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exactly as above and may be omitted. The only change in our work consists of the insertion of a factor x in the integral on the right in (87) and in each of the integrals deriving therefrom, and one arrives at the analogue of (97) for $J'(r, \kappa^2)$ without further ado.

In treating d/dr of the *second* right-hand integral in (42) it is better, when $l = 0$, to replace the path Γ used there by Γ' , shown in figure 8. The formulas (43) and (44) can be used in the resulting integral, and show it to be an analytic function of κ^2 when $r > 0$.

Proof of the theorem is now complete. Before going further, and coming to the end of this paper, it is worthwhile to point out that the development (97), the same as

$$\sum_{j=0}^{\infty} \kappa^{2j} \int_0^1 \frac{e^{-2/x} e^{rx}}{x^{2l+2}} R_j(1/x) dx,$$

is what we would obtain formally if we substituted (90) into the expansion of $e^{\theta(x)}$ in powers of $\theta(x)$, grouped together all the terms involving each power κ^{2j} and, finally, plugged the resulting series into the (meaningless) formal expression

$$\int_0^1 \frac{e^{-2/x} e^{\theta(x)} e^{rx}}{x^{2l+2}} dx.$$

We now recall the conclusions of the discussion pursued at the beginning of this §. According to them, the last theorem has the

COROLLARY. *The asymptotic development (86) holds for each of the functions $\Delta_l(n)$.*

This immediately implies the corresponding development (85) for the quantities $\delta_l(n)$ appearing in (77).

ADDENDUM

At the beginning of §9 and again in §12 it was said that the functions $w_2(r, \kappa^2)$ and $v_2(r, \kappa^2) = r^{-l} w_2(r, \kappa^2)$ – the first given by (40) – are *not analytic in κ^2* at the point $\kappa = 0$. This can be seen by referring to a (complicated) explicit representation of $v_2(r, \kappa^2)$ in terms of known special functions; one may, for instance, consult pp. 181–184 of [4] and especially

formula (2.35) on p. 181 therein. Although the non-analyticity is not actually *used* in the preceding development, it seems worthwhile to see how it can be verified directly, without resorting to special technical material. Let us do that.

It is enough, in light of the observation at the beginning of the proof of Theorem 6 (§ 12), to show that the function $J(r, \kappa^2)$ given by (87), viz.,

$$J(r, \kappa^2) = \int_{\kappa}^1 \left(\frac{x - \kappa}{x + \kappa} \right)^{1/\kappa} \frac{e^{rx}}{(x^2 - \kappa^2)^{l+1}} dx,$$

is not even analytic in κ at the point $\kappa = 0$. For $0 < \kappa < \min(1, 1/l)$ this function has an expansion *in powers of r with coefficients depending on κ* , and it suffices to show that *the latter are not all analytic at $\kappa = 0$* . In fact, the first $2l + 1$ of them *are* (they can be easily computed), and we have to go out to the coefficient of r^{2l+1} in order to observe failure of analyticity. Here we only consider the case where $l = 0$ so as to keep things simple. The treatment for larger values of l is very similar, but *a bit* more involved.

Taking, then, $l = 0$, we look at the value of

$$\frac{\partial J(r, \kappa^2)}{\partial r} - \kappa J(r, \kappa^2) = \int_{\kappa}^1 \left(\frac{x - \kappa}{x + \kappa} \right)^{1/\kappa} \frac{e^{rx}}{x + \kappa} dx,$$

for $r = 0$, that is, at

$$A(\kappa) = \int_{\kappa}^1 \left(\frac{x - \kappa}{x + \kappa} \right)^{1/\kappa} \frac{dx}{x + \kappa}.$$

With $(x - \kappa)/(x + \kappa) = s$, this becomes

$$(98) \quad A(\kappa) = \int_0^{\frac{1-\kappa}{1+\kappa}} \frac{s^{1/\kappa}}{1-s} ds,$$

and we wish to show that the function $A(\kappa)$, so far only defined for $0 < \kappa < 1$, *cannot thence be extended into any neighbourhood of 0 so as to be analytic therein*.

For $0 < \kappa < 1$ we have $0 < (1 - \kappa)/(1 + \kappa) < 1$ and the expansion of $1/(1 - s)$ in powers of s can be substituted into the right side of (98), yielding

$$(99) \quad A(\kappa) = \left(\frac{1 - \kappa}{1 + \kappa} \right)^{1/\kappa} \sum_{n=1}^{\infty} \frac{((1 - \kappa)/(1 + \kappa))^n}{(1/\kappa) + n}.$$

Here,

$$\left(\frac{1 - \kappa}{1 + \kappa} \right)^{1/\kappa} = \exp \left(-2 - \frac{2\kappa^2}{3} - \frac{2\kappa^4}{5} - \dots \right)$$

(cf. in §4), a function obviously analytic (in κ^2) for $|\kappa| < 1$ (with κ complex). Hence $A(\kappa)$ can be extended from $(0, 1)$ so as to be analytic near 0 if and only if

$$(100) \quad B(\kappa) = \sum_{n=1}^{\infty} \frac{((1-\kappa)/(1+\kappa))^n}{(1/\kappa) + n}$$

can be so extended.

The series in (100) converges uniformly on any compact set of (complex) κ in the open right half plane, since $|(1-\kappa)/(1+\kappa)| < 1$ precisely in that region. The function $B(\kappa)$, initially specified only for $0 < \kappa < 1$, thus has an *analytic* extension to the half plane $\operatorname{Re} \kappa > 0$. To ensure analyticity of a corresponding extension of $A(\kappa)$, we should further require $|\kappa| < 1$ (see above); we can thus be sure that $A(\kappa)$ has, at any rate, an analytic extension from $(0, 1)$ to the half-disk

$$\mathcal{D}_+ = \{\kappa; \operatorname{Re} \kappa > 0 \text{ and } |\kappa| < 1\},$$

and continues to be given by (99) therein.

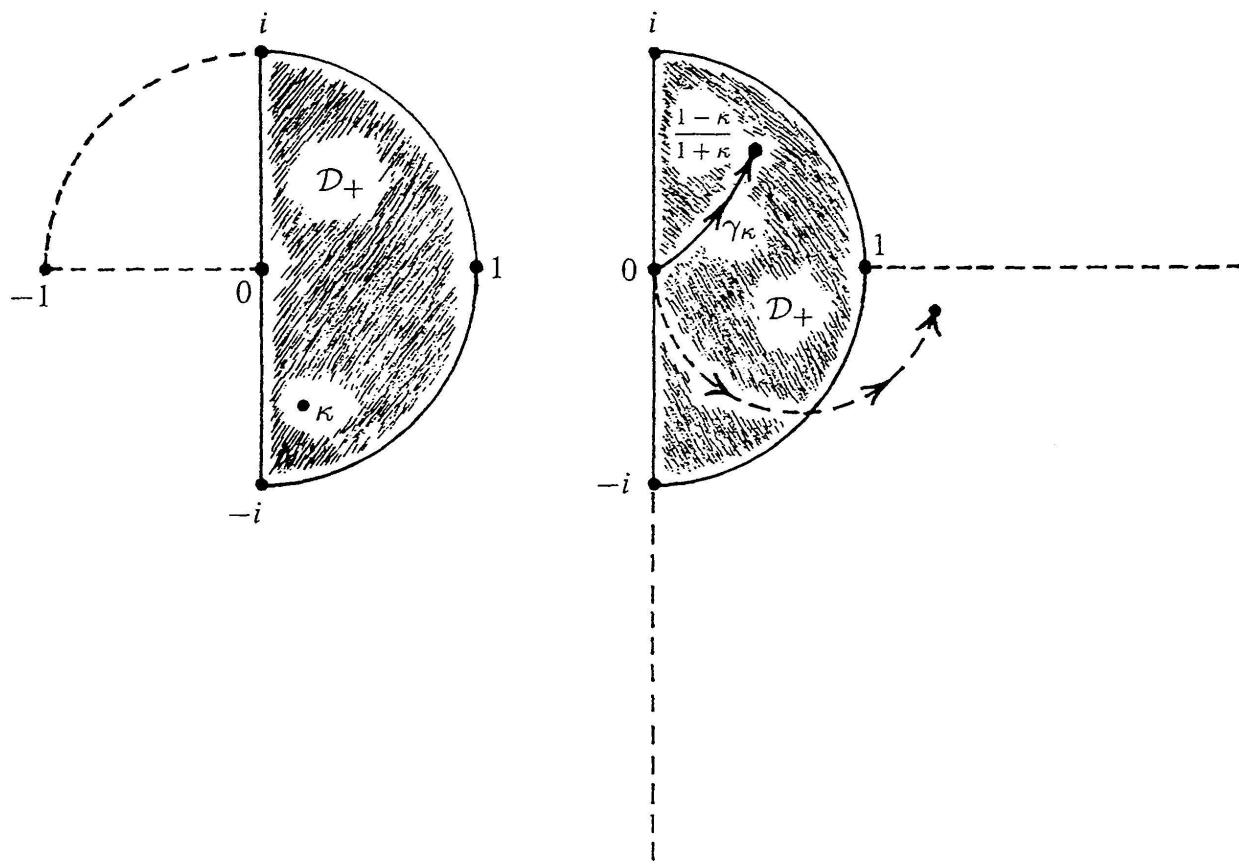


FIGURE 10

The transformation $\kappa \rightarrow (1 - \kappa)/(1 + \kappa)$ takes \mathcal{D}_+ conformally onto itself so, for $\kappa \in \mathcal{D}_+$, we have paths γ_κ *lying in* \mathcal{D}_+ (save for their initial endpoints) and running from 0 out to $(1 - \kappa)/(1 + \kappa)$ (see figure 10). Referring to (99) we see that a version of (98) *holds* for $\kappa \in \mathcal{D}_+$; we have, namely,

$$(101) \quad A(\kappa) = \int_{\gamma_\kappa} \frac{s^{1/\kappa}}{1-s} ds,$$

where γ_κ is any of the paths just described. (In integrals like the one on the right, $s^{1/\kappa}$ is understood to be obtained from the principal branch of $\log s$.)

Take now any integer $m > 1$; then (101) can be rewritten

$$A(\kappa) = \sum_{n=0}^{m-1} \int_{\gamma_\kappa} s^{(1/\kappa)+n} ds + \int_{\gamma_\kappa} \frac{s^{(1/\kappa)+m}}{1-s} ds,$$

that is,

$$(102) \quad A(\kappa) = \left(\frac{1-\kappa}{1+\kappa} \right)^{1/\kappa} \sum_{n=1}^m \frac{((1-\kappa)/(1+\kappa))^n}{(1/\kappa) + n} + \int_{\gamma_\kappa} \frac{s^{(1/\kappa)+m}}{1-s} ds.$$

And this formula, valid for $\kappa \in \mathcal{D}_+$, enables us to *continue* $A(\kappa)$ *analytically across the segment* $(0, i)$, *from* \mathcal{D}_+ *into the intersection of the open unit disk with the second quadrant* (excluding the negative real axis).

Let, indeed, C be any compact set passing, across $(0, i)$, from \mathcal{D}_+ into the second region; then $|1/\kappa|$ will be bounded for $\kappa \in C$ and hence $\text{Re}(1/\kappa)$ *bounded below there*, so, if the integer m in (102) is *large enough*, $\text{Re}(1/\kappa) + m$ will be > -1 on C . For such κ , *on* $(0, i)$ or *beyond* it, $(1 - \kappa)/(1 + \kappa)$ will lie *in the open fourth quadrant*, and there will be paths γ_κ like the dotted one shown in figure 10, lying in the fourth quadrant and going from 0 out to $(1 - \kappa)/(1 + \kappa)$ *while avoiding the point* 1. The *integral* in (102) will thus make sense with such paths γ_κ for $\kappa \in C$, and obviously continue to represent an analytic function of κ there. At the same time, the *sum* in (102) will *remain analytic* for κ in the second quadrant, not on the real axis, and with $|\kappa| < 1$.

It is now claimed that *when* κ , *in the open second quadrant, tends to any point* $-1/p$, $p = 2, 3, \dots$, *the function* $A(\kappa)$, *specified in the way just described, tends to* ∞ . Fixing any such p , we can choose an integer $m > p$ such that (102) will be valid for the κ in question, with indeed

$\operatorname{Re}(1/\kappa) + m > -1$ and bounded away from -1 as $\kappa \rightarrow -1/p$. For the γ_κ we can take *circular arcs* lying in the fourth quadrant, *orthogonal to the real axis* and running from 0 to $(1 - \kappa)/(1 + \kappa)$; these γ_κ will stay away from 1 while $(1 - \kappa)/(1 + \kappa) \rightarrow (p + 1)/(p - 1)$, i.e., while $\kappa \rightarrow -1/p$. Then $|1 - s|$ will be uniformly bounded away from 0 for s on these γ_κ , and the *integral* in (102) thus *remain bounded* as $\kappa \rightarrow -1/p$. At the same time, however, the *sum* in (102) will tend to ∞ like $1/((1/\kappa) + p)$. Hence $A(\kappa)$ will tend to ∞ as $\kappa \rightarrow -1/p$ in the manner described.

This being so for *each* of the points $-1/p$, $p = 2, 3, \dots$, $A(\kappa)$ *can have no analytic continuation from \mathcal{D}_+ into any neighbourhood of 0* , since any such continuation would have to coincide with the one just constructed on the intersection of the open second quadrant with the neighbourhood in question. That is what we needed to prove.

Before concluding, I must again thank my friend Victor Havin for having, during a conversation, expressed a thought which, indirectly, got me onto a path leading to the above argument.

BIBLIOGRAPHY

- [1] SCHIFF, L. I. *Quantum Mechanics*. McGraw-Hill, New York, 1955.
- [2] MARGENAU, H. and G. M. MURPHY. *The Mathematics of Physics and Chemistry*. Van Nostrand, New York, 1943.
- [3] HARTREE, D. R. The wave mechanics of an atom with a non-Coulomb central field. Part III. Term values and intensities in series in optical spectra. *Proc. Camb. Phil. Soc.* 24 (1928), 426–437.
- [4] SEATON, M. J. Quantum defect theory. *Reports Prog. Phys.* 46 (1983), 167–257.
- [5] GALLAGHER, T. F. *Rydberg Atoms*. Cambridge Univ. Press, 1994.
- [6] TITCHMARSH, E. C. *Eigenfunction Expansions*. Oxford, Clarendon Press, 1946.
- [7] HAM, F. S. The quantum defect method. In: *Solid State Physics*, edited by Seitz and Turnbull. Vol. 1 (1955), 127–192. Academic Press, New York.
- [8] MOTT, N. F. and H. S. W. MASSEY. *The Theory of Atomic Collisions*. Oxford, Clarendon Press; 2nd edition, 1949; 3rd edition, 1965.
- [9] FANO, U. and A. R. P. RAU. *Atomic Collisions and Spectra*. Academic Press, Orlando, 1986.
- [10] RAU, A. R. P. and M. INOKUTI. The quantum defect: Early history and recent developments. *Amer. J. Phys.* 65:3 (1997), 221–225.
- [11] INCE, E. L. *Ordinary Differential Equations*. Dover, New York, 1956.