom is in the $1S$ state, and two photons are in the radiation field). This is also the case for two-photon transition matrix elements, provided the final state has the same energy as the initial state, plus the energy of the two absorbed photons (i.e., at resonance; see Refs. [6,8]). For the dynamic polarizability studied in the current article, the resonance condition is always met because relevant matrix elements describe the absorption of a laser photon and the concomitant emission of that same photon. So, the initial state considered in our investigations here has the same energy as the final atomic state, which is in fact identical to the initial state (it has the same number of laser photons, and the same atomic state).

The deeper reason for the "hybrid" gauge invariance of resonant processes lies in the possibility of formulating such energy perturbations in terms of adiabatically switched fields and potentials; the gauge transformation of the initial and final states of the wave function at $t \to \pm\infty$ amounts to the identity transformation because the adiabatically switched fields and potentials vanish in that same limit. Hence, the gauge transformation of the wave function can be omitted. This general picture is confirmed by the investigations presented here, and augmented by the general form of the transition current which has to be added in the velocity gauge.

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