Off-diagonal hydrogenic and generalized Kepler $r^k e^{-qr} {}^{\sin}_{\cos}(pr)$ integrals in closed form

1975 J. Phys. A: Math. Gen. 8 L61

(http://iopscience.iop.org/0305-4470/8/7/001)

J. Phys. A: Math. Gen., Vol. 8, No. 7, 1975. Printed in Great Britain. © 1975

LETTER TO THE EDITOR

Off-diagonal hydrogenic and generalized Kepler $r^k\, \mathrm{e}^{-qr} \,{}^{\sin}_{\cos}(pr)$ integrals in closed form

N Bessis, G Bessis and G Hadinger

Laboratoire de Spectroscopie et de Luminescence, Université Claude Bernard, Lyon I, 69621 Villeurbanne, France

Received 27 May 1975

Abstract. Closed-form expressions of the off-diagonal $\langle nl\gamma|r^k\, \mathrm{e}^{-qr}\,{}^{\sin}_{\cos}(pr)|n'l'\gamma'\rangle$ matrix elements ($n \neq n', l \neq l', \gamma \neq \gamma'$) between generalized Kepler $R^{l+\gamma}_{n+\gamma}(\mu r)$ functions have been obtained from ladder operator considerations. As a particular case ($\gamma = \gamma' = 0$), these integrals reduce to the off-diagonal $r^k\, e^{-qr}\,{}^{\sin}_{\cos}(pr)$ hydrogenic integrals.

It is known (Infeld and Hull 1951) that the generalized Kepler functions $R^{l+\gamma}_{n+\gamma}(\mu r)$, where γ is any constant, are solutions of a factorizable equation. For $\gamma = 0$, they reduce to the usual hydrogenic functions $R^l_n(Zr/n)$. As a consequence of the factorizability, one can apply the 'multi-step' or 'accelerated' operator procedure (Hadinger *et al* 1974) to obtain a closed-form expression of any matrix element in terms of one unique integral which, in most cases of interest in physics, is easily found.

Recently Kumei (1974), using a group theoretic argument, has paid special attention to the hydrogenic $r^k\, \mathrm{e}^{-qr}\,{}^{\sin}_{\cos}(pr)$ integrals and closed-form expressions of the diagonal integrals have been obtained for special cases. As it has been shown elsewhere (Hadinger *et al* 1974), the use of the Infeld–Hull 'artificial' factorization enables one to deal with the current matrix element without having to discriminate between diagonal and off-diagonal cases. In this paper, closed-form expressions for the off-diagonal $r^k\, \mathrm{e}^{-qr}\,{}^{\sin}_{\cos}(pr)$ Kepler integrals are derived.

The Kepler functions are solutions of the (type F) factorizable equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{(l+\gamma)(l+\gamma+1)}{r^2}+\frac{2a}{r}-\frac{a^2}{(n+\gamma)^2}\right)R^{l+\gamma}_{n+\gamma} = 0$$

where a is a parameter. The associated ladder operators and factorization function are

$$H^{\pm}_{l+\gamma} = \frac{l+\gamma}{r}-\frac{a}{l+\gamma}\mp\frac{\mathrm{d}}{\mathrm{d}r} \qquad L(l+\gamma) = -a^2/(l+\gamma)^2 \tag{1}$$

with the quantification condition (class I)

$$n-l-1 = v = \text{integer} \geqslant 0.$$

Consequently, the generalized Kepler functions are solutions of the following pair of differential-difference equations:

$$\left(\frac{l+\gamma+1}{r}-\frac{a}{l+\gamma+1}-\frac{\mathrm{d}}{\mathrm{d}r}\right)R_{n+\gamma}^{l+\gamma} = N_{l+\gamma+1}R_{n+\gamma}^{l+\gamma+1}$$

$$\left(\frac{l+\gamma}{r}-\frac{a}{l+\gamma}+\frac{\mathrm{d}}{\mathrm{d}r}\right)R_{n+\gamma}^{l+\gamma} = N_{l+\gamma}R_{n+\gamma}^{l+\gamma-1}$$

with

$$N_{l+\gamma} = [a^2(n-l)(n+2\gamma+l)]^{1/2}/(n+\gamma)(l+\gamma).$$

In the same way as for the hydrogenic functions, starting from the one-step ladders (1), one can build up a 'v-step' or 'accelerated ladder' operator, involving the artificial parameter $\mu = a/(n+\gamma)$. This operator, when applied to the key function ($v = 0$) generates any Kepler function, and consequently, any matrix element of an operator Q can be expressed in terms of a 'key' parametric integral (see Hadinger *et al* 1974, table 1 for type F)

$$\mathscr{I}_{tt'} = \int_0^\infty r^{l+\gamma+\gamma'+l'+2+t+t'}\,\mathrm{e}^{-(\mu+\mu')r}Q\,\mathrm{d}r.$$

Hence, for $Q = r^k\,\mathrm{e}^{-qr}\,{}^{\sin}_{\cos}(pr)$, one can write

$$\begin{aligned}\langle nl\gamma|r^k\,e^{-qr}\,{}^{\sin}_{\cos}(pr)|n'l'\gamma'\rangle &= CC'\sum_{t=0}^{v}\binom{v}{t}\frac{(-2\mu)^t}{\Gamma(2l+2\gamma+2+t)}\sum_{t'=0}^{v'}\binom{v'}{t'}\frac{(-2\mu')^{t'}}{\Gamma(2l'+2\gamma'+t'+1)}\\ &\quad\times\int_0^\infty r^{K+t+t'-1}\,\mathrm{e}^{-(\mu+q+\mu')r}\,{}^{\sin}_{\cos}(pr)\,\mathrm{d}r \end{aligned} \qquad (2)$$

where

$$K = l+\gamma+l'+\gamma'+k+3$$

$$C = (-1)^{l+1}(2\mu)^{l+\gamma+\frac{3}{2}}\left(\frac{\Gamma(n+l+2\gamma+1)}{v!2(n+\gamma)}\right)^{1/2}. \qquad (3)$$

The integral in (2) can be found in Gradshteyn and Ryzhik (1965). Finally, one gets the following expression:

$$\begin{aligned}\langle nl\gamma|r^k\,\mathrm{e}^{-qr}\,{}^{\sin}_{\cos}(pr)|n'l'\gamma'\rangle &= CC'\sum_{t=0}^{n-l-1}\binom{n-l-1}{t}\frac{1}{\Gamma(2l+2\gamma+2+t)}\left(\frac{-2\mu}{\mu+q+\mu'}\right)^t\\ &\quad\times\sum_{t'=0}^{n'-l'-1}\binom{n'-l'-1}{t'}\frac{(-2\mu')^{t'}}{\Gamma(2l'+2\gamma'+2+t')}\,\frac{\Gamma(K+t+t')}{[(\mu+q+\mu')^2+p^2]^{(K+t+t')/2}}\\ &\quad\times{}^{\sin}_{\cos}\left[(K+t+t')\tan^{-1}\left(\frac{p}{\mu+q+\mu'}\right)\right].\end{aligned}$$

This result is valid for complex q and p if $\mathrm{Re}(\mu+q+\mu') > |\mathrm{Im}\, p|$. The associated conditions for k are:

$$l+\gamma+l'+\gamma'+1 > \begin{cases} -k-3 & \text{for the } r^k\,\mathrm{e}^{-qr}\sin(pr) \text{ integral} \\ -k-2 & \text{for the } r^k\,\mathrm{e}^{-qr}\cos(pr) \text{ integral.} \end{cases}$$

C and K are given by (3).

Of course, when setting $\gamma = 0$, $\mu = Z/n$, one readily obtains the $\langle nl|r^k\,\mathrm{e}^{-qr}\,{}^{\sin}_{\cos}(pr)|n'l'\rangle$ off-diagonal hydrogenic integral.

References

Gradshteyn I S and Ryzhik I M 1965 *Tables of Integrals, Series and Products* (New York and London: Academic Press)

Hadinger G, Bessis N and Bessis G 1974 *J. Math. Phys.* **15** 716

Infeld L and Hull T E 1951 *Rev. Mod. Phys.* **23** 21

Kumei S 1974 *Phys. Rev.* A **9** 2306