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A MODIFICATION OF THE SPHERICAL HARMONICS METHOD IN NEUTRON TRANSPORT THEORY

A. Sauer

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Abstract

The oscillatory character and the consequent poor convergence of the spherical harmonics method which arises when it is applied to a discontinuous problem is remedied by an appropriate modification. The new method is applied to the plane Milne problem, and the results compared with those obtained from both the conventional spherical harmonics method and Yvon's modification.

1. It was shown recently by Kofink[1] in the course of his profound investigations of the spherical harmonics method that the spherical harmonics solution $f^{(L)}(\xi,\mu)$ of the Milne problem does not converge in the limit $L \to \infty$ to the true solution $f(\xi,\mu)$, but instead oscillates about it, intersecting it in a denumerably infinite set of points. The angular distribution at the boundary $\xi = 0$ in particular is correctly given by the spherical harmonics method only in the directions $\mu = \mu_i$, where the μ_i are the roots of the equation $\lim_{L \to \infty} P_{L+1}(\mu_i) = 0$. Although for finite L the points of coincidence are not determined any more exactly by the roots of $P_{L+1}(\mu_i) = 0$, it is nonetheless true that the error of the P_L- approximation consists mostly of the $(L+1)^{st}$ spherical harmonic. This idea will form the basis for the proposed modification of the spherical harmonics method.

2. It is most convenient to illustrate all the methods to be discussed by their application to the Milne problem, in which a scattering medium fills the half space $\xi < 0$, while the half space $\xi > 0$ is empty; the neutrons are supplied by a plane source at $\xi = -\infty$. However, it must be realized that this particular example makes the conventional spherical harmonics method appear in an adverse light and does not bring out its potentialities fairly, since it imposes an excessive demand upon the method, which after all attempts to describe the angular distribution even at the interface by a continuous function. The exact distribution, on the other hand, is discontinuous at $\mu = 0$; $f(\mu > 0)$ gives the finite (and necessarily positive) probability that a particle will emerge in the

1. W. Kofink, Studies of the Spherical Harmonics Method in Neutron Transport Theory, ORNL Report 2358 (1957).

direction μ from the scattering medium, while $f(\mu < 0) = 0$ indicates that back scattering from the vacuum is impossible. The spherical harmonics method, trying to strike a happy mean, will give a continuous angular distribution near $\mu = 0$ which will be too low in the forward direction, while in the backward direction it will be too high. This means that the error of the P_L- approximation changes abruptly at $\mu = 0$ from a negative to a positive value; still, on either side separately it consists mostly of the $(L+1)^{st}$ spherical harmonic.

If we therefore attempt to remove the error by including the next harmonic into the approximation, it will try to oblige both sides, and in the resulting compromise the overall error will not be sizeably decreased. Thus, to obtain a marked improvement it is necessary to permit the amplitude of the $(L+1)^{st}$ harmonic to be different in the forward and backward directions.

3. Our approach is now seen to be somewhat similar to a method due to J. Yvon[2], who uses altogether different expansions in the forward and backward directions. We realize now that this process is quite radical and makes the formalism unduly complicated. In order to reduce the complexity one has to be satisfied with a lower order approximation; but then the gained advantage is partially lost again. It is therefore felt that the proposed approach steers a reasonable middle course between the poorly converging spherical harmonics method and the too ponderous method of Yvon.

---

2. An explicit description of this method can, for instance, be found in a memorandum by J. Bengston, ORNL CF-56-3-170 (1956).

4. The Boltzmann equation of the plane Milne problem is:

$$F(\xi,\mu) = 0 = \mu \frac{\partial f(\xi,\mu)}{\partial \xi} + f(\xi,\mu) - \tfrac{1}{2}(1-\gamma_a)\int_{-1}^{1} d\mu' f(\xi,\mu').$$

We expand $f(\xi,\mu)$ into spherical harmonics and terminate the series arbitrarily after the L^{th} term:

$$f^{(L)}(\xi,\mu) = \sum_{l=0}^{L-1}(2l+1) f_l(\xi) P_l(\mu) + (2L+1) P_L(\mu) \cdot \begin{cases} f_+(\xi), & \mu > 0 \\ f_-(\xi), & \mu < 0 \end{cases}.$$

For the conventional spherical harmonics method, reasonable boundary conditions can only be obtained when L is odd. A similar effect arises in our method; however, here L has to be even. (More generally, we can state that in all spherical harmonics methods reasonable boundary conditions always exist when the number of coefficients $f_i(\xi)$ is even. Thus, Yvon's method is feasible for all orders.) In addition, the equations for the $f_i(\xi)$ themselves become slightly simpler here when L is even, because then the materials constants will enter directly only into the lowest order equations. We shall therefore take L to be even throughout.

Now we have to determine the $f_i(\xi)$. Since there are $L+2$ of them, they will be the solutions of $L+2$ differential equations. $L+1$ equations are obtained by taking the first $L+1$ harmonic moments $\int_{-1}^{1} d\mu\, P_m(\mu)\, F(\xi,\mu) = 0$ of the Boltzmann equation:

$$\sum_{l=0}^{L-1}(2l+1) f_l' \int_{-1}^{1} d\mu\, P_m(\mu)\cdot \mu P_l(\mu) + \sum_{l=0}^{L-1}(2l+1) f_l \int_{-1}^{1} d\mu\, P_m(\mu)\cdot P_l(\mu)$$
$$+ (2L+1)\cdot \tfrac{1}{2}\left[f_+' + (-1)^{m+1} f_-' \right] \cdot 2 \int_{0}^{1} d\mu\, P_m(\mu)\cdot \mu P_L(\mu)$$
$$+ (2L+1)\cdot \tfrac{1}{2}\left[f_+ + (-1)^{m} f_- \right] \cdot 2 \int_{0}^{1} d\mu\, P_m(\mu)\cdot P_L(\mu)$$
$$- 2(1-\gamma_a) f_0\, \delta_{m0} = 0, \qquad m = 0 \ldots L.$$

Another equation is found by forming the expression $\int_0^1 d\mu\, P_L(\mu)\, F(\xi,\mu) - \int_{-1}^0 d\mu\, P_L(\mu)\, F(\xi,\mu) = 0$:

$$\sum_{\ell=0}^{L-1} (2\ell+1) f'_\ell \cdot \tfrac{1}{2}\left[1+(-1)^\ell\right] \cdot 2\int_0^1 d\mu\, P_L(\mu)\cdot\mu\, P_\ell(\mu)$$

$$+ \sum_{\ell=0}^{L-1} (2\ell+1) f_\ell \cdot \tfrac{1}{2}\left[1+(-1)^{\ell-1}\right] \cdot 2\int_0^1 d\mu\, P_L(\mu)\cdot P_\ell(\mu)$$

$$+ (2L+1) f'_L \cdot 2\int_0^1 d\mu\,\mu\, P_L^2(\mu) + (2L+1)\bar{f}_L \cdot 2\int_0^1 d\mu\, P_L^2(\mu) = 0\,,$$

where we have introduced the abbreviations

$$\tfrac{1}{2}(f_+ + f_-) = f_L \quad \text{and} \quad \tfrac{1}{2}(f_+ - f_-) = \bar{f}_L\,.$$

The integrals are all elementary and can be evaluated easily.

$$M_{\alpha\beta} = M_{\beta\alpha} = \int_0^1 d\mu\, P_\alpha(\mu)\, P_\beta(\mu)$$

$$= \begin{cases} 0 & |\alpha-\beta| \text{ even but } \neq 0 \\[1ex] \dfrac{1}{2\alpha+1} & \beta=\alpha \\[1ex] \dfrac{(-1)^{\frac{1}{2}(\alpha+\beta+1)}}{2^{\alpha+\beta-1}}\,\dfrac{1}{(\alpha-\beta)(\alpha+\beta+1)}\,\dfrac{\alpha!\,\beta!}{\left[(\frac{\alpha}{2})!\,(\frac{\beta-1}{2})!\right]^2} & \left.\begin{matrix}\alpha \text{ even}\\ \beta \text{ odd}\end{matrix}\right\} \end{cases};$$

$$N_{\alpha\beta} = N_{\beta\alpha} = \int_0^1 d\mu\,\mu\, P_\alpha(\mu)\, P_\beta(\mu)$$

$$= \begin{cases} 0 & |\alpha-\beta| \text{ odd but } \neq 1 \\[1ex] \dfrac{\alpha}{4\alpha^2-1} & \beta=\alpha-1 \\[1ex] \dfrac{(-1)^{\frac{1}{2}(\alpha+\beta+2)}}{2^{\alpha+\beta}}\,\dfrac{\alpha(\alpha+1)+\beta(\beta+1)}{(\alpha-\beta-1)(\alpha-\beta+1)(\alpha+\beta)(\alpha+\beta+2)}\,\dfrac{\alpha!\,\beta!}{\left[(\frac{\alpha}{2})!\,(\frac{\beta}{2})!\right]^2} & \left.\begin{matrix}\alpha \text{ even}\\ \beta \text{ even}\end{matrix}\right\} \end{cases}.$$

Written down explicitly, our system of equations will then appear as follows:

$$
\left.
\begin{array}{ll}
\boxed{\begin{array}{c}
\dfrac{m}{2m+1} f'_{m-1} + \dfrac{m+1}{2m+1} f'_{m+1} \\[2ex]
+ f_m - (1-\gamma_a) f_0 \delta_{m0} \\[2ex]
m = 0 \dots L
\end{array}}
&
\begin{array}{l}
+ (2L+1) N_{0L} \bar{f}'_L = 0 \\
+ (2L+1) M_{1L} \bar{f}_L = 0 \\
+ (2L+1) N_{2L} \bar{f}'_L = 0 \\
+ (2L+1) M_{3L} \bar{f}_L = 0 \\
\vdots \\
+ (2L+1) M_{L-1,L} \bar{f}_L = 0 \\
+ (2L+1) N_{L,L} \bar{f}'_L = 0
\end{array} \\
1 \cdot N_{L0} f'_0 + 3 M_{L1} f_1 + \dots + (2L+1) N_{L,L} f'_L & + (2L+1) M_{L,L} \bar{f}_L = 0
\end{array}
\right\}
$$

In the box we have the equations of the conventional spherical harmonics method; there the bordering elements all vanish, since one assumes that $f_+ = f_-$, i.e., $\bar{f}_L = 0$. We will now calculate an example and see that actually $\bar{f}_L$ is far from being zero.

5. For $L = 2$, the system of differential equations is

$$
\left.
\begin{array}{lllll}
\gamma_a f_0 & + f_1' & & + \frac{5}{8} \bar{f}_2' & = 0 \\
\frac{1}{3} f_0' & + f_1 & + \frac{2}{3} f_2' & + \frac{5}{8} \bar{f}_2 & = 0 \\
 & \frac{2}{5} f_1' & + f_2 & + \frac{5}{8} \bar{f}_2' & = 0 \\
\frac{1}{8} f_0' & + \frac{3}{8} f_1 & + \frac{5}{8} f_2' & + \bar{f}_2 & = 0
\end{array}
\right\}
$$

If we now put $f_i = A_i e^{\lambda \xi}$, we obtain four linear homogeneous equations for the A_i which have a non-trivial solution only if

$$
\lambda^2 = 3 \gamma_a \frac{1 - \frac{331}{735} \lambda^2}{1 - \frac{9}{49} \lambda^2} .
$$

As long as $\gamma a \ll 1$ the lowest pair of roots is given by

$$\lambda^2 = 3\gamma a \left(1 - \frac{4}{5}\gamma a + \frac{244}{1225}\gamma a^2 \cdots\right) ;$$

we see that the first two coefficients in this expansion are correctly given by this approximation. The next two roots are expressed by

$$\lambda^2 = \frac{49}{9}\left(1 + \frac{4}{5} + \frac{108}{245}\gamma a^2 \cdots\right) .$$

6. Since the lowest root of the secular equation rules the behavior of the approximate solution inside the scatterer, it is instructive to compare how accurately it is given by the different methods. The number of correct coefficients in the expansion $\lambda^2 = \sum_{m=0}^{\infty} \alpha_m \gamma a^m$ is always equal to the number of Legendre polynomials employed in the approximation; thus the conventional P_3-method (which uses the four expansion functions $P_0(\mu) \cdots P_3(\mu)$) gives the first four coefficients $\alpha_0 = 0$, $\alpha_1 = 3$, $\alpha_2 = -\frac{12}{5}$, $\alpha_3 = \frac{12}{175}$ correctly.

On the other hand, the order of the secular equation in λ, which is a fair measure of the complexity of the approximation, is equal to the number of expansion coefficients. Thus the conventional P_L- method, Yvon's $P^2_{\frac{1}{2}(L-1)}$ - method, and our modified P'_{L-1}-method are comparable in complexity. We expect, therefore, that inside a scattering medium with absorption the modified P'_{L-1}-approximation will not be materially worse than the P_L-method, especially for large L, while Yvon's equally complex $P^2_{\frac{1}{2}(L-1)}$-method will trail far behind in accuracy.

For further comparison, we tabulate the lowest root - which is inversely proportional to the mean free path - as given by the different methods of equal complexity for a black absorber.

Table 1. Lowest root λ for a black absorber.

Method	Exact	P_3	P_2'	P_1^2
λ	1.000	1.161	1.199	1.267

7. We shall now complete the solution for the case of a pure scatterer, so that $\gamma_a = 0$. Then the lowest eigen value vanishes, and the corresponding exponential solution degenerates into a straight line. We find

$$f(\xi \leq 0, \mu) = a_0 \xi + \ell_0 - a_0 \mu + A_0 e^{2.3333\xi} \left(1 - 1.0714 P_1(\mu) + P_2(\mu) \cdot \begin{cases} 0.3571 \\ -5.3571 \end{cases}\right),$$

while on the vacuum side

$$f(\xi \geq 0, \mu) = C_1 e^{-1.1989 \cdot \xi} \left(1 + 1.9038 P_1(\mu) + P_2(\mu) \cdot \begin{cases} 4.3133 \\ 1.1217 \end{cases}\right)$$
$$+ C_2 e^{-3.3708 \cdot \xi} \left(1 + 2.0291 P_1(\mu) + P_2(\mu) \cdot \begin{cases} -4.8777 \\ 1.1978 \end{cases}\right).$$

The coefficients of the spherical harmonics in these expressions are essentially the A_i which were calculated from the system of equations in §5.

To obtain the remaining undetermined quantities in the expressions for $f(\xi \geq 0, \mu)$ and $f(\xi \leq 0, \mu)$ we match these at $\xi = 0$, and then compare the coefficients of the different spherical harmonics. Such a procedure is equivalent to an application of Mark's boundary condition which, however, cannot be generalized to cover our case since it is based on a special property of the Legendre polynomials; the effect of Mark's condition is to reduce the system of linear equations for the undetermined coefficients to two separate systems of half as many equations. This is an advantage which we cannot obtain; on the other hand, we do not have to make any partial use of our intuitive knowledge of the behavior of the exact solution. From the system

$$\left.\begin{aligned} b_0 + A_0 &= C_1 + C_2 \\ -a_0 - 1.0714\,A_0 &= 1.9038\,C_1 + 2.0291\,C_2 \\ 0.3571\,A_0 &= 4.3133\,C_1 - 4.8777\,C_2 \\ -5.3571\,A_0 &= 1.1217\,C_1 + 1.1978\,C_2 \end{aligned}\right\}$$

and the normalization condition to unit forward current,

$$1 = 2\pi \int_0^1 d\mu\, \mu\, f(-0,\mu) = -2.0944 a_0 + 3.1416 b_0 + 1.1781 A_0,$$

we find

$$a_0 = -0.2408 \qquad C_1 = 0.07261$$
$$b_0 = 0.1691 \qquad C_2 = 0.06641$$
$$A_0 = -0.03005 \ .$$

This gives us the angular distribution at the boundary

$$f(0,\mu) = 0.1390 + 0.2730\,\mu + P_2(\mu)\begin{cases} -0.0107 \\ 0.1610 \end{cases},$$

and the flux in the medium

$$\phi(\xi) = 2\pi \int_{-1}^{1} d\mu\, f(\xi,\mu) = -0.7565\,\xi + 0.5312 - 0.0944\,e^{2.3333\,\xi} .$$

The back current is 0.86%, and the extrapolation distance

$$\delta = -\frac{\phi_{as}(0)}{\phi'_{as}(0)} = \frac{b_0}{a_0} = 0.7022 .$$

8. The obtained angular distribution is plotted in Figure 1; for comparison, the exact distribution[3] is also shown. It is seen that the agreement is quite excellent in the forward direction. In the backward direction the accuracy of the approximation is less impressive; this is not too surprising, for one could not expect one high harmonic to cancel completely the combined effect of all the others - which are, after all, orthogonal to it.

In Figure 2 the error of the regular P_3- and the modified P_2'- methods are plotted on a larger scale. In both directions the P_2'- method represents a considerable improvement. Incidentally, it can be checked directly by means of this plot that the error of the P_3- approximation consists mostly of the Legendre component $P_4(\mu)$.

For further comparison, we have calculated the mean square error of the different approximations:

Table 2. Mean square error $\sqrt{\int d\mu \, [f^{(L)}(0,\mu) - f^{exact}(0,\mu)]^2}$.

	$\mu > 0$	$\mu < 0$
P_3	$164{,}7 \times 10^{-4}$	392×10^{-4}
P_2'	$13{,}3 \times 10^{-4}$	182×10^{-4}
P_1^2	$20{,}7 \times 10^{-4}$	0

In the forward direction, the P_2'- method is seen to be better than Yvon's method; of course, it cannot compete in the backward direction, where - by an ad hoc construction - Yvon's method is exact. Indeed, it is quite fortuitous that the P_1^2- approximation - which approximates the exact distribution by a straight line on both sides - does not show a larger error. If

3. Taken from Case, DeHoffmann, and Placzek, Introduction to the Theory of Neutron Diffusion I, Los Alamos 1953. (Renormalized to unit current.)

we had included a certain amount of absorption, the true distribution would have been much more strongly peaked forward, and the P_1^2-approximation would have been quite inaccurate, while our method would have given good results since it also includes a quadratic term.

Finally, we tabulate the extrapolation distances obtained by the different methods.

Table 3. Extrapolation distances.

	Exact	P_3	P_2'	P_1^2
δ	0.7104	0.6949	0.7022	0.7113

Here, the P_1^2-method is quite clearly superior.

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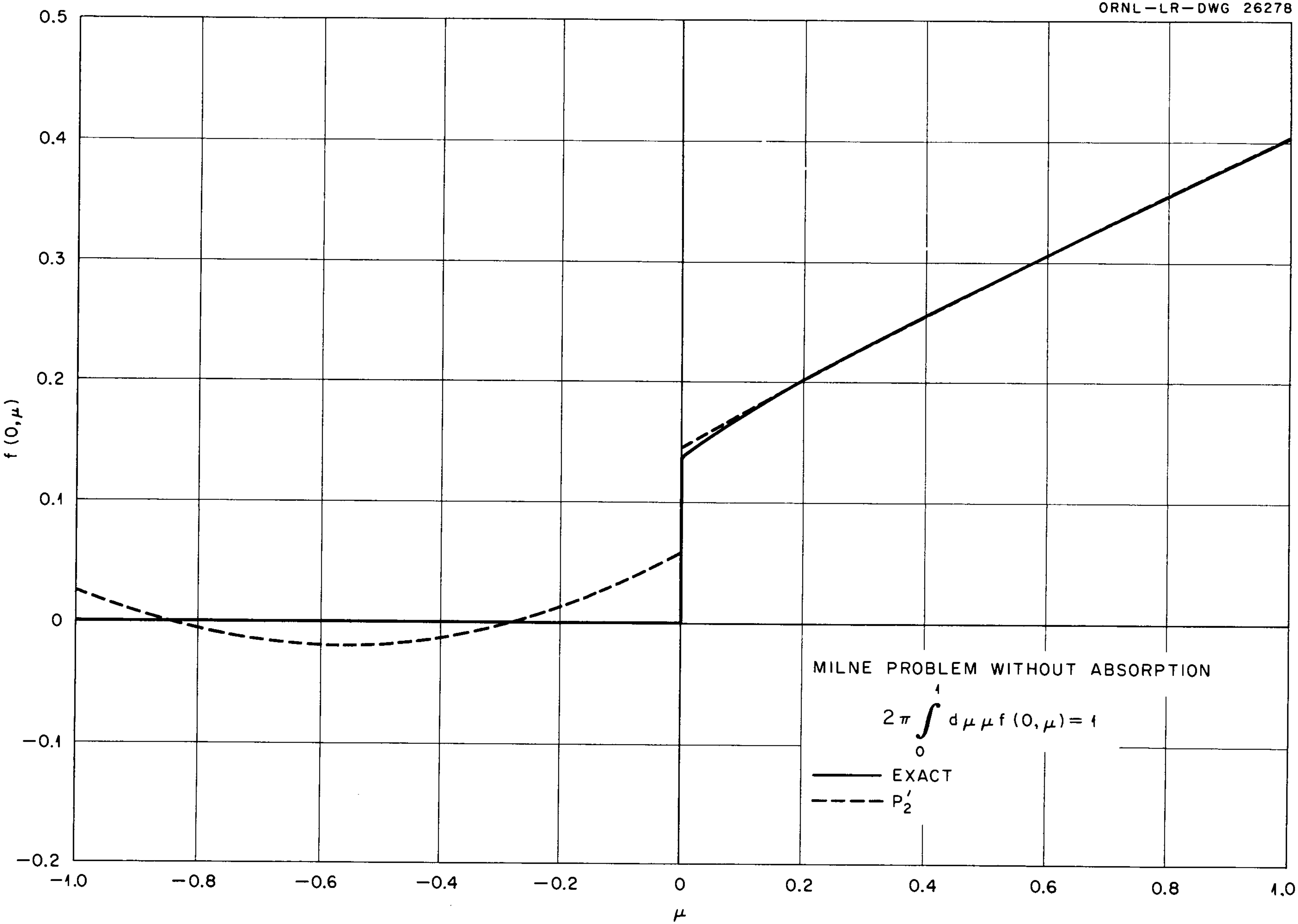

Fig. 1. Angular Distribution at Boundary.

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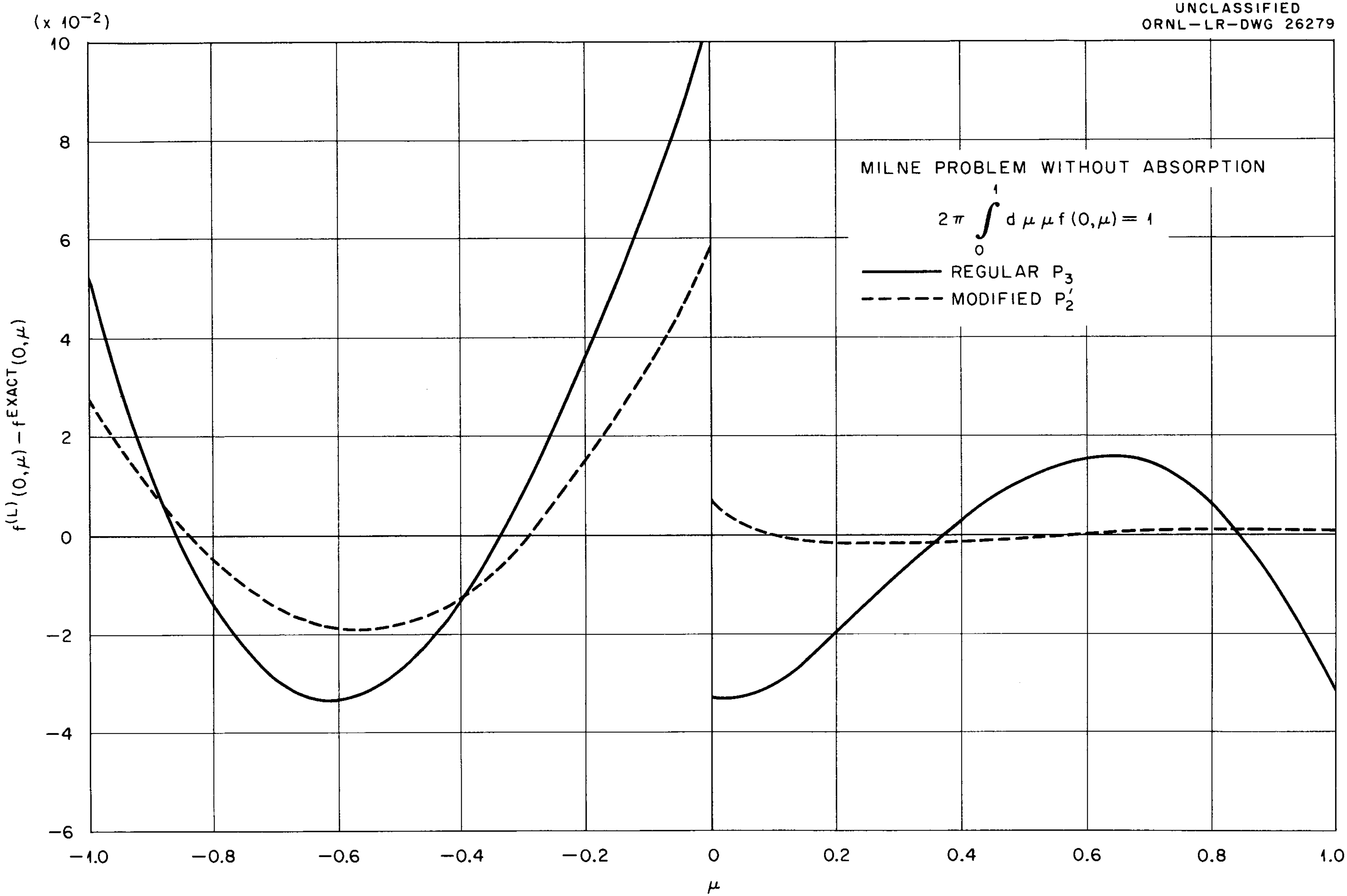

Fig. 2. Error in the Angular Distribution at the Boundary.