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# Singular part of the hydrogen dipole matrix element

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**Abstract.** The singular part of the hydrogen dipole matrix element is exactly calculated. The result can be of interest for both quantum electrodynamics (bremsstrahlung, Rayleigh scattering) and quantum optics (above-threshold ionisation). Comparison with approximate methods is performed.

## 1. Introduction

The hydrogen atom was one of the first problems solved within the framework of quantum mechanics. Its properties, such as the bound-continuum structure of the energy spectrum, are the subject of many fundamental textbooks.

On the other hand, an electron in the hydrogen atom when interacting with the electromagnetic field undergoes transitions between different atomic states. In many physical phenomena (such as bremsstrahlung, Rayleigh scattering, above-threshold ionisation) [1-3] these transitions may also occur between two continuum states. The rate of transition is governed (in the dipole approximation) by the dipole matrix element (DME) $\langle E, l, m|er|E', l', m'\rangle$.

In 1925 Gordon [4] found an exact formula for the DME (both in spherical and cylindrical coordinates) expressed in terms of some numerical factors multiplied by the hypergeometric function. The characteristic property of this formula is that when the initial and final values of energies coincide, i.e. $E = E'$, the DME becomes infinite (this is also referred to as the diagonal singularity). The exact form of this singularity was not important in [4], because of the type of physical problems considered. In most calculations based on the perturbational approach the exact form of this singularity was not important and the off-diagonal values of the DME were sufficient. Recently, however, there appeared a new range of effects such as, for example, cross sections of multiphoton ionisation (including above-threshold ionisation) for which the knowledge of these diagonal singularities becomes necessary [5]. It is the subject of this paper to analyse these singularities. We present an exact method of analytical regularisation of the DME (in our paper we will restrict ourselves to the case of the angular momentum basis $|E, l, m\rangle$ which is determined by the following quantum numbers: energy, angular momentum and its $z$ component). Thus we establish the convenient groundwork for analytical calculations of various integrals, important in applications, containing the DME—especially in the case when the integration domain meets a singularity at the coinciding energies $E = E'$.

The paper is organised as follows. In the appendix we briefly derive the recurrence (similar to the one derived by Gordon in [4]) which forms the basis of our method. In § 2 using this recurrence we calculate the singular part of the DME.

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## 2. Singular part of the hydrogen DME

In this section we calculate the singular part of the DME using the recursion scheme derived in the appendix. We will restrict ourself to the radial part of the DME, since the angular one does not contain any singularities. The radial part of the DME takes the following form [6]:

$$\mathfrak{M}_{kk'l}=\langle k,l|r|k',l-1\rangle=\lim_{\varepsilon\to 0}2^{-2l-3}\mathfrak{N}_{kl}\mathfrak{N}_{k'l-1}J^{1,2}_{2l+2,\varepsilon}\left(l+1+\frac{\mathrm{i}}{k},l+\frac{\mathrm{i}}{k'}\right) \tag{2.1}$$

where

$$\mathfrak{N}_{kl}=\frac{1}{(2l+1)!}(2k)^{l+1}\exp(\pi/2k)\left|\Gamma\left(l+1+\frac{\mathrm{i}}{k}\right)\right|$$

and the last factor on the right-hand side of (2.1) was already defined in (A1) and is equal to

$$\begin{aligned}J^{1,2}_{2l+2,\varepsilon}&\left(l+1+\frac{\mathrm{i}}{k},l+\frac{\mathrm{i}}{k'}\right)\\&=\frac{-2l(2l+1)}{k^2}\left[J^{1,0}_{2l,\varepsilon}\left(l+1+\frac{\mathrm{i}}{k}\,l+\frac{\mathrm{i}}{k'}\right)\right.\\&\quad\left.+J^{1,0}_{2l,\varepsilon}\left(l-1+\frac{\mathrm{i}}{k},l+\frac{\mathrm{i}}{k'}\right)-2J^{1,0}_{2l,\varepsilon}\left(1+\frac{\mathrm{i}}{k},1+\frac{\mathrm{i}}{k'}\right)\right].\end{aligned} \tag{2.2}$$

One can check that the last term on the right-hand side actually appears while considering the normalisation condition of the wavefunction. Thus we can immediately write its contribution to the DME:

$$\mathfrak{M}^{(2)}_{kk'l}=2\pi\frac{|l+\mathrm{i}/k|}{k}\,\delta(k-k'). \tag{2.3}$$

Let us define $\tilde{\mathfrak{M}}_{kk'l}=\mathfrak{M}_{kk'l}-\mathfrak{M}^{(2)}_{kk'l}$. Then the remaining part in our recursion formula may be written as

$$\begin{aligned}\tilde{\mathfrak{M}}_{kk'1}=\lim_{\varepsilon\to 0}2^{-2l-3}\mathfrak{N}_{kl}\mathfrak{N}_{k'l-1}&\frac{-2l(2l+1)}{k^2}\\&\times\left[J^{1,0}_{2l,\varepsilon}\left(l+1+\frac{\mathrm{i}}{k},l+\frac{\mathrm{i}}{k'}\right)+J^{1,0}_{2l,\varepsilon}\left(l-1+\frac{\mathrm{i}}{k},l+\frac{\mathrm{i}}{k'}\right)\right].\end{aligned} \tag{2.4}$$

Now we apply formulae (A5) and (A5′) to obtain the following expression:

$$\begin{aligned}J^{1,0}_{2l,\varepsilon}&\left(l+1+\frac{\mathrm{i}}{k},l+\frac{\mathrm{i}}{k'}\right)\\&=\frac{1}{\frac{1}{4}(k'^2-k^2)-\mathrm{i}\varepsilon k'-\varepsilon^2}\left[\left(-\mathrm{i}k+\frac{2\mathrm{i}\varepsilon}{k'}\right)J^{0,0}_{2l,\varepsilon}\left(l+1+\frac{\mathrm{i}}{k},l+\frac{\mathrm{i}}{k'}\right)\right.\\&\quad\left.-2\varepsilon\left(l+\frac{\mathrm{i}}{k}\right)J^{0,0}_{2l,\varepsilon}\left(l+1+\frac{\mathrm{i}}{k},l+1+\frac{\mathrm{i}}{k'}\right)\right]\end{aligned} \tag{2.5}$$

and in a similar way:

$$J^{1,0}_{2l,\varepsilon}\left(l-1+\frac{i}{k},l+\frac{i}{k'}\right)$$

$$=\frac{1}{\frac{1}{4}(k'^2-k^2)+i\varepsilon k+\varepsilon^2}\left[ik+2\varepsilon\left(1-\frac{i}{k}\right)J^{0,0}_{2l,\varepsilon}\left(l-1+\frac{i}{k},l+\frac{i}{k'}\right)\right.$$

$$\left.+2\varepsilon\left(l-1+\frac{i}{k}\right)J^{0,0}_{2l,\varepsilon}\left(l+\frac{i}{k},l+\frac{i}{k'}\right)\right]. \tag{2.6}$$

The rightmost terms proportional to $\varepsilon$ in (2.5) and (2.6) vanish in the limit $\varepsilon\to 0$. Therefore we obtain

$$J^{1,0}_{2l,\varepsilon}\left(l+1+\frac{i}{k},l+\frac{i}{k'}\right)\simeq\frac{-ik+2i\varepsilon/k'}{\frac{1}{4}(k'^2-k^2)-i\varepsilon k'-\varepsilon^2}J^{0,0}_{2l,\varepsilon}\left(l+1+\frac{i}{k},l+\frac{i}{k'}\right)$$

$$J^{1,0}_{2l,\varepsilon}\left(l-1+\frac{i}{k},l+\frac{i}{k'}\right)\simeq\frac{ik+2\varepsilon(l-i/k)}{\frac{1}{4}(k'^2-k^2)+i\varepsilon k+\varepsilon^2}J^{0,0}_{2l,\varepsilon}\left(l-1+\frac{i}{k},l+\frac{i}{k'}\right) \tag{2.7}$$

where, according to the definition (A2),

$$J^{0,0}_{2l,\varepsilon}\left(l+1+\frac{i}{k},l+\frac{i}{k'}\right)$$

$$=(2l-1)!(\varepsilon+\tfrac{1}{2}i(k+k'))^{1+i/k+i/k'}[\varepsilon+\tfrac{1}{2}i(k'-k)]^{-l-1-i/k}(\varepsilon-\tfrac{1}{2}i(k'-k))^{-l-i/k'}$$

$$\times F\left(l+1+\frac{i}{k},l+\frac{i}{k'},2l,\frac{-kk'}{\varepsilon^2+\frac{1}{4}(k-k')^2}\right) \tag{2.8}$$

and correspondingly

$$J^{0,0}_{2l,\varepsilon}\left(l-1+\frac{i}{k},l+\frac{i}{k'}\right)$$

$$=(2l-1)![\varepsilon+\tfrac{1}{2}i(k+k')]^{-1+i/k+i/k'}$$

$$\times[\varepsilon+\tfrac{1}{2}i(k'-k)]^{-l+1-i/k}[\varepsilon-\tfrac{1}{2}i(k'-k)]^{-l-i/k'}$$

$$\times F\left(l-1+\frac{i}{k},l+\frac{i}{k'},2l,\frac{-kk'}{\varepsilon^2+\frac{1}{4}(k-k')^2}\right). \tag{2.9}$$

Now we do the most tedious part of our work; namely we expand the hypergometric function for $\varepsilon\ll k,k'$ and $|k'-k|\ll k,k'$ [7] and extract the singular part. (By definition the singular part is the one that diverges in the limit $\lim_{\varepsilon\to 0}\lim_{k'\to k}$ or $\lim_{k'\to k}\lim_{\varepsilon\to 0}$.) Here we quote only the final result:

$$(\mathfrak{M}_{kk'l})_{\text{sing}}=\lim_{\varepsilon\to 0}\left\{-\frac{i}{4}\frac{l-i/k}{|l-i/k|}\right.$$

$$\times\left[1-\frac{i(k'-k)}{k^2}\left(\ln k-\gamma+\frac{1}{2}\left(\psi\left(l+1+\frac{i}{k}\right)+\psi\left(l+1-\frac{i}{k}\right)\right)\right)\right]$$

$$\left.\times\frac{1}{[\varepsilon+\frac{1}{2}i(k'-k)]^2}+\text{cc}\right\} \tag{2.10}$$

where $\psi(z)=\Gamma'(z)/\Gamma(z)$ and $\gamma=0.577\,21\ldots$ is the Euler constant. In the formula (2.10) we have omitted all terms which either vanish in the limit $\varepsilon\to 0$ as, for example, $\varepsilon^n/[\varepsilon+\frac{1}{2}i(k-k')]^2$ for $n\geqslant 1$ or are regular as $(k-k')^n/[\varepsilon+\frac{1}{2}i(k-k')]^2$ for $n\geqslant 2$. The last step is to identify the generalised functions in (2.10). Before we do this, we repeat here the well known formulae:

$$\lim_{\varepsilon\to 0}\frac{k'-k}{[\varepsilon\pm\frac{1}{2}\mathrm{i}(k'-k)]^2}=-4\left[P\left(\frac{1}{k'-k}\right)\pm\mathrm{i}\pi\delta(k'-k)\right] \tag{2.11}$$

$$\lim_{\varepsilon\to 0}\frac{1}{[\varepsilon\pm\frac{1}{2}\mathrm{i}(k'-k)]^2}=-4\left[P\left(\frac{1}{(k'-k)^2}\right)\mp\mathrm{i}\pi\delta'(k'-k)\right] \tag{2.12}$$

where $P(1/(k'-k))$ denotes the principal value of the integral and $P(1/(k'-k)^2)$ is defined as follows:

$$P\left(\frac{1}{(k'-k)^2}\right)(f)=\lim_{\delta\to 0}\left(\int_{-\infty}^{-\delta}\mathrm{d}x\frac{f(x)-f(0)}{x^2}+\int_{\delta}^{\infty}\mathrm{d}x\frac{f(x)-f(0)}{x^2}\right). \tag{2.13}$$

Thus, considering (2.10) and performing the limit $\varepsilon\to 0$ we obtain

$$(\tilde{\mathfrak{M}}_{kk'l})_{\mathrm{sing}}=\pi\frac{l-\mathrm{i}/k}{|l-\mathrm{i}/k|}\left\{\delta'(k'-k)\right.$$
$$\left.+\frac{\mathrm{i}}{k^2}\left[\ln k-\gamma+\frac{1}{2}\left(\psi\left(l+1+\frac{\mathrm{i}}{k}\right)+\psi\left(l+1-\frac{\mathrm{i}}{k}\right)\right)\right]\right\}+\mathrm{cc}. \tag{2.14}$$

The formulae (2.3), (2.10) and (2.14) are the main results of our paper. We recall that $\mathfrak{M}_{kk'l}=\mathfrak{M}^{(2)}_{kk'l}+\tilde{\mathfrak{M}}_{kk'l}$. Let us stress that the main singularity, i.e. the term proportional to the $\delta'(k'-k)$ in (2.14), can be obtained from approximate calculations, when we replace the exact wavefunctions by their asymptotic expansion (this result was first obtained in [8]). Since this property also holds in the case of the normalisation constant [9] (which is left as an exercise for the interested reader) it is possible that the leading singularity in these types of integrals can always be easily extracted by simplification based on replacing the integrand by its expansion near the singular point at infinity.

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**Appendix**

Here we will present the recursion relations between different $J^{s,p}_{\gamma,\varepsilon}(\alpha,\alpha')$ where $J^{s,p}_{\gamma,\varepsilon}(\alpha,\alpha')$ is defined as follows:

$$J^{s,p}_{\gamma,\varepsilon}(\alpha,\alpha')=\int_0^\infty \exp(-\varepsilon z)\exp[-\tfrac{1}{2}\mathrm{i}(k+k')z]z^{\gamma-1+s}F(\alpha,\gamma,\mathrm{i}kz)F(\alpha',\gamma-p,\mathrm{i}k'z)\,\mathrm{d}z \tag{A1}$$

where $\gamma+s>0$ and $F$ is the confluent hypergeometric function. Our formula is a simple generalisation of the result obtained by Gordon [4] for the case of regularised integrals. We will follow closely the idea presented in [4].

The starting point of our recurrence can be evaluated directly with the following result:

$$J^{0,0}_{\gamma,\varepsilon}(\alpha,\alpha')=\Gamma(\gamma)[\varepsilon+\tfrac{1}{2}\mathrm{i}(k+k')]^{\alpha+\alpha'-\gamma}[\varepsilon+\tfrac{1}{2}\mathrm{i}(k'-k)]^{-\alpha}[\varepsilon-\tfrac{1}{2}\mathrm{i}(k'-k)]^{-\alpha'}\times F\left(\alpha,\alpha',\gamma,\frac{-kk'}{\varepsilon^2+\frac{1}{4}(k'-k)^2}\right) \tag{A2}$$

where $\Gamma$ denotes the gamma function and $F$ is the hypergeometric function.

Next we remind ourselves of the method of reducing the value of $p$ and $s$ in (A1):

$$J^{s,2}_{\gamma,\varepsilon}(\alpha,\alpha')=\{J^{s,0}_{\gamma-2,\varepsilon}(\alpha,\alpha')-2J^{s,0}_{\gamma-2,\varepsilon}(\alpha-1,\alpha')+J^{s,0}_{\gamma-2,\varepsilon}(\alpha-2,\alpha')\}\frac{-(\gamma-1)(\gamma-2)}{k^2} \tag{A3}$$

$$\begin{aligned}J^{s+1,0}_{\gamma,\varepsilon}(\alpha,\alpha')=&\frac{1}{\frac{1}{4}(k'^2-k^2)-\mathrm{i}\varepsilon k'-\varepsilon^2}\\&\times\{[\mathrm{i}k(\tfrac{1}{2}\gamma-\alpha)-\mathrm{i}k'(\tfrac{1}{2}\gamma-\alpha')-s(\varepsilon+\mathrm{i}k')-\varepsilon(\gamma+s-2\alpha')]J^{s,0}_{\gamma,\varepsilon}(\alpha,\alpha')\\&-2\varepsilon\alpha' J^{s,0}_{\gamma,\varepsilon}(\alpha,\alpha'-1)+s(\gamma+s-1-2\alpha')J^{s-1,0}_{\gamma,\varepsilon}(\alpha,\alpha')\\&+2s\alpha' J^{s-1,0}_{\gamma,\varepsilon}(\alpha,\alpha'-1)\}.\end{aligned} \tag{A4}$$

For application to the calculation of the DME only the case $s=0$ appears. Then the above formula can be written in the following form:

$$\begin{aligned}J^{1,0}_{\gamma,\varepsilon}(\alpha,\alpha')=&\frac{1}{\frac{1}{4}(k'^2-k^2)-\mathrm{i}\varepsilon k'-\varepsilon^2}\\&\times\{[\mathrm{i}k(\tfrac{1}{2}\gamma-\alpha)-\mathrm{i}k'(\tfrac{1}{2}\gamma-\alpha')-\varepsilon(\gamma-2\alpha')]J^{s,0}_{\gamma,\varepsilon}(\alpha,\alpha')\\&-2\varepsilon\alpha' J^{s,0}_{\gamma,\varepsilon}(\alpha,\alpha'-1)\}.\end{aligned} \tag{A5}$$

In our paper we will also use a slightly different form of (A5) which is

$$\begin{aligned}J^{s+1,0}_{\gamma,\varepsilon}(\alpha,\alpha')=&\frac{1}{\frac{1}{4}(k'^2-k^2)+\mathrm{i}\varepsilon k+\varepsilon^2}\\&\times\{[\mathrm{i}k(\tfrac{1}{2}\gamma-\alpha)-\mathrm{i}k'(\tfrac{1}{2}\gamma-\alpha')+s(\varepsilon+\mathrm{i}k)+\varepsilon(\gamma+s-2\alpha)]\\&\times J^{s,0}_{\gamma,\varepsilon}(\alpha,\alpha')+2\varepsilon\alpha J^{s,0}_{\gamma,\varepsilon}(\alpha-1,\alpha')-s(\gamma+s-1-2\alpha)J^{s-1,0}_{\gamma,\varepsilon}(\alpha,\alpha')\\&-2s\alpha J^{s-1,0}_{\gamma,\varepsilon}(\alpha-1,\alpha')\}\end{aligned} \tag{A4$'$}$$

$$\begin{aligned}J^{1,0}_{\gamma,\varepsilon}(\alpha,\alpha')=&\frac{1}{\frac{1}{4}(k'^2-k^2)+\mathrm{i}\varepsilon k+\varepsilon^2}\\&\times\{[\mathrm{i}k(\tfrac{1}{2}\gamma-\alpha)-\mathrm{i}k'(\tfrac{1}{2}\gamma-\alpha')+\varepsilon(\gamma-2\alpha)]J^{s,0}_{\gamma,\varepsilon}(\alpha,\alpha')+2\varepsilon\alpha J^{s,0}_{\gamma,\varepsilon}(\alpha-1,\alpha')\}.\end{aligned} \tag{A5$'$}$$

## References


[1] Akhiezier A I and Berestecki V B 1965 *Quantum Electrodynamics* (New York: Wiley)
Bethe H A and Salpeter E E 1957 *Quantum Mechanics of One and Two-electron Atoms* (Berlin: Springer)

[2] Pratt R H and Feng I J 1985 *Atomic Inner-Shell Physics* (New York: Plenum)

[3] Agostini P, Fabre F, Mainfray G, Petite G and Rahman N H 1979 *Phys. Rev. Lett.* **42** 1127
Fabre F, Petite G, Agostini P and Clement M 1982 *J. Phys. B: At. Mol. Phys.* **15** 1353
Mittleman M H 1982 *Theory of Laser-Atom Interaction* (New York Plenum)
Kruit P, Kimman J, Muller H G and Van der Wiel M J 1983 *J. Phys. Rev.* A **28** 248
Chin S L and Lambropoulos P 1984 *Multiphoton Ionization of Atoms* (New York: Academic)
Delone N B and Krainov V P 1984 *Atoms in Strong Light Fields* (Berlin: Springer)
Faisal F H M 1987 *Theory of Multiphoton Processes* (New York: Plenum)
Crance M 1987 *Phys. Rep.* **144** 119
Eberly J H and Javanainen J 1988 *Eur. J. Phys.* **9** 265
[4] Gordon W 1929 *Ann. Phys.* **2** 1031
[5] Lewenstein M, Mostowski J and Trippenbach M 1985 *J. Phys. B: At. Mol. Phys.* **18** L481
Trippenbach M 1987 *J. Opt. Soc. Am.* B **4** 1429
Trippenbach M, Rzazewski K and Grobe R 1988 *Phys. Rev.* A **37** 4194
[6] Landau L D and Lifshitz H 1958 *Quantum Mechanics* (Oxford: Pergamon)
[7] Bateman H and Erdelyi A 1953 *Higher Transcendental Functions* vol 1 (New York: McGraw-Hill)
[8] Trippenbach M, Rzazewski K, Federov M V and Kazakov A E 1988 *J. Phys. B: At. Mol. Opt. Phys.* submitted
[9] Gottfried K 1986 *Quantum Mechanics* (New York: Benjamin)