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Note

Complex-Plane Methods for Evaluating Integrals with Highly Oscillatory Integrands*

I. Introduction

Complex-plane methods have been very effective in the numerical and analytical evaluation of many integrals of interest in physics. (Typical examples are given in Refs. [1–7].) Of particular importance are integrals that can be evaluated by the methods of steepest descent [1, 2, 4] and of stationary phase [4] and integrals whose integrands have rapid *asymptotic* oscillations [1, 3, 4, 6, 7]. We report briefly here on two general types of highly oscillatory integrals which can be evaluated easily by deforming the contour of integration in the complex plane. Other methods for evaluating special cases of such integrals are given, e.g., in Refs. [8, 9].

A. *Oscillatory Integrands with Exponential Damping*

Consider an integral of the form

$$I^{(+)}(k, a) = \int_0^\infty f^{(+)}(k, a; \chi)\, dx, \tag{1.1}$$

where k and a are oscillation and damping coefficients, respectively, as can be seen from the asymptotic form of $f^{(+)}$,

$$f^{(+)}(k, a; \chi) \xrightarrow[x \to \infty]{} B^{(+)}(x)\, e^{ikx} e^{-ax}, \tag{1.2}$$

and $B^{(+)}(x)$ is a rational function of x. For small values of k (relative to a), the integral can be evaluated by integrating along the real axis, normally by using a standard quadrature scheme. However, if $k \sim a$, the integrand begins to oscillate rapidly, making the real-axis integration very difficult, and for larger values of k, it becomes crucial to use a complex-plane technique to evaluate the integral. We let $x \to z = x + iy$ and deform the contour by rotating the real axis to the line defined by

$$y(x) = \frac{k}{a} x, \tag{1.3}$$

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so that

$$e^{ikz}e^{-az} = e^{-a^{-1}(k^2+a^2)x}, \tag{1.4}$$

which decreases exponentially with *no* oscillatory behavior. The resulting integral along this line now converges very rapidly. Note that the asymptotic oscillations are eliminated for *any* value of k. This method may be used to evaluate numerically a number of simple integrals having highly oscillatory behavior and the high-momentum components of the Fourier and spherical Bessel-function transforms of the Woods–Saxon and Gaussian potentials. It can also be used to evaluate certain types of oscillatory principal-value integrals. For further details, see Ref. [7].

B. *Oscillatory Integrands with No Exponential Damping*

An example of this type is [6–8]

$$I_{ll'L}(kk'p) = \int_0^\infty r^2 j_l(kr)\, j_{l'}(k'r)\, j_L(pr)\, dr, \tag{1.5}$$

where $j_l(x)$ is a spherical Bessel function. This integral cannot be evaluated by numerical integration along the real axis. It can be expressed in terms of a hypergeometric function whose series expansion is much too complicated to be useful. Equation (1.5) does reduce to a closed-form expansion [8] for the case in which l', l', L and k, k', p satisfy certain triangular inequalities. (See Section III.) However, the only general, reliable way to evaluate such an integral is by a complex-plane method [3, 6, 7]. Integrals of this type are the most important examples of the method we are using, and the remainder of this paper will be devoted to the evaluation of the general integral

$$J^{(R,m)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n) = \int_R^\infty r^m \left[\prod_{i=1}^n \chi_{l_i}(k_i r)\right] dr, \tag{1.6}$$

where m and $n > 0$ are arbitrary integers and $\chi_{l_i}(k_i r)$ is a spherical Bessel function, j_{l_i}, or a spherical Neumann function n_{l_i}. Special cases of this integral have been discussed in Refs. [6–8] (for $m = 2$, $n = 3$) and in Ref. [9] (for $m = 0$, $n = 3$).

II. Complex-Plane Method for Evaluating Eq. (1.6)

Consider the integral

$$J^{(m)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n) = \int_0^\infty r^m \left[\prod_{i=1}^n \chi_{l_i}(k_i r)\right] dr, \tag{2.1}$$

which can be separated as

$$J^{(m)}_{l_1l_2\cdots l_n}(k_1k_2k_n) = \int_0^R r^m \left[\prod_{i=1}^{n} \chi_{l_i}(k_ir)\right] dr + J^{(R,m)}_{l_1l_2\cdots l_n}(k_1k_2\cdots k_n). \tag{2.2}$$

We adopt the notation that $J^{(m)}_{l_1l_2\cdots l_n}(k_1k_2\cdots k_n) = I^{(m)}_{l_1l_2\cdots l_n}(k_1k_2\cdots k_n)$ if all of the χ_{l_i}'s are spherical Bessel functions. Note that the first integral in Eq. (2.2) *may* diverge of $m<0$ or for certain combinations of one or more Neumann functions. In any case, we assume that if the first integral exists, it may be evaluated using standard numerical quadrature. See Ref. [6] for a discussion of how to choose R (for $m=2$, $n=3$) in order to avoid either undue oscillations in the first integral in Eq. (2.2) or near singularities in the $J^{(R,m)}_{l_1l_2\cdots l_n}$ function.

We now proceed to evaluate Eq. (1.6). First, expand the product of χ_{l_i}'s in the integrand as

$$\prod_{i=1}^{n} \chi_{l_i}(k_ir) = 2^{-n} t_{l_1} t_{l_2} \cdots t_{l_n} \sum_{\tau_1\tau_2\cdots\tau_n = -1}^{+1} \prod_{i=1}^{n} H^{(\tau_i)}_{l_i}(k_ir), \tag{2.3}$$

where

$$t_{l_i} = \begin{cases} 1 & \text{if } \chi_{l_i} \text{ is a } j_{l_i} \\ -i & \text{if } \chi_{l_i} \text{ is an } n_{l_i}, \end{cases} \tag{2.4}$$

$$H^{(\tau_i)}_{l_i}(k_ir) = \begin{cases} h^{(1)}_{l_i}(k_ir) & \text{for } \tau_i = -1 \\ s_{l_i} h^{(2)}_{l_i}(k_ir) & \text{for } \tau_i = +1, \end{cases} \tag{2.5}$$

and

$$s_{l_i} = \begin{cases} 1 & \text{if } \chi_{l_i} \text{ is a } j_{l_i} \\ -1 & \text{if } \chi_{l_i} \text{ is an } n_{l_i}. \end{cases} \tag{2.6}$$

The functions $h^{(1)}_{l_i}$ and $h^{(2)}_{l_i}$ are spherical Hankel functions having the following asymptotic behavior

$$\begin{aligned} h^{(1)}_l(\rho) &\xrightarrow[\rho\to\infty]{} -\frac{i}{\rho} e^{i(\rho - (1/2)l\pi)} \\ h^{(2)}_l(\rho) &\xrightarrow[\rho\to\infty]{} \frac{i}{\rho} e^{-i(\rho - (1/2)l\pi)}. \end{aligned} \tag{2.7}$$

Note that the τ_i in Eq. (2.3) run over the values -1 and $+1$. Next, examine a particular term in the expansion of Eq. (2.3), namely

$$H^{(\tau_1)}_{l_1}(k_1r)\, H^{(\tau_2)}_{l_2}(k_2r) \cdots H^{(\tau_n)}_{l_n}(k_nr), \tag{2.8}$$

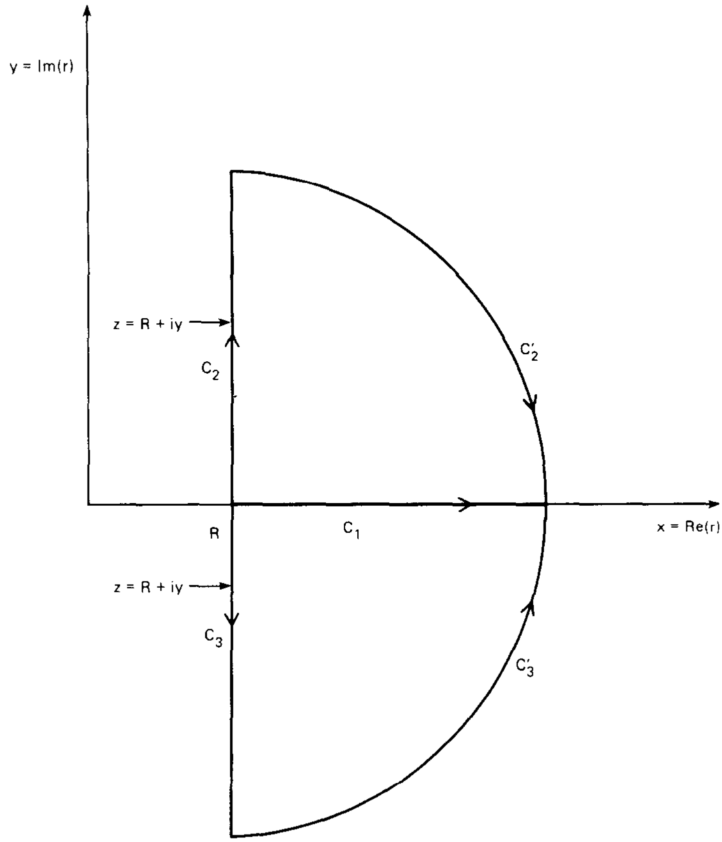

FIG. 1. Contours of integration in the complex r plane ($r \to z = x + iy$) for the evaluation of the integral in Eq. (1.6). Along C_2, $z = R + iy$, $0 \leq y < \infty$, while along C_3, $z = R + iy$, $-\infty < y \leq 0$. The integrals along the sections of infinite semicircles vanish.

for which we define

$$p = \sum_{i=1}^{n} \tau_i k_i. \tag{2.9}$$

From Eq. (2.7), if $p > 0$ then the term, (2.8), is analytic in the upper half-plane of Fig. 1, while if $p < 0$, it is analytic in the lower half-plane. We thus separate Eq. (2.3) as

$$\prod_{i=1}^{n} \chi_{l_i}(k_i r) = \mathscr{U}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n; r) + \mathscr{L}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n; r), \tag{2.10}$$

where $\mathscr{U}_{l_1 l_2 \cdots l_n}$ contains all of the terms analytic in the upper half-plane and $\mathscr{L}_{l_1 l_2 \cdots l_n}$, all of the terms analytic in the lower half-plane. Also, from the analytic properties of the Hankel functions, it can be shown that

$$\mathscr{L}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n; z) = \mathscr{U}^*_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n; z^*). \tag{2.11}$$

Combining Eqs. (1.6), (2.10), and (2.11), we find that

$$J^{(R,m)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n) = -2 \int_0^\infty dy \operatorname{Im}[(R+iy)^m \mathscr{U}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n; R+iy)], \tag{2.12}$$

an integral that converges rapidly and can be evaluated by Guassian quadrature [6].

A useful relation can be derived from Eq. (1.6), namely

$$J^{(R,m)}_{l_1 l_2 \cdots l_n}\left(\frac{k_1}{\lambda}, \frac{k_2}{\lambda^2}, ..., \frac{k_n}{\lambda}\right) = \lambda^{m+1} J^{(R/\lambda,m)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n). \tag{2.13}$$

Thus, if some of the k_i's are very small or very large, the integral may be scaled to a range of k values which is numerically manageable [6].

III. The $I^{(2)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n)$ Function

We conlude with a derivation of an important property of the $I^{(2)}_{l_1 l_2 \cdots l_n}$ function. This occurs in the angular momentum decomposition of

$$\delta^3\left(\sum_{i=1}^n \mathbf{k}_i\right) = (2\pi)^{-3} \int d^3\mathbf{r} e^{i\mathbf{r} \cdot \sum_{i=1}^n \mathbf{k}_i}, \tag{3.1}$$

which after some angular momentum recoupling becomes

$$\delta^3\left(\sum_{i=1}^n \mathbf{k}_i\right) = \frac{2^{n-1}\pi^{(n/2-2)}}{(2l_n+1)} \sum_{l_1 l_2 \cdots l_n} I^{(2)}_{l_1 l_2 l_n}(k_1 k_2 \cdots k_n) \times \prod_{i=1}^n [(2l_i+1)^{1/2} i^{l_i}]\, Q_{l_1 l_2 \cdots l_n}(\hat{k}_1, \hat{k}_2, ..., \hat{k}_n), \tag{3.2}$$

where

$$\begin{aligned} Q_{l_1 l_2 \cdots l_n}(\hat{k}_1, \hat{k}_2, ..., \hat{k}_n) = & \sum_{m_1 m_2 \cdots m_n} \prod_{i=1}^n Y^*_{l_i m_i}(\hat{k}_i) \\ & \times \sum_{\lambda_1 \lambda_2 \cdots \lambda_{n-3}} (-)^{\mu_1+\mu_2+\cdots+\mu_{n-3}} \mathscr{C}(l_1 l_2 \lambda_1; m_1 m_2 \mu_1) \\ & \times \left[\prod_{i=1}^{n-4} \mathscr{C}(\lambda_i, l_{i+2}, \lambda_{i+1}; \mu_i, m_{i+2}, \mu_{i+1})\right] \\ & \times \mathscr{C}(\lambda_{n-3}, l_{n-1}, l_n; \mu_{n-3}, m_{n-1}, -m_n), \end{aligned} \tag{3.3}$$

$Y_{lm}(\hat{k})$ is a spherical harmonic, and $\mathscr{C}(abc;\alpha\beta\gamma)$ is a product of the Clebsch–Gordan coefficients:

$$\mathscr{C}(abc;\alpha\beta\gamma) \equiv \langle ab\alpha\beta; c\gamma\rangle\langle ab00; c0\rangle. \tag{3.4}$$

In the above we have related all vectors to $\mathbf{k}_n$. However, there is nothing special about $\mathbf{k}_n$; thus, these equations can always be rewritten in terms of any one of the $\mathbf{k}_i$. From the properties of the Clebsch–Gordan coefficients, we find that

$$\sum_{i=1, i\neq j}^{n} l_i \geqslant l_j; \qquad j = 1, 2, ..., n \tag{3.5a}$$

and

$$(-)^{l_1+l_2+\cdots+l_n} = 1, \tag{3.5b}$$

which are the angular momentum decompositions of the vector inequalities implied by Eq. (3.1), namely

$$\sum_{i=1, i\neq j}^{n} k_i \geqslant k_j; \qquad j = 1, 2, ..., n. \tag{3.6}$$

Assume that, for a particular $I^{(2)}_{l_1 l_2 \cdots l_n}$ function, Eqs. (3.5) are satisfied but not necessarily Eqs. (3.6). Then, from the relation

$$j_l(-x) = (-)^l j_l(x) \tag{3.7}$$

and Eq. (3.5b), we obtain

$$I^{(2)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n) = \frac{1}{2}\int_{-\infty}^{\infty} x^2 j_{l_1}(k_1 x)\, j_{l_2}(k_2 x) \cdots j_{l_n}(k_n x)\, dx. \tag{3.8}$$

Next, assume that *one* of the Eqs. (3.6) is violated; e.g., $j = \gamma$, with

$$\sum_{i=1, i\neq \gamma}^{n} k_i < k_\gamma. \tag{3.9}$$

However, from Eq. (3.9) it also follows that

$$k_\gamma + \sum_{i=1, i\neq\gamma}^{n} \tau_i k_i > 0, \tag{3.10}$$

with $\tau_i = \pm 1$, and all possible combinations of τ_i's in the sum are allowed, so that Eqs. (3.6) are satisfied for $j \neq \gamma$. Then Eq. (3.8) can be rewritten as

$$I^{(2)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n) = U^{(2)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n) + L^{(2)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n), \tag{3.11}$$

where

$$U^{(2)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n) = \frac{1}{4}\int_{-\infty}^{\infty} x^2\, dx\, h^{(1)}_{l_\gamma}(k_\gamma x) \prod_{\substack{i=1 \\ i\neq\gamma}}^{n} j_{l_i}(k_i x) \tag{3.12a}$$

and

$$L^{(2)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n) = \frac{1}{4}\int_{-\infty}^{\infty} x^2\, dx\, h^{(2)}_{l_\gamma}(k_\gamma x) \prod_{\substack{i=1 \\ i\neq\gamma}}^{n} j_{l_i}(k_i x). \tag{3.12b}$$

The integrands on the right-hand sides of Eqs. (3.12a) and (3.12b) are analytic in the upper and lower half planes, respectively, a result which follows from Eq. (3.10). The only possible pole which can occur in these integrands is at $x = 0$, where we have

$$x^2 h^{(j)}_{l_\gamma}(k_\gamma x) \prod_{\substack{i=1 \\ i\neq\gamma}}^{n} j_{l_i}(k_i x) \underset{x\to 0}{\simeq} x^{2+\alpha}, \tag{3.13}$$

and

$$\alpha = \left[\sum_{i=1, i\neq\gamma}^{n} l_i\right] - l_\gamma \geqslant 0, \tag{3.14}$$

which follows from Eqs. (3.5a) for $j = \gamma$. Thus, there is no pole at the origin and for Eqs. (3.12) we may complete the contours in the upper and lower half planes to obtain

$$I^{(2)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n) = 0.$$

We have established that if Eqs. (3.5) are satisfied, $I^{(2)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n)$ will vanish if one of the vector inequalities in Eqs. (3.6) is violated. This means that $I^{(2)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n)$ is a step function in the k_i's, a property that must be taken into account when using this function in calculations. This behavior, of course, just reflects the angular momentum decomposition of the delta function in Eq. (3.2). Finally, we mention that $I^{(2)}_{l_1 l_2 \cdots l_n}(k_1 k_2 \cdots k_n)$ does not generally vanish if one of the Eqs. (3.6) is violated *and* Eqs. (3.5) are *not* satisfied. For this case, the complex-plane method described in the previous section must be used to evaluate the integral.

References

1. P. M. Morse and H. Feshbach, *Methods of Theoretical Physics, Part I* (McGraw–Hill, New York, 1953), p. 434.
2. W. Gautschi, *SIAM J. Numer. Anal.* 7, 187 (1970).

3. C. M. VINCENT AND H. T. FORTUNE, *Phys. Rev. C* **2**, 782 (1970).
4. J. D. MURRAY, *Asymptotic Analysis* (Oxford Univ. Press, Clarendon, Oxford, 1974), p. 40.
5. C. W. HELSTROM AND S. O. RICE, *J. Comput. Phys.* **54**, 289 (1984).
6. K. T. R. DAVIES, M. R. STRAYER, AND G. D. WHITE, *J. Phys. G, Nucl. Phys.* **14**, 961 (1988).
7. K. T. R. DAVIES, *J. Phys. G, Nucl. Phys.* **14**, 973 (1988).
8. A. D. JACKSON AND L. C. MAXIMAN, *SIAM J. Math. Anal.* **3**, 446 (1972).
9. A. BAEZA, B. WILWES, R. BILWES, J. DIAZ, J. F. FERRERO, AND J. RAYNAL, *Nucl. Phys. A* **437**, 93 (1985).

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