Interaction of the Vibrational and Electronic Motions in Some Simple Conjugated Hydrocarbons

II.: Algebraic Evaluation of the Integrals*

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Die in der Theorie der Wechselwirkungen zwischen den Schwingungs- und Elektronenbewegungen in konjugierten Kohlenwasserstoffen vorkommenden Integrale werden algebraisch und numerisch berechnet.

In the preceeding paper [1] the author has presented the results of a calculation of the intensities of the vibronically (vibrationally-electronically) allowed ${}^1A_{1g} \rightarrow ({}^1B_{1u}, B_{1u})$ benzene spectral transitions. This computation involved the evaluation of a number of integrals not previously reported in the literature. We shall in this note outline the manipulative techniques required for the evaluation of these integrals.

From the definitions of the integrals $I_j(\bar{x})$ **, $(j=0, 1, 2, 3, 4, 5, 6)$ given in reference 1 [see equations (I, A 1 – 10 and 15), (I, A 2 – 5 and 9), and (I, A 3 – 26, 31, and 38)], we may write

$$\begin{aligned}\frac{a_0^2}{Z^2 e^2} I_0(x_{rt}) = {} & J_0(x_{rt}) - 18\, J_2(x_{rt}) + 90\, J_4(x_{rt}) + \tfrac{1}{4}\{72\, J_3(x_{rt}) + 72\, J_{13}(x_{rt}) + 48\, J_{14}(x_{rt}) \\ & + 24\, J_{15}(x_{rt}) + 9\, J_{16}(x_{rt}) + 2\, J_{17}(x_{rt})\} \\ & + \tfrac{1}{4} J_{18}(x_{rt}) - \tfrac{1}{8}\{720\, J_5(x_{rt}) + 720\, J_{26}(x_{rt}) + 360\, J_{27}(x_{rt}) + 120\, J_{28}(x_{rt}) + 30\, J_{29}(x_{rt}) \\ & + 6\, J_{30}(x_{rt}) + J_{31}(x_{rt})\},\end{aligned} \tag{1}$$

$$\begin{aligned}\frac{a_0^2}{Z^2 e^2} I_1(x_{rt}) = {} & \tilde{J}_1(x_{rt}) - 18\, \tilde{J}_3(x_{rt}) + 90\, \tilde{J}_5(x_{rt}) + \tfrac{1}{4}\{72\, J_6(x_{rt}) + 72\, J_1(x_{rt}) + 48\, J_8(x_{rt}) \\ & + 24\, J_9(x_{rt}) + 9\, J_{10}(x_{rt}) + 2\, J_{11}(x_{rt})\} \\ & + \tfrac{1}{4} J_{12}(x_{rt}) - \tfrac{1}{8}\{720\, J_{19}(x_{rt}) + 720\, J_{20}(x_{rt}) + 360\, J_{27}(x_{rt}) + 120\, J_{22}(x_{rt}) + 30\, J_{23}(x_{rt}) \\ & + 6\, J_{24}(x_{rt}) + J_{25}(x_{rt})\},\end{aligned} \tag{2}$$

$$I_2(x_{rt}) = J_{32}(x_{rt}), \tag{3}$$

$$-\frac{2\, a_0}{Z} I_3(x_{rt}) = \tilde{J}_{16}(x_{rt}), \tag{4}$$

$$-\frac{a_0^2}{Z^2 e^2} I_4(x_{rt}) = \tfrac{1}{8}\{J_{36}(x_{rt}) + 4\, J_{35}(x_{rt}) + 12\, J_{34}(x_{rt}) + 16\, J_{33}(x_{rt})\}, \tag{5}$$

$$-\frac{a_0^2}{Z^2 e^2} I_5(x_{rt}) = \tfrac{1}{8}\{16\, J_9(x_{rt}) + 12\, J_{10}(x_{rt}) + 4\, J_{11}(x_{rt}) + J_{12}(x_{rt})\}, \tag{6}$$

$$\frac{a_0}{Z e^2} I_6(x_{rt}) = \tfrac{1}{4}\{J_{40}(x_{rt}) + 4\, J_{39}(x_{rt}) + 12\, J_{38}(x_{rt}) + 16\, J_{37}(x_{rt})\}. \tag{7}$$

Hence the evaluation of the integrals $I_j(x_{rt})$, $(j=0, 1, 2, 3, 4, 5, 6)$ depends explicitly on the evaluation of the forty $J_i(x_{rt})$ integrals and the four $\tilde{J}_i(x_{rt})$ integrals. The author has evaluated the J_i and $\tilde{J}_i$ integrals by several different methods. Only those representations which were found to be most amenable to numerical computations will be given in this paper.

* This paper is based, in part, on a thesis submitted in May, 1955 by the author to the Committee of Chemical Physics, Harvard University, in partial fulfillment of requirements for the Ph. D. degree.

[1] A. D. LIEHR, Z. Naturforschg. 13 a, 311 [1958]; Part I.

** Anm. d. Redaktion: Bei allen folgenden Werten x handelt es sich um das $\bar{x}$ der Arbeit I, wie es auch in Abb. 2 angegeben ist. Der Querstrich wurde aus satztechnischen Gründen weggelassen.

Algebraic Evaluation of the Integrals $J_i(x)$ and $\tilde{J}_i(x)$

The integrals J_i and $\tilde{J}_i$ are most conveniently expressed in terms of the bipolar co-ordinates ϱ_r, α_r, and β defined in reference 1 [see I, Fig. 2, and equation (I, A 1 – 7)]. Upon integration over $d\beta$ from 0 to 2π, the integrals J_i and $\tilde{J}_i$ reduce to the following ($N^2 = 1/32\pi$):

$$
\begin{aligned}
J_0(x_{rt}) &= \pi N^2 \int \varrho_r^2 \sin^2\alpha_r \exp(-\varrho_r) \frac{\cos\alpha_t}{\varrho_t^2} d\sigma_{rt}, \\
J_1(x_{rt}) = J_{14}(x_{rt}) &= \pi N^2 \int \varrho_r^2 \sin^2\alpha_r \exp[-(\varrho_r+\varrho_t)] \frac{\cos\alpha_t}{\varrho_t^2} d\sigma_{rt}, \\
J_2(x_{rt}) &= \pi N^2 \int \varrho_r^2 \sin^2\alpha_r \exp(-\varrho_r) \frac{\cos\alpha_t}{\varrho_t^4} d\sigma_{rt}, \\
J_3(x_{rt}) &= \pi N^2 \int \varrho_r^2 \sin^2\alpha_r \exp[-(\varrho_r+\varrho_t)] \frac{\cos\alpha_t}{\varrho_t^4} d\sigma_{rt}, \\
J_4(x_{rt}) &= \frac{3\pi N^2}{4} \int \varrho_r^4 \sin^4\alpha_r \exp(-\varrho_r) \frac{\cos\alpha_t}{\varrho_t^6} d\sigma_{rt}, \\
J_5(x_{rt}) &= \frac{3\pi N^2}{4} \int \varrho_t^2 \sin^4\alpha_t \exp[-(\varrho_r+\varrho_t)] \frac{\cos\alpha_t}{\varrho_t^4} d\sigma_{rt}, \\
J_{6+m}(x_{rt}) &= \pi N^2 \int \varrho_t^2 \sin^2\alpha_t \exp[-\tfrac{1}{2}(3\varrho_t+\varrho_r)] \frac{\varrho_t^m\cos\alpha_t}{\varrho_t^4} d\sigma_{rt}, \quad (m=0,1,2,3,4,5,6), \\
J_{12+m}(x_{rt}) &= \pi N^2 \int \varrho_t^2 \sin^2\alpha_t \exp[-(\varrho_r+\varrho_t)] \frac{\varrho_t^m\cos\alpha_t}{\varrho_t^4} d\sigma_{rt}, \quad (m=1,2,3,4,5,6), \\
J_{19+m}(x_{rt}) &= \frac{3\pi N^2}{4} \int \varrho_t^2 \sin^4\alpha_t \exp[-\tfrac{1}{2}(3\varrho_t+\varrho_r) \frac{\varrho_t^m\cos\alpha_t}{\varrho_t^4} d\sigma_{rt}, \quad (m=0,1,2,3,4,5,6), \\
J_{25+m}(x_{rt}) &= \frac{3\pi N^2}{4} \int \varrho_t^2 \sin^4\alpha_t \exp[-(\varrho_r+\varrho_t)] \frac{\varrho_t^m\cos\alpha_t}{\varrho_t^4} d\sigma_{rt}, \quad (m=1,2,3,4,5), \\
J_{32}(x_{rt}) &= \pi N^2 \int \varrho_t^2 \sin^2\alpha_t \exp[-\tfrac{1}{2}(\varrho_r+\varrho_t)] d\sigma_{rt}, \\
J_{33+m}(x_{rt}) &= \pi N^2 \int \varrho_t^2 \sin^2\alpha_t \frac{\cos\alpha_t}{\varrho_r} \exp[-(\varrho_r+\varrho_t)] \varrho_r^m d\sigma_{rt}, \quad (m=0,1,2,3), \\
J_{37+m}(x_{rt}) &= \pi N^2 \int \varrho_t^2 \sin^2\alpha_t \frac{\exp[-(\varrho_r+\varrho_t)]}{\varrho_t} \varrho_t^m d\sigma_{rt}, \quad (m=0,1,2,3), \\
\tilde{J}_1(x_{rt}) = 8J_1(\tfrac{1}{2}x_{rt}) &= \pi N^2 \int \varrho_t^2 \sin^2\alpha_t \exp[-\tfrac{1}{2}(\varrho_r+\varrho_t)] \frac{\cos\alpha_t}{\varrho_t^2} d\sigma_{rt}, \\
\tilde{J}_3(x_{rt}) = 2J_3(\tfrac{1}{2}x_{rt}) &= \pi N^2 \int \varrho_t^2 \sin^2\alpha_t \exp[-\tfrac{1}{2}(\varrho_r+\varrho_t)] \frac{\cos\alpha_t}{\varrho_t^4} d\sigma_{rt}, \\
\tilde{J}_5(x_{rt}) = 2J_5(\tfrac{1}{2}x_{rt}) &= \frac{3\pi N^2}{4} \int \varrho_t^2 \sin^4\alpha_t \exp[-\tfrac{1}{2}(\varrho_r+\varrho_t)] \frac{\cos\alpha_t}{\varrho_t^4} d\sigma_{rt}, \\
\tilde{J}_{16}(x_{rt}) = 32J_{16}(\tfrac{1}{2}x_{rt}) &= \pi N^2 \int \varrho_t^2 \sin^2\alpha_t \exp[-\tfrac{1}{2}(\varrho_r+\varrho_t)] \cos\alpha_t \, d\sigma_{rt}.
\end{aligned}
\tag{8}
$$

In equation (8) use has been made of the bipolar relation [1], $\varrho_r \sin\alpha_r = \varrho_t \sin\alpha_t$.

I.

The reduction of integrals of the form

$$\int \varrho_t^l \sin^n\alpha_t \exp(-\varrho_r) \frac{\cos\alpha_t}{\varrho_t^m} d\sigma_{rt}, \quad m > l, \tag{9}$$

is straightforward and will be illustrated by the evaluation of $J_4(x_{rt})$. Since $\varrho_r\cos\alpha_r + \varrho_t\cos\alpha_t$ equals x_{rt}, we can write $J_4(x_{rt})$ as

$$J_4(x_{rt}) = \frac{3\pi N^2}{4} \int \varrho_r^4 \sin^4\alpha_r \exp(-\varrho_r) \frac{(x_{rt}-\varrho_r\cos\alpha_r)\,\varrho_r^2\, d\varrho_r \sin\alpha_r}{(\varrho_r^2+x_{rt}^2-2\varrho_r x_{rt}\cos\alpha_r)^{7/2}} d\alpha_r.$$

Letting μ equal $\cos \alpha_r$ we may reduce the preceeding expression for $J_4(x_{rt})$ to the following:

$$J_4(x_{rt}) = \frac{3\pi N^2}{4} \int_0^\infty \varrho_r^6 \exp(-\varrho_r)\, d\varrho_r \int_{-1}^1 (1-\mu^2)^2\, d\mu \frac{\partial}{\partial x_{rt}} \left\{ \frac{-\frac{1}{3}}{(\varrho_r^2 + x_{rt}^2 - 2\,\varrho_r\, x_{rt}\,\mu)^{5/2}} \right\}.$$

Using the well-known expansion for $(1+h^2-2\,h\,\mu)^{(-|m|)/2}$ (see PAULING and WILSON [2], for example), we have

$$J_4(x_{rt}) = -\frac{3\pi N^2}{20} \int_0^\infty \varrho_r^6 \exp(-\varrho_r)\, d\varrho_r \int_{-1}^1 (1-\mu^2)\, d\mu\, \tfrac{1}{3} \sum_{l=2}^\infty P_l^2(\mu) \left\{ \frac{1}{\varrho_r^5} \left(\frac{x_{rt}}{\varrho_r}\right)^{l-3} (l-2), \quad \varrho_r > x_{rt}. \right.$$
$$\left. - \frac{1}{x_{rt}^6} \left(\frac{\varrho_r}{x_{rt}}\right)^{l-2} (l+3), \quad x_{rt} > \varrho_r. \right\}$$

But since $(1-\mu^2)$ equals $\frac{1}{3} P_2^2(\mu)$ and

$$\int_{-1}^1 P_l^m(\mu)\, P_{l'}^m(\mu)\, d\mu$$

equals [3] $2(l+m)!\,\delta_{l,l'}/(2\,l+1)\,(l-m)!$, we may write

$$J_4(x_{rt}) = \frac{4\pi N^2}{5\,x^6} \int_0^x \varrho_r^6 \exp(-\varrho_r)\, d\varrho_r.$$

Defining $A_n(x)$ as

$$A_n(x) = \int_1^\infty y^n\, e^{-xy}\, dy, \tag{10}$$

we have finally

$$J_4(x_{rt}) = \frac{4\pi\, x_{rt}\, N^2}{5} \left\{ \frac{6!}{x_{rt}^7} - A_6(x_{rt}) \right\}. \tag{11}$$

II.

The integrals of the type

$$\int \varrho_t^l \sin^n \alpha_t \exp[-(\varrho_r + \varrho_t)]\, \frac{\cos \alpha_t}{\varrho_t^m}\, d\sigma_{rt} \tag{12}$$

offer more difficulty that those of (9) when $m > l$, but are still tractable. If $l > m$ equation (12) is trivial to evaluate. For example, consider

$$J_{16}(x_{rt}) = \pi N^2 \int \varrho_t^2 \sin^2 \alpha_t \exp[-(\varrho_r + \varrho_t)] \cos \alpha_t\, d\sigma_{rt}.$$

Using confocal elliptic co-ordinates [4] $(1 \le \lambda \le \infty,\ -1 \le \mu \le 1)$

$$\lambda = \frac{\varrho_t + \varrho_r}{x_{rt}}, \quad \mu = \frac{\varrho_t - \varrho_r}{x_{rt}},$$

$$d\sigma_{rt} = \left(\frac{x_{rt}}{2}\right)^3 (\lambda^2 - \mu^2)\, d\lambda\, d\mu,$$

$$\cos \alpha_t = \frac{1+\lambda\,\mu}{\lambda+\mu}, \quad \sin \alpha_t = \frac{[(\lambda^2-1)(1-\mu^2)]^{1/2}}{\lambda+\mu}, \tag{13}$$

we can write

$$J_{16}(x_{rt}) = \pi N^2 \left(\frac{x_{rt}}{2}\right)^5 \int_1^\infty \exp(-x_{rt}\,\lambda)\,(\lambda^2-1)\, d\lambda$$
$$\cdot \int_{-1}^1 d\mu \{\lambda\,\mu^4 - (\lambda^2-1)\,\mu^3 - 2\,\lambda\,\mu^2 + (\lambda^2-1)\,\mu + \lambda\},$$

$$J_{16}(x_{rt}) = \frac{16\pi N^2}{15} \left(\frac{x_{rt}}{2}\right)^5 \int_1^\infty \exp(-x_{rt}\,\lambda)\,\lambda\,(\lambda^2-1)\, d\lambda.$$

At this point one can use (10), and write

$$J_{16}(x_{rt}) = \frac{16\pi N^2}{15} \left(\frac{x_{rt}}{2}\right)^5 \{A_3(x_{rt}) - A_1(x_{rt})\}, \tag{14}$$

or, one can use the fact that the BESSEL functions $K_{n+1/2}(x)$, $I_{n+1/2}(x)$ are generated by the integrals [5]

$$K_{n+1/2}(x) = \frac{\pi^{1/2}}{n!} \left(\frac{x}{2}\right)^{n+1/2} \int_1^\infty e^{-xy} (y^2-1)^n\, dy,$$

$$I_{n+1/2}(x) = \frac{\pi^{-1/2}}{n!} \left(\frac{x}{2}\right)^{n+1/2} \int_{-1}^1 e^{-xy} (1-y^2)^n\, dy. \tag{15}$$

[2] L. PAULING and E. B. WILSON, JR., Introduction to Quantum Mechanics, McGraw-Hill, New York 1935, p. 128.

[3] E. JAHNKE and F. EMDE, Tables of Functions, Dover, New York 1945.

[4] S. GLASSTONE, Theoretical Chemistry, D. van Nostrand, New York 1944, pp. 73 and 74.

[5] G. N. WATSON, The Theory of BESSEL Functions, University Press, Cambridge 1944.

Differentiating (15) with respect to x yields the desired formulae:

$$K_{n+3/2}(x) = \frac{\pi^{1/2}}{n!}\left(\frac{x}{2}\right)^{n+1/2} \int_1^\infty e^{-xy}\, y\,(y^2-1)^n\, dy\,,$$
$$I_{n+3/2}(x) = \frac{-\pi^{-1/2}}{n!}\left(\frac{x}{2}\right)^{n+1/2} \int_{-1}^{1} e^{-xy}\, y\,(1-y^2)^n\, dy\,. \tag{16}$$

Substitution of (16) into our expression for $J_{16}(x_{rt})$ gives the alternate expression

$$J_{16}(x_{rt}) = \frac{16}{15}\,\pi^{1/2} N^2 \left(\frac{x_{rt}}{2}\right)^{7/2} K_{5/2}(x_{rt})\,. \tag{17}$$

Other integrals which may be evaluated analogously to $J_{16}(x_{rt})$ are those having structures similar to $J_{33+m}(x_{rt})$ and $J_{37+m}(x_{rt})$, $(m=0,\,1,\,2,\,3)$.

III.

The case of $m>l$ in equation (12) is more difficult. We shall illustrate the mode of computation for this case by solving the integral for $J_{26}(x_{rt})$. Using the confocal elliptic co-ordinates of equation (13), we can write

$$J_{26}(x_{rt}) = \frac{3\,\pi\,N^2}{4}\left(\frac{x_{rt}}{2}\right)^2 \int_1^\infty d\lambda\, e^{-xy}(\lambda^2-1)^2 \int_{-1}^{1} \frac{\mu(1-\mu^2)^2\,(\lambda^2-1)+\lambda(1-\mu^2)^3}{(\lambda+\mu)^5}\, d\mu\,.$$

Now there exists an expansion of $(\lambda+\mu)^{-1}$ in terms of LEGENDRE polynomials of the first and second kind. This expansion is [6]

$$\frac{1}{\lambda+\mu} = \sum_{n=0}^\infty (-1)^n\,(2n+1)\,P_n(\mu)\,Q_n(\lambda)\,, \qquad (1<\lambda<\infty\,;\; -1\le\mu\le 1)\,. \tag{18}$$

Upon differentiating (18) with respect to both λ and μ a sufficient number of times, we may substitute (18) into $J_{26}(x_{rt})$ and obtain

$$J_{26}(x_{rt}) = \frac{3\,\pi\,N^2}{4}\left(\frac{x_{rt}}{2}\right)^2 \int_1^\infty d\lambda\, \exp(-x_{rt}\,\lambda)\,(\lambda^2-1)^2 \sum_{n=0}^\infty (-1)^n \frac{(2n+1)}{24}\int_{-1}^{1} d\mu \left\{\frac{d^3P_n(\mu)}{d\mu^3}\,\frac{dQ_n(\lambda)}{d\lambda}\,\lambda(1-\mu^2)^3 + \frac{d^2P_n(\mu)}{d\mu^2}\,\frac{d^2Q_n(\lambda)}{d\lambda^2}\,(\lambda^2-1)\,\mu(1-\mu^2)^2\right\}.$$

Integrating the μ integrals by parts, noticing that the integrated terms vanish due to the $(1-\mu^2)$ factor, we have

$$J_{26}(x_{rt}) = \frac{3\,\pi\,N^2}{96}\left(\frac{x_{rt}}{2}\right)^2 \int_1^\infty d\lambda\, \exp(-x_{rt}\,\lambda)\,(\lambda^2-1)^2 \int_{-1}^{1} d\mu \sum_{n=0}^\infty (-1)^n\,(2n+1)\,P_n(\mu) \cdot\left\{8\,P_3(\mu)\,(\lambda^2-1)\,\frac{d^2Q_n(\lambda)}{d\lambda^2} + 48\,\lambda\,P_3(\mu)\,\frac{dQ_n(\lambda)}{d\lambda}\right\}$$

or

$$J_{26}(x_{rt}) = \frac{3\,\pi\,N^2}{2}\left(\frac{x_{rt}}{2}\right)^2 \int_1^\infty d\lambda\, \exp(-x_{rt}\,\lambda)\,(\lambda^2-1)^2 \left\{-\tfrac{1}{3}\,(\lambda^2-1)\,\frac{d^2Q_3(\lambda)}{d\lambda^2} - 2\,\lambda\,\frac{dQ_3(\lambda)}{d\lambda}\right\}.$$

Since $Q_n(\lambda)$ is given by [3]

$$Q_n(\lambda) = P_n(\lambda)\,Q_0(\lambda) + \sum_{j=0}^{n-1} a_j\,\lambda^j\,, \tag{19}$$

where $P_n(\lambda)$ is the n^{th} LEGENDRE polynomial and

$$Q_0(\lambda) = \tfrac{1}{2}\ln\frac{\lambda+1}{\lambda-1}\,, \tag{20}$$

we can reduce the integrand of $J_{26}(x_{rt})$ to terms involving only $\exp(-x_{rt}\,\lambda)$, $Q_0(\lambda)$, and a suitable power of λ. Defining $F_n(x)$ as

$$F_n(x) = \int_1^\infty e^{-x\lambda}\,\lambda^n\,Q_0(\lambda)\,d\lambda\,, \tag{21}$$

[6] W. MAGNUS and F. OBERHETTINGER, Formulae and Theorems for the Functions of Mathematical Physics, Chelsea, New York 1954

we can at last write $J_{26}(x_{rt})$ as

$$J_{26}(x_{rt}) = \frac{3\pi N^2}{2} x_{rt}^2 \{5 A_6(x_{rt}) - \tfrac{31}{3} A_4(x_{rt}) + 6 A_2(x_{rt}) - \tfrac{2}{3} A_0(x_{rt}) - 5 F_7(x_{rt}) + 12 F_5(x_{rt}) - 9 F_3(x_{rt}) + 2 F_1(x_{rt})\} . \tag{22}$$

IV.

By far the most difficult integrals are those of the type

$$\int \varrho_t^l \sin^n \alpha_t \exp[-\tfrac{1}{2}(3\varrho_t + \varrho_r) \frac{\cos \alpha_t}{\varrho_t^m} \, d\sigma_{rt} . \tag{23}$$

If $l > m$ the integration is relatively simple. For example, consider the integral $J_{25}(x_{rt})$. Using the coordinate transformation of equation (13) we have

$$J_{25}(x_{rt}) = \frac{3\pi N^2}{4} \left(\frac{x_{rt}}{2}\right)^7 \int_1^\infty e^{-x\lambda} (\lambda^2 - 1)^2 \, d\lambda \int_{-1}^1 e^{-(x/2)\mu} (1-\mu^2)^2 \{(\lambda^2-1)\mu + \lambda(1-\mu^2)\} \, d\mu .$$

The application of equations (15) and (16) immediately yields the desired answer

$$J_{25}(x_{rt}) = 18\pi N^2 x_{rt} (2)^{1/2} K_{7/2}(x_{rt}) \, I_{7/2}(\tfrac{1}{2} x_{rt}) . \tag{24}$$

V.

In order to evaluate (23) for the case $m > l$, we make use of the expansion [7]

$$\exp(-\tfrac{1}{2}\varrho_r) = \exp[-\tfrac{1}{2}(\varrho_t^2 + x_{rt}^2 - 2\varrho_t x_{rt} \cos\alpha_t)^{1/2}] = \sum_{n=0}^\infty \frac{(2n+1)}{(\varrho_t x_{rt})^{1/2}} p_n(\tfrac{1}{2}, r_>; r_<) \, P_n(\cos\alpha_t) , \tag{25}$$

where
$$p_n(\tfrac{1}{2}, r_>; r_<) = r_> I_{n+1/2}(\tfrac{1}{2} r_<) K_{n+3/2}(\tfrac{1}{2} r_>) - r_< I_{n-1/2}(\tfrac{1}{2} r_<) K_{n+1/2}(\tfrac{1}{2} r_>) , \tag{26}$$

$r_<$ being the smaller and $r_>$ the greater of x_{rt} and ϱ_t. We shall illustrate the use of (25) on the integrals $J_{6+m}(x_{rt})$. Letting μ equal $\cos\alpha_t$ we may write $J_{6+m}(x_{rt})$ as

$$J_{6+m}(x_{rt}) = \frac{2\pi N^2}{5} \int_0^\infty \exp(-\tfrac{3}{2}\varrho_t) \, \varrho_t^m \, d\varrho_t \int_{-1}^1 d\mu \, \{P_1(\mu) - P_3(\mu)\} \sum_{n=0}^\infty \frac{(2n+1)}{(x_{rt}\varrho_t)^{1/2}} p_n(\tfrac{1}{2}, r_>; r_<) \, P_n(\mu) ,$$

$$J_{6+m}(x_{rt}) = \frac{4\pi N^2}{5 (x_{rt})^{1/2}} \int_0^\infty \exp(-\tfrac{3}{2}\varrho_t) \, \varrho_t^m \frac{d\varrho_t}{(\varrho_t)^{1/2}} \{p_1(\tfrac{1}{2}, r_>; r_<) - p_3(\tfrac{1}{2}, r_>; r_<)\} .$$

Defining the quantity $C_n^m(x_{rt})$ as

$$C_n^m(x_{rt}) = \frac{1}{(x_{rt})^{1/2}} \int_0^\infty \exp(-\tfrac{3}{2}\varrho_t) \, \varrho_t^m \frac{d\varrho_t}{(\varrho_t)^{1/2}} p_n(\tfrac{1}{2}, r_>; r_<) , \tag{27}$$

we have the answer

$$J_{6+m}(x_{rt}) = \frac{4\pi N^2}{5} \{C_1^m(x_{rt}) - C_3^m(x_{rt})\} . \tag{28}$$

VI.

We must yet evaluate the $C_n^m(x)$ integrals. Now from equations (26) and (27), we have

$$C_n^m(x) = \frac{1}{(x)^{1/2}} \int_0^x \exp(-\tfrac{3}{2}\varrho) \, \varrho^m \frac{d\varrho}{(\varrho)^{1/2}} \{x I_{n+1/2}(\tfrac{1}{2}\varrho) K_{n+3/2}(\tfrac{1}{2}x) - \varrho I_{n-1/2}(\tfrac{1}{2}\varrho) K_{n+1/2}(\tfrac{1}{2}x)\}$$

$$+ \frac{1}{(x)^{1/2}} \int_x^\infty \exp(-\tfrac{3}{2}\varrho) \, \varrho^m \frac{d\varrho}{(\varrho)^{1/2}} \{\varrho I_{n+1/2}(\tfrac{1}{2}x) K_{n+3/2}(\tfrac{1}{2}\varrho) - x I_{n-1/2}(\tfrac{1}{2}x) K_{n+1/2}(\tfrac{1}{2}\varrho)\} .$$

[7] N. F. Mott and I. N. Sneddon, Wave Mechanics and Applications, Clarendon Press, Oxford 1948.

Setting ϱ equal to $x\,y$, we have that $C_n{}^m(x)$ becomes

$$C_n{}^m(x) = \frac{1}{(x)^{1/2}} \int_0^\infty e^{-3/2\,\varrho}\,\varrho^m \frac{\mathrm{d}\varrho}{(\varrho)^{1/2}} \{x\,I_{n+1/2}(\tfrac{1}{2}\varrho)\,K_{n+3/2}(\tfrac{1}{2}x) - \varrho\,I_{n-1/2}(\tfrac{1}{2}\varrho)\,K_{n+1/2}(\tfrac{1}{2}x)\}$$

$$+ x^{m+1} \int_1^\infty e^{-3/2\,xy}\,y^m \frac{\mathrm{d}y}{(y)^{1/2}} \{y\,I_{n+1/2}(\tfrac{1}{2}x)\,K_{n+3/2}(\tfrac{1}{2}y) - I_{n-1/2}(\tfrac{1}{2}x)\,K_{n+1/2}(\tfrac{1}{2}xy)\}$$

$$+ x^{m+1} \int_1^\infty e^{-3/2\,xy}\,y^m \frac{\mathrm{d}y}{(y)^{1/2}} \{y\,I_{n-1/2}(\tfrac{1}{2}xy)\,K_{n+1/2}(\tfrac{1}{2}x) - I_{n+1/2}(\tfrac{1}{2}xy)\,K_{n+3/2}(\tfrac{1}{2}x)\}\,.$$

Defining $G_n{}^m(\frac{1}{2}x)$ and $H_n{}^m(\frac{1}{2}x)$ such that

$$G_n{}^m(\tfrac{1}{2}x) = \int_1^\infty e^{-3/2\,xy}\,y^m\,I_{n+1/2}(\tfrac{1}{2}xy)\,\frac{\mathrm{d}y}{(y)^{1/2}}, \qquad H_n{}^m(\tfrac{1}{2}x) = \int_1^\infty e^{-3/2\,xy}\,y^m\,K_{n+1/2}(\tfrac{1}{2}xy)\,\frac{\mathrm{d}y}{(y)^{1/2}}, \tag{29}$$

and using the formula [5]

$$\int_0^\infty e^{-3/2\,\varrho}\,\varrho^m\,I_{n+1/2}(\tfrac{1}{2}\varrho)\,\frac{\mathrm{d}\varrho}{(\varrho)^{1/2}} = \left(\frac{\pi}{2}\right)^{-1/2} (-1)^m\,2^{m+1/2}\,Q_n{}^m(3)\,, \tag{30}$$

where

$$Q_n{}^m(3) = \left.\frac{\mathrm{d}^m Q_n(x)}{\mathrm{d}x^m}\right]_{x=3}, \tag{31}$$

we obtain

$$C_n{}^m(x) = (-2)^m \left(\frac{4\,x}{\pi}\right)^{1/2} \{K_{n+3/2}(x/2)\,Q_n{}^m(3) + (x/2)\,K_{n+1/2}(x/2)\,Q_{n-1}^{m+1}(3)\}$$
$$+ x^{m+1} \left\{\begin{matrix} H_{n+1}^{m+1}(x/2)\,I_{n+1/2}(x/2) - H_n{}^m(x/2)\,I_{n-1/2}(x/2) - G_n{}^m(x/2)\,K_{n+3/2}(x/2) \\ + G_{n-1}^{m+1}(x/2)\,K_{n+1/2}(x/2) \end{matrix}\right\}. \tag{32}$$

Since the Bessel functions take the form [5]

$$K_{n+1/2}(x\,y/2) = \left(\frac{4\pi}{x\,y}\right)^{1/2} \overline{K}_{n+1/2}(x\,y/2), \qquad I_{n+1/2}(x\,y/2) = \frac{2}{(\pi\,x\,y)^{1/2}}\,\overline{I}_{n+1/2}(x\,y/2), \tag{33}$$

where

$$\overline{K}_{n+1/2}(x\,y/2) = \tfrac{1}{2}\,e^{-xy/2} \sum_{j=0}^{n} \frac{(n+j)!}{j!\,(n-j)!\,x^j\,y^j},$$

$$\overline{I}_{n+1/2}(x\,y/2) = \tfrac{1}{2} \sum_{j=0}^{n} \frac{(n+j)!}{j!\,(n-j)!\,x^j\,y^j}\,[(-1)^j\,e^{xy/2} + (-1)^{n+1}\,e^{-xy/2}]\,, \tag{34}$$

we can immediately see that

$$G_n{}^m(x/2) = (\pi\,x)^{-1/2}\,\overline{G_n{}^m}(x/2)\,, \qquad H_n{}^m(x/2) = (\pi/x)^{1/2}\,\overline{H_n{}^m}(x/2)\,, \tag{35}$$

$\overline{G_n{}^m}(x/2)$, $\overline{H_n{}^m}(x/2)$ being the expressions

$$\overline{G_n{}^m}(x/2) = \sum_{j=0}^{n} \frac{(n+j)!}{j!\,(n-j)!\,x^j} \{(-1)^j\,E_{j-m+1}(x) + (-1)^{n+1}\,E_{j-m+1}(2\,x)\}\,,$$
$$\overline{H_n{}^m}(x/2) = \sum_{j=0}^{n} \frac{(n+j)!}{j!\,(n-j)!\,x^j}\,E_{j-m+1}(2\,x)\,. \tag{36}$$

In equation (36) we have used Placzek's notation [8] for the exponential integrals, $E_n(x)$,

$$E_n(x) = \int_1^\infty e^{-xy}\,y^{-n}\,\mathrm{d}y\,. \tag{37}$$

[8] G. Placzek, The Functions $E_n(x)$, National Research Council of Canada, Ontario 1946.

We see that for $n<0$, $n=-m$ $(m>0)$ say, we have the relation

$$E_{-m}(x)=A_m(x)\,, \qquad (m=0,1,2,\ldots)\,, \tag{38}$$

the $A_m(x)$ integrals being defined as in equation (10).

If we substitute (33) and (35) into (32) we obtain the more convenient computational relation

$$\begin{aligned} C_n{}^m(x) = {} & 2x^m[(-1)^m 2(2/x)^m\{\overline{K}_{n+3/2}(x/2)\,Q_n{}^m(3)+(2/x)\,\overline{K}_{n+1/2}(x/2)\,Q_{n-1}^{m+1}(3)\}] \\ & +2x^m\{-\overline{G}_n{}^m(x/2)\overline{K}_{n+3/2}(x/2)+\overline{G}_{n-1}^{m+1}(x/2)\,\overline{K}_{n+1/2}(x/2)-\overline{H}_n{}^m(x/2)\,\overline{I}_{n-1/2}(x/2) \\ & +\overline{H}_{n+1}^{m+1}(x/2)\,\overline{I}_{n+1/2}(x/2)\}\,. \end{aligned} \tag{39}$$

Equations (28), (31), (34), (36), (37), (38), and (39) suffice for the determination of the integrals $J_{6+m}(x_{rt})$, $(m=0,1,2,3,4,5)$.

The results of employing the methods outlined above to the evaluation of all the $J_j(x_{rt})$ integrals are summarized below.

$$J_0(x)=32\pi N^2 x^3\left\{\frac{1}{60}A_1(x)-\frac{1}{24}A_4(x)+\frac{1}{40}A_6(x)+\frac{1}{x^5}-\frac{18}{x^7}\right\}$$

$$J_1(x)=\frac{\pi N^2}{4}x^3\left\{7A_5(x)-\frac{38}{3}A_3(x)+\frac{17}{3}A_1(x)-7F_6(x)+15F_4(x)-9F_2(x)+F_0(x)\right\}$$

$$J_2(x)=\frac{4\pi N^2}{3}x\left\{\frac{24}{x^5}-A_4(x)\right\}$$

$$J_3(x)=\pi N^2 x\left\{5A_3(x)-\frac{13}{3}A_1(x)-5F_4(x)+6F_2(x)-F_0(x)\right\}$$

$$J_4(x)=\frac{4\pi N^2}{5}x\left\{\frac{720}{x^7}-A_6(x)\right\}$$

$$J_5(x)=\frac{3\pi N^2}{4}x\left\{-7A_5(x)+\frac{38}{3}A_3(x)-\frac{27}{5}A_1(x)+7F_6(x)-15F_4(x)+9F_2(x)-F_0(x)\right\}$$

$$J_6(x)=\frac{4\pi N^2}{5}\{C_1{}^0(x)-C_3{}^0(x)\} \qquad J_7(x)=\frac{4\pi N^2}{5}\{C_1{}^1(x)-C_3{}^1(x)\}$$

$$J_8(x)=\frac{4\pi N^2}{5}\{C_1{}^2(x)-C_3{}^2(x)\} \qquad J_9(x)=\frac{4\pi N^2}{5}\{C_1{}^3(x)-C_3{}^3(x)\}$$

$$J_{10}(x)=\frac{4\pi N^2}{5}\{C_1{}^4(x)-C_3{}^4(x)\} \qquad J_{11}(x)=\frac{4\pi N^2}{5}\{C_1{}^5(x)-C_3{}^5(x)\}$$

$$\begin{aligned} J_{12}(x)=4\pi N^2x^2\Big\{&-\frac{7}{x}\overline{K}_{7/2}(x)\,\overline{I}_{5/2}(x/2)-\frac{16}{x}\overline{K}_{5/2}(x)\,\overline{I}_{7/2}(x/2)-2\overline{K}_{3/2}(x)\,\overline{I}_{7/2}(x/2) \\ &+\overline{K}_{5/2}(x)\,\overline{I}_{5/2}(x/2)+\overline{K}_{7/2}(x)\,\overline{I}_{3/2}(x/2)\Big\} \end{aligned}$$

$$J_{13}(x)=\frac{\pi N^2}{2}x^2\{-9A_4(x)+11A_2(x)-2A_0(x)+9F_5(x)-14F_3(x)+5F_1(x)\}$$

$$J_{14}(x)=J_1(x)$$

$$J_{15}(x)=\frac{\pi N^2x^4}{4}\{-A_6(x)+\tfrac{8}{3}A_4(x)-2A_2(x)+\tfrac{1}{3}A_0(x)+F_7(x)-3F_5(x)+3F_3(x)-F_1(x)\}$$

$$J_{16}(x)=\frac{2}{15}\pi N^2x^3\overline{K}_{5/2}(x)=\frac{\pi N^2}{30}x^5\{A_3(x)-A_1(x)\}$$

$$J_{17}(x)=\frac{\pi N^2}{15}x^3\{5\overline{K}_{5/2}(x)+x\overline{K}_{3/2}(x)\}=\frac{\pi N^2}{240}x^6\{5A_4(x)-6A_2(x)+A_0(x)\}$$

$$J_{18}(x)=\frac{\pi N^2}{105}x^4\{21\overline{K}_{7/2}(x)+4x\overline{K}_{5/2}(x)\}=\frac{\pi N^2}{240}x^7\left\{3A_5(x)-\frac{26}{7}A_3(x)+\frac{5}{7}A_1(x)\right\}$$

$$J_{19}(x)=\frac{4\pi N^2}{105}\{5C_5{}^0(x)-14C_3{}^0(x)+9C_1{}^0(x)\} \qquad J_{20}(x)=\frac{4\pi N^2}{105}\{5C_5{}^1(x)-14C_3{}^1(x)+9C_1{}^1(x)\}$$

$$J_{21}(x) = \frac{4\pi N^2}{105}\{5\,C_5^2(x) - 14\,C_3^2(x) + 9\,C_1^2(x)\} \qquad J_{22}(x) = \frac{4\pi N^2}{105}\{5\,C_5^3(x) - 14\,C_3^3(x) + 9\,C_1^3(x)\}$$

$$J_{23}(x) = \frac{4\pi N^2}{105}\{5\,C_5^4(x) - 14\,C_3^4(x) + 9\,C_1^4(x)\} \qquad J_{24}(x) = \frac{4\pi N^2}{105}\{5\,C_5^5(x) - 14\,C_3^5(x) + 9\,C_1^5(x)\}$$

$$J_{25}(x) = 72\,\pi N^2 K_{7/2}(x)\, I_{7/2}(x/2)$$

$$J_{26}(x) = \frac{3\pi N^2}{2} x^2 \left\{5\,A_6(x) - \frac{31}{3}A_4(x) + 6\,A_2(x) - \frac{2}{3}A_0(x) - 5\,F_7(x) + 12\,F_5(x) - 9\,F_3(x) + 2\,F_1(x)\right\}$$

$$J_{27}(x) = \frac{3\pi N^2}{8} x^3 \{-15\,A_7(x) + 37\,A_5(x) - 29\,A_3(x) + 7\,A_1(x) + 15\,F_8(x) - 42\,F_6(x) + 40\,F_4(x) - 14\,F_2(x) + F_0(x)\}$$

$$J_{28}(x) = \frac{3\pi N^2}{32} x^4 \{25\,A_8(x) - \tfrac{227}{3}A_6(x) + 79\,A_4(x) - 31\,A_2(x) + \tfrac{8}{3}A_0(x) - 25\,F_9(x) + 84\,F_7(x) - 102\,F_5(x) + 52\,F_3(x) - 9\,F_1(x)\}$$

$$J_{29}(x) = \frac{3\pi N^2}{64} x^5 \{-11\,A_9(x) + \tfrac{124}{3}A_7(x) - \tfrac{286}{5}A_5(x) + \tfrac{172}{5}A_3(x) - \tfrac{113}{15}A_1(x) + 11\,F_{10}(x) - 45\,F_8(x) + 70\,F_6(x) - 50\,F_4(x) + 15\,F_2(x) - F_0(x)\}$$

$$J_{30}(x) = \frac{3\pi N^2}{64} x^6 \{A_{10}(x) - \tfrac{14}{3}A_8(x) + \tfrac{128}{15}A_6(x) - \tfrac{22}{3}A_4(x) + \tfrac{41}{15}A_2(x) - \tfrac{4}{15}A_0(x) - F_{11}(x) + 5\,F_9(x) - 10\,F_7(x) + 10\,F_5(x) - 5\,F_3(x) + F_1(x)\}$$

$$J_{31}(x) = \tfrac{3}{35}\pi N^2 x^4 K_{7/2}(x) = \frac{3\pi N^2}{560} x^7 \{A_5(x) - 2\,A_3(x) + A_1(x)\}$$

$$J_{32}(x) = \frac{8\pi N^2}{15} x^2 \{10\,K_{5/2}(x/2) + x\,K_{3/2}(x/2)\} = \frac{\pi N^2}{120} x^5 \{5\,A_4(x/2) - 6\,A_2(x/2) + A_0(x/2)\}$$

$$J_{33}(x) = \frac{x^2}{96}K_{3/2}(x) \qquad J_{34}(x) = \frac{x^3}{240}K_{5/2}(x)$$

$$J_{35}(x) = \frac{x^3}{480}\{3\,K_{5/2}(x) + x\,K_{3/2}(x)\} \qquad J_{36}(x) = \frac{x^4}{3360}\{7\,K_{7/2}(x) + 4\,x\,K_{5/2}(x)\}$$

$$J_{37}(x) = \frac{x^2}{96}K_{5/2}(x) \qquad J_{38}(x) = \frac{x^2}{240}\{5\,K_{5/2}(x) + x\,K_{3/2}(x)\}$$

$$J_{39}(x) = \frac{x^3}{480}\{5\,K_{7/2} + x\,K_{5/2}(x)\} \qquad J_{40}(x) = \frac{x^3}{3360}\{105\,K_{7/2}(x) + 35\,x\,K_{5/2}(x) + 4\,x^2 K_{3/2}(x)\}$$

$$\tilde{J}_1(x) = 8\,J_1(\tfrac{1}{2}x) \qquad \tilde{J}_3(x) = 2\,J_3(\tfrac{1}{2}x) \qquad \tilde{J}_5(x) = 2\,J_5(\tfrac{1}{2}x) \qquad \tilde{J}_{16}(x) = 32\,J_{16}(\tfrac{1}{2}x)$$

$$A_n(x) = \int_1^\infty e^{-xy} y^n\,dy = E_{-n}(x) \qquad F_n(x) = \int_1^\infty e^{-xy} y^n Q_0(y)\,dy$$

$$K_{n+1/2}(x) = \frac{1}{n!}\left(\frac{x}{2}\right)^{n+1}\int_1^\infty e^{-xy}(y^2-1)^n\,dy \qquad K_{n+3/2}(x) = \frac{1}{n!}\left(\frac{x}{2}\right)^{n+1}\int_1^\infty e^{-xy}\,y\,(y^2-1)^n\,dy$$

$$I_{n+1/2}(x) = \frac{1}{n!}\left(\frac{x}{2}\right)^{n+1}\int_{-1}^1 e^{-xy}(1-y^2)^n\,dy \qquad I_{n+3/2}(x) = -\frac{1}{n!}\left(\frac{x}{2}\right)^{n+1}\int_{-1}^1 e^{-xy}\,y\,(1-y^2)^n\,dy\,. \quad (40)$$

In equation (40) we have designated x_{rt} by x for convenience. The quantity N^2 is defined as $1/32\,\pi$.

Numerical Computation of the Integrals $J_i(x)$ and $\tilde{J}_i(x)$

As was seen in the previous section, the numerical evaluation of the $J_i(x)$ and $\tilde{J}_i(x)$ integrals involves the extensive tabulation of the auxiliary functions $A_n(x)$, $F_n(x)$, $I_{n+1/2}(x)$, $K_{n+1/2}(x)$, $Q_n^m(3)$, $G_n^m(x)$, $H_n^m(x)$, $C_n^m(x)$, and $E_n(x)$ [recall that $E_{-n}(x)$ equals $A_n(x)$, $n>0$]. There exist tabulations of some

$J_n(x)$	$(1/2\,x_{01})$	$x_{01} = 8.5$	$(7/4)^{1/2}\,x_{01}$	$(3/2)\,x_{01}$	$(3)^{1/2}\,x_{01}$	$(13/4)^{1/2}x_{01}$	$2\,x_{01}$
$J_0\,(x)$	$2.0920 \cdot 10^{-2}$	$1.0520 \cdot 10^{-2}$	$6.7897 \cdot 10^{-3}$	$5.4717 \cdot 10^{-3}$	$4.2306 \cdot 10^{-3}$	$3.9324 \cdot 10^{-3}$	$3.2447 \cdot 10^{-3}$
$J_1\,(x)$	$4.1989 \cdot 10^{-4}$	$1.5902 \cdot 10^{-5}$	$1.4988 \cdot 10^{-6}$	$3.9390 \cdot 10^{-7}$	$6.6373 \cdot 10^{-8}$	$3.8361 \cdot 10^{-8}$	$8.2238 \cdot 10^{-9}$
$J_2\,(x)$	$1.2870 \cdot 10^{-3}$	$1.7732 \cdot 10^{-4}$	$6.1752 \cdot 10^{-5}$	$3.7671 \cdot 10^{-5}$	$2.1263 \cdot 10^{-5}$	$1.8124 \cdot 10^{-5}$	$1.1971 \cdot 10^{-5}$
$J_3\,(x)$	$1.0408 \cdot 10^{-4}$	$2.0368 \cdot 10^{-6}$	$1.4547 \cdot 10^{-7}$	$3.3706 \cdot 10^{-8}$	$4.9130 \cdot 10^{-9}$	$2.7269 \cdot 10^{-9}$	$5.2621 \cdot 10^{-10}$
$J_4\,(x)$	$4.2248 \cdot 10^{-4}$	$3.5500 \cdot 10^{-5}$	$8.2898 \cdot 10^{-6}$	$4.0645 \cdot 10^{-6}$	$1.7516 \cdot 10^{-6}$	$1.3817 \cdot 10^{-6}$	$7.4419 \cdot 10^{-7}$
$J_5\,(x)$	$4.0389 \cdot 10^{-5}$	$7.6098 \cdot 10^{-7}$	$5.3456 \cdot 10^{-8}$	$1.2293 \cdot 10^{-8}$	$1.7763 \cdot 10^{-9}$	$9.8351 \cdot 10^{-10}$	$1.8860 \cdot 10^{-10}$
$J_6\,(x)$		$2.6173 \cdot 10^{-5}$			$1.1980 \cdot 10^{-6}$		$3.8540 \cdot 10^{-7}$
$J_7\,(x)$		$3.4525 \cdot 10^{-5}$			$1.6256 \cdot 10^{-6}$		$5.2547 \cdot 10^{-7}$
$J_8\,(x)$		$6.7938 \cdot 10^{-5}$			$3.3256 \cdot 10^{-6}$		$1.0822 \cdot 10^{-6}$
$J_9\,(x)$		$1.7702 \cdot 10^{-4}$			$9.1123 \cdot 10^{-6}$		$2.9908 \cdot 10^{-6}$
$J_{10}(x)$		$5.7165 \cdot 10^{-4}$			$3.1326 \cdot 10^{-5}$		$1.0393 \cdot 10^{-5}$
$J_{11}(x)$		$2.1929 \cdot 10^{-3}$			$1.2959 \cdot 10^{-4}$		$4.3557 \cdot 10^{-5}$
$J_{12}(x)$		$9.6998 \cdot 10^{-3}$			$6.2652 \cdot 10^{-4}$		$2.1387 \cdot 10^{-4}$

Table 1. Numerical Values of the Integrals $J_n(x)$, $(n=0, 1, \ldots, 12)$.

$J_n(x)$	$(1/2)\,x_{01}$	$x_{01} = 8.5$	$(7/4)^{1/2}\,x_{01}$	$(3/2)\,x_{01}$	$(3)^{1/2}\,x_{01}$	$(13/4)^{1/2}\,x_{01}$	$2\,x_{01}$
$J_{13}(x)$	$1.7696 \cdot 10^{-4}$	$4.6726 \cdot 10^{-6}$	$3.7627 \cdot 10^{-7}$	$9.1968 \cdot 10^{-8}$	$1.4243 \cdot 10^{-8}$	$8.0392 \cdot 10^{-9}$	$1.6199 \cdot 10^{-9}$
$J_{14}(x)$	$4.1989 \cdot 10^{-4}$	$1.5902 \cdot 10^{-5}$	$1.4988 \cdot 10^{-6}$	$3.9390 \cdot 10^{-7}$	$6.6373 \cdot 10^{-8}$	$3.8361 \cdot 10^{-8}$	$8.2238 \cdot 10^{-9}$
$J_{15}(x)$	$1.2378 \cdot 10^{-3}$	$6.9671 \cdot 10^{-5}$	$7.8806 \cdot 10^{-6}$	$2.2562 \cdot 10^{-6}$	$4.2040 \cdot 10^{-7}$	$2.4999 \cdot 10^{-7}$	$5.7756 \cdot 10^{-8}$
$J_{16}(x)$	$4.2704 \cdot 10^{-3}$	$3.6301 \cdot 10^{-4}$	$4.9996 \cdot 10^{-5}$	$1.5712 \cdot 10^{-5}$	$3.2684 \cdot 10^{-6}$	$2.0052 \cdot 10^{-6}$	$5.0292 \cdot 10^{-7}$
$J_{17}(x)$	$1.6664 \cdot 10^{-2}$	$2.1441 \cdot 10^{-3}$	$3.6217 \cdot 10^{-4}$	$1.2544 \cdot 10^{-4}$	$2.9273 \cdot 10^{-5}$	$1.8555 \cdot 10^{-5}$	$5.0710 \cdot 10^{-6}$
$J_{18}(x)$	$7.2032 \cdot 10^{-2}$	$1.3926 \cdot 10^{-2}$	$2.8926 \cdot 10^{-3}$	$1.1061 \cdot 10^{-3}$	$2.9022 \cdot 10^{-4}$	$1.9019 \cdot 10^{-4}$	$5.6739 \cdot 10^{-5}$
$J_{19}(x)$		$1.1010 \cdot 10^{-5}$			$5.0550 \cdot 10^{-7}$		$1.6271 \cdot 10^{-7}$
$J_{20}(x)$		$1.4270 \cdot 10^{-5}$			$6.7531 \cdot 10^{-7}$		$2.1853 \cdot 10^{-7}$
$J_{21}(x)$		$2.7459 \cdot 10^{-5}$			$1.3534 \cdot 10^{-6}$		$4.4112 \cdot 10^{-7}$
$J_{22}(x)$		$6.9692 \cdot 10^{-5}$			$3.6155 \cdot 10^{-6}$		$1.1893 \cdot 10^{-6}$
$J_{23}(x)$		$2.1859 \cdot 10^{-4}$			$1.2064 \cdot 10^{-5}$		$4.0131 \cdot 10^{-6}$
$J_{24}(x)$		$8.1290 \cdot 10^{-4}$			$4.8237 \cdot 10^{-5}$		$1.6263 \cdot 10^{-5}$

Table 2. Numerical Values of the Integrals $J_n(x)$, $(n=13, 14, 15, \ldots, 24)$.

$J_n(x)$	$(1/2)\,x_{01}$	$x_{01} = 8.5$	$(7/4)^{1/2}\,x_{01}$	$(3/2)\,x_{01}$	$(3)^{1/2}\,x_{01}$	$(13/4)^{1/2}\,x_{01}$	$2\,x_{01}$
$J_{25}(x)$		$3.4828 \cdot 10^{-3}$			$2.2458 \cdot 10^{-4}$		$7.6911 \cdot 10^{-5}$
$J_{26}(x)$	$6.4449 \cdot 10^{-5}$	$1.5560 \cdot 10^{-6}$	$1.2004 \cdot 10^{-7}$	$2.8748 \cdot 10^{-8}$	$4.3456 \cdot 10^{-9}$	$2.4359 \cdot 10^{-9}$	$4.8197 \cdot 10^{-10}$
$J_{27}(x)$	$1.4417 \cdot 10^{-4}$	$4.6822 \cdot 10^{-6}$	$4.0855 \cdot 10^{-7}$	$1.0342 \cdot 10^{-7}$	$1.6656 \cdot 10^{-8}$	$9.5004 \cdot 10^{-9}$	$1.9680 \cdot 10^{-9}$
$J_{28}(x)$	$4.0411 \cdot 10^{-4}$	$1.8222 \cdot 10^{-5}$	$1.8403 \cdot 10^{-6}$	$4.9847 \cdot 10^{-7}$	$8.6878 \cdot 10^{-8}$	$5.0677 \cdot 10^{-8}$	$1.1123 \cdot 10^{-8}$
$J_{29}(x)$	$1.3389 \cdot 10^{-3}$	$8.5316 \cdot 10^{-5}$	$1.0136 \cdot 10^{-5}$	$2.9645 \cdot 10^{-6}$	$5.6559 \cdot 10^{-7}$	$3.3868 \cdot 10^{-7}$	$7.9489 \cdot 10^{-8}$
$J_{30}(x)$	$5.0667 \cdot 10^{-3}$	$4.5920 \cdot 10^{-4}$	$6.4858 \cdot 10^{-5}$	$2.0604 \cdot 10^{-5}$	$4.3370 \cdot 10^{-6}$	$2.6693 \cdot 10^{-6}$	$6.7489 \cdot 10^{-7}$
$J_{31}(x)$	$2.1426 \cdot 10^{-2}$	$2.7566 \cdot 10^{-3}$	$4.6565 \cdot 10^{-4}$	$1.6128 \cdot 10^{-4}$	$3.7636 \cdot 10^{-5}$	$2.3856 \cdot 10^{-5}$	$6.5198 \cdot 10^{-6}$
$J_{32}(x)$		$2.5095 \cdot 10^{-1}$			$3.5983 \cdot 10^{-2}$		$1.6144 \cdot 10^{-2}$
$J_{33}(x)$	$1.6577 \cdot 10^{-3}$	$8.5573 \cdot 10^{-5}$	$9.3794 \cdot 10^{-6}$	$2.6501 \cdot 10^{-6}$	$4.8677 \cdot 10^{-7}$	$2.8835 \cdot 10^{-7}$	$6.5980 \cdot 10^{-8}$
$J_{34}(x)$	$4.2704 \cdot 10^{-3}$	$3.6301 \cdot 10^{-4}$	$4.9996 \cdot 10^{-5}$	$1.5712 \cdot 10^{-5}$	$3.2684 \cdot 10^{-6}$	$2.0052 \cdot 10^{-6}$	$5.0292 \cdot 10^{-7}$
$J_{35}(x)$	$1.2394 \cdot 10^{-2}$	$1.7810 \cdot 10^{-3}$	$3.1218 \cdot 10^{-4}$	$1.0973 \cdot 10^{-4}$	$2.6004 \cdot 10^{-5}$	$1.6550 \cdot 10^{-5}$	$4.5680 \cdot 10^{-6}$
$J_{36}(x)$	$3.8703 \cdot 10^{-2}$	$9.6376 \cdot 10^{-3}$	$2.1683 \cdot 10^{-3}$	$8.5523 \cdot 10^{-4}$	$2.3168 \cdot 10^{-4}$	$1.5308 \cdot 10^{-4}$	$4.6597 \cdot 10^{-5}$

Table 3. Numerical Values of the Integrals $J_n(x)$, $(n=25, 26, \ldots, 36)$.

$J_n(x)$	$(1/2\,x_{01})$	$x_{01} = 8.5$	$(7/4)^{1/2}\,x_{01}$	$(3/2)\,x_{01}$	$(3)^{1/2}\,x_{01}$	$(13/4)^{1/2}\,x_{01}$	$2\,x_{01}$
$J_{37}(x)$	$2.5120 \cdot 10^{-3}$	$1.0677 \cdot 10^{-4}$	$1.1116 \cdot 10^{-5}$	$3.0809 \cdot 10^{-6}$		$3.2714 \cdot 10^{-7}$	
$J_{38}(x)$	$7.8421 \cdot 10^{-3}$	$5.0448 \cdot 10^{-4}$	$6.4418 \cdot 10^{-5}$	$1.9677 \cdot 10^{-5}$		$2.4217 \cdot 10^{-6}$	
$J_{39}(x)$	$2.8680 \cdot 10^{-2}$	$2.8040 \cdot 10^{-3}$	$4.4214 \cdot 10^{-4}$	$1.4936 \cdot 10^{-4}$		$2.1418 \cdot 10^{-5}$	
$J_{40}(x)$	$1.1873 \cdot 10^{-1}$	$1.7504 \cdot 10^{-2}$	$3.4126 \cdot 10^{-3}$	$1.2762 \cdot 10^{-3}$		$2.1356 \cdot 10^{-4}$	
$\tilde{J}_1\,(x)$		$3.3591 \cdot 10^{-3}$			$3.2540 \cdot 10^{-4}$		$1.2722 \cdot 10^{-4}$
$\tilde{J}_3\,(x)$		$2.0815 \cdot 10^{-4}$			$1.1993 \cdot 10^{-5}$		$4.0737 \cdot 10^{-6}$
$\tilde{J}_5\,(x)$		$8.0778 \cdot 10^{-5}$			$4.5180 \cdot 10^{-6}$		$1.5220 \cdot 10^{-6}$
$\tilde{J}_{16}(x)$		$1.3665 \cdot 10^{-1}$			$2.4719 \cdot 10^{-2}$		$1.1616 \cdot 10^{-2}$

Table 4. Numerical Values of the Integrals $J_n(x)$, $(n=37, 38, 39, 40)$, and $\tilde{J}_n(x)$, $(n=1, 3, 5, 16)$.

of the functions enumerated above[9-15], but none of these tabulations were extensive enough for our purposes. Practically all of the functions listed above have been computed ab initio from the following formulae[5, 8, 9, 15]:

$$A_n(x) = A_0(x) + \frac{n}{x} A_{n-1}(x), \qquad A_0(x) = \frac{e^{-x}}{x}.$$

$$F_n(x) = F_{n-2}(x) + \frac{1}{x} \{n F_{n-1}(x) - (n-2) F_{n-3}(x) - A_{n-2}(x)\},$$

$$F_0(x) = \tfrac{1}{2} \left\{ (\ln 2x + c) A_0(x) + E_1(2x) \frac{e^x}{x} \right\}, \quad c = 0.5772156649\ldots,$$

$$F_1(x) = \tfrac{1}{2} \left\{ (\ln 2x + c) A_1(x) + E_1(2x) \frac{e^x}{x} \left(-1 + \frac{1}{x} \right) \right\}.$$

$$I_{n+1/2}(x) = I_{n-3/2}(x) - \frac{(2n-1)}{x} I_{n-1/2}(x); \quad I_{-1/2}(x) = \cosh x; \quad I_{1/2}(x) = \sinh x.$$

$$K_{n+1/2}(x) = K_{n-3/2}(x) + \frac{(2n-1)}{x} K_{n-1/2}(x), \; K_{-1/2}(x) = K_{1/2}(x) = \tfrac{1}{2} e^{-x}.$$

$$E_n(x) = \frac{x}{n-1} \{E_0(x) - E_{n-1}(x)\}, \quad E_0(x) = A_0(x) = \frac{e^{-x}}{x}, \quad n > 1;$$

$$E_1(x) = E_0(x) \sum_{j=0}^{\infty} (-1)^j j!/x^j, \quad x \gg 1 \text{ (asymptomatic expansion)};$$

$E_1(x)$ = tabulated for small x[15]. $Q_n^m(3)$ = calculated from definitions (19) and (31)

$G_n^m(x)$ and $H_n^m(x)$ calculated from definitions (36). $C_n^m(x)$ = calculated from definitions (39). (41)

Using the results of performing the calculations indicated in equations (40) and (41) we arrive at the required values of $J_i(x)$ and $\tilde{J}_i(x)$. These values are tabulated in Tables 1 – 4. The result of substituting the numerical values of $J_i(x)$ and $\tilde{J}_i(x)$ into equations (1) through (7) to numerically evaluate the $I_j(x)$. ($j = 0, 1, 2, 3, 4, 5, 6$) has already been given in I.

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