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Radiative orbital electron capture by the atomic nucleus

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The rate for the photon emission accompanying orbital 1S electron capture by the atomic nucleus is recalculated. While a photon can be emitted by the electron or by the nucleus, the use of the length gauge significantly suppresses the nuclear contribution. Our calculations resolve the long standing discrepancy of theoretical predictions with experimental data for $\Delta J = 2$ forbidden transitions. We illustrate the results by comparison with the data established experimentally for the first forbidden unique decays of ^{41}Ca and ^{204}Tl .

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I. INTRODUCTION

Orbital electron capture by the atomic nucleus (EC) is one of the nuclear decay modes governed by weak interactions, a common and well-known type of radioactivity [1]. In this process the released energy Q (equal to the transition energy Q_{EC} minus the binding energy of the captured electron in the daughter atom) is shared between an emitted electron neutrino and the final atom. With a small probability, of the order of 10^{-4} with respect to the normal EC decay, a photon can be emitted together with the neutrino. In such radiative electron capture decay (REC) the energy is shared statistically between three bodies, thus the energy spectrum of these photons is continuous.

The theoretical description of REC was initiated by Morrison and Schiff [2] who neglected the Coulomb field of the nucleus and took into account just 1S electrons and only in nonrelativistic approximation. An advanced and more accurate theory of radiative electron capture was developed by Glauber and Martin in Refs. [3,4]. They included exactly the Coulomb field in the propagation of the electron, took into account relativistic effects as well as screening and considered captures from higher shells. However, they limited themselves to the allowed decays where the nuclear spin changes by $\Delta J = 0, 1$ with no parity change. Predictions of this model were tested in a large number of experiments, and satisfactory agreement was found [1].

A more general theory of REC, extended to any order of forbiddenness (i.e., for arbitrary change of nuclear angular momentum and parity), was developed by Zon and Rapoport in Ref. [5] and Zon in Ref. [6]. For verification of their results, first forbidden unique transitions ($\Delta J = 2, \pi_i \pi_f = -1$) are of special importance because of a cancellation of the nuclear matrix elements in the ratio of radiative to the nonradiative capture rate. Measurements of radiation accompanying the 1S EC decay in the case of ^{41}Ca [7], which belongs to this category, revealed a serious disagreement with results of Refs. [5,6]. The shape of the photon spectrum differed from the prediction, and the total probability of the REC process per ordinary nonradiative decay was found to be *larger* by a factor of 6 than the predicted one. To resolve this discrepancy a possibility of photon emission by the nucleus, in so called

detour transitions, was examined by Kalinowski *et al.* [8,9] following ideas developed by Ford and Martin [10], see Fig. 1.

According to Refs. [8–10], the nuclear contribution to the REC process accompanying forbidden transitions can be substantial. In particular, for the case of ^{41}Ca it was claimed [8,9] that the detour transitions fully account for the missing intensity established by the experiment. However, for another first forbidden unique transition—the 1S EC decay of ^{204}Tl —a different situation was encountered. The measured intensity of the REC spectrum [11] was found to be *smaller* by a factor of 4 than the value predicted by the model of Zon leaving no room for the nuclear contribution, in contradiction with results of Ref. [9].

Although we agree in general with Refs. [9,10] that nuclear radiation takes place, we point out that the separation of radiation emitted by the electron and the nucleus, respectively, is not physical because it depends on the particular gauge used in the description of the electromagnetic field. We argue, that although physical results do not depend on the selected gauge, the so-called *length* gauge is preferred for the actual calculations. First, it suppresses the nuclear contribution, and second, it makes possible important simplifications in the calculations. We note that some formulas of Zon in [6] for $\Delta J = 2$ transition are divergent for the point nucleus. It means that approximations which lead to these formulas may not be correct. For example, an assumption that the radius of the region where the photon emission occurs is much larger than the dimension of the nucleus where the capture takes place, is not valid in the Coulomb (velocity) gauge used by the authors of Refs. [5,6,9].

The failure of the theory of Zon and Rapoport to describe the experimental data for forbidden EC transitions, and the controversy concerning the nuclear contribution to the REC process, motivated us to address these questions theoretically in an independent and different way. In this work we recalculate the radiative electron capture process in the length gauge. We include only the radiation from the electron, as the probability of the photon radiation from the nucleus is $(QR)^2 \approx 10^{-4}$ (with R being the nuclear radius) smaller in this gauge, and thus can safely be neglected. We restrict ourselves to the 1S electron (K-capture), but the extension to other states is straightforward.

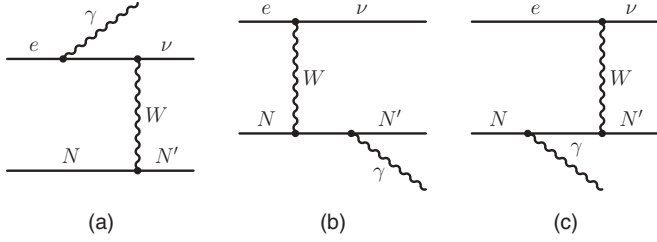


FIG. 1. Diagrams describing radiative orbital electron capture by the nucleus, (a) photon emission by the electron, (b) and (c) photon emission by the nucleus (detour transitions). Probability amplitude for each diagram depends on gauge and we argue that in the so called length gauge, Eqs. (35) and (36), diagrams (b) and (c) can be neglected.

In the following section we describe our calculations in detail. The results, in terms of a dimensionless shape factor, for the case of the first forbidden unique transitions are presented in Sec. III and are compared to the experimental data for ^{41}Ca and ^{204}Tl . Comparison to previous calculations is made in Sec. IV followed by a summary in Sec. V.

II. THEORY

A. Preliminaries

In order to present derivation of the rate for the radiative electron orbital capture, we at first define units, notations and construct wave functions for the electron, the neutrino and the photon in the angular momentum basis. In the following we use natural units $\hbar = c = 1$, $e^2 = 4\pi\alpha$ and set the electron mass $m = 1$. The Hamiltonian for the EC-decay is

$$H_{EC} = \frac{G_F}{\sqrt{2}} [\bar{\psi}_n \gamma_\mu (1 - \lambda \gamma^5) \psi_p] [\bar{\psi}_\nu \gamma^\mu (1 - \gamma^5) \psi_e], \quad (1)$$

where ψ_n , ψ_p , ψ_ν , and ψ_e denote neutron, proton, neutrino, and electron bispinors, respectively, with Fermi constant $G_F = 1.16639(1)10^{-5} \text{ GeV}^{-2}$ and $\lambda = 1.26992(69)$. We use the convention of Björken and Drell [12] for Dirac matrices with $\gamma^5 = \gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3$, namely,

$$\gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \vec{\gamma} = \begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix}, \quad \gamma^5 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad (2)$$

and $\vec{\alpha} = \gamma^0 \vec{\gamma}$.

Matrix elements of H_{EC} in Eq. (1) are calculated with wave functions, having a definite angular momentum. For this reason we introduce spin spherical harmonics χ_κ^m [14]

$$\chi_\kappa^m(\theta, \phi) = \begin{pmatrix} \frac{-\kappa}{|\kappa|} \sqrt{\frac{\kappa+1/2-m}{2\kappa+1}} Y_{|\kappa+1/2|-1/2}^{m-1/2} \\ \sqrt{\frac{\kappa+1/2+m}{2\kappa+1}} Y_{|\kappa+1/2|-1/2}^{m+1/2} \end{pmatrix}, \quad (3)$$

where

$$\kappa = \begin{cases} j + 1/2 & \text{for } j = l - 1/2, \\ -(j + 1/2) & \text{for } j = l + 1/2. \end{cases} \quad (4)$$

They have the following properties:

$$\vec{\sigma} \cdot \hat{r} \chi_\kappa^m = -\chi_{-\kappa}^m, \quad (5)$$

$$\vec{\sigma} \cdot \vec{L} \chi_\kappa^m = -(\kappa + 1) \chi_\kappa^m \quad (6)$$

which are used to solve the Dirac equation. We consider this solution for the left handed neutrino, namely,

$$\frac{1}{2}(1 - \gamma^5)\psi_\nu = \psi_\nu. \quad (7)$$

The wave function ψ_ν with the angular momentum j and the energy q is

$$\psi_\nu(\vec{r}) = \begin{pmatrix} \nu \\ -\nu \end{pmatrix}, \quad (8)$$

$$\nu = q [j_{j-1/2}(qr) \chi_{-(j+1/2)}^m(\theta, \phi) + i j_{j+1/2}(qr) \chi_{j+1/2}^m(\theta, \phi)], \quad (9)$$

with $j_l(x)$ being the spherical Bessel function and ν solution of $\vec{\sigma} \cdot \vec{p} \nu = -q \nu$. The above neutrino wave function is normalized with respect to the energy, namely,

$$\int d^3r \psi_\nu^\dagger(\vec{r}) \psi_\nu(\vec{r}) = 2\pi \delta(q - q'). \quad (10)$$

The next ingredient of Eq. (1) is the electron wave function. It is the solution of the Dirac equation in the Coulomb field $-Z\alpha/r$ [13], which is of the form

$$\psi_e(\vec{r}) = \begin{pmatrix} G(r) \chi_\kappa^m(\theta, \phi) \\ i F(r) \chi_{-\kappa}^m(\theta, \phi) \end{pmatrix}, \quad (11)$$

with the energy $E = E_{n,\kappa}$

$$E_{n,\kappa} = \left(1 + \frac{Z^2 \alpha^2}{(n+1+\gamma)^2} \right)^{-1/2}, \quad (12)$$

where $\gamma = -1 + \sqrt{\kappa^2 - Z^2 \alpha^2}$. The explicit expression for radial wave functions G and F is [13]

$$G_{n,\kappa}(r) = C_{n,\kappa} (2\lambda r)^\gamma e^{-\lambda r} \sqrt{1 + E_{n,\kappa}} [g_{n,\kappa}^{(2)}(r) + g_{n,\kappa}^{(1)}(r)], \quad (13)$$

$$F_{n,\kappa}(r) = C_{n,\kappa} (2\lambda r)^\gamma e^{-\lambda r} \sqrt{1 - E_{n,\kappa}} [g_{n,\kappa}^{(2)}(r) - g_{n,\kappa}^{(1)}(r)], \quad (14)$$

$$g_{n,\kappa}^{(1)}(r) = \sqrt{Z\alpha\lambda^{-1} - \kappa} L_n^{(2+2\gamma)}(2\lambda r), \quad (15)$$

$$g_{n,\kappa}^{(2)}(r) = -(n+2+2\gamma) \sqrt{Z\alpha\lambda^{-1} - \kappa} L_{n-1}^{(2+2\gamma)}(2\lambda r), \quad (16)$$

$$C_{n,\kappa} = \sqrt{\frac{2\lambda^4 n!}{Z\alpha\Gamma(n+3+2\gamma)}}, \quad (17)$$

where $L_n^{(\alpha)}$ are Laguerre polynomials

$$L_n^{(\alpha)}(z) = \sum_{k=0}^n \frac{\Gamma(\alpha + n + 1)}{k!(n-k)!\Gamma(\alpha + k + 1)} (-z)^k, \quad (18)$$

with $L_{-1} \equiv 0$ and $\lambda = \sqrt{1 - E^2}$. In particular, the energy and the wave function of the ground state $n = l = 0$, $\kappa = -1$, and $j = 1/2$ are given by

$$E_{0,-1} = \sqrt{1 - Z^2 \alpha^2} \equiv \mathcal{E}, \quad (19)$$

$$G_{0,-1} = \sqrt{\frac{4Z^3 \alpha^3 (2 + \gamma)}{\Gamma(3 + 2\gamma)}} (2Z\alpha r)^\gamma e^{-Z\alpha r} \equiv \mathcal{G}, \quad (20)$$

$$F_{0,-1} = -\sqrt{\frac{4Z^3 \alpha^3 (-\gamma)}{\Gamma(3 + 2\gamma)}} (2Z\alpha r)^\gamma e^{-Z\alpha r} \equiv \mathcal{F}. \quad (21)$$

For the calculation of radiative transition rates one needs the Dirac-Coulomb Green's function G^D . Its explicit form is [13]

$$G^D(\vec{r}, \vec{r}', E) \equiv \langle \vec{r} | \frac{1}{H - E} | \vec{r}' \rangle = \sum_{\kappa m} G_{\kappa, m}^D(\vec{r}, \vec{r}', E), \quad (22)$$

$$G_{\kappa, m}^D(\vec{r}, \vec{r}', E) = \Theta(r' - r) \psi_{\kappa m}^<(\vec{r}) \otimes \psi_{\kappa m}^>(\vec{r}')^\dagger + \Theta(r - r') \psi_{\kappa m}^>(\vec{r}) \otimes \psi_{\kappa m}^<(\vec{r}')^\dagger, \quad (23)$$

where $\Theta(x)$ is a Heaviside step function, and both $\psi^>$ and $\psi^<$ are of the form Eq. (11) with

$$G_{\kappa}^<(r) = (2\lambda r)^\gamma e^{-\lambda r} \sqrt{1 + E} (f_2 + f_1), \quad (24)$$

$$F_{\kappa}^<(r) = (2\lambda r)^\gamma e^{-\lambda r} \sqrt{1 - E} (f_2 - f_1), \quad (25)$$

$$G_{\kappa}^>(r) = (2\lambda r)^\gamma e^{-\lambda r} \sqrt{1 + E} (f_4 + f_3) \frac{2\lambda \Gamma(a)}{\Gamma(c)}, \quad (26)$$

$$F_{\kappa}^>(r) = (2\lambda r)^\gamma e^{-\lambda r} \sqrt{1 - E} (f_4 - f_3) \frac{2\lambda \Gamma(a)}{\Gamma(c)}, \quad (27)$$

where

$$f_1 = (Z\alpha\lambda^{-1} - \kappa)_1 F_1(a, c, 2\lambda r), \quad (28)$$

$$f_2 = a_1 F_1(a + 1, c, 2\lambda r), \quad (29)$$

$$f_3 = U(a, c, 2\lambda r), \quad (30)$$

$$f_4 = (Z\alpha\lambda^{-1} + \kappa) U(a + 1, c, 2\lambda r), \quad (31)$$

and $a = 1 + \gamma - EZ\alpha\lambda^{-1}$, $c = 3 + 2\gamma$, while ${}_1F_1$ and U are confluent hypergeometric functions regular at the origin and at the infinity, respectively.

Apart from the neutrino and the electron wave function, we need also the photon wave function to describe the radiative capture process. For this reason we introduce vector spherical harmonics [14],

$$\vec{Y}_{JL}^M(\theta, \phi) = \sum_{mq} Y_L^m(\theta, \phi) \vec{e}_q \langle Lm; 1q | L1; JM \rangle, \quad (32)$$

where $\vec{e}_1 = -1/\sqrt{2}(\vec{e}_x + i\vec{e}_y)$, $\vec{e}_0 = \vec{e}_z$, and $\vec{e}_{-1} = 1/\sqrt{2}(\vec{e}_x - i\vec{e}_y)$. The solutions of the Maxwell equations with definite angular momentum and parity are represented by both, the magnetic photon

$$\vec{A}_{JM}^{(M)}(\vec{r}) = \sqrt{2k} j_J(kr) \vec{Y}_{JJ}^M(\hat{r}), \quad (33)$$

$$A_{JM}^{(0(M))}(\vec{r}) = 0, \quad (34)$$

and the electric photon in the length gauge [15,16]

$$\vec{A}_{JM}^{(E)}(\vec{r}) = \sqrt{2k} \sqrt{\frac{2J+1}{J}} j_{J+1}(kr) \vec{Y}_{JJ+1}^M(\hat{r}), \quad (35)$$

$$A_{JM}^{(0(E))}(\vec{r}) = -i\sqrt{2k} \sqrt{\frac{J+1}{J}} j_J(kr) Y_J^M(\hat{r}), \quad (36)$$

while the electric photon in the Coulomb (velocity) gauge is

$$\vec{A}_{JM}^{(E)}(\vec{r}) = \sqrt{2k} \left[\sqrt{\frac{J}{2J+1}} j_{J+1}(kr) \vec{Y}_{JJ+1}^M(\hat{r}) - \sqrt{\frac{J+1}{2J+1}} j_{J-1}(kr) \vec{Y}_{JJ-1}^M(\hat{r}) \right], \quad (37)$$

$$A_{JM}^{(0(E))}(\vec{r}) = 0. \quad (38)$$

These solutions are normalized with respect to energy, so that

$$2k \int d^3r [\vec{A}_{JM}(\vec{r})^* \vec{A}'_{JM}(\vec{r}) - A_{JM}^0(\vec{r})^* A'_{JM}^0(\vec{r})] = 2\pi \delta(k - k'). \quad (39)$$

The difference between both gauges $A_{JM}^\mu(\vec{r})_C - A_{JM}^\mu(\vec{r})_L = \partial^\mu \lambda_{JM}$ is a complete derivative of some function λ_{JM} and therefore physical results do not depend on which A_μ is used. However the use of the length gauge is convenient for performing several simplifications in the calculations of transition rates. Especially important is the possibility to neglect the photon radiation from the nucleus in the length gauge. It is because the photon wave function for small distances from the nucleus behaves like kr in this gauge, what can be seen by inspecting the behavior of the spherical Bessel functions for small x ,

$$j_l(x) \approx x^l / (2l + 1)!! \quad (40)$$

Therefore, the probability of photon radiation from the nucleus is suppressed by a factor $(QR)^2 \approx 10^{-4}$, and thus can be neglected.

B. Electron capture rate

The electron capture rate W is equal to the square of the the matrix element M , summed over final states and averaged over initial states

$$W = \frac{1}{2J_e + 1} \frac{1}{2J_i + 1} \sum_{M_e M_i M_\nu M_f} |M|^2, \quad (41)$$

where

$$M = \langle f | H_{EC} | i \rangle = \int d^3r \frac{G_F}{\sqrt{2}} [\bar{\psi}_f \gamma_\mu (1 - \lambda \gamma^5) \psi_i] \times [\bar{\psi}_\nu \gamma^\mu (1 - \gamma^5) \psi_e]. \quad (42)$$

Although we use single nucleon matrix elements, results can easily be transformed for the nuclear matrix elements, by assuming that ψ_n and ψ_p are field operators, and instead of $\bar{\psi}_f \gamma_\mu (1 - \lambda \gamma^5) \psi_i$ one considers $\langle f | \bar{\psi}_n \gamma_\mu (1 - \lambda \gamma^5) \psi_p | i \rangle$. The tensor decomposition of the matrix element in Eq. (42) leads to

$$M = \frac{G_F}{\sqrt{2}} \int r^2 dr \sum_{JLSM} (-1)^{J+M} (f | T_{JLS}^M (1 - \lambda \gamma^5) | i) \times (\psi_\nu | T_{JLS}^{-M} (1 - \gamma^5) | \psi_e), \quad (43)$$

where

$$T_{JL0}^M = i^L \delta_{JL} Y_L^M, \quad (44)$$

$$T_{JL1}^M = (-1)^{J+L+1} i^L \vec{Y}_{JL}^M \cdot \vec{\alpha}, \quad (45)$$

and (\cdot) denotes the integral over angular coordinates. Each state f, i, ψ_ν and ψ_e has definite angular momentum J, M numbers, so one can use reduced matrix element

$$\langle j, m | T_k^q | j', m' \rangle = (-1)^{j-m} \begin{pmatrix} j & k & j' \\ -m & q & m' \end{pmatrix} \langle j || T_k || j' \rangle, \quad (46)$$

and orthogonality properties of $3j$ symbol [14] to obtain simple formula for the electron capture rate

$$W = \frac{G_F^2}{2} \frac{1}{2J_e + 1} \frac{1}{2J_i + 1} \sum_J \frac{1}{2J + 1} \times \left| \int r^2 dr \sum_{LS} (J_f || T_{JLS} (1 - \lambda\gamma^5) || J_i) \times (J_v || T_{JLS} (1 - \gamma^5) || J_e) \right|^2. \quad (47)$$

The reduced matrix elements of spherical harmonics are given by

$$\langle \kappa_f || Y_l || \kappa_i \rangle = \sqrt{\frac{2l+1}{4\pi}} C_l(\kappa_f, \kappa_i), \quad (48)$$

$$C_l(\kappa_f, \kappa_i) = (-1)^{j_f+1/2} \sqrt{(2j_f+1)(2j_i+1)} \times \begin{pmatrix} j_i & l & j_f \\ 1/2 & 0 & -1/2 \end{pmatrix} \Pi(l_f, l_i, l), \quad (49)$$

$$\Pi(l_f, l_i, l) = \frac{1}{2} [1 + (-1)^{l_f+l_i+l}], \quad (50)$$

and spin spherical harmonics by

$$\langle \kappa_f || \vec{Y}_{JL} \cdot \vec{\sigma} || \kappa_i \rangle = \sqrt{\frac{2J+1}{4\pi}} S_{JL}(\kappa_f, \kappa_i), \quad (51)$$

$$S_{J,J+1}(\kappa_f, \kappa_i) = \sqrt{\frac{J+1}{2J+1}} \left(1 + \frac{\kappa_f + \kappa_i}{J+1} \right) C_J(-\kappa_f, \kappa_i), \quad (52)$$

$$S_{J,J}(\kappa_f, \kappa_i) = \frac{\kappa_i - \kappa_f}{\sqrt{J(J+1)}} C_J(\kappa_f, \kappa_i), \quad (53)$$

$$S_{J,J-1}(\kappa_f, \kappa_i) = \sqrt{\frac{J}{2J+1}} \left(-1 + \frac{\kappa_f + \kappa_i}{J} \right) C_J(-\kappa_f, \kappa_i). \quad (54)$$

With the use of the above formulas for reduced matrix elements, the capture rate W of the 1S electron by the nucleus is

$$W = \sum_J W_J, \quad (55)$$

$$W_0 = \frac{2G_F^2 Q^2}{2J_i + 1} \frac{1}{4\pi} \left| \langle J_f || [T_{000} \mathcal{G}(R) - T_{011} \mathcal{F}(R)] (1 - \lambda\gamma_5) || J_i \rangle \right|^2, \quad (56)$$

$$W_1 = \frac{2G_F^2 Q^2}{2J_i + 1} \frac{1}{4\pi} \left| \langle J_f || [T_{101} \mathcal{G}(R) + (T_{110}/\sqrt{3} + T_{111}\sqrt{2/3}) \mathcal{F}(R)] (1 - \lambda\gamma_5) || J_i \rangle \right|^2, \quad (57)$$

$$W_2 = \frac{2G_F^2 Q^4}{9} \frac{1}{2J_i + 1} \frac{1}{4\pi} \left| \langle J_f || r [T_{211} \mathcal{G}(R) + (T_{220}\sqrt{2/5} + T_{221}\sqrt{3/5}) \mathcal{F}(R)] (1 - \lambda\gamma_5) || J_i \rangle \right|^2, \quad (58)$$

where Q is the energy released in the decay and R is the nuclear radius.

C. Radiative electron capture rate

The probability amplitude for the electron capture with the simultaneous photon emission from the electron is

$$M_R = \int d^3r \frac{G_F}{\sqrt{2}} [\bar{\psi}_f \gamma_\mu (1 - \lambda\gamma^5) \psi_i] [\bar{\psi}_v \gamma^\mu (1 - \gamma^5) \psi'_e], \quad (59)$$

where

$$\psi'_e(\vec{r}) = \langle \vec{r} | \frac{1}{\mathcal{E} - H - k} e^{(A^0 - \vec{\alpha} \cdot \vec{A})} | \psi_e \rangle = - \sum_n \psi'_n(r) \frac{\langle \psi'_n | e^{(A^0 - \vec{\alpha} \cdot \vec{A})} | \psi_e \rangle}{E_n + k - \mathcal{E}}. \quad (60)$$

We use the latter form to perform tensor decomposition of M_R and obtain

$$M_R = \frac{G_F e}{\sqrt{2}} \int r^2 dr \sum_{JLSMM'_e} (-1)^{J+M+1} \times (J_f, M_f | T_{JLS}^M (1 - \lambda\gamma^5) | J_i, M_i) \times \sum_n (J_v, M_v | T_{JLS}^{-M} (1 - \gamma^5) | n, J'_e, M'_e) \frac{1}{E_n + k - \mathcal{E}} \times \langle n, J'_e, M'_e | A_{J_A M_A}^0 - \vec{\alpha} \cdot \vec{A}_{J_A M_A} | J_e, M_e \rangle. \quad (61)$$

The rate for the radiative electron capture W_R is

$$W_R = \int_0^Q dk W_R(k), \quad (62)$$

where

$$W_R(k) = \frac{1}{2J_e + 1} \frac{1}{2J_i + 1} \sum_{M_e M_i M_v M_f M_A} \frac{1}{2\pi} |M_R|^2, \quad (63)$$

with the sum over final state and the average over initial states. The $W_R(k)$ can be expressed in terms of the reduced matrix elements and the summation over magnetic states can be carried out with the aid of the orthogonality of the $3j$ symbols. The result is

$$W_R(k) = G_F^2 \alpha \frac{1}{2J_e + 1} \frac{1}{2J_i + 1} \sum_J \frac{1}{2J + 1} \times \sum_{J'_e} \frac{1}{2J'_e + 1} \left| \sum_n \frac{1}{E_n + k - \mathcal{E}} \times \int r^2 dr \sum_{LS} (J_f || T_{JLS} (1 - \lambda\gamma^5) || J_i) \times (J_v || T_{JLS} (1 - \gamma^5) || J'_e, n) \times \langle n, J'_e || A_{J_A}^0 - \vec{\alpha} \cdot \vec{A}_{J_A} || J_e \rangle \right|^2. \quad (64)$$

We can use now the explicit form of the Dirac-Coulomb Green's function in Eqs. (22)–(31) to replace the sum over intermediate electron states n in Eq. (64) by G^D . Since the electron capture takes place within the nucleus, and the photon radiation in a region of the electron wave function which is several orders of magnitude larger, we apply an identity $\Theta(r' - r) = 1 - \Theta(r - r')$ and neglect $\Theta(r - r')$ in Eq. (23)

completely, so the Green's function becomes

$$G_{\kappa,m}^D(\vec{r}, \vec{r}', E) \approx \psi_{\kappa m}^<(\vec{r}) \otimes \psi_{\kappa m}^>(\vec{r}')^\dagger. \quad (65)$$

In other words, this approximation is allowed, because the integral with $\Theta(r-r')$ gives contribution, which is higher order in the small parameter $\xi = QR$. After this assumption one obtains

$$\begin{aligned} W_R(k) &= \frac{G_F^2}{2} \frac{1}{2J_i+1} \sum_J \frac{1}{2J+1} \sum_{J_e'} \frac{1}{2J_e'+1} \\ &\times \left| \int r^2 dr \sum_{LS} (J_f || T_{JLS} (1 - \lambda\gamma^5) || J_i) \right. \\ &\times (J_v || T_{JLS} (1 - \gamma^5) || J_e' \psi^<) \left. \right|^2 \\ &\times \left\{ \frac{2\alpha}{2J_e+1} |\langle J_e', \psi^> || A_{J_A}^0 - \vec{\alpha} \cdot \vec{A}_{J_A} || J_e \rangle|^2 \right\}. \quad (66) \end{aligned}$$

The approximation in Eq. (65) would not be valid in the Coulomb gauge, as the integral with $\Theta(r-r')$ is of the same order in the parameter ξ , what we discuss in more details in Sec. IV. For similar reason, in the length gauge, we can safely neglect the photon emission by the nucleus, as it is ξ^2 smaller, than emission by the electron.

We consider here transitions with $\Delta J = 0, 1, 2$

$$W_R(k) = W_{R0}(k) + W_{R1}(k) + W_{R2}(k), \quad (67)$$

since no electron radiative capture has been observed for higher multiplicities. Due to the assumption in Eq. (65), transition rate for each value of J can be decomposed into a product of a term corresponding to the photon emission and a term corresponding to the nuclear transition, namely,

$$\begin{aligned} W_{R0}(k) &= W_{M1}(k, S_{1/2} \rightarrow S_{1/2}^>) W_0(Q-k, S_{1/2}^< \rightarrow \nu_{1/2}) \\ &+ W_{E1}(k, S_{1/2} \rightarrow P_{1/2}^>) W_0(Q-k, P_{1/2}^< \rightarrow \nu_{1/2}), \quad (68) \end{aligned}$$

$$\begin{aligned} W_{R1}(k) &= W_{M1}(k, S_{1/2} \rightarrow S_{1/2}^>) W_1(Q-k, S_{1/2}^< \rightarrow \nu_{1/2}) \\ &+ W_{E1}(k, S_{1/2} \rightarrow P_{1/2}^>) W_1(Q-k, P_{1/2}^< \rightarrow \nu_{1/2}), \quad (69) \end{aligned}$$

$$\begin{aligned} W_{R2}(k) &= W_{M1}(k, S_{1/2} \rightarrow S_{1/2}^>) W_2(Q-k, S_{1/2}^< \rightarrow \nu_{3/2}) \\ &+ W_{E1}(k, S_{1/2} \rightarrow P_{1/2}^>) W_2(Q-k, P_{1/2}^< \rightarrow \nu_{3/2}) \\ &+ [W_{E1}(k, S_{1/2} \rightarrow P_{3/2}^>) + W_{M2}(k, S_{1/2} \rightarrow P_{3/2}^>)] \\ &\times W_2(Q-k, P_{3/2}^< \rightarrow \nu_{1/2}) \\ &+ [W_{M1}(k, S_{1/2} \rightarrow D_{3/2}^>) + W_{E2}(k, S_{1/2} \rightarrow D_{3/2}^>)] \\ &\times W_2(Q-k, D_{3/2}^< \rightarrow \nu_{1/2}). \quad (70) \end{aligned}$$

The explicit formulas for the photon emission rate

$$W_{EM} = \frac{2\alpha}{2J_e+1} |\langle J_e', \psi^> || A_{J_A}^0 - \vec{\alpha} \cdot \vec{A}_{J_A} || J_e \rangle|^2 \equiv \frac{\alpha}{\pi} k \mathcal{R}_{EM} \quad (71)$$

are obtained using photon wave function from Eqs. (33)–(36), electron wave function from Eqs. (20) and (21), and the

Dirac-Coulomb Green's function from Eq. (65)

$$\begin{aligned} \mathcal{R}_{M1}(S_{1/2} \rightarrow S_{1/2}^>) &= 2 \left| \int r^2 dr j_1(kr) [G_{-1}^>(\mathcal{E}-k, r) \mathcal{F}(r) \right. \\ &\left. + F_{-1}^>(\mathcal{E}-k, r) \mathcal{G}(r)] \right|^2, \quad (72) \end{aligned}$$

$$\begin{aligned} \mathcal{R}_{M1}(S_{1/2} \rightarrow D_{3/2}^>) &= \left| \int r^2 dr j_1(kr) [G_2^>(\mathcal{E}-k, r) \mathcal{F}(r) \right. \\ &\left. + F_2^>(\mathcal{E}-k, r) \mathcal{G}(r)] \right|^2, \quad (73) \end{aligned}$$

$$\begin{aligned} \mathcal{R}_{M2}(S_{1/2} \rightarrow P_{3/2}^>) &= 3 \left| \int r^2 dr j_2(kr) [G_{-2}^>(\mathcal{E}-k, r) \mathcal{F}(r) \right. \\ &\left. + F_{-2}^>(\mathcal{E}-k, r) \mathcal{G}(r)] \right|^2, \quad (74) \end{aligned}$$

$$\begin{aligned} \mathcal{R}_{E1}(S_{1/2} \rightarrow P_{1/2}^>) &= 2 \left| \int r^2 dr \{ j_1(kr) [G_1^>(\mathcal{E}-k, r) \mathcal{G}(r) \right. \\ &+ F_1^>(\mathcal{E}-k, r) \mathcal{F}(r)] \\ &\left. + 2j_2(kr) G_1^>(\mathcal{E}-k, r) \mathcal{F}(r) \right|^2, \quad (75) \end{aligned}$$

$$\begin{aligned} \mathcal{R}_{E1}(S_{1/2} \rightarrow P_{3/2}^>) &= \left| \int r^2 dr \{ 2j_1(kr) [G_{-2}^>(\mathcal{E}-k, r) \mathcal{G}(r) \right. \\ &+ F_{-2}^>(\mathcal{E}-k, r) \mathcal{F}(r)] \\ &+ j_2(kr) [G_{-2}^>(\mathcal{E}-k, r) \mathcal{F}(r) \\ &\left. - 3F_{-2}^>(\mathcal{E}-k, r) \mathcal{G}(r)] \right|^2, \quad (76) \end{aligned}$$

$$\begin{aligned} \mathcal{R}_{E2}(S_{1/2} \rightarrow D_{3/2}^>) &= 3 \left| \int r^2 dr \{ j_2(kr) [G_2^>(\mathcal{E}-k, r) \mathcal{G}(r) \right. \\ &+ F_2^>(\mathcal{E}-k, r) \mathcal{F}(r)] \\ &\left. + 2j_3(kr) G_2^>(\mathcal{E}-k, r) \mathcal{F}(r) \right|^2, \quad (77) \end{aligned}$$

where $E = E_{0,-1}$, $\mathcal{F}(r) = F_{0,-1}(r)$, and $\mathcal{G}(r) = G_{0,-1}(r)$. The explicit formulas for the electron capture rate are

$$\begin{aligned} W_0(S_{1/2}^< \rightarrow \nu_{1/2}) &= \frac{2G_F^2(Q-k)^2}{2J_i+1} \frac{1}{4\pi} |\langle J_f || [T_{000} G_{-1}^< \\ &(\mathcal{E}-k, R) - T_{011} F_{-1}^<(\mathcal{E}-k, R)] \\ &\times (1 - \lambda\gamma^5) || J_i \rangle|^2, \quad (78) \end{aligned}$$

$$\begin{aligned} W_0(P_{1/2}^< \rightarrow \nu_{1/2}) &= \frac{2G_F^2(Q-k)^2}{2J_i+1} \frac{1}{4\pi} |\langle J_f || [T_{000} F_1^< \\ &(\mathcal{E}-k, R) + T_{011} G_1^<(\mathcal{E}-k, R)] \\ &\times (1 - \lambda\gamma^5) || J_i \rangle|^2, \quad (79) \end{aligned}$$

$$\begin{aligned} W_1(S_{1/2}^< \rightarrow \nu_{1/2}) &= \frac{2G_F^2(Q-k)^2}{2J_i+1} \frac{1}{4\pi} |\langle J_f || [T_{101} G_{-1}^< \\ &(\mathcal{E}-k, R) + (T_{110}/\sqrt{3} + T_{111}\sqrt{2/3}) \\ &\times F_{-1}^<(\mathcal{E}-k, R)] (1 - \lambda\gamma^5) || J_i \rangle|^2, \quad (80) \end{aligned}$$

$$W_1(P_{1/2}^< \rightarrow \nu_{1/2}) = \frac{2G_F^2(Q-k)^2}{2J_i+1} \frac{1}{4\pi} |\langle J_f || [T_{101} F_1^<(\mathcal{E}-k, R) - (T_{110}/\sqrt{3} + T_{111}\sqrt{2/3}) \times G_1^<(\mathcal{E}-k, R)](1 - \lambda\gamma^5) || J_i \rangle|^2, \quad (81)$$

$$W_2(S_{1/2}^< \rightarrow \nu_{3/2}) = \frac{2}{9} \frac{G_F^2(Q-k)^4}{2J_i+1} \frac{1}{4\pi} |\langle J_f || r T_{211} G_{-1}^<(\mathcal{E}-k, R) + (T_{220}\sqrt{2/5} + T_{221}\sqrt{3/5}) \times F_{-1}^<(\mathcal{E}-k, R)](1 - \lambda\gamma^5) || J_i \rangle|^2, \quad (82)$$

$$W_2(P_{1/2}^< \rightarrow \nu_{3/2}) = \frac{2}{9} \frac{G_F^2(Q-k)^4}{2J_i+1} \frac{1}{4\pi} |\langle J_f || r [T_{211} F_1^<(\mathcal{E}-k, R) - (T_{220}\sqrt{2/5} + T_{221}\sqrt{3/5}) \times G_1^<(\mathcal{E}-k, R)](1 - \lambda\gamma^5) || J_i \rangle|^2, \quad (83)$$

$$W_2(P_{3/2}^< \rightarrow \nu_{1/2}) = \frac{G_F^2(Q-k)^2}{(2J_i+1)R^2} \frac{1}{4\pi} |\langle J_f || r [T_{211} G_{-2}^<(\mathcal{E}-k, R) + (T_{220}\sqrt{2/5} + T_{221}\sqrt{3/5}) \times F_{-2}^<(\mathcal{E}-k, R)](1 - \lambda\gamma^5) || J_i \rangle|^2, \quad (84)$$

$$W_2(D_{3/2}^< \rightarrow \nu_{1/2}) = \frac{G_F^2(Q-k)^2}{(2J_i+1)R^2} \frac{1}{4\pi} |\langle J_f || r [T_{211} F_2^<(\mathcal{E}-k, R) - (T_{220}\sqrt{2/5} + T_{221}\sqrt{3/5}) \times G_2^<(\mathcal{E}-k, R)](1 - \lambda\gamma^5) || J_i \rangle|^2. \quad (85)$$

III. RESULTS

Following the generally adopted convention [3,4,9], we calculate the ratio of radiative to nonradiative capture rate. Then, the resulting photon spectrum accompanying the 1S capture is given by

$$\frac{W_R(k)}{W} \equiv \frac{\alpha}{\pi m^2} \left(1 - \frac{k}{Q}\right)^2 k \mathcal{R}, \quad (86)$$

where details of the shape are expressed in terms of the dimensionless shape factor \mathcal{R} .

First, we consider the transitions where $\Delta J = 0, 1$. When the parity of nuclear states does not change, $\pi_i \pi_f = 1$, this transition is allowed. Then, two tensor operators T_{000} and $T_{101}(-\lambda\gamma^5)$ dominate and other operators can be neglected. In the probability ratio the nuclear matrix elements cancel out and the result greatly simplifies:

$$\mathcal{R} = \mathcal{R}_a = \frac{G_{-1}^<(\mathcal{E}-k, R)^2}{\mathcal{G}(R)^2} \mathcal{R}_{M1}(S_{1/2} \rightarrow S_{1/2}^>) + \frac{F_1^<(\mathcal{E}-k, R)^2}{\mathcal{G}(R)^2} \mathcal{R}_{E1}(S_{1/2} \rightarrow P_{1/2}^>). \quad (87)$$

It is worth noting, that in the nonrelativistic limit ($Z\alpha \rightarrow 0$), the shape factor \mathcal{R}_a is equal to 1, what we verified by explicit calculations. If the parity does change, $\pi_i \pi_f = -1$, the transition is first forbidden non unique. Here, all nuclear operators contribute to the transition matrix elements and

the exact expression for \mathcal{R} in general is more complicated. However, one notices that the ratio

$$\frac{F_{\kappa}^<(E, R)}{G_{\kappa}^<(E, R)} = \sqrt{\frac{1-E}{1+E} \frac{\sqrt{\kappa^2 - Z^2\alpha^2} + \kappa - Z\alpha\sqrt{\frac{1+E}{1-E}}}{\sqrt{\kappa^2 - Z^2\alpha^2} - \kappa + Z\alpha\sqrt{\frac{1-E}{1+E}}}} \approx \left(\frac{2\kappa}{Z\alpha}\right)^{\kappa/|\kappa|} \approx -\frac{G_{-\kappa}^<(E, R)}{F_{-\kappa}^<(E, R)}, \quad (88)$$

approximately does not depend on energy E as long as $Z\alpha \ll 1$. Therefore, nuclear matrix elements cancel out and the formula in Eq. (87) holds for nonunique transitions, but only when this approximation is valid. It is important to stress that numerically Eq. (87) yields the same results as those obtained in Refs. [3–5]. Although our results have apparently different and simpler form, they are equivalent to those obtained previously by Glauber, Martin, Zon, and Rapoport for the allowed and first forbidden non unique decays.

The situation is different, however, in the case of the first forbidden unique transition, where $\Delta J = 2$ and $\pi_i \pi_f = -1$. The operator $T_{211}(-\lambda\gamma^5)$ dominates and other nuclear operators are neglected. The resulting shape factor is

$$\mathcal{R}_{1u} = \left(1 - \frac{k}{Q}\right)^2 \mathcal{R}^{(1)} + \frac{k^2}{Q^2} \mathcal{R}^{(2)}, \quad (89)$$

$$\mathcal{R}^{(1)} = \mathcal{R}_a, \quad (90)$$

$$\mathcal{R}^{(2)} = \frac{9}{2k^2 R^2} \frac{G_{-2}^<(\mathcal{E}-k, R)^2}{\mathcal{G}(R)^2} [\mathcal{R}_{E1}(S_{1/2} \rightarrow P_{3/2}^>)] + \frac{9}{2k^2 R^2} \frac{F_2^<(\mathcal{E}-k, R)^2}{\mathcal{G}(R)^2} [\mathcal{R}_{M2}(S_{1/2} \rightarrow P_{3/2}^>)] + \frac{9}{2k^2 R^2} \frac{F_2^<(\mathcal{E}-k, R)^2}{\mathcal{G}(R)^2} \times [\mathcal{R}_{M1}(S_{1/2} \rightarrow D_{3/2}^>) + \mathcal{R}_{E2}(S_{1/2} \rightarrow D_{3/2}^>)]. \quad (91)$$

While the nonrelativistic limit of $\mathcal{R}^{(1)}$ is 1, for the $\mathcal{R}^{(2)}$ function we obtain

$$\lim_{Z \rightarrow 0} \mathcal{R}^{(2)} = 1 + \frac{1}{k} + \frac{2}{k^2}, \quad (92)$$

what we have verified numerically. Although the result of Zon [6] has similar form to Eq. (89), the Coulomb-free limit of the function corresponding to $\mathcal{R}^{(2)}$ is equal to 1, which differs significantly from our result.

Experimentally, the REC process in the first forbidden unique transition was studied so far for two nuclei: ^{41}Ca [7] and ^{204}Tl [11]. The data obtained for ^{41}Ca ($Q_{EC} = 421.3$ keV, $T_{1/2} = 10^5$ years) are shown in Fig. 2 together with theoretical predictions. While the model of Zon and Rapoport [5,6] underestimates the intensity of the REC spectrum by a factor of about 6, the results of our calculations are in excellent agreement with the experiment. The contribution of relativistic and Coulomb effects is evident. The Coulomb-free limit of our result would overestimate the intensity approximately by a factor of 2. The discrepancy between the Zon model and the ^{41}Ca data was used as an argument in favor of nuclear contribution to the REC process [8,9]. In fact, if both, the nuclear and the electron radiation were calculated correctly, the result should agree with Eq. (89), what is explained in the next section.

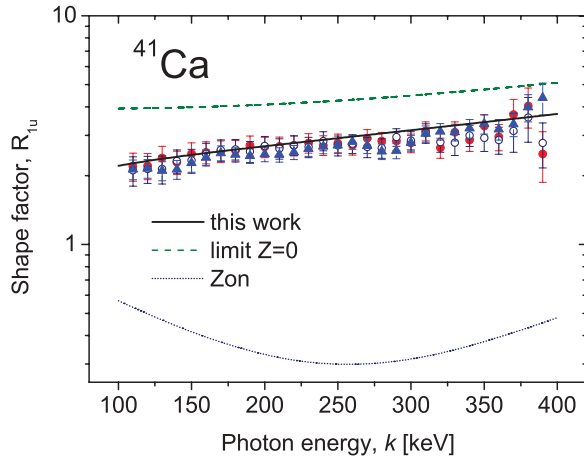


FIG. 2. (Color online) The shape factor for the 1S component of the first forbidden unique REC in ^{41}Ca . The points with error bars represent the experimental values form Ref. [7]. The solid line shows the result of this work as given by Eqs. (86)–(88), while the nonrelativistic limit is shown by the dashed line. The dotted line represents the prediction of the Zon and Rapoport [5,6]. The value of Q is 416.4 keV.

The case of ^{204}Tl ($Q_{EC} = 346.5$ keV, $T_{1/2} = 3.78$ years) is illustrated in Fig. 3. Again, our results perfectly agree with experimental data, while the results of Zon and Rapoport overestimate the spectrum by a factor of about 4 [11]. As expected, the influence of Coulomb field is much stronger in case of thallium ($Z = 81$) than in case of calcium ($Z = 20$). The nonrelativistic limit would overestimate the intensity of the REC spectrum by a factor of about 10.

IV. COMPARISON TO PREVIOUS CALCULATIONS

We have verified numerically that Eq. (87) agrees with former results obtained in Refs. [3–6] for the allowed and

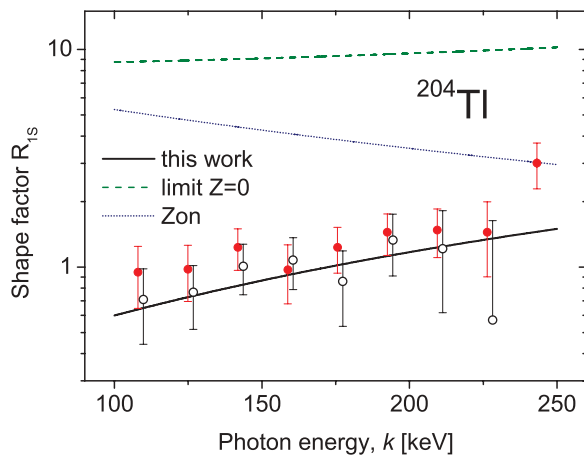


FIG. 3. (Color online) The shape factor for the 1S component of the first forbidden unique REC in ^{204}Tl . The points with error bars represent the experimental values form Ref. [11]. The meaning of theoretical lines is the same as in Fig. 2. The value of Q is 264.0 keV.

first forbidden nonunique EC transitions. However, in contrast to previous works [5,6,9], our results correctly describe the known experimental data for the first forbidden unique decays. The difference, in our opinion, is due to incorrect approximations adopted in the Refs. [5,6]. If we use the Coulomb gauge for the emitted photon, Eqs. (37) and (38), then the approximation of Eq. (65) for the Coulomb Green's function is not valid, because the integral with the neglected remainder, which is proportional to $\Theta(r - r')$ is as important as the integral with the approximated form in Eq. (65). As an consequence of this approximation in the Coulomb gauge, $\mathcal{R}_{E1}(S_{1/2} \rightarrow P_{3/2})$ in Eq. (76) would contain $j_0(kr)$, and the integral would diverge for small values of r , as the integral in the function B_{21} of Ref. [6] does. With the length gauge, Eqs. (35) and (36), where $E1$ photon wave function contains a combination of $j_1(kr)$ and $j_2(kr)$ functions, the r -integral in Eq. (76) is finite, as it should. Moreover, the probability amplitude for the radiation from the nucleus is strongly suppressed, because the photon wave function is kR times smaller within the nucleus. However, we can not exclude completely the nuclear contribution if there are close-lying excited states in the daughter or in the parent nucleus. In such a case, the nuclear radiation should be obtained using the same gauge. Since the photon wavelength is much larger than the size of the nucleus, the dipole approximation is allowed. Then, the coupling of nucleus to the electromagnetic field in the length gauge takes the form $-\vec{d} \cdot \vec{E} - \vec{\mu} \cdot \vec{B}$, and this form should be used for the calculation of the photon radiation from the nucleus.

V. SUMMARY

We have recalculated the rate of radiative orbital electron capture by the atomic nucleus. We applied the length gauge for the radiated photon, because it suppresses the nuclear radiation and substantially simplifies the calculations. By the use of a convenient form of the Dirac-Coulomb Green's function from Ref. [13], the results for the capture of the 1S electron can easily be generalized for the arbitrary state of the captured electron. The results obtained are found to be in good agreement with experimental data for allowed, first forbidden and first forbidden unique transitions, in particular with the results for ^{41}Ca and ^{204}Tl .

There is another case of the first forbidden unique EC transition, the decay of ^{81}Kr , which can be used to verify predictions presented in this paper. An experiment with a sample of ^{81}Kr is being undertaken, and its outcome will be published soon.

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