

Transitions between shifted Landau states and photoionization of the hydrogen atom moving in a strong magnetic field

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Received 29 September 1993, in final form 3 May 1994

Abstract. Motion of a neutral two-body system transverse to a uniform magnetic field breaks the axial symmetry and causes a shift of the wavefunction outward from the Coulomb well. Therefore the preferable position of the centre of the transverse basis for the wavefunction expansion depends on the motion. In strong magnetic fields, the most appropriate is a set of Landau functions which describe the states of free charged particles. We employed this basis shifted with respect to the Coulomb well and considered radiative transitions between eigenstates with different shifts. Transverse parts of the dipole matrix elements are calculated analytically. The expressions obtained enable one to apply the adiabatic approximation to the photoionization of a moving hydrogen atom with the choice of the transverse (Landau) parts of wavefunctions being localized in the Coulomb and magnetic wells for the initial (ground) and final (continuum) states, respectively. Contrary to the usual adiabatic approach, this method gives good agreement with more precise non-adiabatic calculations.

1. Introduction

The two-body problem in the presence of a magnetic field arises in different branches of modern physics. In solid state physics, it is associated particularly with properties of excitons in magnetized crystals and with diamagnetism of hydrogen atoms (see, for example, Ipatova *et al* 1984 and Vincke *et al* 1992, respectively). In astrophysics, photoionization of the hydrogen atom in strong magnetic fields ($B = 10^{12}$ – 10^{13} G) significantly affects formation of thermal spectra of cooling neutron stars (Pavlov *et al* 1994). The latter process has been studied in a number of papers (Hasegawa and Howard 1961, Gnedin *et al* 1974, Schmitt *et al* 1981, Wunner *et al* 1983, Miller and Neuhauser 1991, Potekhin and Pavlov 1993). It has been shown that strong magnetic fields, $\gamma \equiv \hbar^3 B / (m^2 e^3 c) = B / (2.35 \times 10^9 \text{ G}) \gg 1$, change drastically both the atomic structure and radiative transition rates. The atom is compressed transverse to the field, and the photoionization cross sections change their frequency dependence and acquire strong dependence on polarization.

The above-cited papers are based on the *adiabatic approximation* for a non-moving atom. In this approximation, the internal atomic motion transverse to the magnetic field is treated as non-perturbed by the Coulomb interaction and is described by the Landau wavefunctions. Radiative matrix elements are factorized into ‘transverse’ and ‘longitudinal’ parts, the first being calculated analytically.

The situation is much more complicated when atomic motion across the magnetic field is taken into account, which breaks the axial symmetry. The electric field induced in the

atomic rest frame pulls the electron density distribution apart from the Coulomb well in the plane transverse to the magnetic field. The displacement depends on the magnetic field value and the quantum state of atom (Vincke *et al* 1992). It is maximal when the relative electron-to-proton motion wavefunction is localized in the magnetic well, which corresponds to strongly decentred atomic states (Burkova *et al* 1976, Ipatova *et al* 1984). The approaches, at which the transverse basis of the Landau functions may be centred at the Coulomb or magnetic well, are based on the relative Hamiltonians, which are well known in the literature (see, for example, Gorkov and Dzyaloshinsky 1968, Herold *et al* 1981). However, they cannot be optimal for the adiabatic approximation, since the electron density centre actually lies between these two wells.

Recently Vincke *et al* (1992) have applied gauge choice freedom and canonical operator transformations to obtain a Hamiltonian which can be used for constructing the arbitrarily displaced adiabatic wavefunctions. In our paper we also derive a convenient relative Hamiltonian using a more transparent method of explicit coordinate transformation of the wavefunction (section 2). Then we consider radiative transitions between two states, for which appropriate adiabatic solutions correspond to different displacements. The Landau state creation/annihilation operator formalism is presented. It enables us to calculate analytically the transverse parts of radiative matrix elements (section 3). The advantages of the new approach are illustrated in section 4 by a comparison of the adiabatical photoionization cross sections with those calculated more precisely (using the non-adiabatic wavefunction of the initial state).

2. General expressions

Eigenstates of a neutral two-body system of particles with masses, charges and coordinates m_- , $-e$, r_- and m_+ , e , r_+ ($e > 0$), respectively, which move in an uniform magnetic field \mathbf{B} , may be characterized by the generalized momentum $\hbar\mathbf{K}$, which is the eigenvalue of the operator (Gorkov and Dzyaloshinsky 1968)

$$\hat{P}(\mathbf{R}, \mathbf{r}) = -i\hbar \frac{\partial}{\partial \mathbf{R}} - \frac{e}{2c} \mathbf{B} \times \mathbf{r} \quad (1)$$

where $\mathbf{R} = (m_- r_- + m_+ r_+)/M$ and $\mathbf{r} = \mathbf{r}_- - \mathbf{r}_+$ are the centre-of-mass and relative coordinates, respectively, $M = m_- + m_+$ is the total mass, and the cylindric gauge of the vector potential, $\mathbf{A}(\mathbf{r}) = \frac{1}{2} \mathbf{B} \times \mathbf{r}$, is used. The corresponding wavefunction of the system can be presented in the pseudo-factorized form

$$\psi_{\mathbf{K}}(\mathbf{R}, \mathbf{r}) = \exp \left[\frac{i}{\hbar} \left(\hbar\mathbf{K} + \frac{e}{2c} \mathbf{B} \times \mathbf{r} \right) \mathbf{R} \right] \psi_{\mathbf{K}}^{(0)}(\mathbf{r}). \quad (2)$$

The wavefunction of relative motion $\psi_{\mathbf{K}}^{(0)}(\mathbf{r})$ satisfies the Schrödinger equation

$$(\hat{H}_{\mathbf{K}}^{(0)} - E) \psi_{\mathbf{K}}^{(0)}(\mathbf{r}) = 0 \quad (3)$$

with the Hamiltonian

$$\hat{H}_{\mathbf{K}}^{(0)} = \frac{\hbar^2 K^2}{2M} + \frac{\hat{p}_z^2}{2\mu} + \hat{H}_{\perp}(\mathbf{r}_{\perp}) + \frac{e\hbar}{Mc} (\mathbf{K}_{\perp} \times \mathbf{B}) \cdot \mathbf{r}_{\perp} + \hat{V}(\mathbf{r}) \quad (4)$$

where $\hat{p}_z = -i\hbar \partial / \partial z$, the z-axis is directed along \mathbf{B} , $\mu = (m_+ m_-) / M$ is the reduced mass, $\hat{V}(\mathbf{r}) = -e^2 / r$ is the Coulomb potential, and E is the energy of the system.

The Hamiltonian

$$\hat{H}_{\perp}(\mathbf{r}_{\perp}) = \frac{\hat{p}_{\perp}^2}{2\mu} + \frac{e^2 B^2}{8\mu c^2} r_{\perp}^2 + \frac{e}{2c} \left(\frac{1}{m_-} - \frac{1}{m_+} \right) \mathbf{B} \cdot (\mathbf{r}_{\perp} \times \hat{\mathbf{p}}_{\perp}) \quad (5)$$

where $\hat{p}_\perp = -i\hbar\partial/\partial r_\perp$, corresponds to the harmonic motion in the plane perpendicular to the magnetic field. The energies and wavefunctions can be written as

$$\begin{aligned} E_{n,N} &= \hbar\omega_g^-(n + \frac{1}{2}) + \hbar\omega_g^+(N + \frac{1}{2}) \\ \Phi_{n,N}(r_\perp) &= \frac{e^{i(n-N)\varphi}}{\sqrt{2\pi}a_m} F_{n,N}\left(\frac{r_\perp^2}{2a_m^2}\right) \end{aligned} \quad (6)$$

where $n = 0, 1, 2, \dots$ and $N = 0, 1, 2, \dots$ enumerate the Landau levels of the negatively and positively charged particles, respectively, $\omega_g^\mp = eB/(m_\mp c)$ are the gyrofrequencies, r_\perp and φ are the polar coordinates of \mathbf{r}_\perp , $a_m = \sqrt{c\hbar/(eB)}$ is the magnetic length, and the function $F_{n,N}(u)$ is equal to zero if $n < 0$ or $N < 0$, while at $n \geq 0$, $N \geq 0$ it is given by the expression (Kaminker and Yakovlev 1981)

$$F_{n,N}(u) = (-1)^{n-N} F_{N,n}(u) = \left(\frac{n!}{N!} u^{N-n} e^{-u}\right)^{1/2} L_n^{N-n}(u) \quad (7)$$

where $L_n^k(u)$ is the Laguerre polynomial.

The term with $\mathbf{K}_\perp \times \mathbf{B}$ in (5) describes the influence of the electric field generated by the motion transverse to \mathbf{B} on the energy of the system. This term is eliminated by the transformation (Gorkov and Dzyaloshinsky 1968, Herold *et al* 1981)

$$\psi_K^{(0)}(\mathbf{r}) = \exp(i\mathfrak{x}\mathbf{K}_\perp \mathbf{r}_\perp) \psi_K^{(1)}(\mathbf{r} - \mathbf{r}_0) \quad (8)$$

where $\mathfrak{x} = (m_+ - m_-)/(2M)$ and $\mathbf{r}_0 = -(a_m^2/B) \mathbf{K}_\perp \times \mathbf{B}$, which leads to the equation

$$(\hat{H}_K^{(1)} - E) \psi_K^{(1)}(\mathbf{r}) = 0. \quad (9)$$

The transformed Hamiltonian

$$\hat{H}_K^{(1)} = \frac{\hbar^2 K_z^2}{2M} + \frac{\hat{p}_z^2}{2\mu} + \hat{H}_\perp(\mathbf{r}_\perp) + \hat{V}(\mathbf{r} + \mathbf{r}_0) \quad (10)$$

contains the shifted potential of interaction between the particles. A more general transformation reads

$$\psi_K^{(0)}(\mathbf{r}) = \exp(i\eta\mathfrak{x}\mathbf{K}_\perp \mathbf{r}_\perp) \psi_K^{(\eta)}(\mathbf{r} - \eta\mathbf{r}_0) \quad (11)$$

with $\psi_K^{(\eta)}(\mathbf{r})$ satisfying the equation

$$(\hat{H}_K^{(\eta)} - E) \psi_K^{(\eta)}(\mathbf{r}) = 0 \quad (12)$$

where

$$\begin{aligned} \hat{H}_K^{(\eta)} &= \frac{\hbar^2 K_z^2}{2M} + (1-\eta)^2 \frac{\hbar^2 K_\perp^2}{2M} + \frac{\hat{p}_z^2}{2\mu} + \hat{H}_\perp(\mathbf{r}_\perp) + (1-\eta) \frac{e\hbar}{Mc} (\mathbf{K}_\perp \times \mathbf{B}) \mathbf{r}_\perp \\ &\quad + \hat{V}(\mathbf{r} + \eta\mathbf{r}_0). \end{aligned} \quad (13)$$

The Hamiltonian (13) reduces to (5) and (10) at $\eta = 0$ and $\eta = 1$, respectively, and is equivalent to that obtained by Vincke *et al* (1992) on the basis of generalized canonical transformations.

In strong magnetic fields it is convenient to expand the wavefunctions over the transverse basis of the Landau states (6)

$$\psi_{K,i}^{(\eta)}(\mathbf{r}) = \sum_{n',N'} g_{K,i;n',N'}^{(\eta)}(z) \Phi_{n',N'}(\mathbf{r}_\perp) \quad (14)$$

where the coefficients $g_{K,i;n',N'}^{(\eta)}(z)$ are to be calculated numerically. In this approach, the eigenstates of the system $|K, i\rangle \equiv |K, n, N, v\rangle$ are determined by the generalized

momentum $\hbar\mathbf{K}$, the Landau numbers n and N , and by an additional quantum number ν related to the 'longitudinal' energy (either positive or negative). The stronger the magnetic field, the better is the convergence of the expansion (14). If $a_m \ll (m/\mu)a_0$, where $a_0 = \hbar^2/(me^2)$ is the Bohr radius (for the hydrogen atom it means $\gamma \gg 1$), the adiabatic approximation may be applied, in which only the main term with $n' = n$ and $N' = N$ is kept in (14):

$$\psi_{K,i}^{(\eta)}(\mathbf{r}) \simeq g_{K,i}^{(\eta)}(z)\Phi_{n,N}(\mathbf{r}_\perp) \quad (15)$$

where $g_{K,i}^{(\eta)}(z) \equiv g_{K,i;n,N}^{(\eta)}(z)$.

3. Radiative transitions

Let us consider the radiative transition between two eigenstates, $|\mathbf{K}, i\rangle$ and $|\mathbf{K}', f\rangle$, which are determined by the generalized momentum values \mathbf{K} and \mathbf{K}' and by the sets i and f of additional quantum numbers. To obtain the corresponding cross section one should calculate the matrix element \mathcal{D} (see equation (A13)). We shall choose the *length representation* and consider the *dipole approximation* at *different shifts*, η and η' , for the initial and final wavefunctions, respectively. Then

$$\mathcal{D} = \langle \psi_{K',f}^{(\eta')}(\mathbf{r} + \mathbf{r}_*) | \exp(i\alpha(\eta - \eta')\mathbf{K}_\perp \mathbf{r}_\perp) \mathbf{r} | \psi_{K,i}^{(\eta)}(\mathbf{r}) \rangle \quad (16)$$

where $\mathbf{r}_* = (\eta - \eta')\mathbf{r}_0$. Let now in this equation the transverse basis (6) be used for the exact (14) or adiabatic representation (15) of the initial and final wavefunctions. Since the operator \hat{r}_\perp transforms the Landau state $|n, N\rangle$ into the superposition of the neighbouring states $|n-1, N\rangle$, $|n+1, N\rangle$, $|n, N-1\rangle$ and $|n, N+1\rangle$ (see, for example, Hasegawa and Howard 1961, or (21) and (22) below) one comes to the separate problem of calculation of the 'transverse' matrix elements

$$I_{n',N',n,N} = \langle \Phi_{n',N'}(\mathbf{r}_\perp + \mathbf{r}_*) | \exp(i\alpha(\eta - \eta')\mathbf{K}_\perp \mathbf{r}_\perp) | \Phi_{n,N}(\mathbf{r}_\perp) \rangle. \quad (17)$$

In the case of motion ($\mathbf{K}_\perp \neq 0$), if $\eta' \neq \eta$, the direct integration in (17) with the Landau functions (6) is complicated due to the shift \mathbf{r}_* . However, it is possible to use a method which does not employ an explicit form of the wavefunctions. First, the final wavefunction can be written as

$$\Phi_{n',N'}(\mathbf{r}_\perp + \mathbf{r}_*) = \hat{T} \Phi_{n',N'}(\mathbf{r}_\perp) \quad (18)$$

where

$$\hat{T} = \exp\left(\mathbf{r}_* \frac{\partial}{\partial \mathbf{r}_\perp}\right) = \exp\left(\frac{i}{\hbar} \mathbf{r}_* \hat{\mathbf{p}}_\perp\right) \quad (19)$$

is the shift operator. Due to the orthogonality of \mathbf{r}_* and \mathbf{K}_\perp , the arguments of the exponents in (17) and (19) commute, and one may multiply them to obtain the equation

$$I_{n',N',n,N} = \langle n', N' | \exp\left(-\frac{i}{\hbar} \mathbf{r}_* \hat{\mathbf{p}}_\perp + i\alpha(\eta' - \eta)\mathbf{K}_\perp \mathbf{r}_\perp\right) | n, N \rangle \quad (20)$$

in which the wavefunctions are no longer mutually shifted.

For further calculations it is convenient to use the relations

$$\begin{aligned} \hat{x} &= -\frac{a_m}{\sqrt{2}} (\hat{a} + \hat{a}^\dagger - \hat{A} - \hat{A}^\dagger) & \hat{y} &= -\frac{ia_m}{\sqrt{2}} (\hat{a} - \hat{a}^\dagger + \hat{A} - \hat{A}^\dagger) \\ \hat{p}_x &= \frac{i\hbar}{2\sqrt{2}a_m} (\hat{a} - \hat{a}^\dagger - \hat{A} + \hat{A}^\dagger) & \hat{p}_y &= -\frac{\hbar}{2\sqrt{2}a_m} (\hat{a} + \hat{a}^\dagger + \hat{A} + \hat{A}^\dagger) \end{aligned} \quad (21)$$

which determine the creation \hat{a}^+ and \hat{A}^+ , and annihilation operators \hat{a} and \hat{A} of the states with the Landau numbers n and N , respectively,

$$\begin{aligned}\hat{a}|n, N\rangle &= \sqrt{n}|n-1, N\rangle & \hat{a}^+|n, N\rangle &= \sqrt{n+1}|n+1, N\rangle \\ \hat{A}|n, N\rangle &= \sqrt{N}|n, N-1\rangle & \hat{A}^+|n, N\rangle &= \sqrt{N+1}|n, N+1\rangle.\end{aligned}\quad (22)$$

From equation (22) the commutation rules follow:

$$[\hat{a}, \hat{a}^+] = 1 \quad [\hat{A}, \hat{A}^+] = 1 \quad [\hat{a}, \hat{A}] = [\hat{a}, \hat{A}^+] = [\hat{a}^+, \hat{A}] = [\hat{a}^+, \hat{A}^+] = 0. \quad (23)$$

It should be noted that expressions (21) and (22) correspond to the well known matrix elements of the operators \hat{r}_\perp and \hat{p}_\perp in the basis of the Landau states (6), and allow one to present the Hamiltonian \hat{H}_\perp in the form of the superposition of the independent harmonic motions of the particles transverse to the magnetic field,

$$\hat{H}_\perp = \hbar\omega_g^- (\hat{a}^+ \hat{a} + \frac{1}{2}) + \hbar\omega_g^+ (\hat{A}^+ \hat{A} + \frac{1}{2}) \quad (24)$$

the energies $E_{n,N} = \langle n, N | \hat{H}_\perp | n, N \rangle$ of the eigenstates $|n, N\rangle$ being determined by equation (6).

In terms of the creation and annihilation operators the matrix element (20) reduces to the form (B1) (see appendix B), where

$$\alpha = \frac{i}{\sqrt{2}} \frac{m_-}{M} (\eta - \eta') (K_x + iK_y) \quad \beta = \frac{i}{\sqrt{2}} \frac{m_+}{M} (\eta - \eta') (K_x - iK_y). \quad (25)$$

Thus, with the aid of the result (B9) one obtains

$$I_{n', N', n, N} = e^{-i(n' - N' - n + N)\epsilon} F_{n', n}(u_-) F_{N', N}(u_+) \quad (26)$$

where

$$\epsilon = \frac{\pi}{2} + \tan^{-1} \left(\frac{K_y}{K_x} \right) \quad u_\mp = \left(\frac{m_\mp}{M} \right)^2 (\eta - \eta')^2 u \quad u = (a_m K_\perp)^2 / 2. \quad (27)$$

For the adiabatic approximation (15), this leads to the following expressions for the cyclic components ($D_{\pm 1} = (D_x \pm iD_y)/\sqrt{2}$, $D_0 = D_z$) of the vector D :

$$\begin{aligned}D_{+1} &= -a_M e^{-i(n' - N' - n + N)\epsilon} \\ &\quad \times [\sqrt{n+1} F_{n', n+1}(u_-) F_{N', N}(u_+) - \sqrt{N} F_{n', n}(u_-) F_{N', N-1}(u_+)] \{g_{K, f}^{(\eta')} | g_{K, i}^{(\eta)}\} \\ D_{-1} &= -a_M e^{-i(n' - N' - n + N)\epsilon} \\ &\quad \times [\sqrt{n} F_{n', n-1}(u_-) F_{N', N}(u_+) - \sqrt{N+1} F_{n', n}(u_-) F_{N', N+1}(u_+)] \{g_{K, f}^{(\eta')} | g_{K, i}^{(\eta)}\} \\ D_0 &= e^{-i(n' - N' - n + N)\epsilon} F_{n', n}(u_-) F_{N', N}(u_+) \{g_{K, f}^{(\eta')} | z | g_{K, i}^{(\eta)}\}.\end{aligned}\quad (28)$$

It should be noted that the direction of the centre-of-mass motion in the xy -plane affects only the common phase of each component. When the shifts coincide ($\eta' = \eta$ and/or $K_\perp = 0$), we have $u_+ = u_- = 0$, and all F -functions turn to delta-symbols. In this case the transverse parts of D_μ do not depend on the particle masses and for $\mu = \pm 1$ reduce (with accuracy of a phase factor) to the well known matrix elements of r_\pm (see, for example, Hasegawa and Howard 1961).

4. Photoionization of the moving hydrogen atom

Expressions (28) enable one to extend the ranges of the adiabatic approximation applicability. We illustrate this by calculation of photoionization rates for a moving hydrogen atom.

To write the photoionization cross section summed over all final states, take into account that the dependence of the continuum wavefunction on the relative coordinate z along \mathcal{B} at large z has the asymptotic behaviour $\psi_{K',f}^{(\eta')} \sim \exp(ik'z)$, where k' is determined by the (positive) 'longitudinal' energy,

$$E'_{\parallel} \equiv \frac{\hbar^2 k'^2}{2\mu} = E' - \frac{\hbar^2 K_z'^2}{2M} - \hbar\omega_{\mathcal{B}}^-(n' + \frac{1}{2}) - \hbar\omega_{\mathcal{B}}^+(N' + \frac{1}{2}). \quad (29)$$

If L_z is the normalizing length, then $k' = (2\pi/L_z)v'$, and the final state density is equal to $d\rho_f = dv' = (L_z/2\pi)dk'$. In terms of the 'longitudinal' energy we have

$$d\rho_f = \frac{L_z}{4\pi a_{\mathcal{B}}} \sqrt{\frac{\mu}{m}} \frac{dE'_{\parallel}}{\sqrt{E'_{\parallel} \text{Ry}}} \quad (30)$$

where $\text{Ry} = me^4/(2\hbar^2) = 13.6 \text{ eV}$ is the Rydberg energy. Substitution of (30) into (A9) and summation over the sets $[n', N', E'_{\parallel}]$ give

$$\sigma_{K,i}(\omega, q) = \pi \frac{e^2 L_z}{\hbar c a_{\mathcal{B}}} \sqrt{\frac{\mu}{m}} \sum_{n', N'} |eD|^2 \frac{\hbar\omega}{\sqrt{E'_{\parallel} \text{Ry}}} \theta(E'_{\parallel}/\text{Ry}) \quad (31)$$

where E'_{\parallel} is determined by (29) with $E' = E + \hbar\omega$ and $K' = K$ (for the dipole approximation), $\theta(\xi) = 0$ at $\xi \leq 0$ and $\theta(\xi) = 1$ at $\xi > 0$, the factor $\theta(E'_{\parallel}/\text{Ry})$ reflects the threshold character of partial cross sections associated with different final states.

For calculation of the matrix element D in (31), the wavefunctions of the initial $\psi_{K,i}^{(\eta)}$ and final $\psi_{K',f}^{(\eta')}$ states can be expanded over the partially shifted transverse basis according to (14). In strong magnetic fields ($\gamma \gg 1$) the terms $n' \neq 0$ may be omitted from (14) at energies $|E|, |E'| \ll \hbar\omega_{\mathcal{B}}^-$. However, in matrix elements D of radiative transitions this can be done if only the length form is used, in analogy with the case of $K_{\perp} = 0$ (Potekhin and Pavlov 1993). When keeping only one of the remaining N' -terms, one comes to the adiabatic approximation (15), while keeping more terms enables one to describe the wavefunction more accurately. The coefficients $g_{K,i;n',N'}^{(\eta)}$ of the expansion (14) can be found from a set of coupled linear second-order differential equations. Analytical estimates of Ipatova *et al* (1984) and variational results of Vincke *et al* (1992) showed that at transverse momenta $\hbar K_{\perp}$ below some critical value $\hbar K_c$ the ground-state electron is localized near the nucleus. Hence the non-shifted ($\eta = 0$) adiabatic approximation is appropriate at $K_{\perp} < K_c$ for this initial state. On the other hand, only full-shift ($\eta' = 1$) representation ensures the correct K value when an electron is gone far from the nucleus, which is the case of continuum $\psi_{K',f}^{(1)}$ functions.

We treat the continuum wavefunctions adiabatically. Coulomb forces, however, distort them at short distances. This effect may be taken into account approximately by orthogonalization of the final wavefunction with respect to the initial one:

$$\psi_{K',f}^{(\eta')}(\mathbf{r}) \rightarrow \psi_{K',f}^{(\eta')}(\mathbf{r}) - \psi_{K',i}^{(\eta')}(\mathbf{r}) \langle \psi_{K',f}^{(\eta')}(\mathbf{r}) | \psi_{K',i}^{(\eta')}(\mathbf{r}) \rangle \quad (32)$$

with

$$\psi_{K',i}^{(\eta')}(\mathbf{r}) = \exp(i\alpha(\eta - \eta')K_{\perp}r_{\perp}) \psi_{K,i}^{(\eta)}(\mathbf{r} - \mathbf{r}_*). \quad (33)$$

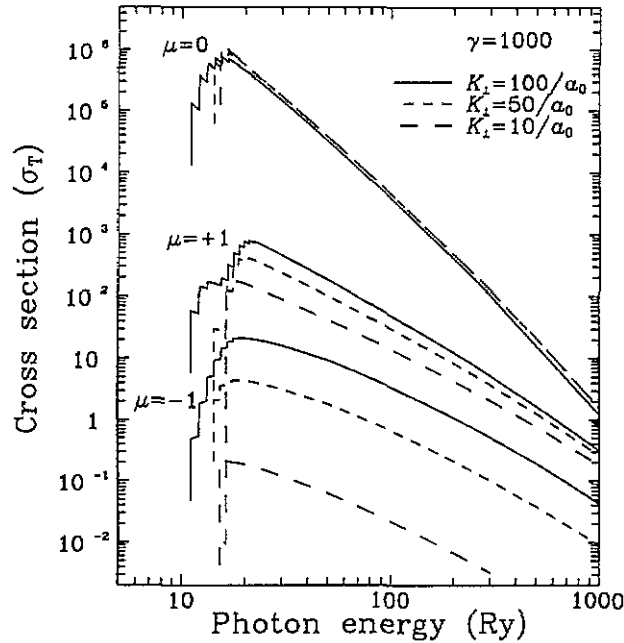


Figure 1. Influence of the motion across the strong magnetic field $B = 2.35 \times 10^{12}$ G on the photoionization cross sections of the hydrogen atom. The cross sections (in units of the Thomson cross section $\sigma_T = 6.65 \times 10^{-25}$ cm²) are plotted as functions of the photon energy (in Ry = 13.6 eV) for the longitudinal ($\mu = 0$), right ($\mu = +1$) and left circular ($\mu = -1$) polarization of the incident radiation. Long-dashed, short-dashed, and full curves correspond to the transverse atomic wave numbers $K_{\perp} = 10/a_0$, $50/a_0$, and $100/a_0$, respectively.

It is equivalent to replacing \mathbf{r} by $\mathbf{r} - \mathbf{r}_{K,i}^{(\eta)}$ in (16), where

$$\mathbf{r}_{K,i}^{(\eta)} = \langle \psi_{K,i}^{(\eta)}(\mathbf{r}) | \mathbf{r} | \psi_{K,i}^{(\eta)}(\mathbf{r}) \rangle \quad (34)$$

is the mean value of \mathbf{r} in the initial state. Since for the adiabatic approximation of $\psi_{K,i}^{(\eta)}(\mathbf{r})$ we have $\mathbf{r}_{K,i}^{(\eta)} = 0$, such a procedure does not change (28).

We have calculated photoionization cross sections of the hydrogen atom moving across the magnetic field using the dipole approximation for \mathbf{D} and representations with equal shifts $\eta' = \eta = 1$ in (14). The initial (bound) state was treated non-adiabatically, with allowance for an admixture of the proton Landau states (see Potekhin 1994 for details). In this case the mean value $\mathbf{r}_{K,i}^{(1)}$ was not equal to zero (but was very close to zero, because the decentring was very small). The corresponding terms were taken into account in the transverse part of the \mathbf{D} expansion. It should be noted that it would be more consistent to treat the final (continuum) state also non-adiabatically. Then the orthogonality of the initial and final wavefunctions could be achieved with an appropriate accuracy and it would not be necessary to resort to the special procedure. Now the treatment involving the effects of the coupling of different Landau orbitals in the continuum is in progress.

Figure 1 shows the numerical results for $\gamma = 1000$ and various $K_{\perp} < K_c$ (where $K_c \sim 150/a_0$, see, for example, Vincke *et al* 1992). Cross sections for longitudinal ($\mu = 0$) and circular ($\mu = \pm 1$, where μ denotes the cyclic components of \mathbf{e}) polarizations of incident radiation are presented. The jumps near the ionization thresholds are due to inclusion of partial transitions to different N channels, all of them being allowed at $K_{\perp} \neq 0$.

Moreover, transitions from the ground state under left-polarized radiation are not forbidden with allowance for motion. Thus the dipole selection rules are broken by the motion, in agreement with the conclusion of Pavlov and Mészáros (1993).

The non-adiabatic results (full curves) for $\mu = 0$ and $\mu = +1$ are compared in figures 2 and 3 with those obtained when $\psi_{K,i}^{(\eta)}$ is treated adiabatically. Long- and short-dashed lines correspond to the different adiabatic approximations, the conventional one ($\eta' = \eta = 1$) and the modified one ($\eta' = 1, \eta = 0$), respectively. Since the first approximation assumes the full decentring of the wavefunction, it fails when such a situation does not occur ($K_{\perp} < K_c$) and the shift value is greater than the transverse size of the wavefunction ($r_0 > a_m$), for example, when $\sqrt{\gamma}/a_0 < K_{\perp} < K_c$. Numerical calculations confirm that under those conditions threshold energies and especially transition rates are strongly underestimated. In contrast to this, the new adiabatic results, calculated from expressions (28) for the case $\eta' = 1, \eta = 0$, are remarkably close to the non-adiabatic ones. The small discrepancy between the tails of the adiabatic and non-adiabatic cross sections is connected with a small decentring of the initial state, which is not taken into account by the adiabatic wavefunction $\psi_{K,i}^{(0)}$. Our numerical tests prove this fact and give the value of corresponding shift ($\eta \simeq 0.2$ for $\gamma = 1000$ and $K_{\perp} = 100/a_0$), which eliminates this deviation when one uses the adiabatic wavefunction $\psi_{K,i}^{(\eta)}$. Therefore, an analytic estimate of the shift $\eta(B, K_{\perp})$ associated with the decentring is thought to be useful. This would give an additional improvement of our adiabatic approach.

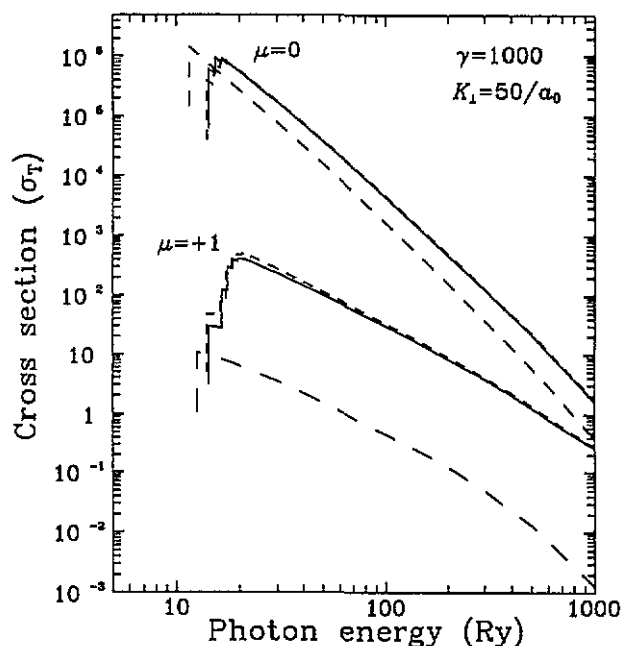


Figure 2. Comparison of the traditional ($\eta' = \eta = 1$, long-dashed curves) and modified ($\eta' = 1, \eta = 0$, short-dashed curves) adiabatic approximations of the photoionization cross sections of the moving hydrogen atom with more precise non-adiabatic cross sections (full curves) for magnetic field $B = 2.35 \times 10^{12}$ G and transverse wavenumber $K_{\perp} = 50/a_0$.

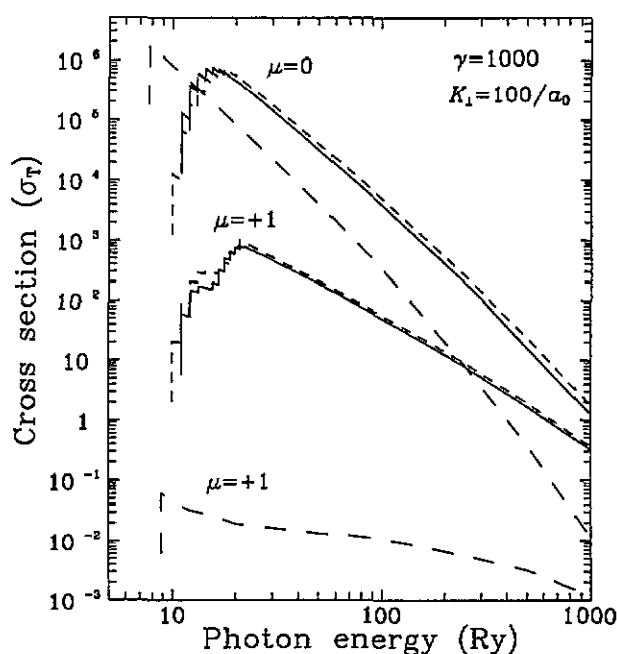


Figure 3. The same as in figure 2 for $K_{\perp} = 100/a_0$.

5. Conclusion

We have considered the family of Hamiltonians (13) for a two-body system moving in a magnetic field, parametrized by the variable η which determines the position of the Coulomb centre in the relative motion coordinate frame. Corresponding eigenfunctions describe internal motion in the system in terms of the shifted relative coordinate $\mathbf{r} = \mathbf{r}_- - \mathbf{r}_+ - \eta \mathbf{r}_0$, and can be expanded over the basis of the Landau states, associated with free relative motion of the particles across the magnetic field. In this case matrix elements for the radiative transitions between differently shifted eigenstates involve 'transverse' parts which are explicitly calculated on the basis of the creation/annihilation operator technique.

For a moving hydrogen atom, the exact ground-state wavefunction exhibits only a small decentering in strong magnetic fields, when the transverse generalized momentum value $\hbar K_{\perp}$ is below some critical one $\hbar K_c$ (Ipatova *et al* 1984, Vincke *et al* 1992). In this case, the non-shifted ($\eta = 0$) adiabatic approximation should be valid. As for the continuum, the full-shifted ($\eta' = 1$) representation should be applied in order to make the Hamiltonian (13) axially symmetric at large z . Therefore, the analytical results obtained for the radiative transition matrix elements enable one to extend the range of the adiabatic approach. This conclusion is illustrated by a good agreement of the adiabatic photoionization cross sections with those calculated with the aid of more precise (non-adiabatic) wavefunctions.

Acknowledgments

We are grateful to G G Pavlov, D G Yakovlev and Y A Shibanov for useful discussions and interest about this work. Our investigations were partly supported by the ESO C and EE programme, grant no A-01-068.

Appendix A. Interaction with radiation

The differential cross section for the radiative transition $|K, i\rangle \rightarrow |K', f\rangle$ caused by the absorption of a photon with frequency ω , wave vector q and polarization unit vector e is determined by the expression

$$d\sigma_{K',f;K,i}(\omega, q) = \frac{4\pi^2 e^2}{c\omega} |e M_{K',f;K,i}(q)|^2 \delta(E' - E - \hbar\omega) \frac{dK'}{(2\pi)^3} d\rho_f \quad (A1)$$

where E and E' are the energies of the initial and final states, respectively, $d\rho_f$ is the density of final states associated with the set of quantum numbers $|f\rangle$,

$$M_{K',f;K,i}(q) = \langle \psi_{K',f}(\mathbf{r}_-, \mathbf{r}_+) | \hat{M}(q) | \psi_{K,i}(\mathbf{r}_-, \mathbf{r}_+) \rangle \quad (A2)$$

is the matrix element of the operator

$$\hat{M}(q) = \frac{\exp(iq\mathbf{r}_-)}{m_-} \left(\hat{p}_- + \frac{e}{2c} \mathbf{B} \times \mathbf{r}_- + \frac{\hbar q}{2} \right) - \frac{\exp(iq\mathbf{r}_+)}{m_+} \left(\hat{p}_+ - \frac{e}{2c} \mathbf{B} \times \mathbf{r}_+ + \frac{\hbar q}{2} \right) \quad (A3)$$

where $\hat{p}_\mp = -i\hbar\partial/\partial\mathbf{r}_\mp$. After introducing the centre-of-mass and relative coordinates and using the form (2) for the eigenfunctions, the integration over \mathbf{R} in (A2) gives the conservation of the generalized momentum

$$M_{K',f;K,i}(q) = (2\pi)^3 L_{f,i}^K(q) \delta(K' - K - q). \quad (A4)$$

Here the matrix element

$$L_{f,i}^K(q) = \langle \psi_{K',f}^{(0)}(\mathbf{r}) | \hat{L}_{(v)}^{(0,0)}(q) | \psi_{K,i}^{(0)}(\mathbf{r}) \rangle \quad (A5)$$

is calculated with the wavefunctions of the relative motion, $K' = K + q$, and

$$\hat{L}_{(v)}^{(0,0)}(q) = \exp\left(i\frac{m_+}{M}q\mathbf{r}\right) \hat{F}_-^{(0)} + \exp\left(-i\frac{m_-}{M}q\mathbf{r}\right) \hat{F}_+^{(0)} \quad (A6)$$

where

$$\hat{F}_\mp^{(0)} = \frac{1}{m_\mp} \left(\hat{p} \pm \frac{e}{2c} \mathbf{B} \times \mathbf{r} \right) \pm \frac{\hbar K}{M} \pm \frac{\hbar q}{2m_\mp}. \quad (A7)$$

The term in parentheses in (A7) gives the momentum operators in the presence of the magnetic field,

$$\hat{\pi} = \hat{p} + \frac{e}{2c} \mathbf{B} \times \mathbf{r} \quad \text{and} \quad \hat{\Pi} = \hat{p} - \frac{e}{2c} \mathbf{B} \times \mathbf{r} \quad (A8)$$

corresponding to negatively and positively charged particles, respectively. Using equation (A4), one can perform summation in (A1) over all the final values of K' and obtain

$$d\sigma_{K,f;i}(\omega, q) = \frac{4\pi^2 e^2}{c\omega} |e L_{f,i}^K(q)|^2 \delta(E' - E - \hbar\omega) d\rho_f. \quad (A9)$$

Equation (A6) represents the *velocity form* of the matrix element $L_{f,i}^K(q)$, which is produced by the operator $\hat{L}_{(v)}^{(0,0)}(q)$. Alternative is the *length form*, which can be obtained on the basis of the relations

$$\begin{aligned} [\hat{H}_K^{(0)}, \mathbf{r}] &= -i\hbar \left(\frac{\hat{\pi}}{m_-} + \frac{\hat{\Pi}}{m_+} \right) \\ [\hat{H}_K^{(0)}, \exp(i\lambda q\mathbf{r})] &= \lambda \hbar q \exp(i\lambda q\mathbf{r}) \left\{ \frac{\hat{p}}{\mu} + \lambda \frac{\hbar q}{2\mu} + \frac{e\mathbf{x}}{c\mu} \mathbf{B} \times \mathbf{r} \right\} \\ \hat{H}_K^{(0)} &= \hat{H}_{K'}^{(0)} - \frac{\hbar q}{M} \left(\hbar K + \frac{\hbar q}{2} + \frac{e}{c} \mathbf{B} \times \mathbf{r} \right) \end{aligned} \quad (A10)$$

and is determined by (A5) with the operator

$$\begin{aligned} \hat{L}_{(0)}^{(0,0)}(\mathbf{q}) = & \exp\left(i\frac{m_+}{M}\mathbf{q}\mathbf{r}\right) \left\{ i\frac{m_+}{M} \left[\omega_{f,i} - \mathbf{q}\hat{F}_-^{(0)} \right] \mathbf{r} + \hat{G}_-^{(0)} \right\} \\ & + \exp\left(-i\frac{m_-}{M}\mathbf{q}\mathbf{r}\right) \left\{ i\frac{m_-}{M} \left[\omega_{f,i} + \mathbf{q}\hat{F}_+^{(0)} \right] \mathbf{r} + \hat{G}_+^{(0)} \right\} \end{aligned} \quad (\text{A11})$$

where

$$\hat{G}_{\mp}^{(0)} = \mp \left[\frac{e}{Mc} \mathbf{B} \times \mathbf{r} + \frac{\hbar \mathbf{K}}{M} + \frac{\hbar \mathbf{q}}{2m_{\mp}} \right] \quad (\text{A12})$$

and $\omega_{f,i} = (E' - E)/\hbar$ is the frequency of the transition. Velocity (A6) and length (A11) forms correspond to (A4) and (A7), respectively, of Potekhin and Pavlov (1993), for the matrix elements

$$D = (i\omega)^{-1} L_{f,i}^K(\mathbf{q}) \quad (\text{A13})$$

at the transverse polarization of radiation, when $e\mathbf{q} = 0$.

For applications it may be convenient to describe the relative motion by the eigenfunctions of the Hamiltonian (13), in general case the values of η and η' being different for the initial and final states, respectively. The expressions for the matrix element $L_{f,i}^K(\mathbf{q})$ and two alternative forms of corresponding operator can be obtained from (A5), (A6) and (A11), if we perform the shift transformations (11) and change the variable of the integration in (A5). This gives

$$L_{f,i}^K(\mathbf{q}) = \langle \psi_{K',f}^{(\eta')}(\mathbf{r} + \mathbf{r}_*) | \hat{L}_{(v,i)}^{(\eta',\eta)}(\mathbf{q}) | \psi_{K,i}^{(\eta)}(\mathbf{r}) \rangle \quad (\text{A14})$$

where $\mathbf{r}_* = (\eta - \eta')\mathbf{r}_0$,

$$\hat{L}_{(v)}^{(\eta',\eta)}(\mathbf{q}) = \exp(i\varphi_-^{(\eta',\eta)}) \hat{F}_-^{(\eta)} + \exp(i\varphi_+^{(\eta',\eta)}) \hat{F}_+^{(\eta)} \quad (\text{A15})$$

for the velocity representation, and

$$\begin{aligned} \hat{L}_{(0)}^{(\eta',\eta)}(\mathbf{q}) = & \exp(i\varphi_-^{(\eta',\eta)}) \left\{ i\frac{m_+}{M} \left[\omega_{f,i} - \mathbf{q}\hat{F}_-^{(\eta)} \right] (\mathbf{r} + \eta\mathbf{r}_0) + \hat{G}_-^{(\eta)} \right\} \\ & + \exp(i\varphi_+^{(\eta',\eta)}) \left\{ i\frac{m_-}{M} \left[\omega_{f,i} + \mathbf{q}\hat{F}_+^{(\eta)} \right] (\mathbf{r} + \eta\mathbf{r}_0) + \hat{G}_+^{(\eta)} \right\} \end{aligned} \quad (\text{A16})$$

for the length representation. Here

$$\begin{aligned} \varphi_{\mp}^{(\eta',\eta)} = & \left[\alpha(\eta - \eta')K_{\perp} \pm \left((1 - \eta')\frac{m_{\pm}}{M} + \frac{\eta'}{2} \right) q_{\perp} \right] (\mathbf{r}_{\perp} + \eta\mathbf{r}_0) \pm \frac{m_{\pm}}{M} q_z z \\ \hat{F}_{\mp}^{(\eta)} = & \frac{1}{m_{\mp}} \left(\hat{\mathbf{p}} \pm \frac{e}{2c} \mathbf{B} \times \mathbf{r} \right) \pm (1 - \eta) \frac{\hbar \mathbf{K}_{\perp}}{M} \pm \frac{\hbar \mathbf{K}_z}{M} \pm \frac{\hbar \mathbf{q}}{2m_{\mp}} \\ \hat{G}_{\mp}^{(\eta)} = & \mp \left[\frac{e}{Mc} \mathbf{B} \times \mathbf{r} + (1 - \eta) \frac{\hbar \mathbf{K}_{\perp}}{M} + \frac{\hbar \mathbf{K}_z}{M} + \frac{\hbar \mathbf{q}}{2m_{\mp}} \right]. \end{aligned} \quad (\text{A17})$$

Equations (A15)–(A17) are simplified in the case $\eta' = \eta = 1$, when

$$\begin{aligned} \varphi_{\mp}^{(1,1)} = & \pm \frac{1}{2} q_{\perp} (\mathbf{r}_{\perp} + \mathbf{r}_0) \pm \frac{m_{\pm}}{M} q_z z \\ \hat{F}_{\mp}^{(1)} = & \frac{1}{m_{\mp}} \left(\hat{\mathbf{p}} \pm \frac{e}{2c} \mathbf{B} \times \mathbf{r} \right) \pm \frac{\hbar \mathbf{K}_z}{M} \pm \frac{\hbar \mathbf{q}}{2m_{\mp}} \\ \hat{G}_{\mp}^{(1)} = & \mp \left[\frac{e}{Mc} \mathbf{B} \times \mathbf{r} + \frac{\hbar \mathbf{K}_z}{M} + \frac{\hbar \mathbf{q}}{2m_{\mp}} \right] \end{aligned} \quad (\text{A18})$$

and for the *dipole approximation* ($q = 0$)

$$\hat{L}_{(v)}^{(\eta', \eta)}(0) = \exp \{ i \alpha (\eta - \eta') K_{\perp} r_{\perp} \} \left(\frac{\hat{\pi}}{m_{-}} + \frac{\hat{\Pi}}{m_{+}} \right) \quad (\text{A19})$$

$$\hat{L}_{(v)}^{(\eta', \eta)}(0) = i \omega_{f,i} \exp \{ i \alpha (\eta - \eta') K_{\perp} r_{\perp} \} (r + \eta r_0).$$

The exponent in (A19) corresponds to the transformation (11) between the wavefunctions $\psi_{K,f}^{*(\eta')}(r + r_*)$ and $\psi_{K,f}^{*(\eta)}(r)$ or between the wavefunctions $\psi_{K,i}^{(\eta)}(r)$ and $\psi_{K,i}^{(\eta')}(r + r_*)$, respectively. Thus the length form of the dipole matrix element can be written, for example, as

$$L_{f,i}^K(q) = \langle \psi_{K,f}^{(\eta)}(r) | r + \eta r_0 | \psi_{K,i}^{(\eta')}(r) \rangle. \quad (\text{A20})$$

Since here the final and initial wavefunctions relate to the same Hamiltonian (13) but correspond to the different energies, $E' \neq E$, they are orthogonal, and the term ηr_0 does not contribute. Therefore this term may be omitted in the expression for the corresponding operator and one may set

$$\hat{L}_{(v)}^{(\eta', \eta)}(0) = i \omega_{f,i} \exp \{ i \alpha (\eta - \eta') K_{\perp} r_{\perp} \} r. \quad (\text{A21})$$

Appendix B. Transverse matrix element

Let us consider the matrix element

$$I_{n', N', n, N} = \langle n', N' | \exp(\alpha \hat{a} - \alpha^* \hat{a}^+ + \beta \hat{A} - \beta^* \hat{A}^+) | n, N \rangle. \quad (\text{B1})$$

Since the creation and annihilation operators, which change the Landau level numbers for different particles, commute, one may write

$$I_{n', N', n, N} = \langle n', N' | \exp(\alpha \hat{a} - \alpha^* \hat{a}^+) \exp(\beta \hat{A} - \beta^* \hat{A}^+) | n, N \rangle. \quad (\text{B2})$$

Using the relation

$$\exp(\hat{A} + \hat{B}) = \exp(\hat{A}) \exp(\hat{B}) \exp\left(-\frac{1}{2}[\hat{A}, \hat{B}]\right) \quad (\text{B3})$$

and the commutation rules (23), it is possible to reduce (B2) to the form with four separated exponents

$$I_{n', N', n, N} = \exp\left(-\frac{1}{2}|\alpha|^2\right) \exp\left(-\frac{1}{2}|\beta|^2\right) \times \langle n', N' | \exp(-\alpha^* \hat{a}^+) \exp(\alpha \hat{a}) \exp(-\beta^* \hat{A}^+) \exp(\beta \hat{A}) | n, N \rangle. \quad (\text{B4})$$

Now each exponent can be expanded over the powers of the operators. Taking into account that

$$\hat{a}^k |n, N\rangle = \begin{cases} \sqrt{\frac{n!}{(n-k)!}} |n-k, N\rangle & k \leq n \\ 0 & k > n \end{cases} \quad (\text{B5})$$

that $(\hat{a}^+)^k$ operates from the right-hand side the state $\langle n', N' |$ in the same way, and that the operators \hat{A}^k and $(\hat{A}^+)^k$ have analogous properties, one reduces (B4) to the sum of the scalar products $\langle n' - k', N' - l' | n - k, N - l \rangle$, which are equal to $\delta_{n'-k', n-k} \delta_{N'-l', N-l}$ due to the normalization property of the transverse basis. This gives

$$I_{n', N', n, N} = I_{n', n}(\alpha, \alpha^*) I_{N', N}(\beta, \beta^*) \quad (\text{B6})$$

where

$$I_{n',n}(\alpha, \alpha^*) = \exp\left(-\frac{1}{2}|\alpha|^2\right) \sum_{k'=0}^{n'} \sum_{k=0}^n \frac{(-\alpha^*)^{k'} (\alpha)^k}{k'! k!} \sqrt{\frac{n'! n!}{(n'-k')! (n-k)!}} \delta_{n'-k', n-k} \quad (\text{B7})$$

and $I_{N',N}(\beta, \beta^*)$ is determined by the same equation. Now it is possible to perform the summation over k' (at $n' > n$) or over k (at $n' < n$) in (B7). The remaining sum in the first case reduces to the Laguerre polynomial

$$L_n^{n'-n}(|\alpha|^2) = \sum_{k=0}^n \frac{n! (-|\alpha|^2)^k}{(n'-n+k)! (n-k)! k!} \quad (\text{B8})$$

while in the second case it reduces to the Laguerre polynomial $L_{n'}^{n-n'}(|\alpha|^2)$.

Finally, independently of a relation between the Landau numbers, one obtains

$$I_{n',N',n,N} = \left(\frac{\alpha^*}{\alpha}\right)^{(n'-n)/2} \left(\frac{\beta^*}{\beta}\right)^{(N'-N)/2} F_{n',n}(|\alpha|^2) F_{N',N}(|\beta|^2) \quad (\text{B9})$$

where the functions $F_{n',n}$ and $F_{N',N}$ are determined by (7). Thus, in spite of the fact that Landau basis (6) is connected with the eigenstates of the relative motion of the particles, result (B9) for matrix element (B1) has the factorized form, which is natural for the non-interactive particles.

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