(X-641-65-460)

NASA TM X-55301

THEORY OF LOW-ENERGY POSITRON-HELIUM SCATTERING

FACILITY FORM 602

N66-10674	
(ACCESSION NUMBER)	(THRU)
21	1
(PAGES)	(CODE)
	24
(NASA CR OR TMX OR AD NUMBER)	(CATEGORY)

BY

RICHARD J. DRACHMAN

GPO PRICE $ ________

CFSTI PRICE(S) $ ________

Hard copy (HC) 1.00

Microfiche (MF) .50

ff 653 July 65

NOVEMBER 1965

GODDARD SPACE FLIGHT CENTER
GREENBELT, MARYLAND

Theory of Low-Energy Positron-Helium Scattering*

Richard J. Drachman
Laboratory for Theoretical Studies
National Aeronautics and Space Administration
Goddard Space Flight Center
Greenbelt, Maryland

10674

A modified adiabatic method, previously tested in positron-hydrogen scattering, has been applied to the case of positron-helium scattering below the positronium threshold (17.8 ev). Since the ratio of the positron's velocity to that of the atomic electrons is about the same as in the hydrogen test case, similar accuracy is expected, the main source of error being due to the approximate atomic wave function used. Phase shifts for L = 0,1,2 are presented, and total and momentum-transfer cross-sections are computed. The latter disagree completely with the only experiments performed to date.

Author

INTRODUCTION

In a recent paper[1], the author applied the exact second-order polarization potential of Dalgarno and Lynn[2] to the scattering of low-energy positrons by atomic hydrogen. Several objections may be brought against this procedure.

First, the polarization potential used is adiabatic, and does not account explicitly for velocity-dependent effects. A comparison of the adiabatic results[1] with the detailed variational s-wave phase shifts of Schwartz[3] indicates that the polarization potential is too attractive, and a semi-empirical modification was introduced to achieve essentially exact agreement. This modification consisted in suppressing most of the short-range (monopole) parts of the potential. Besides the good agreement thereby achieved, the justification for such a modification was based on the fact that an adiabatic method is most likely to be in error near the atomic nucleus, where complicated correlations can occur. The monopole suppression used was energy independent, but nevertheless excellent s-wave phase shifts resulted over the whole energy range up to the positronium threshold (6.8 ev).

Second, the possibility of virtual positronium formation is not explicitly included. Since the positronium atom is a large, loosely bound system, it is not too surprising that s-wave scattering is not seriously affected by this omission, but higher impact parameter (higher angular momentum) scattering should include more virtual positronium. This is borne out by recent $L = 1$ and $L = 2$ lower bound calculations[4], which indicate that the polarization potential method underestimates the attraction in these partial waves. It is apparently not possible to retain the good s-wave agreement and also fit the p- and d- wave phase shifts with a simple, L-independent local potential.

The situation for positron-hydrogen scattering is clear: the modified adiabatic method will underestimate the total cross-sections as the positronium threshold is approached, and will also underestimate the angular dependence of the scattering.

The purpose of the present paper is to apply the polarization potential method to the elastic scattering of positrons by helium atoms. This problem is presently too difficult for rigorous solution, but is much more accessible to experiments. This is due to the relatively high threshold for positronium formation in helium (17.8 ev) compared to that of hydrogen, and also due to the fact that atomic helium is stable. It seems probable that energy resolved positron beams will soon be available[5], and the helium scattering experiment should prove feasible. At the moment, one experimental cross-section value exists[6], although the analysis[7] is rather intricate, since it involves the diffusion of a swarm of positrons through gaseous helium under the influence of an electric field.

It is, thus, of interest to examine the modified adiabatic method as applied to the helium case. To do this with any hope of success, one must first verify that the velocity range of interest is appropriate. For the case of hydrogen, the mean kinetic energy of the atomic electron is 13.6 eV and that of the positron is less than 6.8 eV. For Helium, each electron has an average kinetic energy of 39.5 eV, while that of the positron is less than 17.8 eV. One can see that the positron moves somewhat slower relative to the electron velocity for helium than for hydrogen. Thus the semi-classical criterion for an adiabatic approximation is at least as well satisfied.

To apply the Dalgarno-Lynn[2] potential one must have a hydrogenic ground state for the target atom. Using a shielded, uncorrelated hydrogenic wave function for helium introduces the largest uncontrolled error into the present work, and it remains to be seen how much error in the scattering this approximation causes. The only parameters in the theory are the effective nuclear charge, the monopole suppression factor and one more parameter which can be used to bring the static polarizability into agreement with experiment.

The Modified Adiabatic Calculation

The non-relativistic Hamiltonian for the system consisting of a fixed helium nucleus, two electrons and one positron can be written as follows:

$$H = H_0 + H_{12} + H_x + V \qquad (1)$$

where

$$H_0 = -\sum_{i=1,2}\left[\underset{\sim}{\nabla}_i^{\,2} + \frac{4}{r_i}\right]$$

$$H_{12} = \frac{2}{|\underset{\sim}{r}_1 - \underset{\sim}{r}_2|}$$

$$H_x = -\underset{\sim}{\nabla}_x^{\,2}$$

$$V = 2\sum_{i=1,2}\left[\frac{1}{x} - \frac{1}{|\underset{\sim}{x} - \underset{\sim}{r}_i|}\right].$$

Here, $\underset{\sim}{r}_1$ and $\underset{\sim}{r}_2$ are the position vectors of the two electrons and $\underset{\sim}{x}$ is the position vector of the positron. Atomic units are used with energies in Rydbergs, lengths in units of the Bohr radius, a_0, and momenta in units of a_0^{-1}.

The modified adiabatic method proposes to use a scattering wave function of the form

$$\psi_{\underset{\sim}{k}}(\underset{\sim}{x}, \underset{\sim}{r}_1, \underset{\sim}{r}_2) = \left[1 + C\,(G - G_0) + \alpha\, G_0\right]\chi_{\underset{\sim}{k}}(\underset{\sim}{x})\,\phi(\underset{\sim}{r}_1, \underset{\sim}{r}_2). \qquad (2)$$

In this equation, $\phi(\underset{\sim}{r}_1,\underset{\sim}{r}_2)$ is the ground state wave function of the helium atom and satisfies

$$\left[H_0 + H_{12} - E_0\right] \phi = 0, \tag{3}$$

where E_0 is the ground state energy. The positron scattering function $X_{\underset{\sim}{k}}(\underset{\sim}{x})$ has appropriate boundary conditions, while G and G_0 are the first-order adiabatic correlation function and its monopole part, respectively. They satisfy the equations:

$$\left[G, (H_0 + H_{12})\right] \phi = \left(V - \langle V\rangle\right) \phi \tag{4a}$$

and

$$\left[G_0, (H_0 + H_{12})\right] \phi = \left(V_0 - \langle V_0\rangle\right) \phi, \tag{4b}$$

with

$$\langle Q\rangle \equiv \iint d\underset{\sim}{r}_1\, d\underset{\sim}{r}_2\, \phi^* Q \phi$$

and

$$\langle G\rangle = \langle G_0\rangle = 0$$

As in I, both the potential V and the correlation function G may be understood to be expanded in Legendre polynomials in the angles between $\underset{\sim}{x}$ and $\underset{\sim}{r}_1$ and $\underset{\sim}{r}_2$. The parameter α thus measures the amount of P_0 (monopole) correlation retained in $\Psi_{\underset{\sim}{k}}$, and C will be discussed later.

Assuming that $\Psi_{\underset{\sim}{k}}$ has the correct form to satisfy the Schrödinger equation, one writes [9]

$$\left\langle \left[H - E_0 - k^2 \right] \left[1 + C(G - G_0) + \alpha G_0 \right] \right\rangle \chi_{\underset{\sim}{k}}(\underset{\sim}{x}) = 0 , \tag{5}$$

as the effective Schrödinger equation for the positron.

Using Eqs(4a,b), this becomes

$$\left[H_x - k^2 + \langle V \rangle + C \langle VG \rangle + (\alpha - C) \langle VG_0 \rangle \right] \chi_{\underset{\sim}{k}}(\underset{\sim}{x}) = 0. \tag{6}$$

As in the hydrogen case discussed in I, the various terms can be identified as follows:

$\langle v \rangle$ is the first-order (static) potential $V_1(x)$, $\langle VG \rangle$ is the second-order (polarization) potential $V_2(x)$, and $\langle VG_0 \rangle$ is the second-order monopole polarization potential $V_{20}(x)$. To obtain the phase shifts in this approximation it is necessary to make a partial-wave decomposition of $X_{\underset{\sim}{k}}$, and solve the resulting equations in an entirely straightforward manner.

Of course, the true eigenfunction ϕ describing the helium ground state is not known exactly, and some reasonably simple approximate wave functions must be substituted, in order to evaluate these potentials. (This represents the only extra inaccuracy in the helium case not appearing in the hydrogen case.) In evaluating $V_1(x)$, the two-term analytic approximation to the best Hartree function was chosen. According to Byatt[10], it yields a first order potential

$$V_1(x) = x^{-1} \left(5 e^{-Ax} - e^{-Bx} \right), \tag{7}$$

where

$$A = 2.4915, \; B = 5.4741.$$

A very similar potential was used without polarization by Malik[11]. To evaluate the second-order potentials, an even simpler form is necessary, or else the equations for G and G_0 become intractable. Choosing the uncorrelated, shielded hydrogenic function

$$\phi(\underset{\sim}{r}_1, \underset{\sim}{r}_2) = \pi^{-1} \beta^3 e^{-\beta(r_1 + r_2)}, \tag{8}$$

one can easily show that the second-order potentials can be obtained from the corresponding potentials in the positron-hydrogen case by the following rule:

$$V_2(x)_{\text{Helium}} = 2\, V_2(\beta x)_{\text{Hydrogen}}. \tag{9}$$

The second-order potentials for hydrogen are known[2], and are exhibited in I. It remains to give reasonable values for the three parameters α, β and C.

If it had been possible to use an exact wave function for the helium atom (as was the case for hydrogen), the only parameter in the theory would be α, the amount of monopole distortion retained in the scattering function. This parameter ought to be between zero and unity, and the results of I favor $\alpha \approx 0$. In the present calculation, both extreme values have been tried.

In I the long-range behavior of the polarization potential was shown to be

$$V_2(x)_{\text{Hydrogen}} \longrightarrow -\frac{9}{2x^4}, \tag{10}$$

which shows the correct dipole polarizability, 9/2. In the case of helium, the corresponding limit gives a polarizability of $\frac{9C}{\beta^4}$. The measured[12] polarizability is 1.376, and to obtain this value requires $C/\beta^4 = 0.1529$. Now, if β is determined by a variational calculation, the minimum energy is obtained for $\beta = 27/16$, and then $C = 1.240$. Another approach argues that the energy minimum is very flat and that it is preferable to set $C \equiv 1$, from which it follows that $\beta = 1.5992$. Both of these methods were examined[13].

Results and Discussion

Figs. 1, 2, and 3 show the energy dependence of the phase shift for $L = 0, 1, 2$ up to the threshold for positronium formation ($E = 1.31$). The four curves represent the extreme values of the monopole suppression, and the two methods of adjusting the dipole polarizability discussed above. As the angular momentum increases these curves coalesce, and for $L \geq 3$ an analytic expression[14] involving only the dipole polarizability P is sufficiently accurate, i.e.

$$\delta_L \approx \pi P k^2 / (2L-1)(2L+1)(2L+3) . \tag{11}$$

The total cross section

$$\sigma_T = \frac{4}{k^2} \sum_L (2L+1) \sin^2 \delta_L \tag{12}$$

is shown in Fig. 4, for the same four cases, in units of πa_0^2. In Fig. 5 the momentum-transfer cross-section is similarly displayed. This cross-section, defined as

$$\sigma_{MT} = \int d\Omega \frac{d\sigma}{d\Omega} (1 - \cos\theta) , \tag{13}$$

can be written (in units of πa_0^2) as

$$\sigma_{MT} = \frac{4}{k^2} \sum_L (L+1) \sin^2 (\delta_L - \delta_{L+1}) , \tag{14}$$

and is the particular cross-section which is effective in determining the mean free path for swarm or diffusion measurements. Such a measurement has been made[6] and analyzed[7] under the assumptions that both σ_{MT} and the annihilation rate of free positions in helium are independent of energy, and that positronium formation is very rapid for any positrons attaining the threshold energy. The numerical value derived in this way is $\sigma_{MT} = (0.023 \pm .006)\pi a_0^2$, and is shown in Fig. 5 by the shaded band. It is seen that there is no agreement whatsoever between the experiment and any of the theoretical curves. We have repeated the diffusion analysis of Ref. 7, allowing the cross-section to take the forms given by the present theory, but the disagreement remains. Note that we expect the L = 1 and L = 2 phase shifts to be underestimated by the present calculation; for the diffusion analysis the higher energy range is most important. To estimate the effect on the momentum-transfer cross-section of increasing these two phase shifts one can differentiate Eq. (14) and replace the sine function by its argument. Then

$$\Delta \sigma_{MT} = \frac{8}{k^2}\left[\left(-\delta_0+3\delta_1-2\delta_2\right)\Delta\delta_1+\left(-2\delta_1+5\delta_2-3\delta_3\right)\Delta\delta_2\right]. \tag{15}$$

Inserting the values of the phase shifts at threshold, and assuming $\Delta\delta/\delta \approx 0.5$ (which is justified by comparison with the results of I) one finds that increasing δ_1 and δ_2 makes the agreement with experiment[6,7] even worse than before. The experiment[6] and its analysis[7] are not completely straightforward, and further experiments would seem to be desirable.

One other calculation has been recently carried out[15] which deserves mention. It also employs an effective potential which is actually evaluated in the adiabatic approximation but, in common with similar adiabatic calculations in hydrogen, only a limited number of multipoles (0,1,2) were retained, instead of the complete polarization potential being used. Nevertheless, strong disagreement with experiment still occurs.

Acknowledgment

The numerical calculations reported here were programmed for the Goddard Laboratory for Theoretical Studies IBM 7094 electronic computer by Edward Monasterski, as an extension of his previous work on e^+ - H scattering.

References and Footnotes

*A preliminary report of these results was presented at the 1965 Honolulu meeting of the American Physical Society [Bull. Am. Phys. Soc. 10, 736 (1965)]

1. R. J. Drachman, Phys. Rev. 138, A1582 (1965).
   [Referred to below as I.]
2. A. Dalgarno and N. Lynn, Proc. Phys. Soc. (London) A70, 223 (1957).
3. C. Schwartz, Phys. Rev. 124, 1468 (1961). These results are considered to be definitive.
4. C. J. Kleinman, Y. Hahn and L. Spruch, Phys. Rev. 140, A413 (1965).
5. D. F. Herring (private communication).
6. S. Marder, V. W. Hughes, C. S. Wu, and W. Bennett, Phys. Rev. 103, 1258 (1956).
7. W. B. Teutsch and V. W. Hughes, Phys. Rev. 103, 1266 (1956).
8. A. Dalgarno and J. T. Lewis, Proc. Roy. Soc. (London) A223, 70, (1958).
9. This is essentially the procedure used by A. Temkin, Phys. Rev. 116, 358 (1959), in his method of polarized orbitals, with two differences: He retained only part of G, and included exchange corrections since electron scattering was being treated. See also: R. W. LaBahn and J. Callaway Phys. Rev. 135, A1539 (1964).
10. W. O. Byatt - Phys. Rev. 104, 1298 (1956).
11. F. B. Malik - Z. Naturforsch. 16a, 500 (1961).
12. K. F. Herzfeld and K. L. Wolf, Ann. Physik 76, 71 and 567 (1925). Two recent determinations give higher but discordant values of the polarizability: A. Dalgarno and A. E. Kingston, Proc. Roy. Soc. (London) A259, 424 (1960) obtain the value 1.384, while D. R. Johnston, G. J. Oudemans and R. H. Cole, J. Chem. Phys. 33, 1310 (1960) find the value 1.395. For our purposes these differences are insignificant.

13. A third set of parameters ($\beta = 1.4049$, $C = 0.674$) gives a good approximation to the dipole, quadrupole and octupole polarizabilities, [P. W. Langhoff

and R. P. Hurst, Phys. Rev. 139, A1415 (1965) , but appear to be too far from the energy minimizing values. The scattering thus obtained is not qualitatively different from the other two cases.

14. T. F. O'Malley, L. Rosenberg and L. Spruch, Phys. Rev. 125, 1300 (1962).

15. N. R. Kestner, J. Jortner, M. H. Cohen and S. A. Rice, Phys. Rev. 140, A56 (1965).

Figure Captions

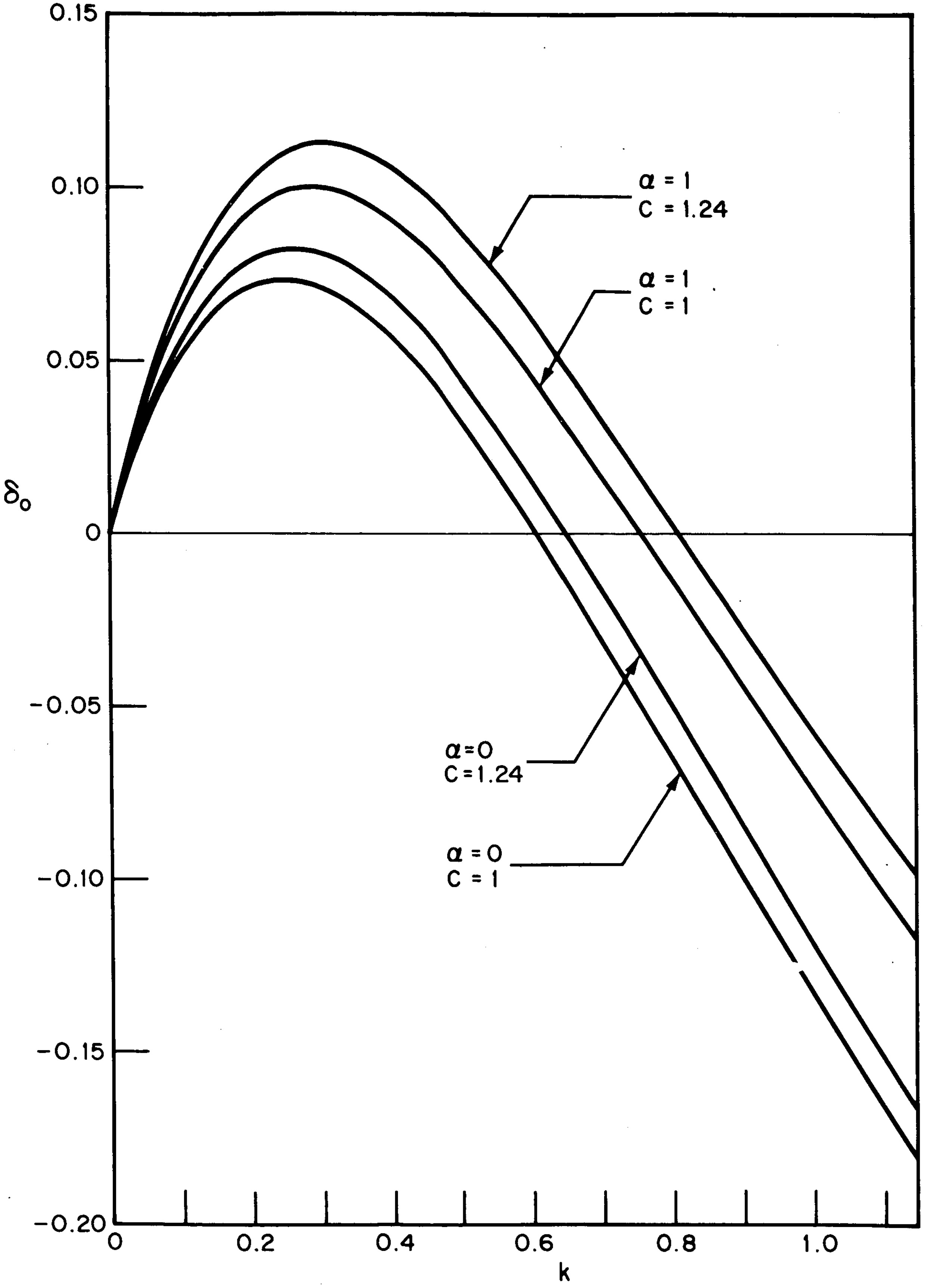
Fig. 1. Phase shifts in radians for s-wave scattering. The four sets of parameters discussed in the text are shown. The abscissa is in atomic units of momentum.

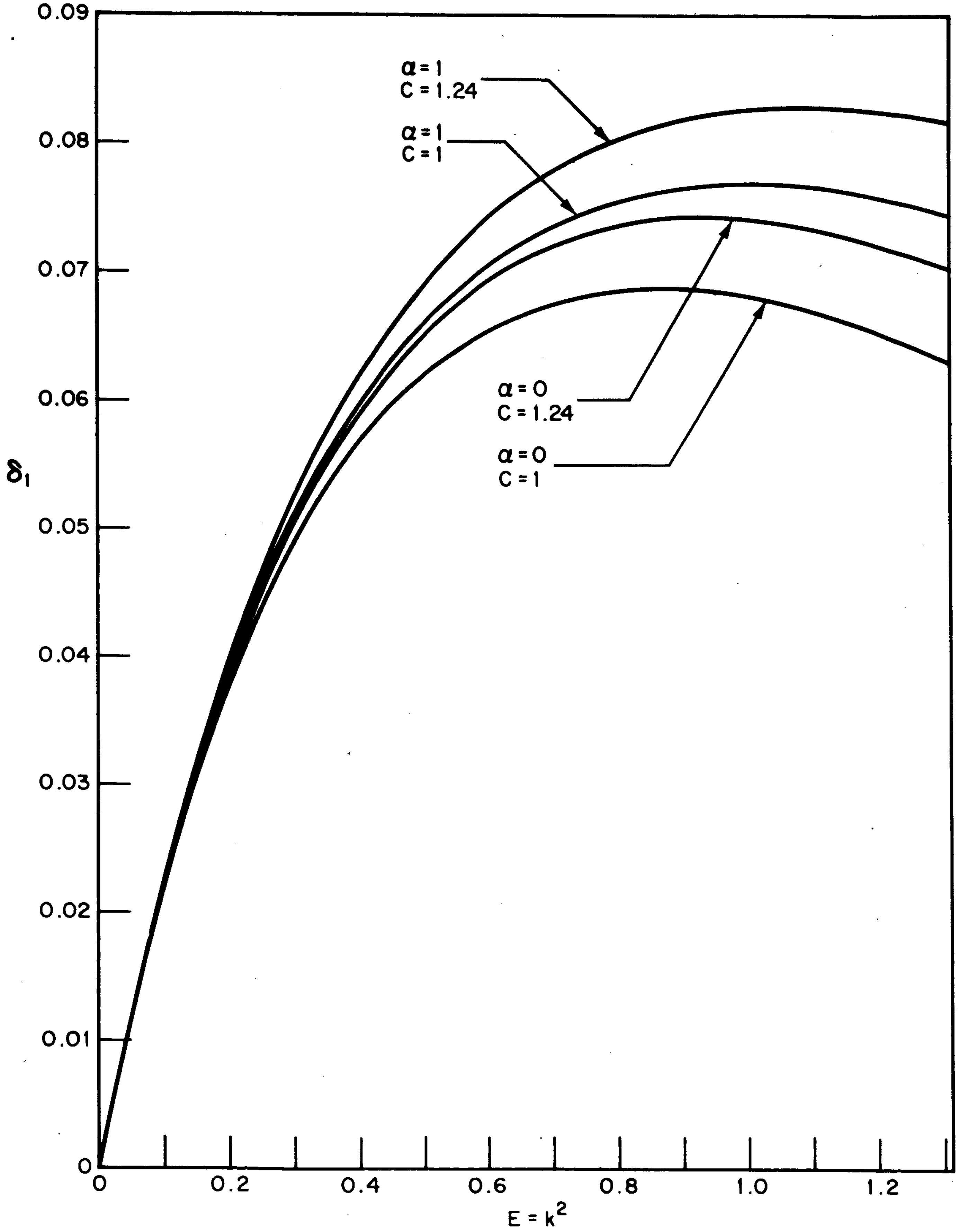
Fig. 2. Phase shifts in radians for p-wave scattering. The four sets of parameters discussed in the text are shown. The abscissa here is in energy units.

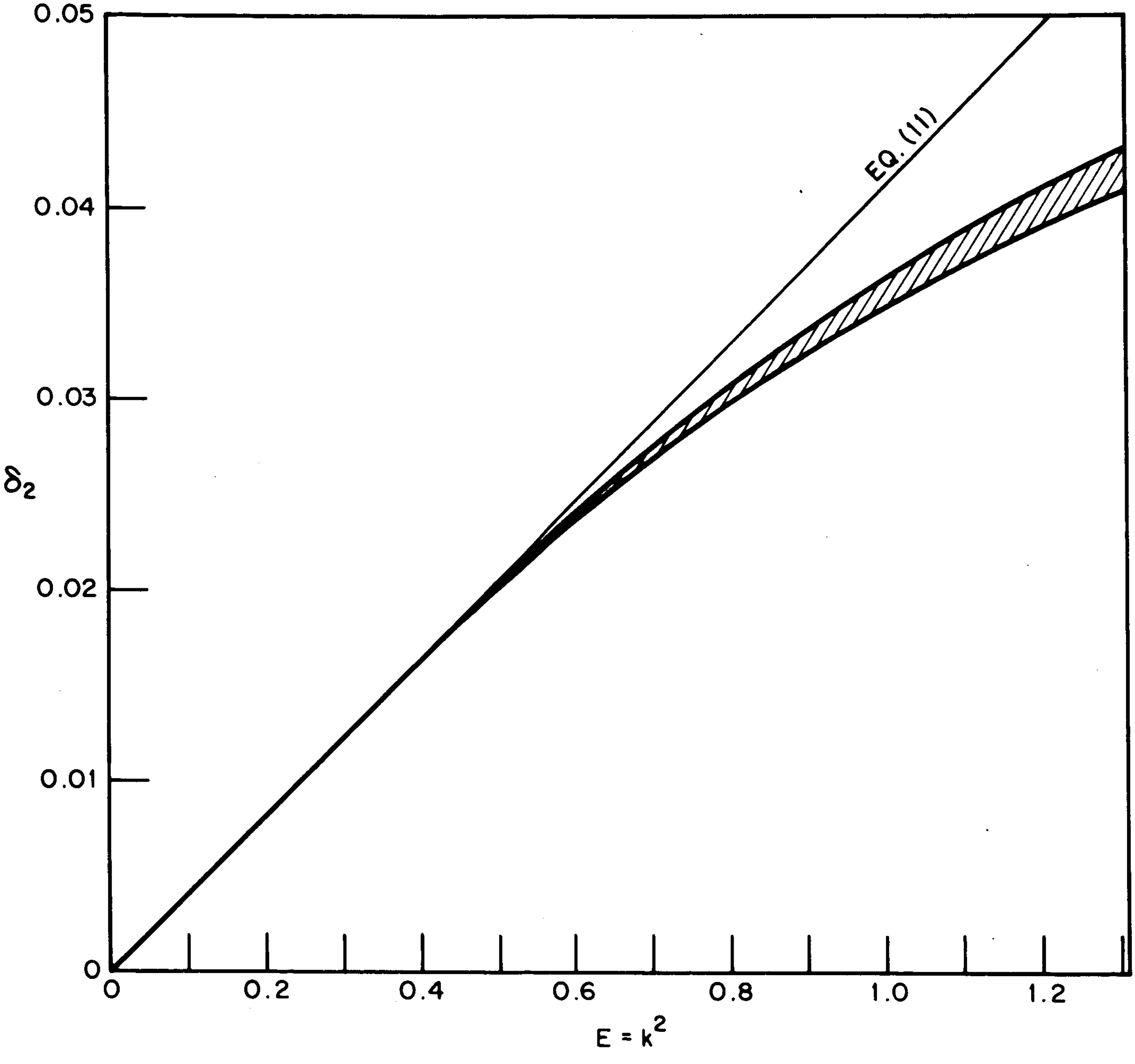
Fig. 3. Phase shifts in radians for d-wave scattering. The four different curves are very close, and are shown as a band. The abscissa again is in energy units, and the linear relation of Eq. (11) is shown to agree well.

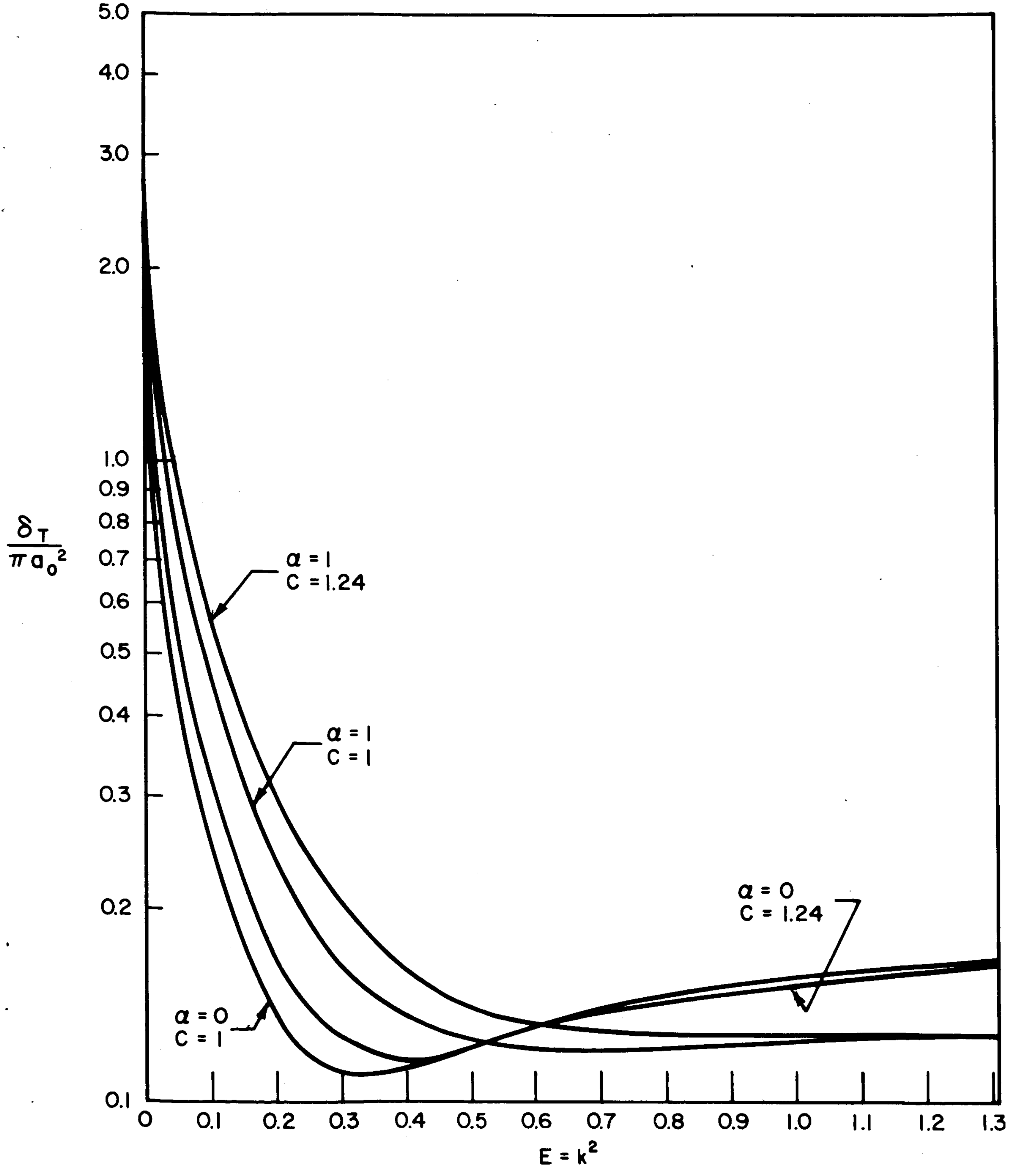
Fig. 4. Total cross-sections in units of πa_0^2, including L = 0,1,2,3 partial waves, for the four cases discussed.

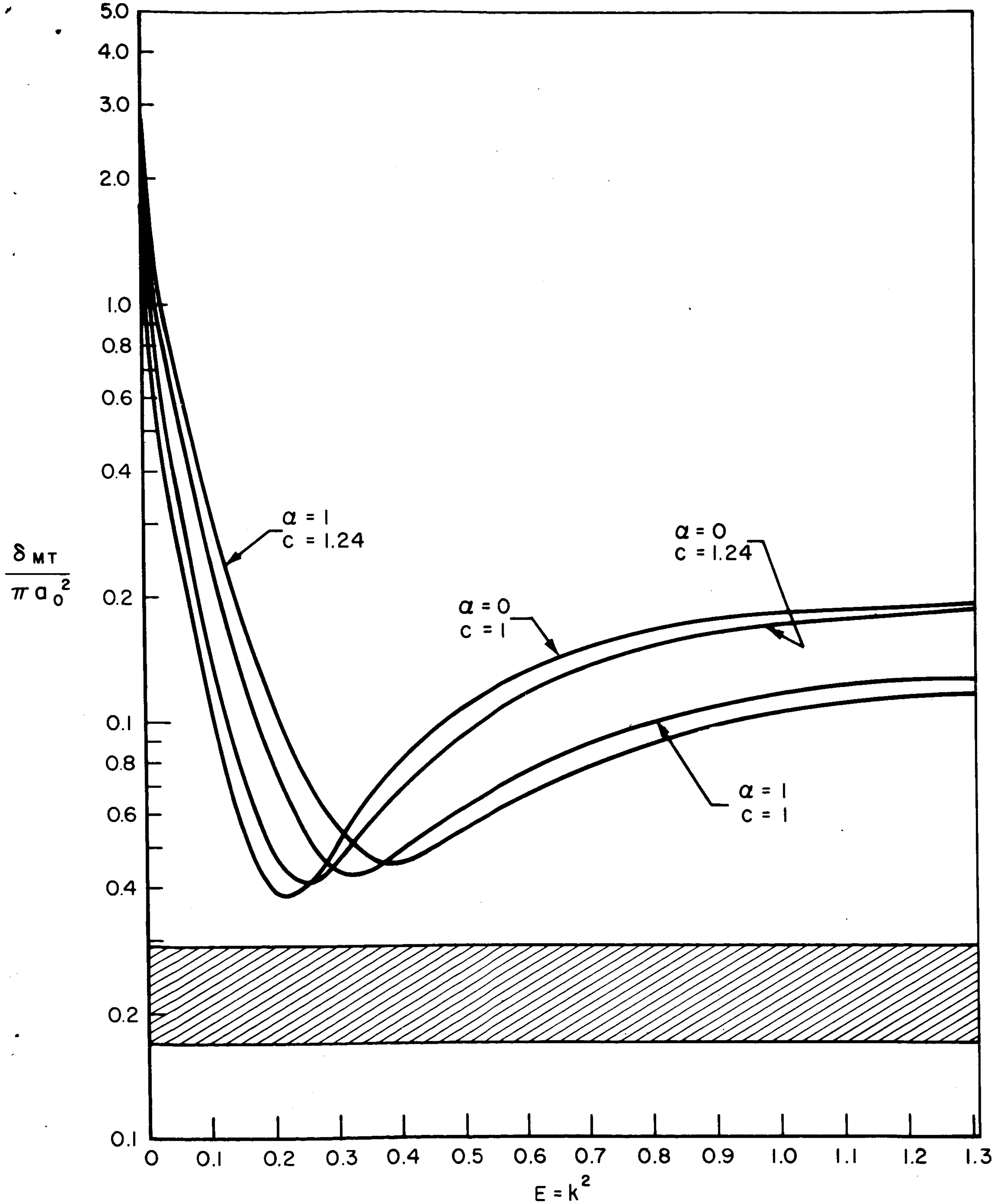
Fig. 5. Momentum-transfer cross-sections in units of πa_0^2, including L = 0,1, 2,3 partial waves, for the four cases discussed. The "experimental result (Ref. 7) is shown by the shaded band.


0.15
0.10
0.05
0
−0.05
−0.10
−0.15
−0.20
δ_o
0
0.2
0.4
0.6
0.8
1.0
k
α = 1
C = 1.24
α = 1
C = 1
α = 0
C = 1.24
α = 0
C = 1


α = 1
C = 1.24
α = 1
C = 1
α = 0
C = 1.24
α = 0
C = 1
δ_1
0.09
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0
0
0.2
0.4
0.6
0.8
1.0
1.2
E = k^2


0.05
0.04
0.03
0.02
0.01
0
δ_2
EQ. (11)
0
0.2
0.4
0.6
0.8
1.0
1.2
$E = k^2$


$\frac{\delta_T}{\pi a_0^2}$
5.0
4.0
3.0
2.0
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
$\alpha = 1$
$C = 1.24$
$\alpha = 1$
$C = 1$
$\alpha = 0$
$C = 1.24$
$\alpha = 0$
$C = 1$
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
$E = k^2$


5.0
4.0
3.0
2.0
1.0
0.8
0.6
0.4
0.2
0.1
0.8
0.6
0.4
0.2
0.1
$\frac{\delta_{MT}}{\pi a_0^2}$
α = 1
c = 1.24
α = 0
c = 1.24
α = 0
c = 1
α = 1
c = 1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
E = k²