A Problematic Set of

Two–Loop Self–Energy Corrections

Ulrich D. Jentschura, Jörg Evers and Christoph H. Keitel

Fakultät Physik der Albert–Ludwigs–Universität, Theoretische Quantendynamik, Hermann–Herder–Straße 3, D–79104 Freiburg, Germany

Krzysztof Pachucki

Institute of Theoretical Physics, University of Warsaw, ul. Hoża 69, 00-681 Warsaw, Poland

Abstract We investigate a specific set of two-loop self-energy corrections involving squared decay rates and point out that their interpretation is highly problematic. The corrections cannot be interpreted as radiative energy shifts in the usual sense. Some of the problematic corrections find a natural interpretation as radiative nonresonant corrections to the natural line shape. They cannot uniquely be associated with one and only one atomic level. While the problematic corrections are rather tiny when expressed in units of frequency (a few Hertz for hydrogenic P levels) and do not affect the reliability of quantum electrodynamics at the current level of experimental accuracy, they may be of importance for future experiments. The problems are connected with the limitations of the so-called asymptotic-state approximation which means that atomic in- and out-states in the S-matrix are assumed to have an infinite lifetime.

PACS numbers 12.20.Ds, 31.15.-p, 31.30Jv.
Keywords quantum electrodynamics - specific calculations;
calculations and mathematical techniques in atomic and molecular physics;
Relativistic and quantum electrodynamic effects in atoms and molecules.

1 Introduction

In view of the rapid progress in ultra-accurate Lamb shift measurements in atomic hydrogen [1,2], it appears useful to investigate the mathematical foundations of the theorems on which our level-shift calculations are based, in addition to the continuing efforts (e.g. [3–7]) of evaluating higher-and-higher order radiative corrections to the bound-state energy levels. Here, we focus on a number of mathematical subtleties connected with the famous theorem of Gell–Mann, Low and Sucher [8, 9] that forms the basis for the derivation of the expressions investigated in level-shift calculations. This theorem has historically proven to be an extremely useful tool in the analysis of bound-state quantum electrodynamics, and it yields formal expressions for the renormalized level shifts whose numerical and analytic evaluation has lead to accurate predictions for the bound-state energy levels that are in agreement with all experiments reported so far in the literature. However, second thoughts about some mathematical subtleties connected with the theorem may be required at the level of accuracy envisaged in projected experiments.

Consider the formula for the energy shift of an atomic state as given by the well-known theorem of Gell–Mann, Low and Sucher [8, 9]

$$\Delta E_n = \lim_{\substack{\varepsilon \to 0^+ \\ \lambda \to 1}} \frac{\mathrm{i}\,\varepsilon\,\lambda}{2} \frac{\partial}{\partial \lambda} \ln \left[\langle n | S_{\varepsilon,\lambda} | n \rangle_c \right] \,, \tag{1}$$

where $|n\rangle$ is an unperturbed asymptotic bound-electron state as given by the Dirac theory. $S_{\varepsilon,\lambda}$ is the infinitesimally damped S matrix given by the time-ordered exponential

$$S_{\varepsilon,\lambda} = \mathrm{T} \exp \left(-\mathrm{i}\lambda \int_{-\infty}^{\infty} \mathrm{d}t \int \mathrm{d}^3 x \, \exp(-\varepsilon|t|) \, \mathcal{H}_{\mathrm{I}}(x) \right) \tag{2}$$

where x denotes the four-vector $(t, \boldsymbol{x})$, and the interaction Hamiltonian density reads

$$\mathcal{H}_{\mathrm{I}}(\boldsymbol{x}) = -\frac{e}{2} \, \hat{A}_\mu(x) \, [\hat{\bar{\psi}}(x), \gamma^\mu \hat{\psi}(x)] - \frac{1}{2} \, \delta m \, [\hat{\bar{\psi}}(x), \hat{\psi}(x)] \,. \tag{3}$$

The interaction Hamiltonian density involves the quantized electromagnetic field $\hat{A}_\mu(x)$, the quantized Dirac field $\hat{\psi}(x)$ in the Furry picture, and the mass counter term δm. The index c in (1) indicates that only connected graphs (see e.g. Ch. 6 of [10]) enter into the expression for the energy shift. Note that in writing down the expression (1), we implicitly assume the physical existence of the asymptotic state $|n\rangle$, i.e. of the unperturbed state $|n\rangle$ with an infinite lifetime. If the interaction with the quantized electromagnetic field (the "vacuum modes") could be "switched off" [as it is assumed for the damped interaction (2) in the distant past and future], then all states would be asymptotic states and could be used to construct S-matrix elements rigorously. While this is – strictly speaking – unphysical, Eq. (2) is still an excellent approximation for most bound-state calculations.

A second-order evaluation of (1) in powers of $\mathcal{H}_{\mathrm{I}}$, which involves the one-loop self-energy, shows that the radiative energy shift of an excited state with nonvanishing angular momentum (say, a P state) has an imaginary part generated by the interaction of the atomic state with the quantized electromagnetic field (which gives the expression for the decay rate Γ). This effect limits the validity of the asymptotic-state approximation which is a good approximation as long as Γ is much smaller than the separation of atomic energy levels [see also the discussion in Ch. XXI of [11], especially Eq. (3.28) on p. 547 *ibid.*].

Certain two-loop self-energy contributions to the hydrogenic energy levels involve the *square* of the imaginary parts of two one-loop insertions, which result in a shift of the real energy eigenvalue. The error initially made in ignoring the decay width of the resonances thus influences the real part of the eigenvalues which theory predicts at two-loop order. This leads to a problem in connection with the asymptotic-state approximation that is originally used in writing down the expression (1). At present, we have no better way to gauge the magnitude of this problematic effect but to evaluate it, according the current formalism, within a theory that *a priori* involves asymptotic states. The effects discussed here touch a certain question regarding the mathematical foundations of bound-state quantum electrodynamics.

This paper is organized as follows: in Sec. 2, we present an evaluation of the problematic two-loop corrections involving the squared decay rates for the 2P state of atomic hydrogen. In Sec. 3, we argue that some of the problematic corrections find a natural interpretation as radiative corrections to the off-resonance effects that influence the line shape in atomic transitions. Conclusions are left to Sec. 4.

2 A Concrete Example

An expression for the two-loop self-energy correction to the energy of a bound hydrogenic state within the formalism of nonrelativistic quantum electrodynamics (NRQED) has been derived in [7] [see Eq. (16) *ibid.*], and we take this equation as the starting point of our investigations. Diagrammatically, the two-loop self-energy can be represented as in Fig. 1. We will investigate the effect within the ϵ-method that involves a scale-separation parameter ϵ for the photon energy (this method is explained in [12] and the Appendix of [13]). For the two photons with energies ω_1 and ω_2, we need two scale-separation parameters ϵ_1 and ϵ_2. These cancel when the high- and the low-energy parts are added, and it is permissible to keep only the divergent and constant terms as both $\epsilon_1 \to 0$ and $\epsilon_2 \to 0$. We therefore keep $\epsilon_{1/2}$ as variables and evaluate only those contributions to the two-loop self-energy integrals that correspond to the square of the residues along the ω_1 and ω_2 integrations (these correspond to the "squared imaginary parts" or "squared decay rates"). We focus on the 2P state of atomic hydrogen and use natural Gaussian ("microscopic") units with $\hbar = c = \epsilon_0 = 1$. The Schrödinger energy of an atomic state is $E_n = -(Z\alpha)^2\, m/(2n^2)$ where n is the principal quantum number, α is the fine-structure constant, and Z is the nuclear charge number.

There is a contribution due to the diagram with crossed loops in Fig. 1 (a),

$$\mathcal{T}_1(2\mathrm{P}) = \lim_{\delta\to 0^+} -\left(\frac{2\,\alpha}{3\,\pi\,m^2}\right)^2 \int_0^{\epsilon_1} \mathrm{d}\omega_1\,\omega_1 \int_0^{\epsilon_2} \mathrm{d}\omega_2\,\omega_2$$
$$\times \left\langle 2\mathrm{P} \left| p^i \,\frac{1}{H - \mathrm{i}\,\delta - E_{2\mathrm{P}} + \omega_1}\, p^j \,\frac{1}{H - E_{2\mathrm{P}} + \omega_1 + \omega_2}\, p^i \,\frac{1}{H - \mathrm{i}\,\delta - E_{2\mathrm{P}} + \omega_2}\, p^j \right| 2\mathrm{P} \right\rangle . \quad (4)$$

Here, the p^i are the momentum operators, and H is the Schrödinger Hamiltonian. We "pick up" only the terms of the "squared-decay" type, i.e. the terms generated by the infinitesimal half-circles around the poles at $\omega_1 = E_{2\mathrm{P}} - E_{1\mathrm{S}}$ and $\omega_2 = E_{2\mathrm{P}} - E_{1\mathrm{S}}$. For the evaluation of these terms, the specification of the infinitesimal imaginary part $-\mathrm{i}\,\delta$ is required in order to fix the sign of the pole contribution. For the contribution $C_1(2\mathrm{P})$ generated by the poles at $\omega_1 = E_{2\mathrm{P}} - E_{1\mathrm{S}}$ and $\omega_2 = E_{2\mathrm{P}} - E_{1\mathrm{S}}$ in $\mathcal{T}_1(2\mathrm{P})$, we obtain

$$\begin{aligned} C_1(2\mathrm{P}) &= \alpha^2\,\frac{4}{27 m^4}\,(E_{2\mathrm{P}} - E_{1\mathrm{S}})^2\; |\langle 1\mathrm{S}|\boldsymbol{p}|2\mathrm{P}\rangle|^2 \left\langle 1\mathrm{S} \left| p^i \,\frac{1}{H + E_{2\mathrm{P}} - 2\,E_{1\mathrm{S}}}\, p^i \right| 1\mathrm{S} \right\rangle \\ &= \frac{2^5}{3^9}\,\alpha^2\,(Z\alpha)^6\, m\,\mathcal{M}_1\,, \end{aligned} \quad (5)$$

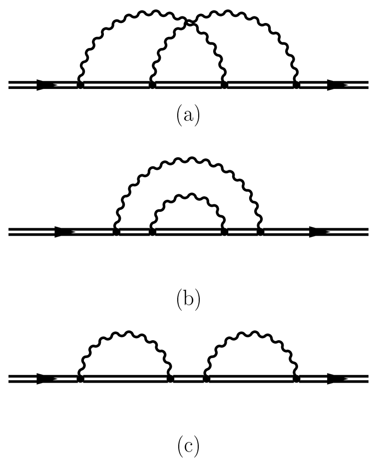

Figure 1: The crossed-loop (a), the rainbow diagram (b) with one loop inside the other, and the loop-after-loop diagram (c) which contribute to the two-loop self-energy for a bound electron. The propagator of the bound electron is denoted by a double line, and the arrow of time is from left to right.

where the summation convention is used and the matrix element $\mathcal{M}_1$ reads

$$\mathcal{M}_1 = \frac{1}{m} \left\langle 1\mathrm{S} \left| p^i \, \frac{1}{H + E_{2\mathrm{P}} - 2\,E_{1\mathrm{S}}} \, p^i \right| 1\mathrm{S} \right\rangle = 0.880 \tag{6}$$

and

$$\left| \left\langle 1\mathrm{S} \left| \frac{\boldsymbol{p}}{m} \right| 2\mathrm{P} \right\rangle \right|^2 = \frac{2^9}{3^8} \, (Z\alpha)^2 \,. \tag{7}$$

Note that the contribution C_1 lacks the factors π in the denominator which are characteristic of other two–loop corrections: these are compensated by additional factors of π in the numerator that characterize the pole contributions.

The rainbow diagram in Fig. 1 (b) with the second loop inside the first does not create squared imaginary contributions. From the irreducible part of the loop-after-loop diagram in Fig. 1 (c) (we exclude the reference state in the intermediate electron propagator), we obtain

$$\begin{aligned} \mathcal{T}_2(2\mathrm{P}) = \lim_{\delta \to 0^+} - \left(\frac{2\,\alpha}{3\,\pi\,m^2} \right)^2 \int_0^{\epsilon_1} \mathrm{d}\omega_1 \, \omega_1 \int_0^{\epsilon_2} \mathrm{d}\omega_2 \, \omega_2 \\ \times \left\langle 2\mathrm{P} \left| p^i \, \frac{1}{H - \mathrm{i}\,\delta - E_{2\mathrm{P}} + \omega_1} \, p^i \left(\frac{1}{H - E_{2\mathrm{P}}} \right)' p^j \, \frac{1}{H - \mathrm{i}\,\delta - E_{2\mathrm{P}} + \omega_2} \, p^j \right| 2\mathrm{P} \right\rangle \,. \end{aligned} \tag{8}$$

Again, picking up only those terms which are generated by the infinitesimal half-circles around the poles at $\omega_1 = E_{2\mathrm{P}} - E_{1\mathrm{S}}$ and $\omega_2 = E_{2\mathrm{P}} - E_{1\mathrm{S}}$, we obtain the contribution $C_2(2\mathrm{P})$ involving squared decay rates,

$$C_2(2\mathrm{P}) = \alpha^2 \frac{4}{27m^4} (E_{2\mathrm{P}} - E_{1\mathrm{S}})^2 \, |\langle 1\mathrm{S}|\boldsymbol{p}|2\mathrm{P}\rangle|^2 \left\langle 1\mathrm{S} \left| p^i \left(\frac{1}{H - E_{2\mathrm{P}}}\right)' p^i \right| 1\mathrm{S} \right\rangle$$

$$= \frac{2^5}{3^9} \alpha^2 (Z\alpha)^6 \, m \, \mathcal{M}_2 \,, \tag{9}$$

where the matrix element $\mathcal{M}_2$ reads

$$\mathcal{M}_2 = \frac{1}{m} \left\langle 1\mathrm{S} \left| p^i \left(\frac{1}{H - E_{2\mathrm{P}}}\right)' p^i \right| 1\mathrm{S} \right\rangle = \frac{6952}{6561} + \frac{4096}{2187} \ln\left(\frac{9}{8}\right) = 1.28 \,. \tag{10}$$

The prime in the reduced Green function indicates that the 2P state is excluded from the sum over intermediate states.

This contribution deserves a more detailed discussion because C_2 can be written as a "second-order perturbation" according to

$$C_2 = \left\langle 2\mathrm{P} \left| \left\{ \mathrm{i}\,\mathrm{Im}\, \Sigma^{(1\mathrm{L})}_{\mathrm{NR}}(E_{2\mathrm{P}}) \right\} \left(\frac{1}{E_{2\mathrm{P}} - H}\right)' \left\{ \mathrm{i}\,\mathrm{Im}\, \Sigma^{(1\mathrm{L})}_{\mathrm{NR}}(E_{2\mathrm{P}}) \right\} \right| 2\mathrm{P} \right\rangle , \tag{11}$$

where $\Sigma^{(1\mathrm{L})}_{\mathrm{NR}}(E)$ denotes the one-loop nonrelativistic self-energy operator with the energy argument E; the matrix elements of this operator read

$$\left\langle \phi_1 \left| \Sigma^{(1\mathrm{L})}_{\mathrm{NR}}(E) \right| \phi_2 \right\rangle = \lim_{\delta \to 0^+} -\frac{2\alpha}{3} \int_0^{\epsilon} \mathrm{d}\omega\, \omega \left\langle \phi_1 \left| \frac{\boldsymbol{p}}{m} \left(\frac{1}{H - \mathrm{i}\,\delta - E + \omega}\right) \frac{\boldsymbol{p}}{m} \right| \phi_2 \right\rangle . \tag{12}$$

In (11) and (12), we pick up only the term corresponding to the square of the two imaginary contributions and obtain the expression

$$\sum_{n \neq 2} \left(-\mathrm{i}\, \frac{2\alpha}{3} \, (E_{2\mathrm{P}} - E_{1\mathrm{S}}) \left\langle 2\mathrm{P} \left| \frac{p^i}{m} \right| 1\mathrm{S} \right\rangle \left\langle 1\mathrm{S} \left| \frac{p^i}{m} \right| n\mathrm{P} \right\rangle \right) \frac{1}{E_{2\mathrm{P}} - E_{n\mathrm{P}}}$$

$$\left(-\mathrm{i}\, \frac{2\alpha}{3} \, (E_{2\mathrm{P}} - E_{1\mathrm{S}}) \left\langle n\mathrm{P} \left| \frac{p^j}{m} \right| 1\mathrm{S} \right\rangle \left\langle 1\mathrm{S} \left| \frac{p^j}{m} \right| 2\mathrm{P} \right\rangle \right) , \tag{13}$$

where the sum covers all P states except the reference state (both discrete and continuum states). Now, we complete the sum over the intermediate states, observing that only P states yield a nonvanishing contribution. After angular averaging over atomic momenta, we obtain a contribution of

$$\frac{4}{27} \alpha^2 \, (E_{2\mathrm{P}} - E_{1\mathrm{S}})^2 \left| \left\langle 1\mathrm{S} \left| \frac{\boldsymbol{p}}{m} \right| 2\mathrm{P} \right\rangle \right|^2 \left\langle 1\mathrm{S} \left| \frac{p^j}{m} \left(\frac{1}{H - E_{2\mathrm{P}}}\right)' \frac{p^j}{m} \right| 1\mathrm{S} \right\rangle \tag{14}$$

in agreement with (9).

From the derivative term (reducible part of the loop-after-loop diagram), we obtain

$$\mathcal{T}_3(2\mathrm{P}) = \lim_{\delta \to 0^+} \left(\frac{2\,\alpha}{3\,\pi\, m^2}\right)^2 \int_0^{\epsilon_1} \mathrm{d}\omega_1\, \omega_1 \int_0^{\epsilon_2} \mathrm{d}\omega_2\, \omega_2$$

$$\times \left\langle 2\mathrm{P} \left| p^i \frac{1}{H - \mathrm{i}\,\delta - E_{2\mathrm{P}} + \omega_1} p^i \right| 2\mathrm{P} \right\rangle \left\langle 2\mathrm{P} \left| p^j \left(\frac{1}{H - \mathrm{i}\,\delta - E_{2\mathrm{P}} + \omega_2}\right)^2 p^j \right| 2\mathrm{P} \right\rangle \tag{15}$$

$$C_3(2\mathrm{P}) = -\alpha^2 \frac{4}{9m^4} (E_{2\mathrm{P}} - E_{1\mathrm{S}}) \, |\langle 1\mathrm{S}|\boldsymbol{p}|2\mathrm{P}\rangle|^4 = -\frac{1}{4} \frac{\Gamma^2_{2\mathrm{P}}}{E_{2\mathrm{P}} - E_{1\mathrm{S}}} = -\frac{2^{17}}{3^{17}} \alpha^2 (Z\alpha)^6 \, m \,, \tag{16}$$

where $\Gamma_{2P} = (2/3)^8\,\alpha\,(Z\alpha)^4\,m$ is the decay width of the 2P state. The last contribution of the "squared-decay" type – it originates from the "seagull term" characteristic of NRQED – reads

$$
\begin{aligned}
\mathcal{T}_4(2P) &= \lim_{\delta\to 0^+} \left(\frac{2\,\alpha}{3\,\pi\,m^2}\right)^2 \int_0^{\epsilon_1} \mathrm{d}\omega_1\,\omega_1 \int_0^{\epsilon_2} \mathrm{d}\omega_2\,\omega_2 \\
&\quad \times \left\langle 2P \left| p^i \,\frac{1}{H - \mathrm{i}\,\delta - E_{2P} + \omega_1}\, \frac{1}{H - \mathrm{i}\,\delta - E_{2P} + \omega_2}\, p^i \right| 2P \right\rangle , \qquad (17)
\end{aligned}
$$

$$
\begin{aligned}
C_4(2P) &= -\alpha^2 \,\frac{4}{9m^3}\,(E_{2P} - E_{1S})^2\, |\langle 1S|\boldsymbol{p}|2P\rangle|^2 = -\frac{3^9}{2^{14}}\,\frac{\Gamma_{2P}^2}{E_{2P} - E_{1S}} \\
&= -\frac{2^5}{3^8}\,\alpha^2\,(Z\alpha)^6\,m\,. \qquad (18)
\end{aligned}
$$

Adding all contributions, we obtain a shift of

$$
\sum_{i=1}^{4} C_i(2P) = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^6\,m}{2^3}\,(-0.188)\,. \qquad (19)
$$

for the 2P level. For atomic hydrogen ($Z = 1$), this correction amounts to -14.9 Hz. Compared to the total Lamb shift of the 2P level, for which a value of $-12\,638\,380(80)$ Hz has been given in [14] (for the $2P_{1/2}$-state), this is a tiny effect. The comparison illustrates the accuracy of the predictions obtained using the Gell–Mann–Low–Sucher theorem (1). The theoretical value of the 2P Lamb shift has been improved in part by the recent numerical evaluation of the one-loop self energy for low Z [15], but the removal of the main theoretical uncertainty will necessitate the complete evaluation of the two-loop self-energy corrections of order $\alpha^2\,(Z\alpha)^6$. Currently, only the double logarithm is known in this order in the $(Z\alpha)$-expansion [16,17], and the groundwork for the evaluation of single-logarithmic and nonlogarithmic corrections has been laid in [7]. In Eq. (19), we write the final result as a contribution to the B_{60} coefficient (for a definition of the analytic B-coefficients of the two-loop self-energy, see e.g. [13]).

For the 3P state, we have to take into account the decays into the 1S and 2S states. For example, the contribution $C_1(3P)$ reads

$$
\begin{aligned}
C_1(3P) &= \alpha^2\,\frac{4}{27m^4} \left\{ (E_{3P} - E_{1S})^2\, |\langle 1S|\boldsymbol{p}|3P\rangle|^2 \left\langle 1S \left| p^i \,\frac{1}{H + E_{3P} - 2\,E_{1S}}\, p^i \right| 1S \right\rangle \right. \\
&\qquad \left. + (E_{3P} - E_{2S})^2\, |\langle 2S|\boldsymbol{p}|3P\rangle|^2 \left\langle 2S \left| p^i \,\frac{1}{H + E_{3P} - 2\,E_{2S}}\, p^i \right| 2S \right\rangle \right\} \\
&\qquad + \alpha^2\,\frac{8}{27m^4}\,\chi\,\mathrm{Re}\left(\langle 3P|p^j|1S\rangle \left\langle 1S \left| p^i \,\frac{1}{H + E_{3P} - E_{2S} - E_{1S}}\, p^i \right| 2S \right\rangle \langle 2S|p^j|3P\rangle \right) \\
&= \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^6\,m}{3^3}\,(0.135)\,, \qquad (20)
\end{aligned}
$$

where $\chi = (E_{3P} - E_{1S})\,(E_{3P} - E_{2S})$. The sum of C_1 – C_4 for the 3P state of atomic hydrogen is

$$
\sum_{i=1}^{4} C_i(3P) = \left(\frac{\alpha}{\pi}\right)^2 \frac{(Z\alpha)^6\,m}{3^3}\,(-0.319)\,. \qquad (21)
$$

For atomic hydrogen, this correction evaluates to -7.47 Hz.

3 Interpretation of the Squared Decay Rate

In this section, we will investigate the question of whether the squared decay rates receive a natural interpretation within the formalism of scattering theory.

We consider the scattering amplitude associated with the diagram in Fig. 2. The hydrogenic atom in the ground state is excited by a laser photon with frequency $\omega_{\rm L}$ that is close to the resonance $\omega_{\rm L} \approx E_{\rm 2P} - E_{\rm 1S}$. Within the resonance approximation, we may restrict the sum over intermediate states to the 2P level only, as indicated by the label "2P" for the electron line. This is the so-called resonance approximation.

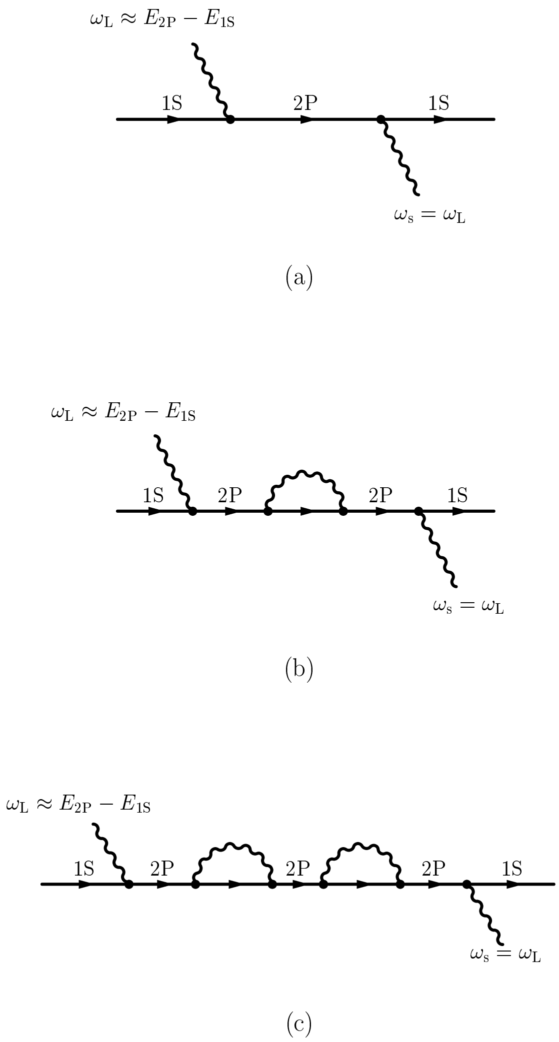

Figure 2: Contributions to the photon scattering cross section near the 2P resonance of atomic hydrogen. The laser photon of frequency $\omega_{\rm L} \approx E_{\rm 2P} - E_{\rm 1S}$ is absorbed, and the dominant contribution to the scattering amplitude is from the virtual 2P state, as indicated by the label on the electron line. The spontaneously emitted photon has a frequency $\omega_{\rm s}$. Figs. (b) and (c) represent radiative corrections to the scattering amplitude. The arrow of time is from left to right.

Fig. 2 (a) represents the dominant Kramers–Heisenberg contribution [18] without radiative corrections. In Fig. 2 (b), we have a one-loop self-energy insertion in the electron propagator. We assume that the absorbed photon is very close to the resonance ($\omega_{\rm L} \approx E_{\rm 2P} - E_{\rm 1S}$) and set the energy argument of the self-energy insertion equal to $E_{\rm 2P}$. Using these approximations, the self-energy insertion, within the resonance approximation, can be described by the diagonal matrix element $\left\langle 2{\rm P} \left| \Sigma^{(1{\rm L})}_{\rm NR}(E_{\rm 2P}) \right| 2{\rm P} \right\rangle$ of the self-energy operator (12). The imaginary part of this matrix element reads

$$
{\rm i}\,{\rm Im} \left\langle 2{\rm P} \left| \Sigma^{(1{\rm L})}_{\rm NR}(E_{\rm 2P}) \right| 2{\rm P} \right\rangle = -{\rm i}\,\frac{\Gamma_{\rm 2P}}{2}\,, \tag{22}
$$

where

$$
\Gamma_{\rm 2P} = \frac{2^8}{3^8} \alpha (Z\alpha)^4\, m \tag{23}
$$

is the well-known decay rate of the 2P state. The diagram in Fig. 2 (c) involves two one-loop self-energy insertions and entails in that sense the "square of the decay rate" of the 2P level within the resonance approximation. This square of the decay is usually not interpreted as an energy shift. Rather, one sums the infinite series of one-loop insertions of which the first terms are shown in the Feynman diagrams in Figs. 2 (a,b,c). We ignore in the sequel the real part of the self-energy operator and define the "decay rate operator" $\hat{\Gamma}$ via the relation

$$
{\rm i}\,{\rm Im} \left\langle \phi_1 \left| \Sigma^{(1{\rm L})}_{\rm NR}(E) \right| \phi_2 \right\rangle = -\frac{\rm i}{2} \left\langle \phi_1 \left| \hat{\Gamma}(E) \right| \phi_2 \right\rangle \tag{24}
$$

so that

$$
-\frac{\rm i}{2} \left\langle 2{\rm P} \left| \hat{\Gamma}(E_{\rm 2P}) \right| 2{\rm P} \right\rangle = -{\rm i}\,\frac{\Gamma_{\rm 2P}}{2}\,. \tag{25}
$$

This leads to the following infinite series representing the electron propagator in the resonance approximation with an infinite number of one-loop self-energy insertions (of which we discard the real part and keep only the imaginary part $-{\rm i}\,\Gamma_{\rm 2P}/2$),

$$
\begin{aligned}
& \frac{|2{\rm P}\rangle\,\langle 2{\rm P}|}{E_{\rm 2P} - (E_{1S} + \omega_{\rm L})} - \frac{|2{\rm P}\rangle}{E_{\rm 2P} - (E_{1S} + \omega_{\rm L})} \left(-{\rm i}\,\frac{\Gamma_{\rm 2P}}{2}\right) \frac{\langle 2{\rm P}|}{E_{\rm 2P} - (E_{1S} + \omega_{\rm L})} \\
& + \frac{|2{\rm P}\rangle}{E_{\rm 2P} - (E_{1S} + \omega_{\rm L})} \left(-{\rm i}\,\frac{\Gamma_{\rm 2P}}{2}\right) \frac{|2{\rm P}\rangle\,\langle 2{\rm P}|}{E_{\rm 2P} - (E_{1S} + \omega_{\rm L})} \left(-{\rm i}\,\frac{\Gamma_{\rm 2P}}{2}\right) \frac{\langle 2{\rm P}|}{E_{\rm 2P} - (E_{1S} + \omega_{\rm L})} + \dots \\
& = \frac{|2{\rm P}\rangle\,\langle 2{\rm P}|}{E_{\rm 2P} - {\rm i}\,\Gamma_{\rm 2P}/2 - (E_{1S} + \omega_{\rm L})}\,.
\end{aligned} \tag{26}
$$

This result expresses the well-known fact that the decay rate term $-{\rm i}\,\Gamma_{\rm 2P}/2$ in the electron propagator denominator is generated by summing an infinite series of Feynman diagrams involving one-loop self-energy insertions; the first three terms in this series are shown in Figs. 2 (a) – (c).

Let us now go beyond the resonance approximation inherent to Eq. (26) and consider off-resonant atomic states (see Fig. 3). We therefore replace

$$
\frac{|2{\rm P}\rangle\,\langle 2{\rm P}|}{E_{\rm 2P} - {\rm i}\,\Gamma_{\rm 2P}/2 - (E_{1S} + \omega_{\rm L})} \to \frac{1}{H - {\rm i}\,\hat{\Gamma}/2 - (E_{1S} + \omega_{\rm L})}\,. \tag{27}
$$

That means that the resonance term involving only the 2P state is replaced by the full Green function of the electron, including the off-resonant states and the "decay rate operator" $\hat{\Gamma}$ defined in Eq. (24). The "energy argument" of $\hat{\Gamma} \equiv \hat{\Gamma}(E)$ is to be taken as $E = E_{1S} + \omega_{\rm L} \approx E_{\rm 2P}$. In Eq. (27), H is *a priori* the Schrödinger Hamiltonian for the bound electron [we have done all calculations in the nonrelativistic (NR) approximation, but the calculations may be generalized to the relativistic case].

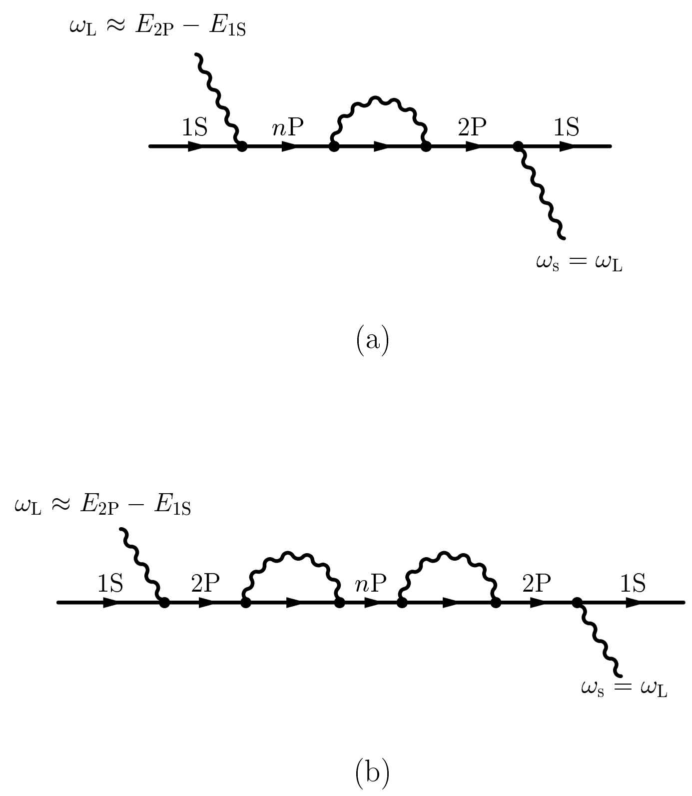

Figure 3: Same as Fig. 2, but with off-resonant virtual states (nP states with $n \neq 2$). The arrow of time is from left to right.

It is now easy to verify by inspection that the amplitudes corresponding to the Feynman diagrams in Figs. 3 (a) and (b) are generated by an expansion of the propagator $1/\{H - {\rm i}\,\hat{\Gamma}/2 - (E_{1S} + \omega_{\rm L})\}$ in powers of $\hat{\Gamma}$. Furthermore, the diagram in Fig. 3 (b) exactly corresponds to the "second-order perturbation" in Eq. (11). So, we conclude that the energy shifts by squared decay rates should rather be interpreted as radiative nonresonant corrections to the photon scattering cross section than energy shifts of individual atomic levels. Specifically, the "second-order perturbation" in Eq. (11), which corresponds to the diagram in Fig. 3 (b), is merely a nonresonant generalization of the resonant diagram Fig. 2 (c). Both diagrams – Fig. 2 (c) and Fig. 3 (b) – can be treated in a natural way by appropriate replacements within the electron propagator denominator. Specifically, we have the replacement $H \to H - {\rm i}\,\hat{\Gamma}/2$ for the infinite series involving the diagrams in Figs. 3 (a) and (b), and the corresponding replacement $E_{\rm 2P} \to E_{\rm 2P} - {\rm i}\,\Gamma_{\rm 2P}/2$ for the propagator denominator in the resonance approximation [see Figs. 2 (b) and (c) and the right-hand side of Eq. (26)]. Both added terms ($-{\rm i}\,\hat{\Gamma}/2$ and $-{\rm i}\,\Gamma_{\rm 2P}/2$) are *not* real energy shifts.

4 Conclusions

We have investigated a problematic set of two-loop self-energy corrections involving the square of the decay rate of the atomic state. These self-energy corrections cannot be interpreted as radiative energy shifts in the usual sense, although the relevant terms are generated by a fourth-order expansion of the Gell–Mann–Low–Sucher theorem (1) in powers of the quantum electrodynamic interaction Lagrangian (3). As explained in Sec. 2, some of the expressions arise naturally if we treat the self-energy leading to the decay rate as a first-order perturbation and consider the resulting second-order perturbation. The same problematic expressions involving squared decay rates result from the alternative formalism for deriving level shifts based on the two-time Green function method [19]. At some risk to over-simplification, we can state that the difficulties are related to the fact that the current methods inadequately address the question of the preparation of the excited atomic states and involve asymptotic states with an infinite lifetime. As explained in Sec. 3, some of the problematic two-loop self-energy corrections find a natural interpretation as radiative nonresonant corrections to the line-shape for atomic transitions which are of second order in the "decay rate operator" $\hat{\Gamma}$ defined in Eq. (24).

For the 2P–level in atomic hydrogen, as shown in Sec. 2, the problematic energy shift by squared decay rates is -14.9 Hz [see Eq. (19)]. For the 3P state of atomic hydrogen, the correction amounts to -7.47 Hz [see Eq. (21)]. It is perhaps interesting to note that the effect discussed here scales as $\alpha^2\,(Z\alpha)^6\,m\,c^2$ (for P states and states with higher angular momenta). The same order-of-magnitude is characteristic of the shift of the peak of the total photon scattering cross section in electric-dipole transitions in atomic hydrogen [20–23]. As is evident from Eqs. (16) and (18), an order-of-magnitude estimate for the problematic two-loop effect is given by the ratio of the square of the decay rate of the atomic state to a typical atomic energy level difference. For the 2S state with a natural line width of 1.3 Hz, the squared decay rate therefore does not represent an appreciable predictive limit in current and future experiments. The situation is different for the 2S–8D transition studied in [1]. Parametrically, the "squared-decay" corrections are of the order of $\alpha^2\,(Z\alpha)^6$ for the 8D state; however, if we assume a typical $1/n^3$-type scaling of the effect (n is the principal quantum number), then we immediately obtain an estimate below 1 Hz for the problematic effect in the 2S–8D transition in atomic hydrogen.

There has recently been a dramatic increase in the accuracy to which atomic energy levels can be measured experimentally [2] and evaluated theoretically (e.g. [3–7]). Tiny nonresonant effects that influence the natural line shape of hydrogenic transitions have received considerable attention [21–23], and it has been pointed out that nonresonant effects are enhanced in differential cross sections as opposed to total cross sections [22,23]. Essentially, the nonresonant effects give rise to a process-dependent new line shape, different from the Lorentzian, which has to be fitted by a number of parameters. By a suitable fit of the line shape, taking into account properly the relevant experimental conditions, it is *in principle* possible to correct the observed peak of the cross section for the nonresonant contributions. The same applies at least in part to the problematic two-loop corrections discussed here (see the discussion in Sec. 3), provided they are interpreted properly as radiative corrections to the off-resonance effects on the line shape. The problematic two-loop corrections illustrate that it is impossible to separate atomic energy levels at the order of $\alpha^2\,(Z\alpha)^6\,m\,c^2$, that is to say to define an energy shift that relates to one and only one level.

In [24], it has been stressed that several important problems associated with the normalization of electronic states and with the infrared catastrophe can be avoided if we consider the electron in a free state as obtained by ionization of a bound state (for example, by ionization of the atomic *ground* state which does not decay at all and is therefore the only "true" asymptotic state). The considerations presented in [24] imply that infrared divergences of free-electron quantum electrodynamics originate because one "disregards the methods of obtaining and detecting these (free) states". It has been shown that in special cases, the spontaneous emission from a certain "well" constructed state is exactly exponential [24]. We have mentioned above that the interpretation of the energy shift by squared decay rates is problematic because it is calculated as a matrix element evaluated on the excited atomic state. Within the formalism introduced in [24], we can argue that this procedure of evaluating the energy shift of the excited atomic state according to the current formalism is inconsistent because it disregards the fact that according to [24], the only "proper" way of defining the excited state is to view this state as having been obtained by excitation from the ground state.

Acknowledgements

The authors acknowlegde insightful discussions with Professor Jean Zinn–Justin. U.D.J., J.E. and C.H.K. gratefully acknowledge funding by the Deutsche Forschungsgemeinschaft (Nachwuchsgruppe within the Sonderforschungsbereich 276), and K.P. acknowledges support from the Polish Committee for Scientific Research under contract no. 2P03B 057 18.

References

[1] B. de Beauvoir, F. Nez, L. Julien, B. Cagnac, F. Biraben, D. Touahri, L. Hilico, O. Acef, A. Clairon, and J. J. Zondy, Phys. Rev. Lett. **78**, 440 (1997).

[2] M. Niering, R. Holzwarth, J. Reichert, P. Pokasov, T. Udem, M. Weitz, T. W. Hänsch, P. Lemonde, G. Santarelli, M. Abgrall, P. Laurent, C. Salomon, and A. Clairon, Phys. Rev. Lett. **84**, 5496 (2000).

[3] K. Pachucki, Phys. Rev. Lett. **72**, 3154 (1994).

[4] U. D. Jentschura, P. J. Mohr, and G. Soff, Phys. Rev. Lett. **82**, 53 (1999).

[5] K. Melnikov and T. v. Ritbergen, Phys. Rev. Lett. **84**, 1673 (2000).

[6] V. A. Yerokhin, Phys. Rev. Lett. **86**, 1990 (2001).

[7] K. Pachucki, Phys. Rev. A **63**, 042503 (2001).

[8] M. Gell-Mann and F. Low, Phys. Rev. **84**, 350 (1951).

[9] J. Sucher, Phys. Rev. **107**, 1448 (1957).

[10] C. Itzykson and J. B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, NY, 1980).

[11] A. Bohm, *Quantum Mechanics – Foundations and Applications* (Springer, New York, 1979).

[12] K. Pachucki, Ann. Phys. (N. Y.) **226**, 1 (1993).

[13] U. D. Jentschura and K. Pachucki, J. Phys. A **35**, 1927 (2002).

[14] U. D. Jentschura and K. Pachucki, Phys. Rev. A **54**, 1853 (1996).

[15] U. D. Jentschura, P. J. Mohr, and G. Soff, Phys. Rev. A **64**, 042512 (2001).

[16] S. G. Karshenboim, J. Phys. B **29**, L29 (1996).

[17] U. D. Jentschura and I. Nandori, e-print hep-ph/0205019.

[18] W. Kramers and W. H. Heisenberg, Z. Phys. **31**, 681 (1925).

[19] V. M. Shabaev, Phys. Rep. **356**, 119 (2002).

[20] F. Low, Phys. Rev. **88**, 53 (1952).

[21] L. N. Labzowsky, D. A. Solovyev, G. Plunien, and G. Soff, Phys. Rev. Lett. **87**, 143003 (2001).

[22] U. D. Jentschura and P. J. Mohr, e-print physics/0110053 (Can. J. Phys., in press, 2002).

[23] L. N. Labzowsky, D. A. Solovyev, G. Plunien, and G. Soff, e-print physics/0201067.

[24] K. Pachucki, Phys. Rev. A **44**, 5407 (1991).