Center-of-mass corrections to the electromagnetic transitions of hydrogen atoms in strong magnetic fields

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The influence of center-of-mass corrections on transition probabilities in the hydrogen spectrum is studied in a homogeneous magnetic field with the help of canonical transformations. To a good approximation, only energy differences are modified but in an unexpected way for electric quadrupole transitions. Center-of-mass corrections mainly affect the lifetimes of the tightly bound states with m < 0. Dipole transitions remain dominant for reduced fields γ up to at least 1000. Quadrupole transitions should dominate the lifetimes of even-parity m=0 states at higher fields.

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I. INTRODUCTION

In a magnetic field, the center-of-mass (c.m.) separation is not a trivial problem, even for the hydrogen atom. The separation can be performed analytically when the field is uniform [1-5], but its physical consequences are not fully understood yet. Except in the unlikely case where the hydrogen-atom motion is perfectly parallel to the field, the internal properties of the atom depend on a collective constant of motion, the total pseudomomentum [1]. The most spectacular effect of the coupling between internal and collective motions is that binding energies may significantly be modified in strong fields [4,5]. States may even become unstable because of c.m. effects [4,6]. The strong-field regime is characterized by values larger than unity of the parameter

$$\gamma = \hbar e B / 2m_1 \mathcal{R} \quad (1)$$

where B is the magnetic field strength, m_1 is the electron mass, and \mathcal{R} is the Rydberg energy.

How does c.m. separation affect electromagnetic transitions? To answer this question, we apply the linearcanonical-transformation formalism described in Refs. [4] and [5] to the calculation of transition probabilities. We assume that the collective motion of the atom in a direction transverse to the field is initially weak. The study of important transverse motions is rather delicate but is in progress.

Electric dipole transitions in the hydrogen spectrum are studied with high accuracy from weak to very strong fields by Forster *et al.* [7] (see also Ref. [8] for a physical discussion in the adiabatic approximation). These authors assume that the effect of the finite proton mass can be taken into account by a simple scaling law [9]. As shown below, this assumption is correct but its correctness is rather fortuitous, since c.m. corrections on quadrupole transitions are counterintuitive.

Here, we calculate transition probabilities with the simple variational basis of Ref. [10]. Since extensive data already exist for low-lying states [7], we concentrate on the influence of c.m. corrections. The validity of the electric dipole approximation is also discussed, since energy differences are much larger in very strong fields.

In Sec. II, formulas for dipole and electric quadrupole transition probabilities are derived with a correct account of c.m. separation. In Sec. III, some transition probabilities are displayed and discussed. Concluding remarks are presented in Sec. IV.

II. CENTER-OF-MASS CORRECTIONS IN TRANSITION PROBABILITIES

In a homogeneous magnetic field **B**, the Hamiltonian of the hydrogen atom reads [4]

$$H = \frac{\pi_0^2}{2m_0} + \frac{\pi_1^2}{2m_1} - \frac{e^2}{|\mathbf{r}_0 - \mathbf{r}_1|} , \qquad (2)$$

where m_0 is the proton mass. With the arbitrary gauge $A(\mathbf{r})$ for the external field, the kinetic momenta π_i are given by

$$\boldsymbol{\pi}_i = \mathbf{p}_i - \boldsymbol{q}_i \, \mathbf{A}(\mathbf{r}_i) \,, \tag{3}$$

where \mathbf{r}_i , \mathbf{p}_i , and q_i are, respectively, the coordinate, momentum, and charge of particle i ($q_0 = -q_1 = e$). The Hamiltonian describing the interaction with the radiation field reads in the Coulomb gauge [11]

$$H_i = -(q_0/m_0)\pi_0 \cdot \mathbf{A}_r(\mathbf{r}_0) - (q_1/m_1)\pi_1 \cdot \mathbf{A}_r(\mathbf{r}_1) , \quad (4)$$

with the vector potential

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(5)

$$\mathbf{A}_{r}(\mathbf{r}) = \mathcal{A}_{0} \boldsymbol{\epsilon} \exp(-i\mathbf{k} \cdot \mathbf{r}) ,$$

where **k** is the photon wave vector, $\boldsymbol{\epsilon}$ its polarization with the property $\boldsymbol{\epsilon} \cdot \mathbf{k} = 0$, and $\mathcal{A}_0 = (\hbar/2\epsilon_0 kc)^{1/2}$.

The Hamiltonian (2) possesses the exact constant of motion [1]

$$\mathbf{K} = \mathbf{k}_0 + \mathbf{k}_1 , \qquad (6)$$

where the pseudomomenta \mathbf{k}_i are given by

$$\mathbf{k}_i = \boldsymbol{\pi}_i + \boldsymbol{q}_i \mathbf{B} \times \mathbf{r}_i \ . \tag{7}$$

For a neutral system, the components of K commute with each other. With the total pseudomomentum K, one defines the canonical transformation [4]

$$\mathbf{r}_{0}^{\prime} = M^{-1}(m_{0}\mathbf{r}_{0} + m_{1}\mathbf{r}_{1}), \quad \mathbf{r}_{1}^{\prime} = \mathbf{r}_{1} - \mathbf{r}_{0}$$

$$\mathbf{p}_{0}^{\prime} = \mathbf{K}, \quad \boldsymbol{\pi}_{1}^{\prime} = \boldsymbol{\pi}_{1} - (m_{1}/M)\mathbf{K} , \qquad (8)$$

where $M = m_0 + m_1$. In (8), we display the physical variables \mathbf{r}'_0 and \mathbf{p}'_0 for the neutral global system, and \mathbf{r}'_1 and π'_1 for the charged light pseudoparticle. The Hamiltonian becomes

$$H' = (2M)^{-1} \mathbf{p}_0'^2 + eM^{-1} (\mathbf{p}_0' \times \mathbf{B}) \cdot \mathbf{r}_1' + H'_{\text{int}} , \qquad (9)$$

with the internal Hamiltonian

$$H'_{\text{int}} = \frac{{\pi'_1}^2}{2m_1} + \frac{{\bf k}_1'^2}{2m_0} - \frac{e^2}{r'_1} \ . \tag{10}$$

In (9), the second term of H' corresponds to the motional Stark effect [12] and couples the internal and collective motions. This term modifies the binding energies of the atomic states [4,5]. The second term in H'_{int} provides an intrinsic correction to the internal energies [2,3]. The operator

$$\mathcal{L}_{1\parallel}^{\prime} = \frac{1}{2} \widehat{\mathbf{B}} \cdot \mathbf{r}_{1}^{\prime} \times (\boldsymbol{\pi}_{1}^{\prime} + \mathbf{k}_{1}^{\prime}) = -(2eB)^{-1} (\mathbf{k}_{1}^{\prime 2} - \boldsymbol{\pi}_{1}^{\prime 2}) \qquad (11)$$

is a constant of motion of H'_{int} , which reduces to the parallel component of the orbital momentum in the symmetric gauge [4].

When applied to the interaction Hamiltonian (4), the canonical transformation (8) yields

$$H'_{i} = e \mathcal{A}_{0} \exp[-i\mathbf{k} \cdot (\mathbf{r}'_{0} - \boldsymbol{M}^{-1}\boldsymbol{m}_{1}\mathbf{r}'_{1})] \\ \times \boldsymbol{\epsilon} \cdot \{-\boldsymbol{M}^{-1}[1 - \exp(-i\mathbf{k} \cdot \mathbf{r}'_{1})]\mathbf{p}'_{0} + \boldsymbol{m}_{0}^{-1}\mathbf{k}'_{1} \\ + \boldsymbol{m}_{1}^{-1}\exp(-i\mathbf{k} \cdot \mathbf{r}'_{1})\boldsymbol{\pi}'_{1}\}.$$
(12)

The transformed interaction Hamiltonian H'_i appears in transition matrix elements involving initial and final wave functions of the two-body system. Since \mathbf{p}'_0 is an exact constant of motion of (9), the eigenfunctions of H' factorize into an internal wave function $\Psi_{\mathbf{K}_{\perp}}(\mathbf{r}'_1)$ and a factor $\exp(i\pi^{-1}\mathbf{K}\cdot\mathbf{r}'_0)$, where \mathbf{K} is an eigenvalue of the total pseudomomentum \mathbf{p}'_0 . Notice that the internal function only depends on the transverse part of \mathbf{K} . In a perturbation expansion with respect to \mathbf{K}_{\perp} , the zeroth-order approximation of $\Psi_{\mathbf{K}_{\perp}}$ is given by the common eigenfunctions of H'_{int} and \mathcal{L}'_{\parallel} [4].

Together with the c.m. factors of the initial and final

wave functions, the factor $exp(-i\mathbf{k}\cdot\mathbf{r}'_0)$ in (12) provides the conservation law [1]

$$\mathbf{K}_{f} = \mathbf{K}_{i} - \hbar \mathbf{k} \ . \tag{13}$$

The photon wave vector is proportional to the difference between the initial and final *pseudomomenta*. From now on, we consider effective transition operators without the factor $\exp(-i\mathbf{k}\cdot\mathbf{r}'_0)$ and with \mathbf{p}'_0 replaced by its eigenvalue \mathbf{K}_i (or equivalently \mathbf{K}_f), in matrix elements involving only internal states.

In the long-wavelength approximation, $\mathbf{k} \cdot \mathbf{r}'_1$ is small and H'_i provides the electric dipole Hamiltonian

$$H_{E1}' = e \mathcal{A}_0 \boldsymbol{\epsilon} \cdot (\boldsymbol{m}_0^{-1} \mathbf{k}_1' + \boldsymbol{m}_1^{-1} \boldsymbol{\pi}_1')$$
(14)

$$= ie \hbar^{-1} \mathcal{A}_0[H'_{\text{int}}, \boldsymbol{\epsilon} \cdot \mathbf{r}'_1] .$$
(15)

The apparently small term $m_0^{-1}\mathbf{k}'_1$ cannot be neglected in (14). Indeed, (14) and (15) lead, respectively, to the equivalent velocity and length forms of the electric dipole approximation. Neglecting $m_0^{-1}\mathbf{k}'_1$ would correspond to replacing H'_{int} in (15) by its infinite-mass approximation. In strong fields, such a replacement would lead to smaller energy differences and would significantly modify the transition probabilities.

From (14) and (15), one deduces electric dipole transition probabilities per unit time, since ψ_{K_1} is to an excellent approximation an eigenfunction of H'_{int} (see also Sec. III). For example, the length version reads

$$W = \frac{1}{6} \alpha^4 (c / a_0) (\Delta E_{\text{int}})^3 \sum_q |\langle \Psi_{\mathbf{K}_f} | r_q | \Psi_{\mathbf{K}_i} \rangle|^2 , \qquad (16)$$

where α is the fine-structure constant, a_0 is the Bohr radius and $r_{\pm 1} = (1/\sqrt{2})(x \pm iy)$, $r_0 = z$, and where energies are expressed in Ry and lengths in a_0 . In (16), the photon wave number is eliminated by using

$$\hbar ck = E_i - E_f \simeq E_{\text{int},i} - E_{\text{int},f} = \Delta E_{\text{int}} , \qquad (17)$$

where the approximation [4] is valid for $K_i \ll m_0 c$. The most important feature in (16) is the occurrence of the third power of ΔE_{int} . Let us recall that [2]

$$\Delta E_{\rm int}(\gamma) \simeq \Delta E_{H\infty}(\gamma) - 2(m_1/m_0)\gamma \Delta m , \qquad (18)$$

where we have neglected a small scaling correction. Only $\Delta m \neq 0$ transitions are affected. Employing in that case the infinite-mass approximation would lead to an important error (see Sec. III). Expression (16) is correctly guessed in Ref. [9], and employed in Ref. [7]. However, one should not believe that any energy difference in transition probabilities is of the form ΔE_{int} . We illustrate this point on quadrupole transitions.

By assuming that $K_{i\perp}$ is small enough and by neglecting a term proportional to $(m_1/m_0)^2 \mathbf{k}'_1$, one obtains after symmetrization [13] the electric quadrupole operator

$$H'_{E2} = -\frac{1}{2}ie\mathcal{A}_0 m_1^{-1} [(\boldsymbol{\epsilon} \cdot \boldsymbol{\pi}'_1)(\mathbf{k} \cdot \mathbf{r}'_1) + (\boldsymbol{\epsilon} \cdot \mathbf{r}'_1)(\mathbf{k} \cdot \boldsymbol{\pi}'_1)]$$
(19)

$$= \frac{1}{2} e \, \hbar^{-1} \mathcal{A}_0[H'_{\infty}, (\boldsymbol{\epsilon} \cdot \mathbf{r}'_1)(\mathbf{k} \cdot \mathbf{r}'_1)] \,. \tag{20}$$

In spite of the fact that the magnetic field enhances energy differences, when $K_{i\perp}$ is small, the final pseudomomentum $K_{f\perp}$ also remains small. Notice the occurrence in (20) of the infinite-mass internal Hamiltonian obtained from (10) with $m_0 = \infty$. In the quadrupole case, c.m. corrections to (19) are proportional to $(m_1/m_0)^2 \gamma$ and remain negligible even when the correction $(m_1/m_0)\gamma$ to the dipole term plays an important role.

The operator H'_{∞} is identical to $H'_{\mu} = H'_{\text{int}} + (eB/m_0)\mathcal{L}'_{1\parallel}$, except for the replacement of m_1 by the reduced mass μ of the system. Replacing H'_{∞} by H'_{μ} in (20) scales H'_{E2} by a negligible amount. Since to an excellent approximation $\Psi_{\mathbf{K}_{\perp}}$ is an eigenfunction of H'_{μ} , an eigenvalue difference appears that can be accurately [4] approximated by $\Delta E_{H_{\infty}}$. The length version of the transition probability then reads

$$W = \frac{1}{320} \alpha^{6} (c / a_{0}) (\Delta E_{\text{int}})^{3} (\Delta E_{H_{\infty}})^{2} \sum_{q} |\langle \Psi_{\mathbf{K}_{f}} | \mathbf{r}_{q}^{(2)} | \Psi_{\mathbf{K}_{i}} \rangle|^{2} ,$$
(21)

where $r_{\pm 2}^{(2)} = (r_{\pm 1})^2$, $r_{\pm 1}^{(2)} = \sqrt{2}r_{\pm 1}r_0$, and $r_0^{(2)} = \sqrt{3/2}(r_0^2 - r_{\pm 1}r_{-1})$. Here the energy difference appears in two different forms. Only photon energies provide ΔE_{int} . The commutator in (20) leads to energy differences $\Delta E_{H\infty}$ of the infinite-mass approximation.

Finally, let us briefly discuss magnetic dipole transitions. Replacing plus in (19) by minus provides the operator

$$H'_{M1} = \frac{1}{2} i e \mathcal{A}_0 m_1^{-1} (\boldsymbol{\epsilon} \times \mathbf{k}) \cdot (\mathbf{r}'_1 \times \boldsymbol{\pi}'_1) . \qquad (22)$$

Notice that $\mathbf{r}'_1 \times \boldsymbol{\pi}'_1$ differs in a magnetic field from the operator \mathcal{L}'_1 appearing in (11). Hence, M1 transitions do not vanish in this approximation as in the field-free case, since the initial and final states are not eigenstates of the interaction operator. The transition probability is given by

$$W = \frac{1}{24} \alpha^{6} (c / a_{0}) (\Delta E_{\text{int}})^{3} \sum_{q} |\langle \Psi_{\mathbf{K}_{f}}| (\mathbf{r}_{1}^{\prime} \times \boldsymbol{\pi}_{1}^{\prime})_{q} |\Psi_{\mathbf{K}_{i}} \rangle|^{2} ,$$
(23)

and does not show c.m. effects besides the modification of the photon energy.

III. TRANSITION PROBABILITIES IN A SIMPLE VARIATIONAL BASIS

Even when $K_{i\perp}=0$, the orthogonal component $K_{f\perp}$ of the final pseudomomentum does not vanish because of the conservation law (13). We have employed a firstorder perturbation expansion of $\Psi_{K_{f\perp}}$ as a function of $K_{f\perp}$ to evaluate the importance of the recoil effect. We have found that the resulting corrections to the transition probabilities satisfy the same selection rules as quadrupole transitions. However, between $\gamma = 1$ and 1000, they are at least two orders of magnitude smaller than quadrupole transition probabilities. Therefore, in the following, we display our results without any recoil effect in the wave functions. Center-of-mass effects only arise in the energy factors appearing in (16), (21), or (23).

When K_{\perp} vanishes, the internal part $\Psi_{\mathbf{K}_{\perp}}$ of the eigenstates of H' possesses the same good quantum numbers as the eigenstates of H'_{int} , i.e., the magnetic quantum number *m* corresponding to $\mathcal{L}'_{i\parallel}$ and the *z* parity *p*. In Ref. [10], we showed that simple approximations of these states can be obtained with the variational expansion

$$\Psi_{n}^{mp}(\mathbf{r}) = \sum_{\nu=0}^{N} \phi_{\nu m}(\mathbf{r}_{\perp}) \sum_{j=1}^{M} C_{\nu m n}^{j} z^{(1-p)/2} \exp(-\beta_{j} |z|) , \qquad (24)$$

where ϕ_{vm} is a Landau state. The β_j are given for M = 18 in Eq. (A5) and Table 2 of Ref. [10] and the C_{vmn}^j are variational constants. Accurate results are already obtained for N = 5 in (24). The quantum number *n* labels the energies and corresponds here to the total number of nodes of the v=0 z component in (24). It is related to n_z in Ref. [10] by $n = 2n_z - \frac{1}{2}(1-p)$. The value of p is therefore uniquely given by $(-)^n$ in the present notation.

fore uniquely given by $(-)^n$ in the present notation. When both $K_{i\perp}$ and $K_{f\perp}$ remain small, *m* is approximately a good quantum number for both the initial and final states, *q* in (16), (21), and (23) then takes the value $\Delta m = m_f - m_i$, and one obtains the selection rule $|\Delta m| \leq 1$ [8] for dipole transitions or $|\Delta m| \leq 2$ for quadrupole transitions.

Writing the operators $r_{\pm 1}$ as a function of creation and annihilation operators [14] leads to simple expressions for the matrix elements with the present basis. The calculations are very easy. However, dipole transitions are already studied in the literature [7]. Therefore, we focus here on c.m. effects and on the validity of the dipole approximation. Obviously, the lifetimes of the tightly bound states (which correspond to $\Delta m = 1$ transitions) are modified by the c.m. corrections at very high fields [see Eq. (18)]. For other states, the lifetimes will only be affected if $\Delta m \neq 0$ transitions contribute significantly to the total probability. As exemplified below, this is not the case. Indeed, the $\Delta m = 0$ transitions are dominant because of the elongation of the atom in the field direction.

Total E1 transition probabilities are displayed in Fig. 1 for different m = 0 states. Even-*n* results are represented as solid lines and odd-n results as dashed lines. The accuracy of the E1 transition probabilities can be checked by comparing them with accurate results [7]. At $\gamma = 1$, the poorest accuracy (15%) is observed for states that decay towards the ground state (odd-n states). This is not surprising because the symmetry of the tightly bound ground state is not dominantly cylindrical below $\gamma = 20$ [15]. At $\gamma = 10$, the agreement is better than 1%. Beyond $\gamma = 100$, the agreement is excellent. The wave functions (24) become better than those of Ref. [15], as suggested in Ref. [16]. Magnitudes as well as γ dependences of the probabilities present a clear odd-even effect. Transition probabilities from odd-n states are larger and steadily increase with γ . The even-*n* probabilities reach a maximum between $\gamma = 10$ and 100. Indeed, $\Delta m = 0$ transitions require a z-parity change. Therefore, only odd-n states can decay directly towards the tightly bound



FIG. 1. Total electric dipole transition probabilities from 0 *n* states (in s⁻¹) as a function of the reduced magnetic field γ : even z parity (solid lines) and odd z parity (dashed lines).

ground state and be enhanced by large energy differences. For even-*n* states, $\Delta m = 0$ transitions still dominate but $\Delta m = -1$ transitions represent 20-50% of the total probability at $\gamma = 1$, 4-10% at $\gamma = 10$ and 1-5% at $\gamma = 100$ and 1000. The shape of the curves arises from the fact that the increase due to energy differences is counterbalanced by a decrease of the matrix elements.

Three electric quadrupole transitions to the ground state corresponding to different Δm values are displayed in Fig. 2 and are compared with the total E1 transition probabilities from the initial state. Let us first comment on the E1 curves. The 0.2 probability is already displayed in Fig. 1. The -11 probability is much larger because of the large decay probability to the tightly bound -10 state. The -11 state becomes unstable with respect to dissociation near $\gamma = 880$ [4]. The -20 state can only decay to the -10 state and has therefore a small transition probability. Its rise at large fields is due to a c.m. effect as shown by the dashed curve, where $(\Delta E_{int})^3$ is replaced by $(\Delta E_{H\infty})^3$. Let us now consider the quadrupole transitions. The $-2 \rightarrow 0$ transition probability is very weak and decreases with increasing γ . The $\Delta m = 1$ transition is much stronger and increases with γ . The dominant transition probability again corresponds to $\Delta m = 0$ and displays a fast increase with γ . At $\gamma = 1000$, it represents a 3.5% correction to the total transition probability of the 0.2 state. Since E1 transition probabilities of even-*n* states decrease when γ increases, quadrupole transitions should become the dominant mode at higher fields. As shown by Fig. 1, only even-n lifetimes will be affected.



FIG. 2. E2 and M1 transition probabilities from m n to m'n' (in s⁻¹) as a function of the reduced magnetic field γ compared with total E1 transition probabilities from the initial state. The dashed line represents a calculation where c.m. effects are neglected.

In a magnetic field, M1 transitions are not forbidden at lowest order. However, they remain small with respect to E2 transitions. For $\Delta m = 0$, they vanish in the adiabatic approximation. Therefore, the E2-to-M1 ratio strongly increases with the field for $\gamma > 1$ (see Fig. 2). For $\Delta m = 1$, M1 transition probabilities are about one order of magnitude smaller than E2 probabilities and are thus negligible.

IV. CONCLUSION

Linear canonical transformations provide a simple formalism for establishing rigorous formulas for electromagnetic transition probabilities. This simplicity is illustrated here in the dipole and electric quadrupole cases. Whereas the E1 formula takes the form assumed and employed by Wunner, Ruder, and Herold [9] and Forster et al. [7], the quadrupole formula shows that intuitive transpositions might be unsafe. The $(\Delta E_{H\infty})^2$ factor reflects the fact that c.m. effects are almost negligible in the transition operator and only show up in the energy of the emitted photon. The same comment can be made for magnetic transitions. Anyway, the expressions for the transition probabilities remain very simple as long as the atom does not present an important motion in the direction transverse to the magnetic field. From a practical point of view, transition probabilities are affected by c.m. corrections only through a modification of energy differences. However, the correction to the c.m energy differences is proportional to Δm , and $\Delta m = 0$ transitions are favored. Therefore, the lifetimes of most states are not affected. The only states for which the correction is not negligible are the physically important tightly bound states with n = 0 and m < 0.

In the field range considered here, electric dipole tran-

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sitions are dominant. The total decay probabilities strongly depend on the z parity of the state. States with even z parity have much longer lifetimes than odd zparity states. Quadrupole transitions are in general negligible but $\Delta m = 0$ transitions exhibit a fast increase with the magnetic field. The lifetime of even z-parity states should be dominated by quadrupole transitions at higher fields. Magnetic transitions remain negligible at large fields.

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