Relativistic recoil in radiative atomic transitions

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A modified time-dependent perturbation theory for single-photon emission is proposed, which yields the exact photon energy for a relativistically recoiling atom. The relevant unperturbed "Hamiltonian" has stationary eigenvalues E^2. Its form is generalized here to hydrogenic atoms of arbitrary nuclear spins.

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When an atom of mass M emits or absorbs a single photon of momentum $\hbar\boldsymbol{k}$, it suffers a recoil, which is used for example in laser cooling. In emission from an atom at rest, the nonrelativistic recoil energy is $P^2/2M$. From momentum conservation $\boldsymbol{P}+\hbar\boldsymbol{k}=0$ and with $k=\omega/c$, the corresponding photon energy $\hbar\omega$ is $\Delta E-(\Delta E)^2/2Mc^2$, where $\Delta E=E-E'$ is the difference of the initial and final atomic energy levels. More precisely, E' is the total energy of the final atomic state in its own rest frame, which for the ground state is just Mc^2 (c^2 times the sum of the masses of its constituents, minus the total binding energy). Another nonrelativistic expression for $\hbar\omega$ is thus $\Delta E-(\Delta E)^2/2E'$. However, relativistic energy conservation requires $E=\hbar\omega+(E'^2+\hbar^2\omega^2)^{1/2}$, which leads to

$$\hbar\omega=(E^2-E'^2)/2E=\Delta E-(\Delta E)^2/2E. \tag{1}$$

This formula is well known in the kinematics of radiative decays of elementary particles. It is missed by the standard time-dependent perturbation theory based on $i\hbar\partial_t\psi=H\psi$ [1], even if H reproduces the stationary eigenvalues E and E'.

In this report, a modified time-dependent equation is proposed in the variable t/E, which provides relativistic energy conservation in atomic transitions and thus reproduces (1). To remove the awkward dimension of $\partial/\partial(t/E)$, we multiply it by the product of the electron and nuclear masses, m_e and m_N, and add a factor c^2,

$$\tau=\mu t,\quad \mu=m_e m_N c^2/E,\quad i\hbar\partial_\tau\psi=h\psi. \tag{2}$$

The "little Hamiltonian" h is dimensionless. In order to arrive at (1), its stationary part h^0 must have eigenvalues E^2 instead of E. The dimensionless form of E^2 is $E/\mu c^2$. Again, for notational convenience, a factor of $1/2$ is included and a constant is subtracted,

$$h^0\psi^{(0)}=(\epsilon/\mu)\psi^{(0)},\quad \epsilon/\mu=\tfrac{1}{2}(E^2/c^4-m_N^2-n_e m_e^2)/m_e m_N, \tag{3}$$

where n_e is the number of electrons. In the relativistic theory of hydrogenic atoms (including positronium), ϵ is a reduced energy and μ is a reduced mass (see below).

The remaining steps of τ-dependent perturbation theory are analogous to those of time-dependent perturbation theory. For a given mode ω of the electromagnetic field, h is split into h^0 and a time-dependent perturbation as follows:

$$h=h^0+h_{\rm per}e^{i\omega t},\quad \omega t=\omega\tau/\mu \tag{4}$$

(for photon absorption, $e^{i\omega t}$ is replaced by $e^{-i\omega t}$). The wave function $\psi(\tau)$ is expanded in a complete set of unperturbed states $\psi_n^{(0)}$,

$$\psi=\sum_n c_n(\tau)\psi_n^{(0)}e^{-i\tau(\epsilon/\mu)_n}. \tag{5}$$

The desired coefficient c_f of the final state is isolated from the sum by means of the orthogonality relations. For Nth order perturbation theory, one expands $c_n=\Sigma_N c_n^{(N)}$, $c_n^{(0)}=\delta_{ni}\Theta(\tau-\tau_0)$. Setting $\hbar=c=1$ in the following, the first order gives

$$c_f(\tau)^{(1)}=-i\int^\tau d\tau'\langle f|h_{\rm per}|i\rangle e^{i\tau'[\omega/\mu_i-(\epsilon/\mu)_i+(\epsilon/\mu)_f]}, \tag{6}$$

with $E_i=E$, $E_f=E'$ in the notation of (1). The constant part of ϵ/μ disappears in (6). The differential decay rate follows as

$$d(E_i\Gamma_{if})=(2\pi)^{-3}d^3k|\langle\boldsymbol{k},\lambda,f|m_e m_N h_{\rm per}|i\rangle|^2\delta(E_i\omega-E_i^2/2+E_f^2/2), \tag{7}$$

where λ denotes the photon helicity. The δ function produces the desired relation (1). When the exponents in (5) are shifted from the imaginary axis by amounts $E_n\Gamma_n\tau/2$, the line shape is a Lorentzian,

$$dW_{if}/d\omega=(2\pi)^{-1}E_i^2\Gamma_{if}[(E_i\omega-E_i^2/2+E_f^2/2)^2+(E_i\Gamma_i)^2/4]^{-1}. \tag{8}$$

The general formalism ends here. h^0 is presently known for leptonium (positronium and muonium), for hydrogen (including recoil corrections of the anomalous magnetic moment), and less precisely for hydrogenic atoms with a spinless nucleus [2]. The relativistic center-of-mass system (c.m.s.) two-body kinematics of two free particles of arbitrary spins leads to the equation

$$(\epsilon^2-\mu^2-\boldsymbol{p}^2)\psi=0,\quad \boldsymbol{p}=\boldsymbol{p}_1=-\boldsymbol{p}_2=-i\boldsymbol{\nabla}. \tag{9}$$

Relativistic kinematics has been developed over the past century, which may excuse quoting a textbook [3]. From the nonrelativistic eigenvalue,

$$E \approx m_{12} - Z^2\alpha^2\mu_{nr}/2n^2, \quad m_{12} = m_1 + m_2 = m_e + m_N, \tag{10}$$

one sees that μ in (2) is in fact close to the nonrelativistic reduced mass μ_{nr}.

The dimensionless forms of the bound-state equations for two fermions and for a single electron are nearly identical,

$$h^0 = \beta + \boldsymbol{\alpha}\boldsymbol{p}_\rho + V(\rho) + h_{hf}, \quad \boldsymbol{\rho} = \mu\boldsymbol{r},\ \boldsymbol{p}_\rho = \boldsymbol{p}/\mu. \tag{11}$$

The hyperfine operator h_{hf} is different, however. Writing $\boldsymbol{\alpha} = \gamma^5\boldsymbol{\sigma}_1$, it is to the order $(Z\alpha)^4$ and to all orders m_e/m_N for leptonium,

$$h_{hf} = i\gamma^5(\boldsymbol{\sigma}_1 \times \boldsymbol{s}_2)V(\rho)\boldsymbol{p}_\rho m_c m_N/m_{12}^2, \tag{12}$$

where $\boldsymbol{s}_2$ is the nuclear-spin operator (leptonium has $\boldsymbol{s}_2 = \boldsymbol{\sigma}_2/2$). The replacement of $1/m_N$ by m_N/m_{12}^2 in the static Dirac equation is due to Breit (at the order $(Z\alpha)^6$, m_{12}^{-2} is replaced by E^{-2} [4,5], which requires new orthogonality relations in the variable $\boldsymbol{r}_E = E\boldsymbol{r}$ [2]). The standard hyperfine operator contains only the Hermitian part $[V,\boldsymbol{\nabla}]/2$ of $V\boldsymbol{\nabla}$; the anti-Hermitian part $\{V,\boldsymbol{\nabla}\}/2$ contributes to hyperfine mixing (in the 16-component formalism, the mixing arises from the retardation part of the Breit operator). A "hyperfine Hermiticity" may be defined in which also the Hermitian adjoint of (11) appears, $h^\dagger\chi = \epsilon\chi$. It is based on the scalar product

$$\int d^3\rho\chi_f^\dagger\psi_i = \delta_{if}, \tag{13}$$

but is needed only for nonperturbative hyperfine interactions. (In the 16-component formalism, ψ and χ are eigenstates of the total chirality $\gamma_1^5\gamma_2^5$, with eigenvalues +1 and −1, respectively. This operator commutes with the parity matrix $\beta = \beta_1\beta_2$.) To demonstrate that h_{hf} does not make E^2 complex, it is sufficient to show that (12) is real: The Dirac spinor ψ is decomposed into large components, $\psi_g = g(r)\chi_{l,S}^{f,m_f}$ and small ones $\psi_f = if(r)\chi_{\tilde{l},S'}^{f,m_f}$, with $\tilde{l} = l \pm 1$ and S = total spin. In this basis, $\gamma^5\boldsymbol{\sigma}_1\boldsymbol{p} = -i\gamma^5\boldsymbol{\sigma}_1\boldsymbol{\nabla}$ is not only Hermitian, but also real, as the matrix elements of $i\gamma^5$ and $\boldsymbol{\sigma}_1\boldsymbol{\nabla}$ are all real. From the commutator algebras of $\boldsymbol{\sigma}_1 = 2\boldsymbol{s}_1$ and $\boldsymbol{s}_2$, one verifies $i\boldsymbol{s}_1 \times \boldsymbol{s}_2 = -[\boldsymbol{s}_1, \boldsymbol{s}_1\boldsymbol{s}_2] = [\boldsymbol{s}_2, \boldsymbol{s}_1\boldsymbol{s}_2]$. The eigenvalues of $2\boldsymbol{s}_1\boldsymbol{s}_2$ for $S = s_2 \pm 1/2$ are s_2 and $-s_2 - 1$, respectively. The explicit matrix elements of $i\boldsymbol{\sigma}_1 \times \boldsymbol{s}_2$ are thus

$$\langle s', m_S'|i\boldsymbol{\sigma}_1 \times \boldsymbol{s}_2|S, m_S\rangle = (S' - S)(s_2 + 1/2)\langle S', m_S'|\boldsymbol{\sigma}_1|S, m_S\rangle, \tag{14}$$

for arbitrary magnetic quantum numbers m_S, m_S'. They vanish for $S' = S$, as required for a matrix that is both real and anti-Hermitian.

The vector potential $\boldsymbol{A}(\boldsymbol{r})$ appears in h_{per} in the combinations $q_i\boldsymbol{A}(\boldsymbol{\rho}_i)/\mu$, with $\boldsymbol{\rho}_i = \mu\boldsymbol{r}_i$. For binary atoms, the transition to the relative and c.m.s. coordinates, $\boldsymbol{r}$ and $\boldsymbol{R}$, brings a factor $e^{i(\boldsymbol{k}+\boldsymbol{P})\cdot\boldsymbol{R}}$ for $\langle f|h_{per}|i\rangle$, which results in the already mentioned momentum conservation. In general,

$$\langle f|h_{per}|i\rangle = \Pi_i \int d^3\boldsymbol{\rho}_i\chi_f^\dagger h_{per}\psi_i. \tag{15}$$

For electric-dipole radiation, one may replace in $h\boldsymbol{p}_\rho$ by $\boldsymbol{p}_\rho + e_{dip}\mu\boldsymbol{A}(\boldsymbol{\rho} = \boldsymbol{0})$, where $e_{dip} = e[1 + (Z-1)m_1/M]$ is the effective dipole charge, as in the nonrelativistic two-body Schrödinger equation.

To conclude, it has been shown that the eigenvalue E^2 of the new equation for "binary" atoms reproduces exact energy conservation in radiative transitions. The argument of the δ function in (7) will slightly change that part of the Lamb shift which is connected to photon emission by a dispersion relation. This remains to be calculated.

For n-particle-bound states ($n = n_e + 1$ in atoms), one has always assumed that the noninteracting part of the Hamiltonian is the sum of single-particle Hamiltonians, $H^0 = \Sigma H_i^0$, because $H^0\psi = E\psi$ remains valid in the asymptotic region of vanishing interactions. Now, instead, one must add the $n(n-1)/2$ Hamiltonians h_{ij} for pairs of noninteracting particles, each in its own c.m.s., with eigenvalues $E_{ij}^2 - m_i^2 - m_j^2$. In terms of the free-particle four-momenta k_i^μ and k_j^μ, $E_{ij}^2 = (k_i + k_j)^2$. Surprisingly, this seemingly odd procedure does lead to an eigenvalue E^2 apart from a constant, because of $E^2 = (\Sigma_i k_i)^2 = \Sigma_{i<j}(k_i + k_j)^2 - \Sigma m_i^2$. The constant is that of (3).

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