Positiveness and monotonicity of continuum-continuum Coulomb dipole matrix elements

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We present a proof that there are no zeros in nonrelativistic Coulomb continuum-continuum transition dipole matrix elements. There is a positive singularity in these matrix elements as the case of equal energies is approached. Considering one energy as fixed, matrix elements are monotonically increasing (decreasing) functions of the other energy below (above) the singular case. This is an extension of our earlier demonstration that the Coulomb dipole matrix elements, connecting a *bound* state to a state of greater energy, never vanish and are monotonic. For the present proof, we utilize asymptotic expansions of the matrix elements for large angular momentum, together with fixed energy recursion relations between pairs of successive angular momentum states (l, l+1) and (l-1, l).

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We wish to report a proof that nonrelativistic Coulomb dipole matrix elements connecting two continuum states are always positive, with a positive singularity as the case of equal energies is approached, and are monotonic functions of either energy above and below the singularity, increasing with ε for $\varepsilon < \varepsilon'$, decreasing with ε for $\varepsilon > \varepsilon'$. We have presented similar demonstrations earlier that Coulomb dipole matrix elements, connecting a bound state to a state of greater energy, never vanish [1] and decrease monotonically as the transition energy increases [2]. These transition matrix elements from a bound state are related to the continuum case through an analytic continuation in energy, so it is natural to ask whether the continuum-continuum dipole matrix elements are also positive and monotonic. Our previous proofs are not directly generalizable, since they relied on the fact that there is a maximum allowed angular momentum associated with bound states of a given energy. Here we will instead utilize asymptotic large angular momentum expansions associated with a given continuum energy.

Recently there has been considerable interest in continuum-continuum dipole matrix elements which represent the quantum mechanisms responsible for such varied phenomena as the chaotic ionization of dynamical atomic system [3,4], the above-threshold ionization of atoms by high-power lasers [5,6], and the autoionization of Rydberg states [7]. Explicit expressions for bound and continuum dipole matrix elements associated with the nonrelativistic hydrogenic atom were obtained by Gordon [8]. However, the analytic structure of the exact dipole matrix elements is fairly complex and not easy to discern from the explicit expressions. In recent years semiclassical formulas [9,10] for the continuumcontinuum Coulomb dipole matrix elements have been obtained, exhibiting simpler analytic structure (and so clarifying certain features of the matrix elements in regimes for which the approximation is appropriate). A large l dependence may be discerned in the semiclassical

work of Kramers [11]; simple features were observed by Tseng and Pratt [12] in a numerical examination of the relativistic case. Here we prove certain mathematical properties of the exact continuum-continuum Coulomb dipole matrix elements: namely, that they are always positive and monotonic.

The ordinary radial wave function of the Schrödinger equation, which we now call $R_{\varepsilon l}^{(1)}$, is analytic in energy except for a normalization factor B_{ε} according to Poincaré's theorem [13]. In the Coulomb case, $R_{\varepsilon l}^{(1)}$ can be written as

$$\boldsymbol{R}_{sl}^{(1)}(\boldsymbol{r}) = \boldsymbol{g}_{sl}^{(1)} \boldsymbol{\overline{R}}_{sl}(\boldsymbol{r}) , \qquad (1)$$

where

$$\begin{split} g_{\varepsilon l}^{(1)}(r) &= \tilde{N}_{\varepsilon l} / B_{\varepsilon} , \\ \overline{R}_{\varepsilon l}(r) &= r^{l} e^{i \sqrt{\varepsilon} r} F(l+1-i / \sqrt{\varepsilon}, 2l+2; -2i \sqrt{\varepsilon} r) , \end{split}$$

with

$$\tilde{N}_{\varepsilon l} = \frac{2^{l+1}}{(2l+1)!} \prod_{s=1}^{l} (1+\varepsilon s^2)^{1/2} ,$$

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

 $\overline{R}_{\varepsilon l}(r) \equiv R_{\varepsilon l}^{(0)}$ is normally called the reduced radial wave function. (In Gordon's work [8] for continuum states, B_{ε} is replaced by $\varepsilon^{1/4}B_{\varepsilon}$.) Here r is in units of Za_0 with a_0 the Bohr radius, and ε is the energy in units of Z^2 Ry; $\varepsilon = -1/n^2$ with integer principal quantum number n for bound states and $\varepsilon = p^2/Z^2$ with p the momentum for continuum states. The branch cut in the energy plane is along the negative real axis and real negative energy is approached from the upper plane. We also define an additional radial wave function $R_{\varepsilon l}^{(2)} = g_{\varepsilon l}^{(2)} \overline{R}_{\varepsilon l}(r)$ with $g_{\varepsilon l}^{(2)} = (\widetilde{N}_{\varepsilon l})^2$; this leads to a type of dipole matrix element which we used in the proof of monotonicity of bound-

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continuum transition dipole matrix element in our previous work [2].

We now define general dipole matrix elements for a transition from a state (ε, l) to (ε', l') ,

$$\boldsymbol{M}^{(i)}(\boldsymbol{\varepsilon},\boldsymbol{l}\,;\boldsymbol{\varepsilon}',\boldsymbol{l}') = \int \boldsymbol{R}_{\boldsymbol{\varepsilon}\boldsymbol{l}}^{(i)}(\boldsymbol{r})\,\boldsymbol{r}^{3}\boldsymbol{R}_{\boldsymbol{\varepsilon}'\boldsymbol{l}'}^{(i)}(\boldsymbol{r})d\boldsymbol{r} , \qquad (2)$$

representing an ordinary dipole matrix element $D_{\varepsilon,\varepsilon'}^{l,l'}$ for i = 1, an alternative dipole matrix element $\tilde{D}_{\varepsilon,\varepsilon'}^{l,l'}$ for i = 2, and a reduced dipole matrix element $\bar{D}_{\varepsilon,\varepsilon'}^{l,l'}$ for i = 0 with $g_{\varepsilon l}^{(0)} = 1$. Note these matrix elements are symmetric under the interchange of initial and final states; Eq. (2) also represents the matrix element for a transition from a state (ε', l') to (ε, l) .

In our previous work [1,2] for the matrix elements of the transitions from a bound state, we have used the recursion relations for $D_{\varepsilon,\varepsilon'}^{l,l'}$ given by Infeld and Hull [14] and we also developed related recursion relations for $\tilde{D}_{\varepsilon,\varepsilon'}^{l,l'}$ for our proof of monotonicity [15]. Related recursion relations for $\overline{D}_{\varepsilon,\varepsilon'}^{l,l'}$ can also be obtained similarly. These three versions of recursion relations, all of which we will use here, can be expressed in the compact fashion:

$$d_{i}M^{(i)}(\varepsilon, l-1; \varepsilon', l) = a_{i}(2l+1)M^{(i)}(\varepsilon, l; \varepsilon', l+1) + b_{i}M^{(i)}(\varepsilon, l+1; \varepsilon', l) ,$$

$$f_{i}M^{(i)}(\varepsilon, l; \varepsilon', l-1) = a_{i}M^{(i)}(\varepsilon, l; \varepsilon', l+1) + b_{i}(2l+1)M^{(i)}(\varepsilon, l+1; \varepsilon', l) ,$$
(3)

with

$$(d_{i}, f_{i}, a_{i}, b_{i}) = \begin{cases} (1, 1, C_{\varepsilon'l+1}/P_{l}, C_{\varepsilon,l+1}/P_{l}) & \text{for } i = 0\\ (2lA_{\varepsilon}^{l}, 2lA_{\varepsilon'}^{l}, A_{\varepsilon'}^{l+1}, A_{\varepsilon}^{l+1}) & \text{for } i = 1\\ (C_{\varepsilon l}, C_{\varepsilon' l}, 1, 1) & \text{for } i = 2 \end{cases}$$

Here $A_{\varepsilon}^{l} = (1 + \varepsilon l^{2})^{1/2}/l$ is always real and positive for $\varepsilon > -1/l^{2} (l > 0)$;

$$C_{\varepsilon l} = \frac{2(1+\varepsilon l^2)}{l(2l+1)(2l+3)} ,$$

$$P_l = 4l(l+1)(2l+1)/(2l+5) .$$

(We note that Price and Harmin [16] have recently converted the i = 1 recursion relations into a differential equation in l, valid for small ε and ε' .) We can use any of these sets of recursion relations to show the positiveness of the continuum-continuum dipole matrix elements because the coefficients d_i , f_i , a_i , and b_i are positive for all three cases. To prove the monotonic character in energy, we use the recursion relations of $\widetilde{D}_{\varepsilon,\varepsilon'}^{l,l'}$ ($\overline{D}_{\varepsilon,\varepsilon'}^{l,l'}$) for the energies $\varepsilon > \varepsilon'$ ($\varepsilon < \varepsilon'$) with the fixed energy ε' , using the fact that all the coefficients are also monotonic nondecreasing functions of ε .

In the case of dipole matrix elements from a bound state, we obtained an explicit proof that all Coulomb dipole matrix elements of finite transition energy $\varepsilon - \varepsilon' \neq 0$ are positive by showing that the top dipole matrix element of a sequence of angular momentum transitions for fixed energies $D_{\varepsilon,\varepsilon'}^{n-1,n}$ with $\varepsilon = -1/n^2$ is positive; $D_{\varepsilon,\varepsilon'}^{n,n-1}=0.$ (The recursion relations for fixed ε and ε' connect one pair of $l \rightarrow l \pm 1$ channels to the next pair $\overline{l} \rightarrow \overline{l} \pm 1$ with $\overline{l} = l - 1.$) Since the coefficients in the recursion relation are positive, if any pair of $l \rightarrow l \pm 1$ matrix elements is positive, all succeeding pairs are positive. (A similar argument, utilizing $\widetilde{D}_{\varepsilon,\varepsilon'}^{l,l'}$, demonstrated monotonicity.)

It does not look possible at first glance to use a similar procedure to show that Coulomb dipole matrix elements between continuum states are always positive, since there is now no definite top angular momentum matrix element of the chain for given energy, unlike in the case of bound state *n* where the maximum *l* is given by n = l + 1. However, what we can do is to take the matrix elements for asymptotic large *l* and recur down. If we can show that the asymptotic large *l* dipole matrix elements for the transitions from continuum states (ε, l) to $(\varepsilon', l - 1)$ and from $(\varepsilon, l - 1)$ to (ε', l) are positive, independent of the relative magnitude of $\varepsilon \neq \varepsilon'$, each pair of $(\varepsilon, \varepsilon')$ matrix elements are positive since the coefficients A_{ε}^{l} of the recursion relations are positive. We can use analogous arguments for monotonicity.

We can obtain asymptotic large *l* dipole matrix elements starting from the explicit full expressions of Gordon [8]. Separate expressions for bound-bound, bound-continuum, and continuum-continuum reduced dipole matrix elements $\overline{D}_{\varepsilon,\varepsilon'}^{l,l-1}$ $(k = \sqrt{\varepsilon}, k' = \sqrt{\varepsilon'})$ are analytic continuations of the common expression, valid for $\varepsilon \neq \varepsilon'$,

$$\overline{D}_{\varepsilon,\varepsilon'}^{l,l-1} = -\frac{i(2l+1)!(-1)^{l-\alpha'}}{2k(k+k')^{2(l+1)}} u^{i/k-i/k'} \times [F(\alpha,\alpha';2l;1-u^{-2}) -u^2F(\alpha-2,\alpha';2l;1-u^{-2})], \quad (4)$$

where $\alpha = l + 1 - i/k$, $\alpha' = l + i/k'$, and u = (k + k')/(k' - k). The continuum reduced dipole matrix elements $\overline{D}_{\varepsilon,\varepsilon'}^{l-1,l}$ can be obtained from Eq. (4) by simply interchanging ε and ε' . (The $\widetilde{N}_{\varepsilon l}$, but not the B_{ε} , are also analytic functions of energy.) This equation can be rewritten for continuum-continuum reduced Coulomb dipole matrix elements using the relation

$$F(a,b;c;x) = (1-x)^{c-1}F(c-a,b;c;x)$$

and the fact that, in this continuum-continuum case, u is real, denoting $\varepsilon_{>}$ as the larger of ε and ε' , as

$$\overline{D}_{\varepsilon,\varepsilon'}^{l,l-1} = \frac{(2l+1)!e^{-\pi/\sqrt{\varepsilon_{>}}}}{\sqrt{\varepsilon}(\sqrt{\varepsilon}+\sqrt{\varepsilon'})^{2(l+1)}} \operatorname{Im} S$$
(5)

with

$$S = -|u|^{i/\sqrt{\varepsilon'}-i/\sqrt{\varepsilon}}$$

× F(l+1+i/\sqrt{\varepsilon}, l-i\sqrt{\varepsilon'}; 2l; 1-1/u^2).

Remembering that $\varepsilon, \varepsilon' > 0$ and so, also, $\varepsilon_>$, the sign of the matrix element in Eq. (5) is determined by the sign of ImS. The asymptotic large *l* value of S, S (we will generally use corresponding script letters for the asymptotic large l limit of a quantity) can be obtained from Watson's results [17] for the asymptotic expansion of hypergeometric functions for large parameters, obtained with the method of steepest descents. The hypergeometric function of concern here is of the form

$$F(a+l,a+l-c+1,a-b+2l+1;2/(1-z)).$$

[Here a, b, and c are $1+i/\sqrt{\epsilon}$, $2+i/\sqrt{\epsilon}$, and $2+i/\sqrt{\epsilon}+i/\sqrt{\epsilon'}$, respectively, and z is $-(\epsilon+\epsilon')/(2\sqrt{\epsilon\epsilon'})$.] Let ξ be defined by $z+\sqrt{z^2-1}=e^{-\xi}$, together with the requirement that $\operatorname{Re}(\xi)>0$.

Then the absolute value of $e^{-\xi}$ is less than one:

$$\begin{split} \varepsilon^{-\xi} &= -\frac{\varepsilon + \varepsilon'}{2(\varepsilon \varepsilon')^{1/2}} + \left[\frac{(\varepsilon - \varepsilon')^2}{4\varepsilon \varepsilon'}\right]^{1/2} \\ &= -\left[\frac{\varepsilon_{<}}{\varepsilon_{>}}\right]^{1/2}, \end{split}$$

where $\varepsilon_{>}$ and $\varepsilon_{<}$ represent the larger and the smaller of ε and ε' . Thus, from the first equation on p. 289 of Ref. [17] and Stirling's formula for Γ functions,

$$\mathcal{F}(l+1+i/\sqrt{\varepsilon},l-i\sqrt{\varepsilon'};2l;2/(1-z)) = 2^{2(l+1+i/\sqrt{\varepsilon})}\sqrt{l/\pi}e^{-\xi(l+1+i/\sqrt{\varepsilon})}$$

$$\times \left[\frac{z-1}{2}\right]^{l+1+i/\sqrt{\varepsilon}}(1-e^{-\xi})^{-(3/2)-i/\sqrt{\varepsilon}-i/\sqrt{\varepsilon'}}$$

$$\times (1+e^{-\xi})^{-(3/2)-i/\sqrt{\varepsilon}+i/\sqrt{\varepsilon'}}\sum_{s=0}^{\infty}\frac{C'_s\Gamma(s+\frac{1}{2})}{l^{s+1/2}}$$

with $C'_0 = 1$ and coefficients C'_s defined in Ref. [17]. In this asymptotic case we may write

$$\mathscr{S} = \left[\frac{\sqrt{\varepsilon} + \sqrt{\varepsilon'}}{\sqrt{\varepsilon_{>}}}\right]^{2l-1} \left|\frac{\sqrt{\varepsilon} + \sqrt{\varepsilon'}}{\sqrt{\varepsilon} - \sqrt{\varepsilon'}}\right|^{3/2} \mathscr{S}' \tag{6}$$

with

$$S' = -\operatorname{Im} \sum_{s=0}^{\infty} \frac{(2s)!}{(4l)^{s}s!} C'_{s}$$
$$= -\frac{1}{2l} \operatorname{Im} \left[C'_{1} + \frac{3}{2l} C'_{2} + \cdots \right].$$

The C'_1 term is given on p. 285 of Ref. [17] and, in our case,

$$ImC'_{1} = \begin{cases} -4/\sqrt{\varepsilon} & \text{if } \varepsilon > \varepsilon' ,\\ 0 & \text{if } \varepsilon < \varepsilon' . \end{cases}$$
(7a)

Similarly the C'_2 term can be computed for the case $\varepsilon < \varepsilon'$, giving

$$ImC'_{1} = \begin{cases} -4/\sqrt{\varepsilon} & \text{if } \varepsilon > \varepsilon' \\ 0 & \text{if } \varepsilon < \varepsilon' \end{cases}$$
(7a)

The resulting expressions for the dipole matrix element between continuum states are

$$\overline{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l,l-1} = \begin{cases} \overline{\mathcal{D}}_{0} & \text{if } \varepsilon > \varepsilon' \\ \overline{\mathcal{D}}_{0}X & \text{if } \varepsilon < \varepsilon' \end{cases} \\
\overline{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l-1,l} = \begin{cases} \overline{\mathcal{D}}_{0}X & \text{if } \varepsilon > \varepsilon' \\ \overline{\mathcal{D}}_{0} & \text{if } \varepsilon < \varepsilon' \end{cases}$$
(8)

with

$$\overline{D}_{0} = \frac{8\sqrt{\pi l} (2l/e)^{2l} e^{-\pi/\sqrt{\varepsilon_{>}}}}{\varepsilon_{>}^{l+1/2} |\varepsilon - \varepsilon'|^{3/2}}, \quad X = \frac{\varepsilon_{>}}{2l|\varepsilon - \varepsilon'|} .$$

We may verify the consistency of the result in Eq. (8) with the recursion relations in Eq. (3). In the asymptotic

limit, the recursion relations for i=0 may first be simplified to

$$4l^{2}\overline{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l-1,l} = \varepsilon'\overline{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l,l+1} + \frac{\varepsilon}{2l}\overline{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l+1,l},$$

$$4l^{2}\mathcal{D}_{\varepsilon,\varepsilon'}^{l,l-1} = \frac{\varepsilon'}{2l}\overline{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l,l+1} + \varepsilon\overline{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l+1,l},$$
(9)

using $\mathcal{P}_l = 4l^2$ and $\mathcal{O}_{\varepsilon,l} = \mathcal{O}_{\varepsilon,l+1} = \varepsilon/2l$, where only the leading term in *l* should be kept. It is easy to find from Eq. (8) that

$$\overline{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l,l'} = \frac{4l^2}{\varepsilon_{>}} \overline{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l-1,l'-1} \quad \text{for both } l' = l \pm 1 .$$
(10)

Inserting these forms in Eq. (9) yields

$$\frac{\overline{\mathcal{D}}_{\varepsilon_{>}\varepsilon_{<}}^{l,l-1}}{\overline{\mathcal{D}}_{\varepsilon_{>}\varepsilon_{<}}^{l-1,l}} = \frac{2l}{\varepsilon_{>}} |\varepsilon - \varepsilon'| .$$
(11)

Equation (11) is indeed consistent with the asymptotic values of $\overline{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l,l'}$ given in Eq. (8).

We now can complete an explicit proof that nonrelativistic Coulomb dipole matrix elements between continuum states are positive. Namely, the coefficients d_i , f_i , a_i , and b_i are all positive and both $\mathcal{D}_{\varepsilon,\varepsilon'}^{l,l-1}$ and $\mathcal{D}_{\varepsilon,\varepsilon'}^{l-1,l}$ are positive:

$$\mathcal{D}_{\varepsilon,\varepsilon'}^{l,l-1} = \begin{cases} \frac{D_0}{\sqrt{\varepsilon'}} & \text{if } \varepsilon > \varepsilon' \\ \frac{D_0}{\sqrt{\varepsilon'}} X & \text{if } \varepsilon < \varepsilon' \\ \end{cases}$$

$$\mathcal{D}_{\varepsilon,\varepsilon'}^{l-1,l} = \begin{cases} \frac{D_0}{\sqrt{\varepsilon}} X & \text{if } \varepsilon > \varepsilon' \\ \frac{D_0}{\sqrt{\varepsilon}} & \text{if } \varepsilon < \varepsilon' \\ \frac{D_0}{\sqrt{\varepsilon}} & \text{if } \varepsilon < \varepsilon' \end{cases}$$
(12)

with

$$D_{0} = \frac{4e^{(\pi/2)|(1/\sqrt{\varepsilon}) - (1/\sqrt{\varepsilon}')|}}{\sqrt{\pi l} |\varepsilon - \varepsilon'|^{3/2}} \left(\frac{\varepsilon}{\varepsilon}\right)^{l/2 + 1/4}$$

Hence, using the recursion relations for i = 1, all pairs of D's will be positive. The same argument for positiveness can be made for the other two kinds of dipole matrix elements.

To discuss the monotonicity in ε of the matrix elements in the energy region $\varepsilon > \varepsilon'$ for fixed continuum energy ε' , we consider

$$\tilde{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l,l-1} = \frac{2}{\sqrt{\pi l^3}} \left[\tilde{\mathcal{N}}_{\varepsilon',l-1} \right]^2 \frac{l - e^{-2\pi/\sqrt{\varepsilon}}}{(\varepsilon - \varepsilon')^{3/2}} ,$$

$$\tilde{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l-1,l} = \frac{4}{\sqrt{\pi l}} \left[\tilde{\mathcal{N}}_{\varepsilon',l} \right]^2 \frac{1 - e^{-2\pi/\sqrt{\varepsilon}}}{(\varepsilon - \varepsilon')^{5/2}} ,$$
(13)

where

$$\widetilde{\mathcal{N}}_{\varepsilon l} = \left[\frac{\sinh \pi / \sqrt{\varepsilon}}{2\pi} \frac{\varepsilon^{l+1/2}}{l^2} \right]^{1/2} \left[\frac{e}{2l} \right]^l$$

 $(\widetilde{D}_{\varepsilon,\varepsilon'}^{l,l'}$ for $\varepsilon < \varepsilon'$ can be obtained by interchanging ε and ε' in the above equations.) We can easily see from Eq. (13) that $\widetilde{D}_{\varepsilon,\varepsilon'}^{l,l'}$ is monotonically decreasing as the energy ε increases, for $\varepsilon > \varepsilon'$. Referencing the recursion relations for i=2 in Eq. (3), since d_2 and f_2 are monotonically nondecreasing in ε , if the right-hand side pair of $M^{(2)}(\varepsilon,l,\varepsilon',l')$ is monotonically decreasing, so is the left-hand pair. Thus, the fact that the asymptotic large l pairs of $M^{(2)}(\varepsilon,l,\varepsilon',l')$ are monotonically decreasing combined with the recursion relations tell us that all $M^{(2)}(\varepsilon,l,\varepsilon',l')$ are monotonically decreasing for $\varepsilon > \varepsilon'$. The ordinary matrix elements $D_{\varepsilon,\varepsilon'}^{l,l'}$ and the reduced dipole matrix elements $\widetilde{D}_{\varepsilon,\varepsilon'}^{l,l'}$ are also decreasing since $\widetilde{N}_{\varepsilon l}$ and $\widetilde{N}_{\varepsilon l}B_{\varepsilon}$ are

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monotonically increasing [2].

Similarly, we can establish the monotonicity in ε for $\varepsilon < \varepsilon'$ by considering $\overline{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l,l'}$ and the recursion relations for i = 0 in Eq. (3). From Eq. (8), $\overline{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l,l'}$ is monotonically increasing in this regime, and the recursion relations then show that all $\overline{\mathcal{D}}_{\varepsilon,\varepsilon'}^{l,l'}$ have this property. The ordinary matrix elements $\mathcal{D}_{\varepsilon,\varepsilon'}^{l,l'}$ are also increasing since $\widetilde{N}_{\varepsilon l}/B_{\varepsilon}$ is monotonically increasing.

As the transition energies approach each other $(\varepsilon = \varepsilon')$, the dipole matrix elements become singular for any fixed l, increasing as the singularity is approached from both above and below. We can show that the ordinary dipole matrix element $D_{\varepsilon,\varepsilon}^{l,l-1}$ approaches

$$\frac{1}{\sqrt{\varepsilon(1+\varepsilon l^2)}}\frac{1}{\pi}\lim_{\varepsilon\to\varepsilon'}\frac{1}{(\sqrt{\varepsilon}-\sqrt{\varepsilon'})^2}$$

in agreement with Veniard and Piraux [5], by calculating the dipole matrix element in Eq. (4) in the limit as $\varepsilon \rightarrow \varepsilon'$. Note this is different from the value one obtains from Eq. (12), where $|\varepsilon - \varepsilon'|$ was fixed as we took the asymptotic large *l* limit.

Thus, combining our previous and present work, we conclude that Coulombic dipole matrix elements for a transition from any bound or continuum state to a continuum state are positive. Further, for a fixed energy of the lower state, they are monotonically decreasing as the energy of the higher-energy state increases. We have also shown that continuum-continuum Coulomb dipole matrix elements are monotonically increasing, for fixed energy of the higher state, as the energy of the lower-energy state increases.

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