Forbidden transitions in the helium atom

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Nonrelativistically forbidden, single-photon transition rates between low-lying states of the helium atom are rigorously derived within quantum electrodynamics theory. Equivalence of velocity and length gauges, including relativistic corrections is explicitly demonstrated. Numerical calculations of matrix elements are performed with the use of high-precision variational wave functions and compared to former results.

DOI: 10.1103/PhysRevA.64.042510

PACS number(s): 31.30.Jv, 12.20.Ds, 32.70.Cs, 31.15.Md

The existence of nonrelativistically forbidden transitions in helium, for example between the singlet and triplet states, indicates the presence of relativistic effects. The calculation of these effects in atoms or ions is a highly nontrivial task. Depending on the magnitude of nuclear charge Z, one performs various approximations. Here we study light atoms, so the expansion in the small parameter $Z \alpha$ is the most appropriate. Forbidden transitions have already been studied for many light atoms and especially for helium (for a review, see [1]). Historically, the first but approximate calculations of S-*P* forbidden transitions were performed by Elton in [2]. Since the dominant part comes from $2^{3}P_{1}$ and $2^{1}P_{1}$ mixing, he included in the calculation only these states. Drake and Dalgarno in [3] were the first to include higher excited states, which led to much higher precision. Moreover, Drake later [4] accounted for corrections to S-state wave functions. Although these calculations were correct, there was no proof that they are complete. As an example, may serve the $2^{3}S_{1}$ -1 $^{1}S_{0}$ M1 transition. Feinberg and Sucher [5] derived an effective operator for this transition and showed the cancellation of electron-electron terms. However, the calculations of Drake in [6] were performed earlier with the implicit assumption that these terms are absent. In a completely different approach based on relativistic many-body perturbation theory (RMBPT), Johnson et al. [1] and Derevianko et al. [7] studied forbidden transition in both velocity and length gauge. They pointed out the significance of negative energy states. However, not all results were in agreement with the nonrelativistic approach based on the Breit Hamiltonian. It is the purpose of this paper to systematically derive matrix elements for forbidden transitions in helium within quantum electrodynamics theory. The equivalence of length and velocity gauges for E1 transitions, including relativistic corrections, is explicitly shown. With the use of optimized numerical wave functions, the amplitudes and transition probabilities for $2^{3}P_{2}-1^{1}S_{0}$, $2^{3}P_{1}-1^{1}S_{0}$, $2^{1}P_{1}$ $-2^{3}S_{1}$, $2^{3}S_{1}-1^{1}S_{0}$, and $3^{3}S_{1}-2^{3}S_{1}$ are calculated with high precision and compared to former results.

The nonrelativistic helium atom interacting with the electromagnetic field is described by the Schrödinger-Pauli Hamiltonian

$$H = \frac{(\vec{p}_1 - e\vec{A})^2}{2m} + \frac{(\vec{p}_2 - e\vec{A})^2}{2m} + \frac{\alpha}{r} - \frac{Z\alpha}{r_1} - \frac{Z\alpha}{r_2}.$$
 (1)

The single-photon transition amplitude T between two eigenstates ϕ and ψ , in the electric dipole approximation is

$$T^{i} = \left\langle \phi \left| \frac{(p_{1} + p_{2})^{i}}{m} \right| \psi \right\rangle = i(E_{\phi} - E_{\psi}) \left\langle \phi \right| (r_{1} + r_{2})^{i} | \psi \rangle,$$
(2)

and the transition probability \mathcal{A} is

$$\mathcal{A} = 2 \alpha |E_{\phi} - E_{\psi}| T^{i} T^{*j} \left(\delta^{ij} - \frac{k^{i} k^{j}}{k^{2}} \right).$$
(3)

In the effective Hamiltonian approach, relativistic corrections enter in two ways, as corrections to the wave functions ϕ and ψ and the correction $\delta \vec{j}$ to the current \vec{p}/m

$$\vec{T} = \langle \phi | \delta \vec{j} | \psi \rangle + \left\langle \phi \left| \frac{\vec{p}_1 + \vec{p}_2}{m} \frac{1}{(E - H)'} \delta H \right| \psi \right\rangle + \left\langle \phi \left| \delta H \frac{1}{(E - H)'} \frac{\vec{p}_1 + \vec{p}_2}{m} \right| \psi \right\rangle.$$
(4)

The correction to the wave function is given by the Breit Hamiltonian. The part responsible for singlet-triplet transition is

$$\delta H = \left[\frac{Z \,\alpha}{4 \,m^2} \left(\frac{\vec{r}_1}{r_1^3} \times \vec{p}_1 - \frac{\vec{r}_2}{r_2^3} \times \vec{p}_2 \right) + \frac{\alpha}{4 \,m^2} \frac{\vec{r}}{r^3} \\ \times (\vec{p}_1 + \vec{p}_2) \right] \frac{\vec{\sigma}_1 - \vec{\sigma}_2}{2} \\ \equiv \vec{h} \cdot \frac{\vec{\sigma}_1 - \vec{\sigma}_2}{2}.$$
(5)

Corrections to the current are given by several time-ordered diagrams, shown in Fig. 1. The corresponding expression is calculated as follows. The first diagram is



FIG. 1. Time-ordered diagrams for corrections to the current. The dashed line is a Coulomb photon; the wavy line is the transverse photon.

$$\delta \vec{j}_{1} = u^{+}(p')\vec{\alpha}u(p) = \frac{1}{2m}(\vec{p}'+\vec{p}) - \frac{i}{2m}[(\vec{p}'-\vec{p})\times\vec{\sigma}] - \frac{1}{16m^{3}}(p'^{2}+3p^{2})(\vec{p}+i\vec{p}\times\vec{\sigma}) - \frac{1}{16m^{3}}(p^{2}+3p'^{2}) \times(\vec{p}'-i\vec{p}'\times\vec{\sigma}),$$
(6)

where u(p) is a normalized plane-wave solution of the free Dirac equation. For considered transitions, one may leave spin-dependent terms only. In position representation, it takes a form

$$\delta \vec{J}_{1} = \frac{i}{2m} \vec{\sigma} \times [\vec{p}, e^{i\vec{k}\cdot\vec{r}}] + \frac{i}{16m^{3}} \{\vec{p} \times \vec{\sigma} e^{i\vec{k}\cdot\vec{r}} p^{2} + 3\vec{p} \\ \times \vec{\sigma} p^{2} e^{i\vec{k}\cdot\vec{r}} - p^{2} e^{i\vec{k}\cdot\vec{r}} \vec{p} \times \vec{\sigma} - 3e^{i\vec{k}\cdot\vec{r}} \vec{p} \times \vec{\sigma} p^{2} \}.$$
(7)

The photon momentum k is of order $m(Z \alpha)^2$, while r is of order $(m Z \alpha)^{-1}$. This means that $e^{i \vec{k} \cdot \vec{r}}$ can be expanded in powers of $\vec{k} \cdot \vec{r}$. After adding contributions from both electrons, the $(Z \alpha)^2$ correction takes the form

$$\delta \vec{J}_1 = \frac{1}{2 m} (\vec{k} \cdot \vec{r}_1) \vec{k} \times \vec{\sigma}_1 + \frac{1}{2 m} (\vec{k} \cdot \vec{r}_2) \vec{k} \times \vec{\sigma}_2.$$
(8)

The next diagram involves one electron-positron pair and the corresponding expression is

$$\delta \vec{J}_{2} = -\frac{Z e^{2}}{q^{2}} \frac{1}{2 m} u^{+}(p') [\vec{\alpha} \Lambda_{-}(p+q) + \Lambda_{-}(p'-q)\vec{\alpha}] u(p)$$
$$= \frac{i}{2 m^{2}} \frac{Z e^{2}}{q^{2}} \vec{q} \times \vec{\sigma} \to -\frac{1}{2 m^{2}} \frac{Z \alpha}{r^{3}} \vec{r} \times \vec{\sigma} e^{i \vec{k} \cdot \vec{r}}, \qquad (9)$$

where Λ_{-} is a projection operator into the negative energy subspace and *q* is a momentum exchange between electron and the nucleus. The $(Z \alpha)^2$ correction from both electrons becomes

$$\delta \vec{j}_2 = -\frac{1}{2 m^2} \frac{Z \alpha}{r_1^3} \vec{r}_1 \times \vec{\sigma}_1 - \frac{1}{2 m^2} \frac{Z \alpha}{r_2^3} \vec{r}_2 \times \vec{\sigma}_2.$$
(10)

The remaining diagrams in Fig. 1 involve electron-electron terms. The last two diagrams are of higher order, so they will not be considered here. The expression for diagram 3 can be obtained from Eq. (9) by the replacements $-Z \alpha \rightarrow \alpha$. In this way, one obtains

$$\delta \vec{J}_3 = \frac{1}{2 m^2} \frac{\alpha}{r^3} \vec{r} \times \vec{\sigma}_1 e^{i \vec{k} \cdot \vec{r}_1} + (1 \leftrightarrow 2), \qquad (11)$$

where \vec{r} denotes here $\vec{r} \equiv \vec{r_{12}} = \vec{r_1} - \vec{r_2}$. The $(Z \alpha)^2$ correction is

$$\delta \vec{J}_{3} = \frac{1}{2 m^{2}} \frac{\alpha}{r^{3}} \vec{r} \times (\vec{\sigma}_{1} - \vec{\sigma}_{2}).$$
(12)

The expression for diagram 4 in Fig. 1 is

$$\delta J_{4}^{i} = -\frac{1}{2 m} \frac{e^{2}}{q^{2}} \left(\delta^{jk} - \frac{q^{j}q^{k}}{q^{2}} \right) u^{+}(p_{2}') \alpha^{k} u(p_{2}) u^{+}(p_{1}') \\ \times [\alpha^{i} \Lambda_{-}(p_{1}+q) \alpha^{j} + \alpha^{j} \Lambda_{-}(p_{1}'-q) \alpha^{i}] u(p_{1}) \\ + (1 \leftrightarrow 2).$$
(13)

The term in the second line equals 2 δ^{ij} and that in the first line has already appeared in Eq. (6), so it becomes

$$\delta \vec{j}_4 = \frac{i}{2m} \frac{e^2}{q^2} \vec{q} \times \vec{\sigma}_2 + (1 \leftrightarrow 2) \rightarrow \frac{1}{2m^2} \frac{\alpha}{r^3} \vec{r} \times \vec{\sigma}_2 e^{i\vec{k} \cdot \vec{r_1}} + (1 \leftrightarrow 2).$$
(14)

The $(Z \alpha)^2$ correction is

$$\delta \vec{j}_4 = -\frac{1}{2 m^2} \frac{\alpha}{r^3} \vec{r} \times (\vec{\sigma}_1 - \vec{\sigma}_2), \qquad (15)$$

and cancels out with that from diagram 3, Eq. (12). The final expression for the relativistic correction to the current of order $O(Z \alpha)^2$ is the sum of Eqs. (8) and (10)

$$\delta \vec{J} = \frac{1}{2 m} (\vec{k} \cdot \vec{r}_1) \vec{k} \times \vec{\sigma}_1 + \frac{1}{2 m} (\vec{k} \cdot \vec{r}_2) \vec{k} \times \vec{\sigma}_2 - \frac{1}{2 m^2} \frac{Z \alpha}{r_1^3} \vec{r}_1 \times \vec{\sigma}_1 - \frac{1}{2 m^2} \frac{Z \alpha}{r_2^3} \vec{r}_2 \times \vec{\sigma}_2.$$
(16)

This δj could be also derived through the Fouldy-Wouythusen transformation of $\alpha^i e^{i \vec{k} \cdot \vec{r}}$, however, in this way, possible electron-electron terms are omitted, which happens to be correct for just this case. Having δj and δH , the transition amplitude T^i in Eq. (4) will be transformed to the length gauge with the use of identity

$$\frac{\vec{p}_1 + \vec{p}_2}{m} = i[H, \vec{r}_1 + \vec{r}_2], \qquad (17)$$

and the fact the terms in T^i proportional to k^i do not contribute to the transition rate, as can be seen from Eq. (3). After performing simple algebraic transformations, the result is

$$T^{i} = i(E_{\phi} - E_{\psi}) \left\{ \left\langle \phi | (r_{1}^{i} + r_{2}^{i}) \frac{1}{(E_{\psi} - H)'} \delta H | \psi \right\rangle + \left\langle \phi | \delta H \frac{1}{(E_{\psi} - H)'} (r_{1}^{i} + r_{2}^{i}) | \psi \right\rangle \right\} + \frac{1}{2 m} \epsilon^{ijk} \left\langle \phi | k^{j} T^{kl} k^{l} | \psi \right\rangle,$$
(18)

where

$$T^{kl} = \frac{1}{2} \left[r^k \frac{(\sigma_1 - \sigma_2)^l}{2} + r^l \frac{(\sigma_1 - \sigma_2)^k}{2} - \frac{2}{3} \,\delta^{kl} \vec{r} \cdot \frac{(\vec{\sigma}_1 - \vec{\sigma}_2)}{2} \right]. \tag{19}$$

The first term in Eq. (18) corresponds to electric dipole, and the second one to magnetic quadrupole transitions. It is worth noting that for electric dipole transitions, as given in length gauge, relativistic corrections enter only through corrections to the Hamiltonian δH .

So far, we have considered only forbidden transitions with spin change between *S* and *P* states, namely $2 {}^{3}P_{2} \rightarrow 1 {}^{1}S_{0}$, $2 {}^{3}P_{1} \rightarrow 1 {}^{1}S_{0}$ and $2 {}^{1}P_{1} \rightarrow 2 {}^{3}S_{1}$. However, even more forbidden *M*1 transitions $2 {}^{3}S_{1} \rightarrow 1 {}^{1}S_{0}$ and $3 {}^{3}S_{1} \rightarrow 2 {}^{3}S_{1}$ arrive at the order $O(Z \alpha)^{3}$, so they are not described by the expression in Eq. (16). No second-order type of terms contribute and in the calculation of δj_{M} , one takes the next corresponding term in the expansion of $e^{i \vec{k} \cdot \vec{r}}$ in Eqs. (6), (9), (12), and (16)

$$\delta \vec{J}_{M} = \frac{i}{2m} \frac{(\vec{k} \cdot \vec{r}_{1})^{2}}{2} \vec{k} \times \vec{\sigma}_{1} + \frac{i}{4m^{3}} p_{1}^{2} \vec{k} \times \vec{\sigma}_{1}$$
$$+ \frac{i}{4m^{3}} (\vec{k} \cdot \vec{p}_{1}) \vec{p}_{1} \times \vec{\sigma}_{1} - \frac{i}{2m^{2}} (\vec{k} \cdot \vec{r}_{1}) \frac{Z\alpha}{r_{1}^{3}} \vec{r}_{1} \times \vec{\sigma}_{1}$$
$$+ \frac{i}{2m^{2}} (\vec{k} \cdot \vec{r}) \frac{\alpha}{r} \vec{r} \times \vec{\sigma}_{1} + (1 \leftrightarrow 2).$$
(20)

This result agrees with the former one, obtained by Feinberg and Sucher in [5]. For M1 transition between $2^{3}S_{1}$ and $1^{1}S_{0}$ it could be further simplified to

$$\delta \vec{J}_{M} = \frac{i}{m} \vec{k} \times \frac{(\vec{\sigma}_{1} - \vec{\sigma}_{2})}{2} \left[\frac{k^{2}}{12} (r_{1}^{2} - r_{2}^{2}) + \frac{1}{3 m^{2}} (p_{1}^{2} - p_{2}^{2}) - \frac{1}{6 m} \left(\frac{Z \alpha}{r_{1}} - \frac{Z \alpha}{r_{2}} \right) \right].$$
(21)

 k^2 in the above can be replaced by

$$k^{2}r_{1}^{2} \rightarrow [H, [H, r_{1}^{2}]] = \frac{2}{m} \frac{Z \,\alpha}{r_{1}} - \frac{2}{m^{2}} p_{1}^{2} - \frac{2}{m} \frac{\alpha}{r^{3}} \vec{r} \cdot \vec{r}_{1}, \quad (22)$$

in this way, one obtains for δj_M another simple expression

$$\delta \vec{J}_{M} = \frac{i}{m} \vec{k} \times \frac{(\vec{\sigma}_{1} - \vec{\sigma}_{2})}{2} \left[\frac{1}{6 m^{2}} (p_{1}^{2} - p_{2}^{2}) - \frac{1}{6 m} \frac{\alpha}{r^{3}} (r_{1}^{2} - r_{2}^{2}) \right].$$
(23)

The analogous expression for the $3 {}^{3}S_{1} - 2 {}^{3}S_{1}$ transition reads

$$\delta \vec{J}_M = \frac{i}{m} \vec{k} \times \frac{(\vec{\sigma}_1 + \vec{\sigma}_2)}{2} \left[\frac{1}{3 m} \left(\frac{Z \alpha}{r_1} + \frac{Z \alpha}{r_2} \right) - \frac{1}{6 m} \frac{\alpha}{r} \right].$$
(24)

We now consider the spin algebra in the calculation of the transition probability, as given by Eqs. (3) and (18). One sums up over final states and averages out over initial states. The appropriate formulas are

$$|{}^{1}S_{0}\rangle\langle{}^{1}S_{0}| = |{}^{1}S\rangle\langle{}^{1}S|\left(1 - \frac{s^{2}}{2}\right),$$
 (25)

$$\frac{1}{3} \sum_{m} |{}^{3}S_{1}, m\rangle \langle {}^{3}S_{1}, m| = |{}^{3}S\rangle \langle {}^{3}S| \frac{s^{2}}{6}, \qquad (26)$$

$$|{}^{3}P_{0}\rangle\langle{}^{3}P_{0}| = |{}^{3}P^{i}\rangle\langle{}^{3}P^{j}|\Big(\delta^{ij}\frac{s^{2}}{2} - s^{j}s^{i}\Big),$$
 (27)

$$\frac{1}{3} \sum_{m} |{}^{3}P_{1}, m\rangle \langle {}^{3}P_{1}, m| = |{}^{3}P^{i}\rangle \langle {}^{3}P^{j}| \frac{1}{2} s^{i} s^{j}, \qquad (28)$$

$$\frac{1}{5} \sum_{m} |{}^{3}P_{2},m\rangle \langle {}^{3}P_{2},m| = |{}^{3}P^{i}\rangle \langle {}^{3}P^{j}| \frac{1}{10} (2 s^{2} \delta^{ij} - 3 s^{i} s^{j} + 2 s^{j} s^{i}), \qquad (29)$$

$$\frac{1}{3} \sum_{m} |{}^{1}P_{1}, m\rangle \langle {}^{1}P_{1}, m| = |{}^{1}P^{i}\rangle \langle {}^{3}P^{j}| \,\delta^{ij} \left(1 - \frac{s^{2}}{2}\right), \quad (30)$$

where $s = \sigma_1/2 + \sigma_2/2$ and the following normalization is utilized: $\langle P^i | P^j \rangle = \delta^{ij}/3$. Moreover, for these calculations one needs two formulas for spin product

$$(\sigma_1 - \sigma_2)^i \left(1 - \frac{s^2}{2}\right) (\sigma_1 - \sigma_2)^j = 2 \,\delta^{ij} s^2 - 4 s^j s^i,$$
 (31)

$$(\sigma_1 - \sigma_2)^i s^2 (\sigma_1 - \sigma_2)^j = 8 \,\delta^{ij} \left(1 - \frac{s^2}{2}\right),$$
 (32)

and the following set of formulas for spin traces:

$$\mathrm{Tr}\,s^i = 0, \tag{33}$$

$$\operatorname{Tr} s^{i} s^{j} = 2 \,\delta^{ij},\tag{34}$$

$$\operatorname{Tr} s^{i} s^{j} s^{k} = i \, \boldsymbol{\epsilon}^{ijk}, \tag{35}$$

$$\operatorname{Tr} s^{i} s^{j} s^{k} s^{l} = \delta^{ij} \delta^{kl} + \delta^{jk} \delta^{il}.$$
(36)

With the help of the above formulas, one obtains for transition probabilities (for simplicity we put m = 1) the following expressions:

$$\mathcal{A}({}^{3}P_{1} \rightarrow {}^{1}S_{0}) = \frac{2}{9} \alpha k^{3} \left| \epsilon^{ijk} \left\langle {}^{3}P^{k} \right| h^{i} \frac{1}{E_{P} - H} (r_{1} + r_{2})^{j} + (r_{1} + r_{2})^{j} \frac{1}{E_{S} - H} h^{i} \right| {}^{1}S \right\rangle \right|^{2},$$
(37)

$$\mathcal{A}({}^{3}P_{2} \to {}^{1}S_{0}) = \frac{1}{30} \alpha \, k^{5} |\langle {}^{3}P^{i} | r^{i} | {}^{1}S \rangle|^{2}, \qquad (38)$$

$$\mathcal{A}({}^{1}P_{1} \rightarrow {}^{3}S_{1}) = \frac{2}{9} \alpha k^{3} \left| \epsilon^{ijk} \left\langle {}^{1}P^{k} \right| h^{i} \frac{1}{E_{P} - H} (r_{1} + r_{2})^{j} + (r_{1} + r_{2})^{j} \frac{1}{E_{S} - H} h^{i} \right| {}^{3}S \right\rangle \right|^{2} + \frac{1}{18} \alpha k^{5} |\langle {}^{1}P^{i} | r^{i} | {}^{3}S \rangle|^{2},$$
(39)

$$\mathcal{A}({}^{3}S_{1} \rightarrow {}^{1}S_{0}) = \frac{4}{3} \alpha k^{3} \left| \left\langle {}^{1}S \left| \frac{1}{6} (p_{1}^{2} - p_{2}^{2}) - \frac{1}{6} \frac{\alpha}{r^{3}} (r_{1}^{2} - r_{2}^{2}) \right| {}^{3}S \right\rangle \right|^{2},$$
(40)

$$\mathcal{A}({}^{3}S_{1} \rightarrow {}^{3}S_{1}) = \frac{4}{3} \alpha k^{3} \left| \left\langle {}^{3}S \right| \frac{1}{3} \left(\frac{Z \alpha}{r_{1}} + \frac{Z \alpha}{r_{2}} \right) - \frac{1}{6} \frac{\alpha}{r} \left| {}^{3}S \right\rangle \right|^{2}, \tag{41}$$

where $k = |\Delta E|$, and h^i is defined by Eq. (5). It is worth noting that ${}^1P_1 \rightarrow {}^3S_1$ is not only a *E*1 transition but also *M*2, which has not yet been recognized in the literature.

Once transition probabilities are expressed in terms of matrix elements between nonrelativistic wave functions, they can be calculated numerically with high precision. In the numerical calculation, we follow an approach developed by Korobov [8]. The wave function is expressed in terms of exponentials

$$\phi_{S} = \sum_{i} c_{i} [e^{-\alpha_{i}r_{1} - \beta_{i}r_{2} - \gamma_{i}r} + (r_{1} \leftrightarrow r_{2})], \qquad (42)$$

$$\vec{\phi}_P = \sum_i c_i [\vec{r}_1 e^{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r} \mp (r_1 \leftrightarrow r_2)], \qquad (43)$$

$$\vec{\phi}_{P+} = \sum_{i} \vec{c_i r_1} \times \vec{r_2} [e^{-\alpha_i r_1 - \beta_i r_2 - \gamma_i r_1} \mp (r_1 \leftrightarrow r_2)]. \quad (44)$$

The parameters $\alpha_i, \beta_i, \gamma_i$ are chosen randomly between some minimal and maximal values, which were found by minimization of energy of a specified state. The maximal dimension of this basis set was 600. Lower values were used

TABLE I. Transition rates in helium in units s^{-1} ; $[n] \equiv 10^n$.

transition	ΔE in atomic units	rate \mathcal{A}
$E1 + M2: 2 {}^{1}P_{1} \rightarrow 2 {}^{3}S_{1}$	0.051 386 291 7	1.548 945
E1: $2^{3}P_{1} \rightarrow 1^{1}S_{0}$	0.770 560 686 3	1.775 771[2]
$M2: 2 {}^{3}P_{2} \rightarrow 1 {}^{1}S_{0}$	0.770 560 686 3	3.270 326[-1]
$M1: 2 {}^{3}S_{1} \rightarrow 1 {}^{1}S_{0}$	0.728 4949 988	1.272 426[-4]
$M1: 3 {}^{3}S_{1} \rightarrow 2^{3}S_{1}$	0.106 5403 10 8	6.484 690[-9]

for checking convergence. The advantage of this basis set is simplicity of matrix elements, which are expressed in terms of integral

$$\frac{1}{16 \pi^2} \int d^3 r_1 d^3 r_2 \frac{e^{-\alpha r_1 - \beta r_2 - \gamma r}}{r_1 r_2 r} = \frac{1}{(\alpha + \beta)(\beta + \gamma)(\gamma + \alpha)}.$$
(45)

For some more singular matrix elements, an additional integral with respect to corresponding parameters has to be performed. The disadvantage of this basis set is the necessity of using quadruple precision for N>100. Moreover, the second-order terms require more careful tuning of parameters due to the singularity of δH and large mixing of $2^{3}P_{1}$ and $2^{1}P_{1}$ states. These, which involve odd parity intermediate *P* states, are much larger than those that involve even parity *P* states, by approximately three orders of magnitude. It is due to the fact that energies of even parity *P* states lie beyond the ionization level. Most often, these small secondorder terms were neglected in the former calculations. However, they are not neglected here. Our numerical results for forbidden transitions between low-lying states are presented in Table I.

In the comparison with former work, we start with the M1 transition $2^{3}S_{1} \rightarrow 1^{1}S_{0}$. This transition was measured by Moos and Woodworth in [9] with the result A $= 1.10(33) \times 10^{-4}$ s⁻¹ and Berry from Notre Dame is currently preparing a more precise measurement [10]. The first (correct) theoretical result obtained by Drake in [6] 1.272 $\times 10^{-4}$ s⁻¹ is in agreement with the experimental value. However, as pointed out by Feinberg and Sucher in [5], Drake has not considered electron-electron terms, which happened to cancel out for this transition. Later, Johnson et al. [1] used RMBPT to calculate forbidden transitions for any heliumlike ions and obtained a result for Z=2, which is 1.266×10^{-4} s⁻¹. It differs slightly from the result obtained here, 1.272426×10^{-4} s⁻¹, due to inclusion in [1] of some higher-order terms, while electron correlations were not well accounted for. Moreover, there are unknown radiative corrections and exchange type of diagrams of order $\alpha/(2\pi)$, the last two in Fig. 1, to any of these transitions. Therefore, only the first three digits are physically significant. Numerical results are presented with higher precision for the purpose of comparison with former results. Next, the M1 transition $3 {}^{3}S_{1} \rightarrow 2 {}^{3}S_{1}$ rate was obtained only by Derevianko *et al.* in [7]. Their result, 1.1710^{-8} s⁻¹, disagrees with ours, $6.484\,690\,10^{-9}$ s⁻¹. The reason of this discrepancy is left unexplained. It may indicate the loss of accuracy of RMBPT

due to strong numerical cancellation. This discrepancy does not have an experimental impact since this rate is too small for Z=2 to be measured. However, calculations should be verified for higher Z, where this transition rate grows with Z^{10} and becomes measurable at some value of Z. The next considered transition is $M2: 2 {}^{3}P_{2} \rightarrow 1 {}^{1}S_{0}$. It was first obtained by Drake [4]: $\mathcal{A}=0.327 {}^{s^{-1}}$, and later by Johnson et al. [1] $\mathcal{A} = 0.3271$ s⁻¹, in agreement with our result \mathcal{A} = 0.3270326 s⁻¹. The calculation of the intercombination E1 transition $2^{3}P_{1} \rightarrow 1^{1}S_{0}$ was a little more elaborate, since it involves infinite summation over intermediate states. In former works, the second term in Eq. (37) involving even parity P states was neglected. Indeed, calculations show it is smaller than 1%. The first complete result by Drake [4] is $\mathcal{A}=176.4 \text{ s}^{-1}$. RMBPT calculations of Johnson *et al.* [1] including negative energy states is $A = 175.7 \text{ s}^{-1}$ and our result A = 177.5771 s⁻¹ agrees within 1%. The last transition $2^{1}P_{1} \rightarrow 2^{3}S_{1}$ is a sum of E1 and M2. The result \mathcal{A} = 1.55 s⁻¹ obtained by Drake includes only E1 transition.

Our result is A = 1.548945 s⁻¹ and the magnetic transition happened to be negligible, 0.000019, due to small energy splitting.

In summary, we have presented a rigorous derivation of rates for nonrelativistically forbidden transitions. We demonstrated equivalence of length and velocity gauges including relativistic correction for forbidden transitions. We confirmed the commonly used fact that in the length gauge, relativistic corrections enters only through corrections to wave function as given by the Breit Hamiltonian. We verified that the M2 $2 {}^{1}P_{1} \rightarrow 2 {}^{3}S_{1}$ transition is much smaller than E1, which was implicitly assumed in former works. Our numerical calculations using simple exponential functions confirmed former results with the exception of the $3 {}^{3}S_{1} \rightarrow 2 {}^{3}S_{1}$ transition, where our result is approximately twice as small as [7].

ACKNOWLEDGMENT

The work of K.P. was supported by the Polish Committee for Scientific Research under Contract No. 2P03B 057 18.

- W.R. Johnson, D.R. Plante, and J. Sapirstein, Adv. At., Mol., Opt. Phys. 35, 255 (1995).
- [2] R.C. Elton, Astrophys. J. 148, 573 (1967); R.C. Elton and W.W. Koppendorfer, Phys. Rev. 160, 194 (1967).
- [3] G.W.F. Drake and A. Dalgarno, Astrophys. J. 157, 459 (1969).
- [4] G.W.F. Drake, J. Phys. B 9, L169 (1976).
- [5] G. Feinberg and J. Sucher, Phys. Rev. Lett. 26, 681 (1971).
- [6] G.W.F. Drake, Phys. Rev. A 3, 908 (1971).

- [7] A. Derevianko, I.M. Savukov, and W.R. Johnson, Phys. Rev. A 58, 4453 (1998).
- [8] V.I. Korobov, Phys. Rev. A 61, 064503 (2000).
- [9] H.W. Moos and J.R. Woodworth, Phys. Rev. A 12, 2455 (1975).
- [10] Physical constants are from [11]: $m \alpha^2 \rightarrow (2 \pi) 2 \operatorname{R} c$ = 4.134 137 33 \cdot 10¹⁶ s⁻¹, α^{-1} = 137.035 999 6.
- [11] P.J. Mohr and B.N. Taylor, Rev. Mod. Phys. 72, 351 (2000).