Calculation of the Decay Rate for $2^3S_1 \rightarrow 1^1S_0$ + One Photon in Helium*

G. Feinberg
Department of Physics, Columbia University, New York, New York 10027

and

J. Sucher
Center for Theoretical Physics, Department of Physics and Astronomy, University of Maryland, College Park, Maryland 20742
(Received 16 February 1971)

The amplitude for the one-photon transition $2^3S_1 \rightarrow 1^1S_0$ in helium is shown, from quantum electrodynamics, to be computable in terms of the nonrelativistic wave functions. Numerical evaluation gives a decay rate of 1.2×10^{-4} sec^{-1}.

One-photon radiative transitions of He and He-like ions of the type $n^3S_1 \rightarrow 1^1S_0$ have attracted considerable interest recently, from a variety of points of view: astrophysics,[1] solar physics,[2] and laboratory experiments.[3] The theory of this decay has, however, been a subject of some controversy; the problem is delicate because the decay amplitude M is of order α^4, so that its computation requires a treatment of the atom which takes into account relativistic effects to rather high accuracy. It is tempting to use as the starting point for such a calculation the Dirac-Breit Hamiltonian

$$H_{DB} = (\vec{\alpha}_1\cdot\vec{p}_1 + \beta_1 m) + (\vec{\alpha}_2\cdot\vec{p}_2 + \beta_2 m) + V_1 + V_2 + V_{12} + B,$$

where $V_i = -Ze^2/r_i$, $V_{12} = e^2/r_{12}$, and

$$B = (-e^2/2r_{12})(\vec{\alpha}_1\cdot\vec{\alpha}_2 + \vec{\alpha}_1\cdot\hat{r}_{12}\vec{\alpha}_2\cdot\hat{r}_{12})$$

is the Breit operator; however, as is well known, use of B beyond first-order perturbation theory leads to quantitatively incorrect results for fine-structure splitting.[4] Although it is possible to base a consistent treatment of this problem on the four-dimensional Bethe-Salpeter equation, we have found a more transparent and simpler approach, which starts directly with the external-field Hamiltonian H of quantum electrodynamics. Our method is based on the observation that in atoms, those effects of the Coulomb interactions which involve the virtual creation of electron-positron pairs lead to level shifts which are of order $\alpha^4 m$ or $Z^2\alpha^4 m$ and hence may ultimately be treated as perturbations, together with the interaction with transverse photons. We show that, to the required accuracy, M may be computed as the matrix element of simple operators, taken between eigenstates φ of the completely nonrelativistic two-electron–atom Hamiltonian H_{nr}:

$$H_{nr}\varphi = (\vec{p}_1^{\,2}/2m + \vec{p}_2^{\,2}/2m + V_1 + V_2 + V_{12})\varphi = W\varphi. \quad (1)$$

We define $H_{ex}^{n.p.}$ and $H_C^{n.p.}$ as the no-pair parts of the interaction H_{ex} with the external field and the Coulomb interaction H_C obtained by dropping all terms corresponding to virtual pair creation or annihilation, and write $H = H^{n.p.} + H'$, with $H^{n.p.} = H_{free} + H_{ex}^{n.p.} + H_C^{n.p.}$ and $H' = H_T + (H_{ex} - H_{ex}^{n.p.}) + (H_C - H_C^{n.p.})$, where H_T is the interaction with the transverse radiation field. $H^{n.p.}$ has normalizable eigenstates Ψ in the two-electron, no-photon sector of Fock space; with

$$\psi(\vec{p}_1, \vec{p}_2) = \sum_{\sigma_1,\sigma_2} u_{\sigma_1}(\vec{p}_1)u_{\sigma_2}(\vec{p}_2)\langle\vec{p}_1, \sigma_1; \vec{p}_2, \sigma_2 | \Psi\rangle,$$

where the u's are positive-energy Dirac spinors, the eigenvalue problem reduces, with $V = V_1 + V_2 + V_{12}$, to

$$H_0\psi \equiv (E_1 + E_2 + \Lambda_{++}V\Lambda_{++})\psi = E\psi. \quad (2)$$

Here $E_i = E(\vec{p}_i) \equiv (\vec{p}_i^{\,2} + m^2)^{1/2}$ and Λ_{++} is the product of positive-energy projection operators: $\Lambda_{++} = \Lambda_+(\vec{p}_1)\Lambda_+(\vec{p}_2)$ with $\Lambda_\pm(\vec{p}) = [E(\vec{p}) \pm (\vec{\alpha}\cdot\vec{p} + \beta m)]/2E(\vec{p})$.

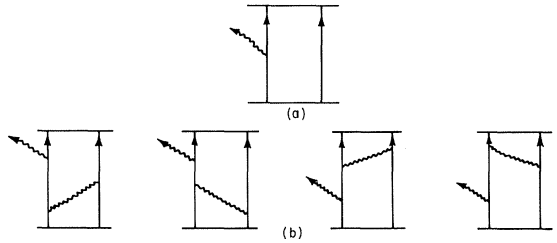

FIG. 1. Time-ordered Feynman-like diagrams contributing to M. The wavy and solid vertical lines represent photons and electrons, respectively; the solid horizontal lines indicate integrations over initial and final atomic-wave functions. (a) $M_a^{(1)}$, the lowest-order term; (b) $M_b^{(1)}$, the leading no-pair, transverse-photon corrections to $M_a^{(1)}$.

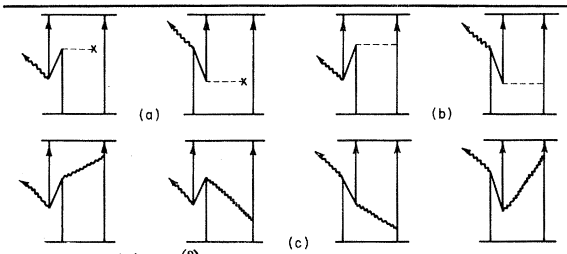

FIG. 2. (a) $M_a^{(2)}$, one-pair, external Coulomb-field corrections; (b) $M_b^{(2)}$, one-pair, electron Coulomb-field corrections; (c) $M_c^{(2)}$, leading one-pair, transverse photon corrections.

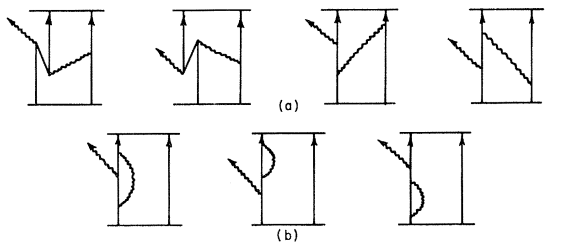

FIG. 3. (a) $M_a^{(3)}$, nonleading transverse photon corrections; (b) $M_b^{(3)}$, radiative corrections to $M_a^{(1)}$.

The matrix element for a transition from a state $|\psi_i\rangle$ to a state $|\psi_f;\vec{k},\vec{\epsilon}\rangle$ containing a photon of momentum $\vec{k}$ and polarization $\vec{\epsilon}$, induced by H', is given by

$$\mathfrak{M}=\langle\psi_f;\vec{k},\epsilon|H'+H'\mathcal{G}_0H'+H'\mathcal{G}_0H'\mathcal{G}_0H'+\cdots|\psi_i\rangle$$

with $\mathcal{G}_0=(E-H^{n.p.}+i\epsilon)^{-1}$, $E=E_i=E_f+k$. The various contributions to $\mathfrak{M}$ are conveniently symbolized by time-ordered Feynman-like diagrams shown in Figs. 1-3; more complicated diagrams, involving creation of more than one transverse photon, may be neglected. We write $\mathfrak{M}=e(2k)^{-1/2}M$ and $M=M^{(1)}+M^{(2)}+M^{(3)}+\cdots$. Corresponding to Fig. 1(a), we have

$$M_a^{(1)}=\langle\psi_f|\vec{\alpha}_1\cdot\vec{\epsilon}\eta_1+\vec{\alpha}_2\cdot\vec{\epsilon}\eta_2|\psi_i\rangle=2\langle\psi_f|\vec{\alpha}_1\cdot\vec{\epsilon}\eta_1|\psi_i\rangle, \tag{3a}$$

with $\eta_i=\exp(-i\vec{k}_i\cdot\vec{r}_i)$ in coordinate space. From Fig. 1(b) we get

$$M_b^{(1)}\approx 2\langle\psi_f|\vec{\alpha}_1\cdot\vec{\epsilon}\eta_1G_0\Lambda_{++}B+B\Lambda_{++}G_0\vec{\alpha}_1\cdot\vec{\epsilon}\eta_1|\psi_i\rangle, \tag{3b}$$

where $G_0=(E-H_0+i\epsilon)^{-1}$ and B is the Breit operator. To arrive at 3(b) we have neglected recoil in the two-electron, one-virtual-photon intermediate state, i.e., neglected $E(\vec{p}_1)+E(\vec{p}_2-\vec{k}')-2m$ relative to the energy k' of the photon; since the major contributions come from $k'\sim\alpha m$, this only introduces an error of relative order α. From Figs. 2(a) and 2(b) we get, respectively,

$$M_a^{(2)}\approx 2\langle\psi_f|\vec{\alpha}_1\cdot\vec{\epsilon}\eta_1\Lambda_-(\vec{p}_1)(V_1/2m)+(V_1/2m)\Lambda_-(\vec{p}_1)\eta_1\vec{\alpha}_1\cdot\vec{\epsilon}|\psi_i\rangle, \tag{4a}$$

$$M_b^{(2)}\approx 2\langle\psi_f|\vec{\alpha}_1\cdot\epsilon\eta_1\Lambda_-(\vec{p}_1)(V_{12}/2m)+(V_{12}/2m)\Lambda_-(\vec{p}_1)\eta_1\vec{\alpha}_1\cdot\vec{\epsilon}|\psi_i\rangle; \tag{4b}$$

here we have neglected the photon and electron kinetic energies relative to $2m$ in the energy denominators, which only introduces an error of order α^2. With similar approximations we get, from Fig. 2(c), correct to relative order α,

$$M_c^{(2)}\approx 2\langle\psi_f|\vec{\alpha}_1\cdot\vec{\epsilon}\eta_1\Lambda_-(\vec{p}_1)(B/2m)+(B/2m)\Lambda_-(\vec{p}_1)\eta_1\vec{\alpha}_1\cdot\vec{\epsilon}|\psi_i\rangle. \tag{4c}$$

The terms arising from Fig. 3(a) are all down by a factor of α from those arising from Fig. 2(c), since there are pairs present in each intermediate state and there is no semismall energy denominator proportional to $k'\sim\alpha m$. Thus, $M_a^{(3)}=O(\alpha)M_c^{(2)}$ may be neglected. Finally, close examination of the radiative corrections exhibited in Fig. 3(b), the off-mass-shell contributions of which on first inspection threaten to be large, i.e., of order α^4, shows that cancelations occur which lead to the result $M_b^{(3)}=O(\alpha^5\ln\alpha)$, which we also neglect.

From 3(a) and 3(b) we see that $M_b^{(1)}$ is essentially a wave-function correction to $M_a^{(1)}$; it is convenient to treat terms together, by defining a new wave function Φ, satisfying

$$[E_1+E_2+\Lambda_{++}(V+B)\Lambda_{++}]\Phi=E\Phi \tag{5}$$

so that $\Phi\approx(1+G_0\Lambda_{++}B)\psi$. In terms of Φ we may write, to the requisite accuracy,

$$M^{(1)}\equiv M_a^{(1)}+M_b^{(1)}\approx 2\langle\Phi_f|\vec{\alpha}_1\cdot\vec{\epsilon}\eta_1|\Phi_i\rangle. \tag{6}$$

Since $\Lambda_+(p_i)\Phi=\Phi$, we have

$$\Phi=(1+\vec{\alpha}_1\cdot\vec{\xi}_1)(1+\vec{\alpha}_2\cdot\vec{\xi}_2)\Phi^{++},$$

where $\Phi^{++}=\frac{1}{4}(1+\beta_1)(1+\beta_2)\Phi$ are the "large components" of Φ and $\vec{\xi}_i=\vec{p}_i/(E_i+m)$; the equation satisfied

by Φ^{++} is $(H_{nr}+H_{f.s.}')\Phi^{++}=E\Phi^{++}$, where $H_{f.s.}'$ is an operator whose diagonal matrix elements, taken between eigenstates of H_{nr} [Eq. (1)], correctly reproduce the fine-structure level shifts, to leading order $\alpha^4 m$. It is both fortunate and remarkable that (6) may be evaluated, to sufficient accuracy, completely in terms of the extreme nonrelativistic approximation $\tilde{\varphi}=\varphi(\vec{r}_1,\vec{r}_2)\chi$ to Φ^{++}, with φ a solution of (1) and χ a spin eigenfunction. To see this we note first that, since $\vec{\alpha}$ is a $J=1$ negative-parity operator and we are interested in a transition from a 1^+ to 0^+ state, in the spherical-harmonic expansion of

$$\eta_1=\textstyle\sum_l(2l+1)(-i)^l j_l(kr_1)P_l(\hat{k}\cdot\hat{r}_1),$$

only the $l=1$ term contributes and we may replace η by

$$\eta_{eff}=-3ij_1(kr_1)P_1(\hat{k}\cdot\hat{r}_1)=-i\vec{k}\cdot\vec{r}_1(1-\tfrac{1}{10}k^2r_1^2+\cdots)$$

everywhere. On using also the expansion $\vec{\xi}_1(\vec{p}_1/2m)(1-\vec{p}_1^{\,2}/4m^2+\cdots)$ and expressing Φ in terms of Φ^{++}, (6) reduces to a sum of terms involving operators explicitly of order α^4, taken between $\Phi_i{}^{++}$ and $\Phi_f{}^{++}$ (which may therefore immediately be replaced by $\tilde{\varphi}_i$ and $\tilde{\varphi}_f$), and a "dangerous" term proportional to $D=(i/2m')\vec{\epsilon}'\times\vec{k}\cdot\langle\Phi_f{}^{++}|\vec{L}|\Phi_i{}^{++}\rangle$, where $\vec{L}$ is the orbital angular momentum operator. However, with $|L,S\rangle$ denoting a simultaneous eigenstate of $\vec{L}^2$ and $\vec{S}^2$, we have

$$|\Phi_i{}^{++}\rangle=a_0|0,1\rangle+a_1|1,1\rangle+a_2|2,1\rangle+a_3|1,0\rangle$$

and

$$|\varphi_f{}^{++}\rangle=b_0|0,0\rangle+b_1|1,1\rangle,$$

with $a_i/a_0=O(\alpha^2)$ and $b_1/b_0=O(\alpha^2)$, the additional terms being induced by the fine-structure operator $H_{f.s.}'$. It follows that $D\sim(k/m)b_1a_1=O(\alpha^6)$, which may be neglected; the remaining terms entering the evaluation of $M^{(1)}$ may be combined to give

$$M^{(1)}\approx\frac{2iK_1}{3m^2}\left\langle\varphi_f\left|\frac{\vec{p}_1^{\,2}}{m}+\frac{mk^2r_1^2}{4}\right|\varphi_i\right\rangle, \tag{7}$$

with $K_1=\langle\chi_f|\vec{\sigma}_1\cdot\vec{k}\times\vec{\epsilon}|\chi_i\rangle$. A similar reduction may be carried out for $M^{(2)}=M_a{}^{(2)}+M_b{}^{(2)}+M_c{}^{(2)}$. Here no dangerous terms arise and one finds

$$M^{(2)}\approx(-2iK_1/6m^2)\langle\varphi_f|r_1V_1'+\vec{r}_1\cdot\hat{r}_{12}V_{12}'+(e^2/r_{12}^2)\vec{r}_1\cdot\hat{r}_{12}|\varphi_i\rangle, \tag{8}$$

the three terms in (8) representing, in order, the contribution of $M_a{}^{(2)}$, $M_b{}^{(2)}$, and $M_c{}^{(2)}$, respectively; we have written the result in a form valid for arbitrary potentials $V_1=V_1(r_1)$ and $V_{12}=V_{12}(r_{12})$ and the prime indicates a derivative. For the case at hand, $V_1'r_1=-V_1$ and $V_{12}'=-e^2/r_{12}^2$ so that the contributions of $M_b{}^{(2)}$ and $M_c{}^{(2)}$ cancel exactly, to this order; and adding (7) and (8) we get

$$M\approx\frac{2iK_1}{3m^2}\left\langle\varphi_f\left|\frac{\vec{p}_1^{\,2}}{m}+\frac{V_1}{2}+\frac{mk^2r_1^2}{4}\right|\varphi_i\right\rangle, \tag{9}$$

which involves only one-electron operators.[5]

For the purpose of numerical computation, it is convenient to rewrite the matrix element (9) in another form, which is equivalent for exact wave functions φ_i, φ_f, and is expected to be closely equal to (9) for the approximate wave functions we shall use. We use the commutator identity,

$$\langle\varphi_f|k^2r_1^2|\varphi_i\rangle=\langle\varphi_f|[H_{nr},[H_{nr},r_1^2]]|\varphi_i\rangle=\left\langle\varphi_f\left|\left(-\frac{2p_1^2}{m^2}-\frac{2V_1}{m}-\frac{2}{m}\frac{e^2}{r_{12}^3}\vec{r}_1\cdot\vec{r}_{12}\right)\right|\varphi_i\right\rangle,$$

to eliminate the p_1^2 term and then use the fact that $|\varphi_i\rangle$ is odd under particle exchange, while $|\varphi_f\rangle$ is even. We can then rewrite (9) as

$$M=(2iK_1/3m^2)I, \tag{9'}$$

with

$$I=\left\langle\varphi_f\left|\left\{\frac{Ze^2}{4}\left(\frac{1}{r_1}-\frac{1}{r_2}\right)+\frac{e^2}{2r_{12}^3}(r_2^2-r_1^2)+\frac{mk^2}{8}(r_2^2-r_1^2)\right\}\right|\varphi_i\right\rangle. \tag{10}$$

Using $\mathfrak{M}=e(2k)^{-1/2}M$, the decay rate R is then given by

$$R=\tfrac{16}{27}\alpha(k^3/m^4)I^2. \quad (11)$$

We have evaluated I using six-parameter variational helium wave functions computed by Huang.[6] The result obtained is $I=-(\frac{1}{4}\alpha^2 m)(1.87)$. Using $kc=2.99\times10^{16}$ Hz, we then get $R=1.2\times10^{-4}$ sec^{-1} or a helium lifetime

$$\tau=8.4\times10^{3} \text{ sec}. \quad (12)$$

We have also evaluated the decay rate in the limit of heliumlike ions with very high Z, where the wave functions are taken as products of hydrogenic wave functions, and find

$$R=\tfrac{4}{2187}Z^8\alpha^9 k. \quad (13)$$

We thank Dr. Dennis Sciama and Dr. Hans Griem for stimulating our interest in this problem, and Mr. Ralph Grishman for aid in the numerical calculations. One of us (J.S.) would like to thank Dr. E. Henley and the Physics Department of the University of Washington for their hospitality during the summer of 1970 when part of this work was done.

*Work supported in part by the U. S. Air Force Office of Scientific Research under Grant No. AFOSR 68-1453MOD# C and the U. S. Atomic Energy Commission.

[1]See M. J. Rees and D. W. Sciama, Comm. Astrophys. Space Phys. 1, 35 (1969).

[2]A. H. Gabriel and C. Jordan, Nature 221, 947 (1969); H. R. Griem, Astrophys. J. 156, L103 (1969), and 161, L155 (1970).

[3]R. W. Schmieder and R. Marrus, Phys. Rev. Lett. 25, 1245 (1970).

[4]See, e.g., H. Bethe and E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer, Berlin, 1957), p. 173. In addition, it is questionable whether H_{DB} has any normalizable eigenstates at all because of the nondenumerable degeneracy of the spectrum in the absence of electron-electron interaction.

[5]After this work was completed, we were informed of the work of G. Drake (to be published) who also has obtained (9) and has carried out numerical evaluations of (9) with many-parameter wave functions for a variety of values of Z. However, this author's starting point is a Hamiltonian containing both the Breit operator B and H_T which has no theoretical foundation; in fact, it gives the wrong fine structure, since H_T is the source of B and transverse photon effects are being counted twice. Drake's numerical result for helium is in substantial agreement with ours.

[6]S. Huang, Astrophys. J. 108, 354 (1948).

X-Ray Parametric Conversion

P. Eisenberger and S. L. McCall
Bell Telephone Laboratories, Murray Hill, New Jersey 07974
(Received 30 December 1970)

The observation of x-ray parametric conversion is reported. Results are in accord with the calculated nonlinear x-ray susceptibility. The appropriate nonlinear mechanisms are described in terms of classical free electrons.

An x-ray nonlinear optical effect has been observed and the corresponding second-order susceptibility measured. Parametric conversion is the absorption of a photon at frequency ω_p with the resultant emission of two photons of frequencies ω_1 and ω_2, where $\omega_1+\omega_2=\omega_p$. At visible wave lengths,[1,2] this phenomena has been observed and measured in a number of materials. Motivated by Freund and Levine's proposal and calculations,[3] we have observed the analogous phenomena in the x-ray regime.

As shown in Fig. 1, the filtered and collimated output of a 2-kW x-ray tube emitting characteristic molybdenum radiation at 17 keV intercepted a beryllium crystal almost oriented for $(11\bar{2}0)$ Bragg scattering. The outgoing radiation was analyzed for coincident photon pairs with energy near 8.5 keV. The observed coincident counting rates were peaked in directions determined by energy-momentum conservation. The measured cross section is in accord with calculations.[3]

Electrons may be regarded as free if $\hbar\omega_p$, $\hbar\omega_1$, $\hbar\omega_2 \gg E_B$, where E_B is a typical electron binding energy. Relativistic effects are small if $\hbar\omega_p \ll mc^2$. In the experiment described here, $\hbar\omega_p = 17$ keV, and $E_B \sim 100$ eV.

Optical nonlinear[4] phenomena depend qualitatively on such material properties as inversion asymmetry and resonances. In contrast, nonlinear x-ray mechanisms involving only x-ray photons depend primarily on the properties of free electrons. Gross material properties, such as