Internal Conversion Coefficients for M4 Transition in Tellurium*

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Abstract

Theoretical results of β_4 for the subshells including M-subshells are presented in the 81.78 KeV transition of ^{121m}Te. Numerical results for gamma energy equal to 0.15 mc^2 are also presented, and compared with the earlier calculations of Rose, and Sliv and Band. Atomic screening and the finite nuclear size effects are included accurately. The experimental data of Chu and Perlman compares favourably with the new theoretical results. The calculated eigenvalues are also found to be in reasonable agreement with the experimental binding energies.

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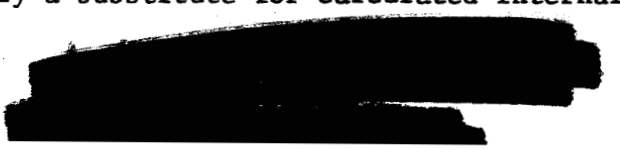
1. Introduction

There are two pioneering efforts in the preparation of internal conversion coefficient tables; one by Rose[1] and his collaborators, and the second by Sliv and Band.[2] In both these calculations, static effects arising due to the finite nuclear size and atomic screening by statistical model of Thomas-Fermi-Dirac are included. The calculations of Sliv and Band include what can be termed as minimal penetration, based on the nuclear currents restricted to the nuclear surface. There have been some differences in these published tables. To understand these differences, and report on an independent calculation is one motivation of the present investigation.

The second motivation of this work arises from the following considerations. A large number of internal conversion coefficients measurements for the M-subshells indicate a significant discrepancy (by factors as large as three) between the available calculations and the experimental data.[3] The only detailed published calculations for the M-subshells are those of Rose and his collaborators,[1] for a point nucleus and unscreened coulomb potential. Sliv and Band[2] did not calculate for the M-subshells. Because of the relatively small magnitude of the radial functions for the principal quantum equal to three at the nucleus, the finite nuclear size effects are not expected to be of any significance. However, the screening corrections for the bound state and the continuum radial wave functions cannot be ignored. An empirical procedure by including an effective screening constant has recently been proposed by Chu and Perlman.[4] Whereas such an empirical scheme is useful especially when results of calculations are not available, this is hardly a substitute for calculated internal



conversion coefficients based on a realistic model. Recently, the author[5,6] calculated and presented preliminary results for the M-subshells. The results for other subshells are completed using a different screening model from earlier calculations.[1,2] In contrast to the statistical Thomas-Fermi-Dirac model for screening used in references (1) and (2), we have used the screening potential corresponding to the non-relativistic Hartree-Fock model. The Slater exchange approximation is used. It would be desirable to have completely relativistic self-consistent solution.[7] However, it is expected that calculated internal conversion coefficients would at the most be influenced by less than one per cent. Such calculations are in progress to establish quantitatively this effect. Because of some existing differences in the two available detailed tables of internal conversion coefficients, it was felt essential to perform an independent calculation. The purpose of this paper is to document the bases of our calculations and discuss results for the 81.78 KeV transition in Tellurium.

The numerical procedure is discussed in Section 2, followed by numerical results. Section 4 contains a discussion and conclusions.

2. Formulation of the Problem

In the calculations of internal conversion coefficients, one needs to calculate the relativistic bound state and the appropriate continuum state radial wave functions. A brief summary is presented to facilitate the discussion of our calculation as well as to remove any ambiguity in the matrix-elements which are tabulated in this paper.

A. Relevant Formulas

The pertinent formulas for magnetic multipoles of order L are

$$\beta_L(\text{subshell}) = \frac{\pi \alpha k}{L(L+1)(2L+1)} \sum_{\kappa} B_{\kappa\kappa'} \left| R_{\kappa}(m) \right|^2 \qquad (1)$$

where the matrix-element

$$R_{\kappa}(m) = \int_{\rho}^{\infty} h_L(kr)\,(f_{\kappa}\, g_{\kappa} + g_{\kappa}\, f_{\kappa'})\, r^2\, dr$$

$$+ \int_{0}^{\rho} X_L(kr)\,(f_{\kappa}\, g_{\kappa'} + g_{\kappa}\, f_{\kappa'})\, r^2\, dr \qquad (2)$$

k is the γ-ray energy in mc^2, ρ is nuclear radius in $\hbar/mc$, f_{κ} and g_{κ} are the continuum radial functions and the primed κ's are for the bound state. κ specifies both the total angular momentum ($|\kappa| - \frac{1}{2}$) as well as the orbital angular momentum. $h_L(kr)$ is the hankel function and $X_L(kr)$ is defined below. There are two major effects; one, the so-called static effect and second, the dynamic effects. The static effects, which arise only because of the nonsingular potential inside the nucleus, can easily be taken into account by standard techniques. The dynamical effect, on the other hand, depends on the detailed nature of nuclear wave functions. In the surface current model used by Sliv and Band, it turns out that the contributions inside the nucleus can be calculated without the detailed knowledge of the nuclear matrix elements. In the penetration model of Rose, one takes $X_L(kr) = h_L(kr)$. The surface current model leads to

$$X_L(kr) = h_L(k\rho)\; J_L(kr)/J_L(k\rho)$$

It has been pointed out in the literature how the penetration effects,[8] which become significant especially for highly retarded gamma transitions, can be treated. For the M-subshells these penetration effects are expected to be of little consequence. The major effort involved in the calculations of internal conversion coefficients reduces to obtaining accurately the relevant bound state wave function and the continuum state radial function for the permissible values of κ.

B. Bound State Wave Functions

In relativistic units: $\hbar = m = c = 1$

$$\left[-\alpha \cdot p - \beta + V(r)\right] \psi_\kappa = W \psi_\kappa \tag{3}$$

W is the total energy in mc^2 units. κ is an integer.

$$\psi_\kappa^\mu = \begin{pmatrix} -i f_\kappa \chi_{-\kappa}^\mu \\ g_\kappa \chi_\kappa^\mu \end{pmatrix} \tag{4}$$

The radial functions obey the following first order coupled differential equation.

$$\frac{dF}{dr} = \frac{\kappa}{r} F - (W - 1 - V) G \tag{5a}$$

$$\frac{dG}{dr} = (W + 1 - V) F - \frac{\kappa}{r} G \tag{5b}$$

where $F = rf$ and $G = rg$.

In contrast to a statistical Thomas-Fermi-Dirac model, we use V(r) given by eqs. (6) for the numerical integration of eqs. (5)

$$V(r) = -\frac{\alpha Z}{2\rho}\left[3 - \left(\frac{r}{\rho}\right)^2\right] \qquad r \lesssim \rho \qquad (6a)$$

$$V(r) = \text{Hartree-Fock Potential (Non-relativistic)} \qquad r \gtrsim \rho \qquad (6b)$$

In eqs. (6), α is the fine structure constant (1/137.037), Z is the atomic number and the nuclear radius, ρ, is equal to $0.42585\ \alpha\ A^{1/3}\ \hbar/mc$.

The standard technique of integrating eqs. (5) from $r \approx 0$ to a match point, close to the classical radius was used. This was accomplished since F/G can be calculated in terms of a highly convergent series. Similarly, F/G at large is also known to be equal to $-\left[1 - W/1 + W\right]^{\frac{1}{2}}$. Backward integration to the match point was performed. If the eigenvalue guess is not correct, the iteration was continued until

$$\left|\frac{y_L - y_R}{y_R}\right| \lesssim 10^{-6} \qquad (7)$$

y_L = (F/G) at r = match point when integration was started from the origin.

y_R = F/G at the match point for the backward integration.

In earlier calculations the ratio defined in eq. (7) was taken to be $\lesssim 10^{-4}$. One test of the calculated wave functions using any screened potential is reflected in the deviations of the calculated eigenvalues from the experimental binding energies. Table I contains a comparison of our calculated eigenvalues with the experimental electron binding energies. It is clear from this comparison that the deviations from the experimental binding energies for the inner most shells is within a few tenths of 1% and less than 4% for the M-subshells. Such an agreement is considered

excellent and definitely better than it is expected from the statistical model used in references 2 and 3. Several precautions were taken to assure accuracy in the present calculations. For example, a large number of points (6000) were used in the numerical integration to minimize the errors introduced by mesh-size. Furthermore, a node count in the large component was used to assure the identification of all orbitals. Double precision was used in treating the W - 1 term because of the small magnitude in particular for the outer shells.

C. Continuum State

Two modifications were made in numerical integration of eqs. (5). First, the potential in eq. (6b) was modified to take into account the absence of the conversion electron and, second, total energy, W, was taken to be equal to the difference in the γ-ray energy and the binding energy of the conversion electron. For continuum radial functions, F/G was calculated at the nuclear surface. Integration of eqs (6) was continued for large distances. The essential feature of the present calculation is the accuracy achieved in the normalization factor, A(r).

$$F \rightarrow - A(r) \sqrt{(W - 1)/\pi p} \quad \sin(pr + \delta)$$

$$G \longrightarrow A(r) \sqrt{(W + 1)/\pi p} \quad \cos(pr + \delta)$$

$A^2(r)$, calculated for the preceding equations, is an oscillating function converging to the correct normalization factor. In our calculations, $A^2(r)$ was assured to have at least 20 points in one cycle. An accuracy of at least one part in ten thousand was accomplished. In earlier calculations[1,2] this accuracy was not achieved because of the computer considerations.

Once the continuum state and the bound state functions were calculated, the internal conversion coefficients were calculated for the M4 transition in Tellurium. The numerical results are given next.

3. Numerical Results

In order to minimize the mesh-size corrections, 6000 points were used in the calculations of β_4. Numerical results for the 81.78 KeV transitions in Te^{121m} are presented in Table II. The experimental value of $\beta_4(k)$ was normalized to the present calculations. Interpolated values from tables of Rose, are also given. Except for the M-subshells, which are not tabulated by Sliv and Band, the interpolated values from the tables of Sliv and Band were in agreement with those of Rose. The M-subshell internal conversion coefficients (of Rose) are for a point nucleus and unscreened coulomb field. The comparison of our calculated results with the experimental values shows clearly an excellent agreement.

It is well known that interpolation of tabulated internal conversion coefficients can lead to 1 - 2% error in particular for low gamma energies. To eliminate this uncertainty, new calculations were also performed for k equal to 0.15 mc^2, which does correspond to the published results. Results of the present calculations are compared with those in Ref. (1) and Ref. (2) in Table III. Table IV contains the matrix-elements for K and L shells. There are only small differences in the matrix-elements calculated by using a surface current model and penetration model of Rose.

4. Discussion and Conclusions

The differences in our calculated results and those of Rose, and Sliv and Band for $\beta_4(k)$ and β_4(L-subshells) are not surprising. It is to be

noted that we have used a more realistic screening model in contrast to the statistical Thomas-Fermi-Dirac model. A major criterion of a realistic potential is the agreement of calculated electron binding energies with the experimental data. It is clear from Table I that our calculated eigenvalues agree within a few tenths of one per cent for the inner orbitals, and the most by a few per cent for the M-subshells. It is known that comparatively large differences result for the Thomas-Fermi-Dirac model. It is expected that the calculated results for very low lying states may be drastically influenced by the screening model.[9])

A few remarks about the internal conversion coefficients for M-subshells is now in order. There is a significant reduction in the values of internal conversion coefficients for M-subshells when a screened potential is used. This fact, originally observed by a comparison of experimental M-subshell coefficients with unscreened values, is not surprising. Figures 2 and 3 give a comparison of rg_{-1} (large component) and rf_{-1} (small component) for 3S bound state of Tellurium for a screened and unscreened coulomb potential. It is clear from these figures, as it is to be expected, that the coulomb radial functions are pulled towards the nucleus as compared to the screened radial functions. Even the qualitative arguments that the electrons are less tightly bound in any screened field when compared to a pure coulomb potential. This change of the wave functions has a more pronounced effect on the calculated internal conversion coefficients when the weighting factor (the appropriate hankel function) is large. This is in fact the case for M4 transitions.

Inasmuch as the surface current model and the penetration model are concerned for M4 transitions, it is to be noted from the numerical results presented here that insignificant differences appear in the two cases. This is because of the relatively small magnitudes of the combinations of appropriate radial functions for M-subshells in the vicinity of a nucleus.

In conclusion, the present calculations show that the present screening model is adequate and our calculated internal conversion coefficients for all the subshells including M-subshells are in agreement with the experimental data.

It is a pleasure to thank Dr. W. R. Garrett for stimulating discussions concerning the Hartree-Fock treatment. The author is also indebted to Professor M. E. Rose and Dr. R. L. Graham for their interest and encouragement. Private communications from Drs. Chu and Perlman are gratefully acknowledged.

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Table I Comparison of calculated and experimental binding energies for Z = 52 (Rydbergs)

Sub-Shell	Hagstrom et al.[a]	Present Calculations[b]
1S	2338.3	2350.6
2S	363.03	365.507
$2P_{1/2}$	338.99	344.529
$2P_{3/2}$	319.07	323.714
3S	73.943	74.2256
$3P_{1/2}$	63.947	65.224
$3P_{3/2}$	60.125	61.281
$3D_{3/2}$	42.777	45.021
$3D_{5/2}$	42.043	44.174

a) S. Hagstrom, C. Nordling and K. Siegbahn, in Alpha-Beta-and-Gamma-Ray Spectroscopy, Vol. 1, p. 845 (1965).

b) Hartree-Fock (non-relativistic) Potential, with finite nuclear size effects.

Table II Comparison of calculated and experimental internal conversion coefficients for M4 transition in Te^{121m} (81.78 keV)

Sub-Shell	Experiment[a]	Present Calculations	Rose (Sliv)[b]
K	[692.3 ± 13]	692.3	660
L_I	310 ± 16	280.1	270
L_{II}	67 ± 5	64.5	62.5
L_{III}	518 ± 16	521.2	500
ΣL	895 ± 22	866	833
M_I	66 ± 5	64.6	133
M_{II}	123 ± 7	15.7	29.7
M_{III}		125.5	314
M_{IV}	5.0 ± 0.9	2.1	10.4
M_V		3.4	14.9
$\sum_i M$	194 ± 8	211	502

a) Chu and Perlman, Phys. Rev. 135 (1964) B319.
Values given are normalized to that for the K-line of the present calculations.

b) Interpolated values. For K- and L subshells, Rose, and Sliv and Band give the same results. M-subshells are for the unscreened Coulomb potential, as tabulated by Rose.

Table III Comparison of New Calculations with Earlier Work for β_4, $Z = 52$, $k = 0.15\ mc^2$

Identification	K	L_I	L_{II}	L_{III}	$K/\sum_i L_i$	L_I/L_{III}
Surface Current Model[a]	917.6	405.5	91.98	803.5	0.7053	0.5046
Penetration Model[b]	925.6	409.2	92.06	808.4	0.7068	0.5061
Rose[c]	882	390	88	758	0.7136	0.5145
Sliv and Band[d]	887	385	85.9	762	0.7194	0.5052
% Difference from c)	-4.9	-4.9	-4.6	-6.6	+1.0	+1.7
% Difference from d)	-3.4	-5.3	-7.1	-5.4	+2.0	+0.1

a) Present calculations based on Sliv's surface current model.

b) Present calculations based on Rose's penetration model.

c) M. E. Rose, Internal Conversion Coefficients (North-Holland Publishing Company, 1958).

d) L. A. Sliv and I. M. Band in Alpha-Beta-and-Gamma Ray Spectroscopy (North-Holland Publishing Company, 1965).

Table IV Matrix Elements for M4 Transitions ($Z = 52.0$, $k = 0.15\ mc^2$)

Subshell	$\lvert R_\kappa \rvert^2$	
K	$\lvert R_{-4}\rvert^2 = 0.23951$ E6 $\lvert R_5\rvert^2 = 0.79906$ E3	Surface Current Model[a]
	$\lvert R_{-4}\rvert^2 = 0.24164$ E6 $\lvert R_5\rvert^2 = 0.79914$ E3	Penetration Model[b]
L_I	$\lvert R_{-4}\rvert^2 = 0.10610$ E6 $\lvert R_5\rvert^2 = 0.24824$ E2	Surface Current Model
	$\lvert R_{-4}\rvert^2 = 0.10707$ E6 $\lvert R_5\rvert^2 = 0.24838$ E2	Penetration Model
L_{II}	$\lvert R_4\rvert^2 = 0.23910$ E5 $\lvert R_{-5}\rvert^2 = 0.20347$ E3	Surface Current Model
	$\lvert R_4\rvert^2 = 0.23931$ E5 $\lvert R_{-5}\rvert^2 = 0.20349$ E3	Penetration Model
L_{III}	$\lvert R_{-3}\rvert^2 = 0.16349$ E6 $\lvert R_4\rvert^2 = 0.76641$ E4	Surface Current Model
	$\lvert R_{-3}\rvert^2 = 0.16449$ E6 $\lvert R_4\rvert^2 = 0.76645$ E4	Penetration Model

a) Present calculations based on Sliv's surface current model.

b) Present calculations based on Rose's penetration model.

Captions to Figures

Fig. 1 Product of r and the large component for 3S bound state in Tellurium versus distance in Bohr radius. The dashed and the solid curves are respectively for the pure Coulomb and the self-consistent Hartree-Fock-Slater potentials.

Fig. 2 Product of r and the small component for 3S bound state in Tellurium versus distance in Bohr radius. The dashed and the solid curves are respectively for the pure Coulomb and the self-consistent Hartree-Fock-Slater potentials.

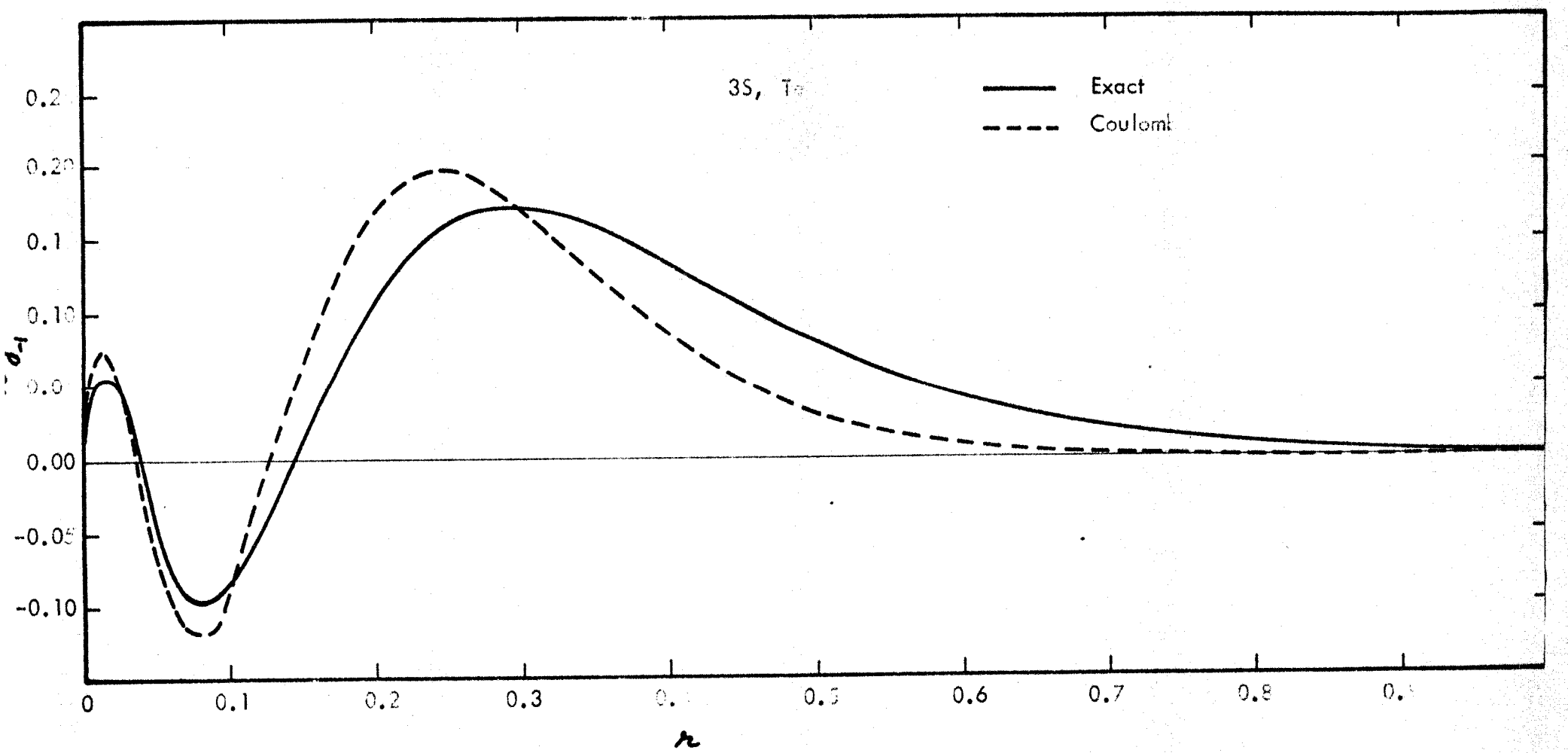

Fig.1, BHALLA

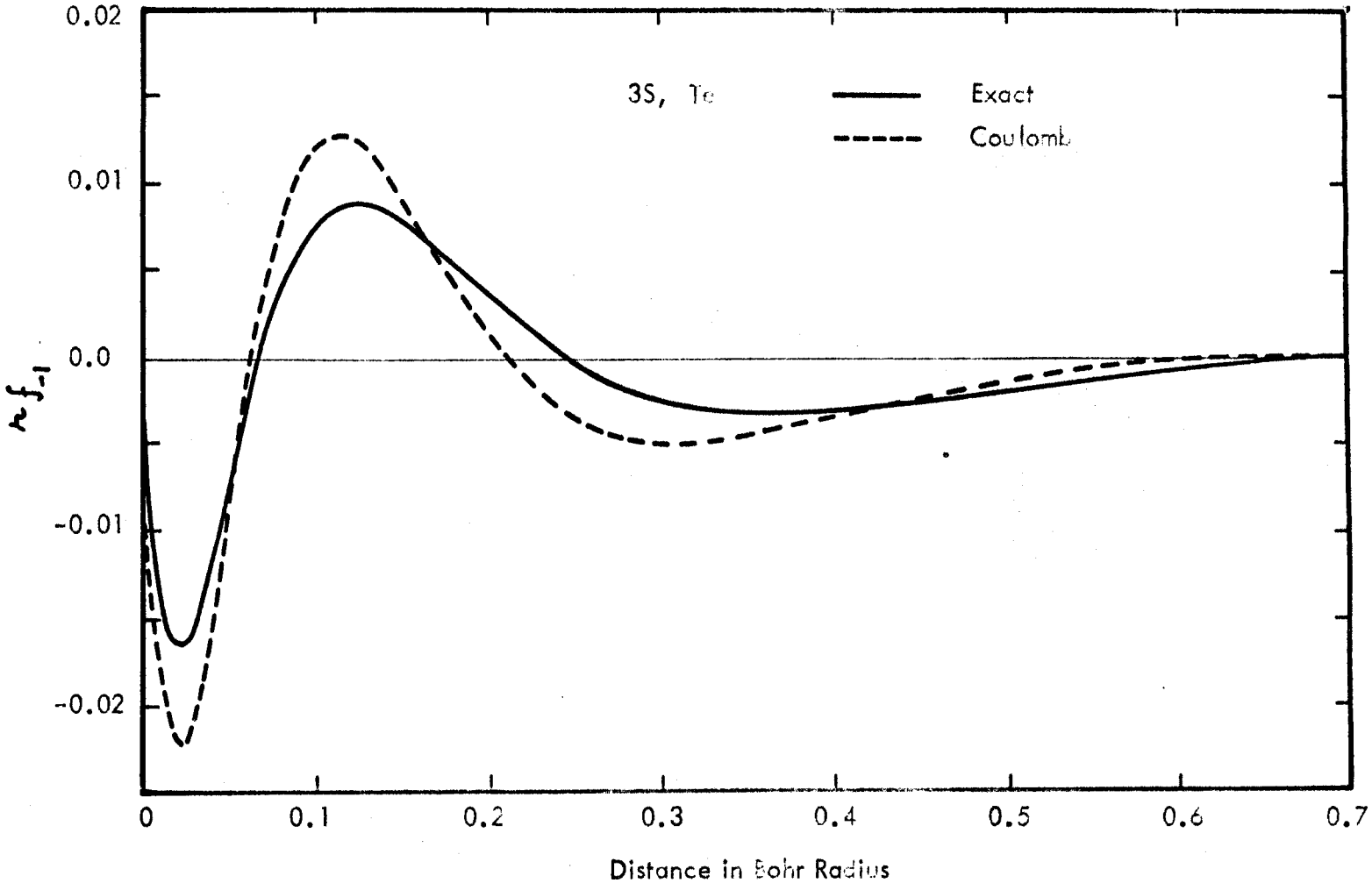
0.02
0.01
0.0
-0.01
-0.02
3S, Te
Exact
Coulomb
$r f_{-1}$
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
Distance in Bohr Radius

Fig.2. Bhalla