Monotonicity of Coulomb dipole matrix elements

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We present a proof that nonrelativistic Coulomb dipole matrix elements are monotonically decreasing functions of transition energy, for transitions from any given bound state to states of greater energy, including bounded and unbounded negative-energy states and positive-energy continuum states. (By an unbounded negative-energy state we mean a solution of the Schrödinger equation, regular at the origin, which is unbounded and therefore is not an eigenstate.) The proof applies both to reduced matrix elements (normalization constants factored out so that for small distances wave functions behave as Cr^2 with $C \simeq 1$) and to full analytic matrix elements (including bound-state normalizations and their analytic continuations). It also applies to the full bound-free matrix element (including the complete continuum normalization) and to the bound-free cross section. The method of proof is related to our recent demonstration that there are no zeros in nonrelativistic Coulomb dipole matrix elements. Our result follows from a new recursion relation, simply related to the Infeld-Hull recursion relation utilized in our previous demonstration.

We have recently given a proof that allowed Coulomb dipole matrix elements never vanish.[1] Here we wish to report that with similar methods we can show that allowed Coulomb dipole matrix elements decrease monotonically as the transition energies increase.

Our previous proof was based on the recursion relations, for fixed initial and final energies ϵ and ϵ',

$$\begin{aligned} 2l A_{\epsilon}^{l} D_{\epsilon,\epsilon'}^{l-1,l} &= (2l+1) A_{\epsilon'}^{l+1} D_{\epsilon,\epsilon'}^{l,l+1} + A_{\epsilon}^{l+1} D_{\epsilon,\epsilon'}^{l+1,l} , \\ 2l A_{\epsilon'}^{l} D_{\epsilon,\epsilon'}^{l,l-1} &= A_{\epsilon'}^{l+1} D_{\epsilon,\epsilon'}^{l,l+1} + (2l+1) A_{\epsilon}^{l+1} D_{\epsilon,\epsilon'}^{l+1,l} , \end{aligned} \tag{1}$$

of Infeld and Hull[2] for successive pairs of dipole matrix elements, $D_{\epsilon,\epsilon'}^{l,l'}$ where

$$D_{\epsilon,\epsilon'}^{l,l'} = \int_0^\infty R_{\epsilon' l'} r^3 R_{\epsilon l}\, dr ,$$

describing a transition from initial energy and angular momentum (ϵ, l) to final (ϵ', l'). Here, the radial Schrödinger wave function $R_{\epsilon l}$, in the point Coulomb potential, is simply

$$N_{\epsilon l} r^l e^{i\sqrt{\epsilon} r} F(l+1-i/\sqrt{\epsilon}, 2l+2; -2i\sqrt{\epsilon} r) ,$$

where r is in units of Za_0 with a_0 the Bohr radius, and ϵ the energy in units of Z^2 Ry. (Here $\epsilon = -1/n^2$ with integer principal quantum number n for bound states and $\epsilon = P^2/Z^2$ with P the momentum for continuum states.) A_{ϵ}^{l} is $(1+\epsilon l^2)^{1/2}/l$ and is real and positive for $\epsilon > -1/l^2$ $(l \geq 1)$. $N_{\epsilon l}$ is a normalization constant which can be written as $N_{\epsilon l} = \tilde{N}_{\epsilon l}/B_{\epsilon}$, with

$$\tilde{N}_{\epsilon l} = \frac{2^{l+1}}{(2l+1)!} \prod_{S=0}^{l} (1+\epsilon s^2)^{1/2} . \tag{2}$$

Here

$$B_{\epsilon} = \begin{cases} (-\epsilon)^{-3/4} & \text{for bound states} \\ (1-e^{-2\pi/\sqrt{\epsilon}})^{1/2} & \text{for continuum states .} \end{cases}$$

$\tilde{N}_{\epsilon l}$ is an analytic function of energy in the finite energy plane, which is monotonically increasing for $\epsilon > -1/l^2$. Also $1/B_{\epsilon}$ is monotonically increasing for $\epsilon > 0$, so that $N_{\epsilon l}$ is monotonically increasing in the continuum states. Note that $R_{\epsilon l}$ is real for real ϵ even when $\epsilon > 0$; for small r $R_{\epsilon l} \simeq N_{\epsilon l} r^l$.

That each pair of dipole matrix elements are positive follows from the same property of the previous pair and that the coefficients A_{ϵ}^{l} of the recursion relations are positive. In our paper[1] we also commented that the reduced dipole matrix element (omitting normalization factors), $\bar{D}_{\epsilon,\epsilon'}^{l,l'} = D_{\epsilon,\epsilon'}^{l,l'}/(N_{\epsilon l} N_{\epsilon' l'})$, is a continuous function of energy ϵ' for $\epsilon' - \epsilon > 0$, even when the energy ϵ' corresponds to an unbound negative-energy state. (Such a state is a solution of the Schrödinger equation regular at the origin, but since it is unbounded it is not an eigenstate.) This followed from the analyticity of $R_{\epsilon' l'}/N_{\epsilon' l'}$, which is due to Poincaré's theorem.[3] This continuity of $\bar{D}_{\epsilon,\epsilon'}^{l,l'}$ in ϵ' is also true in screened potentials and was essential for our recent discussion of the oddness (eveness) of the number of zeroes of the matrix element.[4]

The recursion relations in Eq. (1) are not suitable for a proof of monotonicity. Even if a pair of $D_{\epsilon,\epsilon'}^{l,l'}$ on the right-hand side in Eq. (1) are monotonically decreasing with energy ϵ', the $A_{\epsilon'}^{l}$ are monotonically increasing with ϵ', and so no statement can be made for the $D_{\epsilon,\epsilon'}^{l,l'}$ on the left-hand side. In addition, the $D_{\epsilon,\epsilon'}^{l,l'}$ are not defined for negative energies ϵ' (except bound states) so their monotonicity cannot be discussed in this regime. However, we can rewrite the recursion relations in terms of redefined continuous matrix elements [continuous functions of ϵ'

for $(\epsilon'-\epsilon)>0$] with coefficients which are energy independent. These new matrix elements, $\tilde{D}^{\,l,l'}_{\epsilon,\epsilon'}$ are defined by

$$\tilde{D}^{\,l,l'}_{\epsilon,\epsilon'}=(\epsilon'-\epsilon)\tilde{N}^{\,2}_{\epsilon l}\tilde{N}^{\,2}_{\epsilon' l'}\bar{D}^{\,l,l'}_{\epsilon,\epsilon'} ,$$
$$=(\epsilon'-\epsilon)B_\epsilon B_{\epsilon'}\tilde{N}_{\epsilon l}\tilde{N}_{\epsilon' l'}D^{l,l'}_{\epsilon,\epsilon'} , \quad (3)$$

where $\tilde{N}_{\epsilon l}=B_\epsilon N_{\epsilon l}$. $\tilde{D}^{\,l,l'}_{\epsilon,\epsilon'}$, like $\bar{D}^{\,l,l'}_{\epsilon,\epsilon'}$ is a continuous function of ϵ' for $\epsilon'>\epsilon$ because $\tilde{N}_{\epsilon' l'}$ also has that property. [The extra factor $(\epsilon'-\epsilon)$ is included here in anticipation of our subsequent proof of the monotonicity of the photoeffect cross sections.] With these new continuous matrix elements, the recursion relations in Eq. (1) can be rewritten as

$$C_{\epsilon l}\tilde{D}^{\,l-1,l}_{\epsilon,\epsilon'}=(2l+1)\tilde{D}^{\,l,l+1}_{\epsilon,\epsilon'}+\tilde{D}^{\,l+1,l}_{\epsilon,\epsilon'} ,$$
$$C_{\epsilon' l}\tilde{D}^{\,l,l-1}_{\epsilon,\epsilon'}=\tilde{D}^{\,l,l+1}_{\epsilon,\epsilon'}+(2l+1)\tilde{D}^{\,l+1,l}_{\epsilon,\epsilon'} , \quad (4)$$

where

$$C_{\epsilon l}=\frac{2l(2l+1)}{(2l+3)}\left[\frac{\tilde{N}_{\epsilon l}}{\tilde{N}_{\epsilon l-1}}\right]^2=\frac{2(1+\epsilon l^2)}{l(2l+1)(2l+3)} .$$

Note that all coefficients of the right-hand sides in Eqs. (4) are positive and energy independent. If a given pair of $\tilde{D}^{\,l,l'}_{\epsilon,\epsilon'}$ on the right-hand sides is monotonically decreasing, the entire right-hand sides are monotonically decreasing and therefore likewise the left-hand sides are monotonically decreasing. Since $C_{\epsilon l}$ is energy independent and $C_{\epsilon' l}$ is monotonically increasing with ϵ', it follows that the pair of $\tilde{D}^{\,l,l'}_{\epsilon,\epsilon'}$ on the left-hand side are also monotonically decreasing. Thus, with the recursion relations in Eq. (4), the monotonic decreasing character of one pair of $\tilde{D}^{\,l,l'}_{\epsilon,\epsilon'}$'s generates the same character for the next pair. In the first pair, due to the fact that $D^{n,n-1}_{\epsilon,\epsilon'}$ vanishes,[1] where n is the principal quantum number of the initial bound state, $\tilde{D}^{\,n,n-1}_{\epsilon,\epsilon'}$ also vanishes. Thus all $\tilde{D}^{\,l,l\pm 1}_{\epsilon,\epsilon'}$'s are monotonically decreasing, for any l, if $\tilde{D}^{\,n-1,n}_{\epsilon,\epsilon'}$ is monotonically decreasing.

From the expression for $D^{n-1,n}_{\epsilon,\epsilon'}$ in Eq. (4) of Ref. 1 (see Ref. 5), $\tilde{D}^{\,n-1,n}_{\epsilon,\epsilon'}$ can be easily obtained as

$$\tilde{D}^{\,n-1,n}_{\epsilon,\epsilon'}=\frac{2^{4n+3}(-\epsilon)^{n-1}}{(2n-1)!(2n+1)!}\frac{\prod_{s=0}^{n-1}(1+\epsilon' s^2)}{(\epsilon'-\epsilon)^n}\times\left[\frac{1-\sqrt{\epsilon'/\epsilon}}{1+\sqrt{\epsilon'/\epsilon}}\right]^{1/\sqrt{-\epsilon}} , \quad (5)$$

which is positive for $\epsilon<0$ and $\epsilon'-\epsilon>0$. To investigate the monotonicity of $\tilde{D}^{\,n-1,n}_{\epsilon,\epsilon'}$, we calculate its logarithmic derivative with respect to ϵ', which we denote as

$$X=-\frac{n}{\epsilon'-\epsilon}+\sum_{s=0}^{n-1}f(s)+g_{\epsilon'}-\frac{1}{\epsilon'}\frac{\sqrt{-\epsilon}}{(\epsilon'-\epsilon)} ,$$

where

$$f(s)=s^2/(1+\epsilon' s^2)$$

and

$$g_{\epsilon'}=\frac{1}{2\epsilon'\sqrt{-\epsilon'}}\ln\left[\frac{1+\sqrt{\epsilon'/\epsilon}}{1-\sqrt{\epsilon'/\epsilon}}\right] .$$

Since $\tilde{D}^{\,n-1,n}_{\epsilon,\epsilon'}$ is positive, it will be monotonic if $X<0$. The first and last terms in our expression for X are negative. We note that

$$\sum_{s=0}^{n-1}f(s)=\sum_{s=0}^{n-1}\int_s^{s+1}f(s)dk<\sum_{s=0}^{n-1}\int_s^{s+1}f(k)dk$$
$$=\int_0^n f(k)dk=\frac{n}{\epsilon'}-g_{\epsilon'} ,$$

where in the inequality we have utilized the fact that $f(k)$ is a monotonically increasing function of k. Thus X is negative and hence $\tilde{D}^{\,n-1,n}_{\epsilon,\epsilon'}$ is monotonically decreasing.

Now let us discuss the monotonicity of ordinary and reduced dipole matrix elements, and of cross sections. From Eq. (3), since $\tilde{D}^{\,l,l'}_{\epsilon,\epsilon'}$ is monotonically decreasing and $\tilde{N}_{\epsilon' l'}$ and $(\epsilon'-\epsilon)$ are monotonically increasing, it follows that the reduced dipole matrix element $\bar{D}^{\,l,l'}_{\epsilon,\epsilon'}$ (which is also continuous in ϵ') is also monotonically decreasing. In the continuum, with $\epsilon>0$, B_ϵ is monotonically decreasing. However, we can show that $\tilde{N}_{\epsilon' l'}B_{\epsilon'}(\epsilon'-\epsilon)$ is monotonically increasing, and hence from Eq. (3) the ordinary continuum dipole matrix element $D^{l,l'}_{\epsilon,\epsilon'}$ is monotonically decreasing. In fact, since we will need it subsequently, we will prove the stronger statement that $\tilde{N}_{\epsilon' l'}B_{\epsilon'}(\epsilon'-\epsilon)^{1/2}$ is monotonically increasing. We have already noted that $(\epsilon'-\epsilon)^{1/2}$ is monotonically increasing. This is generally also true for $\tilde{N}_{\epsilon' l'}B_{\epsilon'}$. To show that $\tilde{N}_{\epsilon' l'}B_{\epsilon'}$ is monotonically increasing, we show that its derivative is positive. Using Eq. (2),

$$\frac{d}{d\epsilon'}\tilde{N}_{\epsilon' l'}B_{\epsilon'}=a_{\epsilon'}\tilde{N}_{\epsilon' l'}B_{\epsilon'} ,$$

where

$$a_{\epsilon'}=\tfrac{1}{2}\sum_{s=0}^{l'}f(s)+b_{\epsilon'} ,$$

with

$$b_{\epsilon'}=-\frac{\pi}{2(\epsilon')^{3/2}}\frac{1}{e^{2\pi/\sqrt{\epsilon'}}-1} ,$$

the logarithmic derivative of $B_{\epsilon'}$. Since

$$e^{2\pi/\sqrt{\epsilon'}}-1>\left[1+\frac{2\pi}{\sqrt{\epsilon'}}+\frac{1}{2}\frac{(2\pi)^2}{\epsilon'}+\frac{1}{6}\frac{(2\pi)^3}{(\epsilon')^{3/2}}\right]-1$$
$$>\frac{2\pi}{(\epsilon')^{1/2}}\left[1+\frac{1}{6}\frac{(2\pi)^2}{\epsilon'}\right]>\frac{2\pi}{(\epsilon')^{3/2}}(\epsilon'+1) ,$$
$$b_{\epsilon'}>-\frac{1}{4}\frac{1}{(1+\epsilon')} .$$

Thus for $l'>0$, noting that $f(1)=1/(1+\epsilon')$,

$$a_{\epsilon'}>\tfrac{1}{2}f(1)+b_{\epsilon'}>\frac{1}{4}\frac{1}{1+\epsilon'}>0 .$$

Since $(\tilde{N}_{\epsilon' l'}B_{\epsilon'})$ is positive, $a_{\epsilon'}>0$ means that it is monotonically increasing. For $l=0$, $\tilde{N}_{\epsilon' l'}$ is independent of ϵ' and does not compensate the monotonic decreasing behavior of $B_{\epsilon'}$. This is achieved due to the remaining factor $(\epsilon'-\epsilon)^{1/2}$:

$$\frac{d}{d\epsilon'}(\epsilon'-\epsilon)^{1/2}B_{\epsilon'}=d_{\epsilon'}(\epsilon'-\epsilon)^{1/2}B_{\epsilon'} ,$$

where

$$d_{\epsilon'}=\frac{1}{2}\frac{1}{\epsilon'-\epsilon}+b_{\epsilon'}>\frac{1}{2(\epsilon'-\epsilon)}-\frac{1}{4(\epsilon'+1)}$$

$$\geq\frac{1}{2(\epsilon'+1)}-\frac{1}{4(\epsilon'+1)}>0 ,$$

since $\epsilon\geq -1$, the most deeply bound level. Thus we have shown that $\tilde{N}_{\epsilon' l'}B_{\epsilon'}(\epsilon'-\epsilon)$ is monotonically increasing, and therefore the $D^{l,l\pm 1}_{\epsilon,\epsilon'}$'s are all monotonically decreasing for any l.

Finally we consider the monotonicity of the cross section $\sigma^{l,l'}_{\epsilon,\epsilon'}$ for an electron in an initial (ϵ,l) state which makes a transition to a final (ϵ',l') state,

$$\sigma^{l,l'}_{\epsilon,\epsilon'}=\frac{128\pi^4}{3}l_>(\epsilon'-\epsilon)\,|\,D^{l,l'}_{\epsilon,\epsilon'}\,|^2$$
$$=\frac{128\pi^4}{3}\frac{l_>}{\epsilon'-\epsilon}\left|\frac{\tilde{D}^{\,l,l'}_{\epsilon,\epsilon'}}{B_\epsilon B_{\epsilon'}\tilde{N}_{\epsilon l}\tilde{N}_{\epsilon' l'}}\right|^2 , \tag{6}$$

where now we are restricting ourselves to the case that the final state is in the continuum. Here the cross section is in units of $(Za_0)^2$ and $l_>$ is the larger of l and l'. From Eq. (6) we can see that the bound-free cross section is also a monotonically decreasing function of energy, since $\tilde{D}^{\,l,l'}_{\epsilon,\epsilon'}$ is monotonically decreasing and $B_{\epsilon'}\tilde{N}_{\epsilon' l'}(\epsilon'-\epsilon)^{1/2}$ is monotonically increasing. We have thus shown that, for for continuum energy ϵ', $\bar{D}^{\,l,l\pm 1}_{\epsilon,\epsilon'}$, $D^{l,l\pm 1}_{\epsilon,\epsilon'}$, and $\tilde{D}^{\,l,l\pm 1}_{\epsilon,\epsilon'}$ and $\sigma^{l,l\pm 1}_{\epsilon,\epsilon'}$ all monotonically decrease as the transition energy increases for any l; the statement also applies to negative energies ϵ' such that $\epsilon'-\epsilon>0$ in the case of $\bar{D}^{\,l,l\pm 1}_{\epsilon,\epsilon'}$ and $\tilde{D}^{\,l,l\pm 1}_{\epsilon,\epsilon'}$, which are continuous functions of ϵ' in this domain.

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[1]Sung Dahm Oh and R. H. Pratt, Phys. Rev. A **34**, 2486 (1986).

[2]L. Infeld and T. E. Hull, Rev. Mod. Phys. **23**, 31 (1951). We have further rewritten this notation from Ref. 1, indexing states by energy in order to make clear the analytic continuation in energy.

[3]L. I. Schiff, *Quantum Mechanics*, 3rd ed. (McGraw-Hill, New York, 1968), p. 345.

[4]R. H. Pratt, R. Y. Yin, and Xiaoling Liang, Phys. Rev. A **35**, 1450 (1987).

[5]There is a typographical error in the equation; $(nn')^{n+3}$ should be replaced by $(nn')^{2n+3}$.