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Note

Optimum Numerical Calculation of JWKB Phase Shifts

I. Introduction

In recent years, with the advent of fast computers, it has become practical, and in many cases, routine, to sum the Rayleigh–Faxen–Holtzmark series out to hundreds, and even thousands, of partial waves. Of course, in order to perform this summation, it is necessary to have sufficiently accurate phase shifts which may be exact phase shifts [1] or, where applicable, JWKB phase shifts. In evaluating the JWKB phase shifts, there are two possible methods, both of which are equivalent. First, if one has the classical deflection function, its integral with respect to angular momentum will give the JWKB phase shift [2]. Second, one can evaluate the integral of the inverse compton wavelength for the lth partial wave from the classical turning point, r_0, to infinity, then the phase shift is given by

$$\eta_l = \tfrac{1}{2}\pi(l - \tfrac{1}{2}) - kr_0 - \int_{r_0}^{\infty} (k - 1/\lambda_l)\, dr \tag{1}$$

where k is the wavenumber [3].

Although there is, in general, no difficulty in evaluating Eq. (1) for a small number of phase shifts, if one is interested in evaluating several hundred phase shifts by the second method, extreme care must be used. To see this, consider the requirements for evaluating the phase shift to within an accuracy of a milliradian at $l = 0$ and at $l = 1000$. At $l = 0$, one only needs to evaluate the integral to three or four significant figures. But at $l = 1000$, it is necessary to evaluate the integral to at least three more significant figures, for a total of six or seven, since at least the three first figures will be canceled when the integral is substracted from the $\frac{1}{2}\pi(l + \frac{1}{2}) - kr_0$ terms. Thus, unless the relative accuracy of the integral is increased as l increases, one eventually reaches a point where the subtraction will give a result with *no* significant figures. But, if one does require an increase in the relative accuracy as l increases, one is then faced with the disadvantage of increased computational time as l increases.

In order to overcome these difficulties, we have used another approach, which is to rewrite Eq. (1) so that the strong cancellation which occurs at large l values is done *before* an integral is evaluated. In this manner, we need to evaluate an integral only to the desired number of significant figures. Furthermore, as l

increases past the point where the phase shift is monotonically decreasing in magnitude, we need to evaluate an integral to *less and less* significant figures for a fixed absolute accuracy in the phase shift. Also, upon using this method, we were very pleasantly surprised to find that our computational time was dramatically decreased, whereas before we were averaging around six seconds per phase shift, now we were averaging around 250 msec per phase shift.

II. Optimum Method

We start with a general form of the JWKB phase shift, by rewriting Eq. (1) as

$$\eta_l = \int_{\rho_0}^{\infty} [F(\rho/\rho_0) - 1]\, d\rho - \int_{j}^{\infty} [G(\rho/j) - 1]\, d\rho + (j - \rho_0), \tag{2}$$

where

$$\rho \equiv kr, \tag{3a}$$

$$j \equiv l + \tfrac{1}{2} \tag{3b}$$

$$k \equiv (2mE)^{1/2}, \tag{3c}$$

$$G(x) \equiv (1 - 1/x^2)^{1/2}, \tag{3d}$$

$$F(\rho/\rho_0) \equiv (1 - j^2/\rho^2 - U(\rho/\rho_0))^{1/2}, \tag{3e}$$

$$U(x) \equiv V(\rho_0 x/k)/E, \tag{3f}$$

and $r_0 \equiv \rho_0/k$ is the last classical turning point of the potential $V(r)$, and thus $\rho = \rho_0$ is the last zero of $F(\rho/\rho_0)$.

First, since for large ρ, $(F - 1)$ and $(G - 1)$ will be difficult to calculate in this manner without loss of significant figures, we will replace them by $(F^2 - 1)/(F + 1)$ and $(G^2 - 1)/(G + 1)$, and use Eqs. (3d) and (3e) for reducing the numerator. Then changing the limits on both integrals to be from 1 to ∞ gives

$$\eta_l = -\rho_0 \int_1^{\infty} \frac{U(x)\, dx}{1 + F(x)} + (j - \rho_0) + j \int_1^{\infty} \frac{dx}{x^2} \left[\frac{1}{1 + G(x)} - \frac{j/\rho_0}{1 + F(x)}\right], \tag{4}$$

where x is a dummy variable, proportional to ρ. Now we use the identity

$$\begin{aligned} 1/(1 + F(x)) &= 1/(1 + G(x)) + (G(x) - F(x))/([1 + F(x)][1 + G(x)]), \\ &= x^2[1 - G(x)] \\ &\quad + (U(x) + (j^2/\rho_0^2 - 1)/x^2)/([1 + F(x)][1 + G(x)][G(x) + F(x)]), \end{aligned} \tag{5}$$

which gives us

$$\eta_l = (\rho_0 - j)[(j/\rho_0)(\pi/2 - 1) - 1] - \rho_0 \int_1^\infty \frac{dx}{1 + F(x)} \left[U(x) + \frac{U(x) + (j^2/\rho_0^2 - 1)/x^2}{x^2[1 + G(x)][G(x) + F(x)]}\right]. \quad (6)$$

To obtain the final form for calculational purposes, we define

$$\Delta\rho \equiv \rho_0 - j, \quad (7)$$

which may be calculated by iteration to the desired number of significant figures from

$$\Delta\rho = (j + \Delta\rho)^2 V[(j + \Delta\rho)/k]/((2j + \Delta\rho)E). \quad (8)$$

Then letting $x = 1/y$ in the integral gives

$$\eta_l = \Delta\rho \left[\frac{j}{\rho_0}\left(\frac{\pi}{2} - 1\right) - 1\right] - \rho_0 \int_0^1 \frac{dy}{1 + F(y^{-1})} \left\{W(y) + y^2 \frac{W(y) - \Delta\rho(j + \rho_0)/\rho_0^2}{[1 + G(y^{-1})][F(y^{-1}) + G(y^{-1})]}\right\}. \quad (9)$$

where $W(y) \equiv U(y^{-1})/y^2$.

The advantage of Eq. (9) over Eq. (1) for numerical calculations is obvious. Every individual term in Eq. (9) vanishes as the potential vanishes. Such is not the case for Eq. (1). Rather, the first integral approaches $j(\pi/2 - 1)$ which *diverges* as j becomes very large. This does not happen in Eq. (9). Instead, both $\Delta\rho$ and W approach zero. Consequently, one needs to evaluate this integral only to the number of significant figures desired in the JWKB phase shift.

REFERENCES

1. DAVID J. KAUP, *J. Comp. Phys.* **9** (1972), 254–72, and references therein.
2. R. B. BERNSTEIN, *J. Chem. Phys.* **36** (1962), 1403.
3. "Molecular Beams," (John Ross, ed.) p. 91, Interscience, New York, 1966.

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