Consistent analytical approach for the quasi-classical radial dipole matrix elements

B Kaulakys†

Institute of Theoretical Physics and Astronomy, A Goštauto 12, 2600 Vilnius, Lithuania

Abstract. A consistent analytical approach for calculation of the quasi-classical radial dipole matrix elements in the momentum and coordinate representations is presented. Very simple but relatively precise expressions for the matrix elements are derived in both representations. All analytical expressions contain only one special function—the Anger function and its derivative. They generalize and increase the accuracy of some known quasi-classical expressions. The small difference between the two forms of the expressions for the dipole matrix elements indicates the applicability of the simple expressions given by the consistent quasi-classical approach even for low atomic states.

1. Introduction

Calculation of transition probabilities, oscillator strengths and dipole matrix elements for atomic transitions is stimulated by investigations in spectroscopy, plasma physics, chaotic dynamics of non-linear systems and other fundamental and applied fields. Accurate calculation of these atomic characteristics are very time consuming and in some cases involve certain difficulties, especially for transitions between high states. Therefore, recent attention has been paid to quasi-classical calculations of the dipole matrix elements and oscillator strengths for atomic $nl \rightarrow n'l'$ transitions (Heim *et al* 1989, Delone *et al* 1989, 1994, Kaulakys 1991, D'yachkov and Pankratov 1991, 1994, Pankratov and Meyer-ter Vehn 1992, Nana *et al* 1995). In the review paper by Delone *et al* (1994) the set of analytical formulae for the dipole matrix elements between quasi-classical states is presented. However, this review paper does not reflect the results from the last five-year period by Heim *et al* (1989), Kaulakys (1991), D'yachkov and Pankratov (1991, 1994) Pankratov and Meyer-ter Vehn (1992) and others, and contains some inconsistencies. As a result, the main formulae of the paper contain terms with erroneous sign and do not agree with the exact results, e.g. when $s = \nu' - \nu$ is an integer number and when $s \rightarrow 0$ with ν and ν' being the effective principal quantum numbers of the initial and final states, respectively.

Here, a consistent analytical approach for the quasi-classical dipole coupling of the electron with the electromagnetic field is presented, taking into account a peculiarity of the radial quasi-classical matrix elements: radial wavefunctions of the initial and final states for transitions with $\Delta l \neq 0$ correspond to different effective Hamiltonians and, therefore, we cannot use the usual correspondence between the quasi-classical matrix elements and the Fourier components of the appropriate classical variable (see e.g. Landau and Lifshitz

† E-mail: kaulakys@itpa.fi.lt

1985). So, we should start from the definition of the quantum matrix elements using the quasi-classical radial wavefunctions.

The direct way of coupling a radiation field to the electron Hamiltonian is through the $A \cdot p$ interaction (see, e.g. Bethe and Salpeter 1957, Landau and Lifshitz 1985) where A is the vector potential of the electromagnetic field and $p = -i\hbar\nabla$ is the momentum operator. When the radiation wavelength is long compared with the atomic dimension, as is the case for optical or microwave transitions, the variation of the vector potential within the atom can be neglected. In this case the electric field is also uniform over the extent of the atom. So the electric dipole moment is the only atomic multipole coupled to the field in the multipolar approximation to the interaction operator and the interaction of the electron with the field may also be expressed through the $E \cdot r$ term, where E is the electric field strength and r is the electron's coordinate. As a matter of fact, the two forms of the interaction Hamiltonian in the dipole approximation are equivalent due to the gauge invariance of the field.

Usually one calculates the radial dipole matrix elements in the coordinate form (see Heim *et al* 1989, Delone *et al* 1989, 1994, Kaulakys 1991, D'yachkov and Pankratov 1991, 1994, Pankratov and Meyer-ter Vehn 1992, Nana *et al* 1995 and references therein). For precise wavefunctions of the $|a\rangle$ and $|b\rangle$ states the relation between the matrix elements of p and r operators

$$p_{a,b} = -im\omega_{b,a}r_{a,b} \tag{1}$$

holds. Here m and $\omega_{b,a} = (E_b - E_a)/\hbar$ are the electron mass and the angular frequency of the corresponding transition, respectively. However, when one uses approximate wavefunctions in the evaluation of the matrix elements, the length and velocity forms in general yield different results and the relationship (1) holds only roughly or even fails (see, e.g., Crossley 1969). If asymptotically correct wavefunctions are used, the r-form of the dipole matrix elements is preferable as it stresses the contributions to the integral from the large r region. On the other hand, for wavefunctions correct at small and medium r the velocity form should be used as it puts more weight on the integral at small and medium r. The quasi-classical wavefunctions in the classically allowed region of motion are not correct asymptotically as well as for very small r but are relatively accurate for the medium r between the two turning points of the classical orbit. Therefore, it is likely that the velocity form of the quasi-classical matrix elements is as much (or, maybe, even more) accurate as the length form.

2. Radial dipole matrix elements for any spherical potential

Calculation of the angular part of the matrix elements is a simple problem and, therefore, we restrict ourselves to the radial part. The radial dipole matrix element in the momentum representation is given by†

$$D_{nl}^{n'l\pm1} = \frac{1}{\omega} \int P_{nl}(r) \left(\frac{dP_{n'l\pm1}(r)}{dr} \pm l_{\max} \frac{P_{n'l\pm1}(r)}{r} \right) dr \tag{2}$$

where $P_{nl}(r) = rR_{nl}(r)$ is the solution of the radial Schrödinger equation, $\omega = E_{n'l'} - E_{nl}$ is the transition frequency and $l_{\max} = \max(l, l\pm1)$. The quasi-classical radial wavefunction P_{nl} can be expressed as

$$P_{nl} = \frac{2}{\sqrt{T v_r(r)}} \cos \Phi_{nl}(r) \tag{3}$$

† Further in the paper we will use the atomic units, $\hbar = m = e = 1$.

in the classically allowed region of motion and some exponentially decreasing function outside this region. Here, T is the period of classical rotation, the radial velocity of the electron, v_r, is given by

$$v_r(r) = \left(2E_{nl} - 2U(r) - \frac{(l+\frac{1}{2})^2}{r^2}\right)^{1/2} \tag{4}$$

and the phase Φ_{nl} is defined as

$$\Phi_{nl}(r) = \int_{r_1}^{r} v_r(r) \, dr - \tfrac{1}{4}\pi \tag{5}$$

with $U(r)$ being the effective potential which defines the motion of the Rydberg electron and the roots of the radial velocity $v_r(r)$, r_1 and r_2, are the two classical turning points given by $v_r(r_1) = v(r_2) = 0$.

Further calculations of the matrix elements (2) are similar to those by Heim *et al* (1989) and Kaulakys (1991). Substituting equation (3) into equation (2) and neglecting the rapidly oscillating sine and cosine of the sum of the phases Φ_{nl} and $\Phi_{n'l'}$ one finally finds that

$$D_{nl}^{n'l\pm1} = \frac{2}{\omega\sqrt{TT'}} \int_0^{T_c/2} (-\dot{r}\sin\Delta\Phi(t) \pm r\dot{\varphi}\cos\Delta\Phi(t)) \, dt$$

$$= \frac{2}{\omega\sqrt{TT'}} \int_0^{T_c/2} [-\dot{x}\sin\omega t \pm \dot{y}\cos\omega t] \, dt \tag{6}$$

where φ is the polar angle while x and y are Cartesian coordinates of the electron, dots denote the derivatives with respect to time and T_c is some mean period to be defined later. In the derivation of equation (6) we have used the fact that $r^{-1}l_{\max} = r^{-1}\overline{(l+\frac{1}{2})} = r^{-1}(l+l'+1)/2 = r^{-1}(r^2\dot{\varphi}) = r\dot{\varphi}$ and that, according to equations (4) and (5), linear expansion of the difference of the phases in powers of ω and $\Delta l = l' - l$ is

$$\Delta\Phi \equiv \Phi_{n'l'} - \Phi_{nl} \simeq \omega t - \Delta l\varphi + \cdots \tag{7}$$

Integration of equation (6) by parts yields to the r-form of the radial dipole matrix element

$$R_{nl}^{n'l\pm1} \equiv \langle nl \, | r \, | n'l \pm 1 \rangle = \frac{2}{\sqrt{TT'}} \int_0^{T_c/2} r(t) \cos\Delta\Phi(t) \, dt$$

$$= \frac{2}{\sqrt{TT'}} \int_0^{T_c/2} [x(t)\cos\omega t \pm y(t)\sin\omega t] \, dt. \tag{8}$$

Here we have used the quasi-classical quantization conditions (see Kaulakys 1991 for details) and facts, such that

$$\Delta\Phi(0) \simeq 0 \qquad \Delta\Phi(T_c/2) = \Delta n_r\pi \qquad \omega T_c/2 = \Delta n\pi$$

$$r(0) = x(0) = r_1 \qquad y(0) = y(T_c/2) = 0 \qquad \varphi(0) = 0 \qquad \varphi(T_c/2) = \pi \tag{9}$$

where $n_r = n - l - 1$ is the radial quantum number and Δn and Δn_r are integers. Note, that equation (8) may also be derived from the definition of the radial dipole matrix element in the coordinate representation and using expression (3) for the quasi-classical radial wavefunction (see Kaulakys 1991).

It follows from equations (6)–(8) that only for $\Delta l = 0$ the quasi-classical matrix elements of the module of the radius vector, r, coincide with the Fourier components of the classical variable $r(t)$ and may be expressed through the Fourier components of the classical variable $\dot{r}(t)$, i.e.

$$\langle nl \,|\, r \,|\, n'l \rangle = \frac{2}{\sqrt{TT'}} \int_0^{T_c/2} r(t) \cos \omega t \, dt = \frac{1}{\sqrt{TT'}} \oint r(t) e^{-i\omega t} \, dt$$

$$= -\frac{2}{\omega\sqrt{TT'}} \int_0^{T_c/2} \dot{r}(t) \sin \omega t \, dt = \frac{-i}{\omega\sqrt{TT'}} \oint \dot{r}(t) e^{-i\omega t} \, dt. \tag{10}$$

For the dipole transitions with $\Delta l = \pm 1$ the radial wavefunctions P_{nl} and $P_{n'l'}$ of the initial and final states are solutions of the radial Schrödinger equation with different effective potentials $V_{eff}(r) = U(r) + (l + \frac{1}{2})^2/2r^2$ and $V'_{eff}(r) = U(r) + (l' + \frac{1}{2})^2/2r^2$, respectively. This results in the additional term in the phase difference (7) and the second term in equations (6) and (8).

Note, that the radial dipole matrix elements $D_{nl}^{n'l\pm 1}$ and $R_{nl}^{n'l\pm 1}$ according to equations (6) and (8) may also be expressed as

$$D_{nl}^{n'l\pm 1} = \frac{-i}{\omega\sqrt{TT'}} \oint (\dot{x}(t) \pm \dot{y}(t)) \, e^{-i\omega t} \, dt \tag{11}$$

and

$$R_{nl}^{n'l\pm 1} = \frac{1}{\sqrt{TT'}} \oint (x(t) \pm y(t)) \, e^{-i\omega t} \, dt. \tag{12}$$

It is of interest to note the connection between the expressions for the dipole matrix elements (6)–(10) and the energy change of the classical atom in a monochromatic field (see Gontis and Kaulakys 1987, Kaulakys 1991). The mapping equations of motion for the classical hydrogen atom in an oscillating electric field derived on the basis of the velocity form of interaction are suitable for investigation of the transition to chaotic behaviour and ionization of Rydberg atoms even in the low frequency field when the strength of the external field is comparable with the Coulomb field of the atom (Kaulakys and Vilutis 1995).

Until now we did not use the explicit form of the potential $U(r)$. Therefore, equations (1)–(12) are valid for any spherical potential. Further we will apply this theory for non-hydrogenic atoms.

3. The non-hydrogenic atom

The potential $U(r)$ which defines the motion of the Rydberg electron of a non-hydrogenic atom or ion may be expressed as a sum of two terms—the Coulomb potential $-Z/r$ of the ion core with charge $Z = Z_{ion} + 1$ and the perturbation potential $\Delta U(r)$ due to the deviation from the Coulomb approximation, i.e.

$$U(r) = -Z/r + \Delta U(r). \tag{13}$$

For the non-hydrogenic atom, the perturbation potential $\Delta U(r)$ is short-range and results in the non-Coulomb scattering phase, δ_l, related to the quantum defect, μ_l, by the relationship $\delta_l = \pi \mu_l$. The energy, E_{nl}, of the $|\,nl\rangle$ state is related to the effective principal quantum number, ν, and the quantum defect, μ_l, in the usual way .

$$E_{nl} = Z^2/2\nu^2 \qquad \nu = n - \mu_l. \tag{14}$$

Significant contributions to the integrals (6) and (8) arise from the regions with relatively large r where the potential $U(r)$ is well represented by the Coulomb potential $V(r) = -Z/r$. The additional potential $\Delta U(r)$ results mainly from the non-Coulomb scattering phaseshift, δ_l (see Kaulakys 1991). Thus, the phase (5) and the phase difference (7) in the region of the main contribution to the dipole matrix element may be represented as

$$\Phi_{nl}(r) = \int_{r_1^c}^{r} v_r^c(r)\,dr + \delta_l - \tfrac{1}{4}\pi \tag{15}$$

and

$$\Delta\Phi \simeq \omega t - \Delta l\varphi \simeq \Delta + \omega t_c - \Delta l\varphi_c \tag{16}$$

where v_r^c is the radial velocity for the Coulomb potential, $\Delta = \delta_{l'} - \delta_l$ and it is convenient to introduce the parametric equations of motion for the Coulomb potential

$$
\begin{aligned}
r &= \left(v_c^2/Z\right)(1 - e\cos\xi) & t_c &= \left(v_c^3/Z^2\right)(\xi - e\sin\xi) \\
x &= \left(v_c^2/Z\right)(\cos\xi - e) & y &= \left(v_c^2/Z\right)\left(1 - e^2\right)^{1/2}\sin\xi \\
\varphi_c &= \arccos\left(\frac{\cos\xi - e}{1 - e\cos\xi}\right) & e &= \left(1 - \left(\frac{l + l' + 1}{2v_c}\right)^2\right)^{1/2}.
\end{aligned}
\tag{17}
$$

Here, e denotes the eccentricity of the classical orbit with the period $T_c = 2\pi v_c^3/Z^2$ and the turning points $r_{1,2}^c = \left(v_c^2/Z\right)(1 \mp e)$. The centred effective principal quantum number v_c is defined from the requirement that the phase difference (16) at the turning point r_2 has to be consistent with the quasi-classical quantization conditions, i.e.

$$\Delta\Phi\left(r_2^c\right) = \Delta + \tfrac{1}{2}\omega T_c - \Delta l\pi = \Delta n_r\pi . \tag{18}$$

which, together with the relationship $\Delta n_r\pi = \Delta v\pi + \Delta - \Delta l\pi$, results in the expression (see also D'yachkov and Pankratov 1991, 1994)

$$v_c^3 = \frac{Z^2\Delta v}{\omega} = \frac{2\left(vv'\right)^2}{v + v'}. \tag{19}$$

More precisely, the non-Coulomb phase shifts, δ_l and $\delta_{l'}$, and, consequently the phase difference, $\Delta = \delta_{l'} - \delta_l$, are some functions of r and time, t (see Kaulakys 1991). However, for non-hydrogenic atoms, the phase difference $\Delta(r)$ increases in the region $r \simeq r_1 \simeq r_1^c$ from $\Delta = 0$ to $\Delta = \delta_{l'} - \delta_l =$const in the very narrow interval of the coordinate r, while the main contributions to the radial integrals (6) and (8) occur at large distances, $r \sim v^2$. Thus, in equations (6) and (8) the phase ωt may be replaced by the expression $\Delta + \omega t_c$, while $\varphi \simeq \varphi_c$. Keeping this in mind and substituting equations (16)–(19) into equations (6) and (8) we have

$$D_{nl}^{n'l\pm1} = (-1)^{\Delta n}\frac{v_c^5}{Z\left(vv'\right)^{3/2}}D_p^{\pm}(e,s) \tag{20}$$

$$D_p^{\pm} = \frac{1}{s}\left(J'_{-s}(es) \pm \sqrt{e^{-2} - 1}\left(J_{-s}(es) - \frac{\sin\pi s}{\pi s}\right)\right) \tag{21}$$

$$R_{nl}^{n'l\pm1} = (-1)^{\Delta n}\frac{v_c^5}{Z\left(vv'\right)^{3/2}}D_r^{\pm}(e,s) \tag{22}$$

$$D_r^{\pm} = D_p^{\pm} + \frac{1 - e}{\pi s}\sin\pi s \qquad s = \Delta v = v' - v. \tag{23}$$

Here, $J_{-s}(z)$ and $J'_{-s}(z)$ are the Anger function defined as

$$J_{-s}(z) = \frac{1}{\pi} \int_0^\pi \cos(s\xi + z\sin\xi)\,d\xi \tag{24}$$

and its derivative with respect to the argument z, respectively. Note the properties of the Anger function: $J_{-s}(z) = J_s(-z)$ and $J'_{-s}(z) = -J'_s(-z)$ which result in the symmetry of the matrix elements (21) and (23)

$$D^\pm(e, -s) = D^\mp(e, s). \tag{23'}$$

To the best of our knowledge, equations (20) and (21) are derived for the first time, while equations (22) and (23) within the accuracy of factor $(v_c/\sqrt{vv'})^5$ coincide with equation (16) in the paper by Kaulakys (1991) and are close to the corresponding expressions given by D'yachkov and Pankratov (1991) and by Pankratov and Meyer-ter-Vehn (1992) (see also Nana *et al* 1995). Note, that for the first time the dipole matrix elements in the coordinate representation have been expressed *through the Anger function and its derivative* (however, with some erroneous signs) by Davydkin and Zon (1981).

In the derivation of equations (22) and (23) one integrates equation (8) by parts using the approximate expression $\omega t \simeq \Delta + \omega t_c$. This yields equation (6) with the additional term

$$R_{nl}^{n'l\pm1} - D_{nl}^{n'l\pm1} = -\frac{2r_j^c}{\omega\sqrt{TT'}}\sin\Delta = (-1)^{\Delta n}\frac{v_c^5(1-e)\sin\pi s}{Z(vv')^{3/2}\pi s}. \tag{25}$$

Thus, the difference between the quasi-classical dipole matrix elements in the r- and p-forms, the second term in equation (23), results from the replacement of the electron's motion in the *effective potential $U(r)$ by the motion in the Coulomb potential with the additional phase δ_l.* Therefore, the quasi-classical radial dipole matrix element in the coordinate representation (22)–(23) may contain some additional inaccuracy. On the other hand, the difference (25) between two forms of the dipole matrix elements may be a criterion of the exactness of the quasi-classical approximation. As a rule, the additional term (25) is small because of the small factor $(1-e)$ for states with low l and of the small factor, $\sin\pi s$, for states with larger l but small quantum defects and, consequently, with $s = \Delta v \simeq \Delta n$ close to the integer. In expansion of the dipole matrix elements in terms of $\alpha = \sqrt{1-e^2} = (l+l'+1)/2v_c$ (see Kaulakys 1991 for analogy)

$$D_p^\pm = \frac{1}{s}\left(J'_{-s}(s) \pm \alpha\left(J_{-s}(s) - \frac{\sin\pi s}{\pi s}\right) + \frac{\alpha^2}{2}\left(J'_{-s}(s) + \frac{2\sin\pi s}{\pi s}\right)\right) \tag{26}$$

$$D_r^\pm = D_p^\pm + \frac{\alpha^2}{2}\frac{\sin\pi s}{\pi s} \tag{27}$$

this additional term makes up less than half of the third, proportional to α^2, expansion term. This points to the relatively high (up to several per cent) accuracy of the very simple quasi-classical approximation (20)–(23) for the dipole matrix elements even for the low atomic states. The extensive analysis of such an approach and comparison with the numerical Hartree–Fock calculations will be presented elsewhere. Here we will present only the limiting forms of the dipole matrix elements.

4. Special cases of the parameters

Using the expansions of the functions $J_{-s}(es)$ and $J'_{-s}(es)$ in powers of s (Kaulakys 1991)

$$J_{-s}(es) \simeq 1 - \left(\tfrac{1}{6}\pi^2 + e + \tfrac{1}{4}e^2\right)s^2$$

$$J'_{-s}(es) \simeq -\left(1 + \tfrac{1}{2}e\right)s, s \ll 1 \tag{28}$$

we have from equations (20)–(23)

$$D_{nl}^{n'l\pm1} = (-1)^{\Delta n+1} \frac{v^2}{Z}\left(1 + \tfrac{1}{2}e\right) \tag{29}$$

$$R_{nl}^{n'l\pm1} = (-1)^{\Delta n+1} \frac{3}{2}\frac{v^2}{Z}e \qquad s \ll 1. \tag{30}$$

For hydrogenic atoms with $n' = n$, equation (30) results in the exact expression

$$R_{nl}^{n'l\pm1} = -\frac{3}{2}\frac{n^2}{Z}e. \tag{31}$$

Substitution of the asymptotic, $s \gg 1$, forms of functions $J_{-s}(s)$ and $J'_{-s}(s)$ (Kaulakys 1991)

$$J_{-s}(s) = \frac{2a}{\sqrt{3}s^{1/3}}\cos\left(\pi s - \tfrac{1}{6}\pi\right) \qquad a \simeq 0.447$$

$$J'_{-s}(s) = \frac{2b}{\sqrt{3}s^{2/3}}\cos\left(\pi s + \tfrac{1}{6}\pi\right) \qquad b \simeq 0.411 \tag{32}$$

into equations (26) and (27) yields

$$D_{p,r}^{\pm} \simeq \frac{2b}{\sqrt{3}s^{5/3}}\cos\left(\pi s + \tfrac{1}{6}\pi\right) \pm \frac{2\alpha a}{\sqrt{3}s^{4/3}}\cos\left(\pi s - \tfrac{1}{6}\pi\right). \tag{33}$$

From equation (33), the Bethe rule can be seen: principal and orbital quantum numbers change prevailing in the same direction but only when α and l are not small and $\cos\left(\pi s + \tfrac{1}{6}\pi\right)$ and $\cos\left(\pi s - \tfrac{1}{6}\pi\right)$ are of the same sign, e.g. when s is close to the integer. In the latter case ($s = \Delta n$) we have the improved result of Goreslavsky *et al* (1982) for the removed states

$$D_{nl}^{n'l\pm1} \simeq R_{nl}^{n'l\pm1} \simeq \frac{v_c^5}{Z(vv')^{3/2}}\left(\frac{b}{(\Delta n)^{5/3}} \pm \frac{\alpha a}{(\Delta n)^{4/3}}\right)$$

$$= Z^{7/3}\left(b \pm \alpha a (\Delta n)^{1/3}\right)/\omega^{5/3}(vv')^{3/2} \qquad \Delta n \gg 1. \tag{34}$$

On the other hand, for large $s = \Delta n$, the Anger function and its derivative may be expressed through the Airy function and its derivative or through the McDonald functions. As a result we have from equations (20)–(23)

$$D_{p,r}^{\pm} = (-1)^{\Delta n} \frac{\sqrt{2}\zeta^{3/4}\left(1 - e^2\right)^{1/4}}{\pi\sqrt{3}e\Delta n}\left(K_{2/3}\left(\tfrac{2}{3}s\zeta^{3/2}\right) \pm K_{1/3}\left(\tfrac{2}{3}s\zeta^{3/2}\right)\right) \tag{35}$$

where

$$\tfrac{2}{3}\zeta^{3/2} = \ln\frac{1 + \sqrt{1 - e^2}}{e} - \sqrt{1 - e^2} \tag{36}$$

and $K_\nu(z)$ are the McDonald functions.

For $1 - e^2 = \alpha^2 \ll 1$ it yields from equations (35) and (36)

$$D_{p,r}^{\pm} = (-1)^{\Delta n} \frac{\alpha^2}{\pi\sqrt{3}e\Delta n}\left(K_{2/3}\left(\tfrac{1}{3}\alpha^3\Delta n\right) \pm K_{1/3}\left(\tfrac{1}{3}\alpha^3\Delta n\right)\right). \tag{37}$$

In the limit $\tfrac{1}{3}\alpha^3\Delta n \ll 1$, equation (37) results in the expression (34).

The dipole matrix elements for transitions between states with large, $l \sim n$, orbital quantum numbers, as follows from equations (20)–(23) or (35) and (36) when $e \to 0$, are

exponentially small. Moreover, the Bethe rule in this case is enhanced: transitions with the change of principal and orbital quantum numbers in opposite directions are strongly suppressed in comparison with transitions when n and l change in the same direction.

Thus, the very simple expressions (20)–(23) cover all known quasi-classical non-relativistic results for the dipole matrix elements. They generalize and increase the accuracy of some earlier derived expressions. Extension of the present approach to the continuum states is rather straightforward (see Kaulakys 1991 for analysis in the r-representation).

5. Conclusions

A consistent analytical approach for calculation of the quasi-classical radial dipole matrix elements in the momentum and coordinate representations is presented and very simple but relatively precise expressions for the matrix elements are derived in both representations. All analytical expressions for the quasi-classical radial matrix elements in both representations contain only one special function—the Anger function and its derivative. They generalize and increase accuracy of some known quasi-classical expressions. The small difference between the two forms of the expressions for the dipole matrix elements indicates the applicability of the simple expressions given by the consistent quasi-classical approach even for low atomic states.

It is important to note that the dipole matrix elements *as the analytical functions* (even for the hydrogenic atom) *are expressed through the Anger but not through the Bessel functions*. It is another thing that the Anger functions $J_\nu(z)$ of the integer order $\nu = m$ coincide with the Bessel functions $J_m(z)$, i.e. $J_m(z) = (-1)^m J_{-m}(z) = J_m(z)$. Expression of the dipole matrix elements through the Bessel function $J_s(es)$ or through the Anger function of the positive order and positive argument $J_s(es)$ (see, e.g. Delone *et al* 1994) results in the erroneous limit when $s \rightarrow 0$ and to another inaccuracies.

Acknowledgments

References

Bethe H A and Salpeter E E 1957 *Quantum Mechanics of One- and Two-Electron Atoms* (Berlin: Springer)
Crossley R J S 1969 *Adv. At. Mol. Phys.* 5 237
Davydkin V A and Zon B A 1981 *Sov. Phys.–Opt. Spectrosc.* 51 13
Delone N B, Goreslavsky S P and Krainov V P 1989 *J. Phys. B: At. Mol. Opt. Phys.* 22 2941
——1994 *J. Phys. B: At. Mol. Opt. Phys.* 27 4403
D'yachkov L G and Pankratov P M 1991 *J. Phys. B: At. Mol. Opt. Phys.* 24 2267
——1994 *J. Phys. B: At. Mol. Opt. Phys.* 27 461
Goreslavsky S P, Delone N K and Krainov V P 1982 *Sov. Phys.–JETP* 55 1032
Gontis V and Kaulakys B 1987 *J. Phys. B: At. Mol. Phys.* 20 5051
Heim T M, Trautmann D and Baur G 1989 *J. Phys. B: At. Mol. Opt. Phys.* 22 727
Kaulakys B 1991 *J. Phys. B: At. Mol. Opt. Phys.* 24 571
Kaulakys B and Vilutis G 1995 *Chaos—The Interplay between Stochastic and Deterministic Behaviour* ed P Garbaczewski, M Wolf and A Weron *Springer Lecture Notes in Physics* vol 457 (Berlin: Springer) pp 445-50
Landau L D and Lifshitz E M 1985 *Quantum Mechanics* (New York: Pergamon)

Nana E S G, Owono O L C, Dada J P, Waha N L, Kwato N M G, Oumarou B and Motapon O 1995 *J. Phys. B: At. Mol. Opt. Phys.* 28 2333
Pankratov P and Meyer-ter Vehn J 1992 *Phys. Rev. A* 46 5500