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The elastic positron scattering from mercury in the relativistic polarized orbital method

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Abstract. The results of relativistic calculations on the elastic positron scattering from mercury atoms for incident positron energies of up to 100 eV are presented. The polarization potential applied in the calculations was obtained by solving the coupled Dirac-Hartree-Fock equations. The values of scattering length, phaseshifts, total elastic cross sections and elastic momentum transfer cross sections are compared with theoretical results of other authors.

1. Introduction

In a previous paper (Szmytkowski 1991, to be referred to as I) the relativistic polarized orbital theory of elastic electron and positron scattering from closed-shell atoms, based on the coupled Dirac-Hartree-Fock (CDHF) equations, has been formulated. In the present paper we illustrate an application of the theory studying the positron scattering from mercury atoms for which relativistic effects in a polarization potential are expected to be very important.

There are only four earlier theoretical papers concerning the positron scattering from mercury and all of them deal with the elastic scattering only. Sin Fai Lam (1980) used the Dirac-Hartree-Fock (DHF) static potential together with a model polarization potential in calculations based on the Schrödinger equation. Jaskólski (1985) used the same potentials in his investigation of the relative importance of direct and indirect relativistic effects. Hasenburg (1986) used again the DHF static potential and a different model polarization potential and discussed reasons for the extremely small values of the spin polarizations of scattered positrons. Recently, Sienkiewicz and Baylis (1991) have performed calculations on e^+-Hg scattering in the DHF framework treating the positron as the electron with a negative energy below $-mc^2$. Also in these calculations the distortion of the atomic charge cloud has been described by a model polarization potential. In view of the model character of all the above mentioned calculations it should be emphasized that below we study the positron scattering from mercury for the first time in a fully *ab initio* manner. Unfortunately, it has been impossible to compare the present results with the experiment because no measurements on e^+-Hg scattering have been published so far.

The paper is organized in the following way. In section 2 methods of solution of the CDHF equations and computational details of the scattering problem are described. In section 3 we present results of calculations for the polarizaton potential, scattering length, phaseshifts, differential, total elastic and elastic momentum transfer cross

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sections and compare them with results of other calculations. The results are briefly summarized in section 4.

The notation (I.- -) refers to equation (- -) in I.

2. Computational methods

2.1. Coupled Dirac-Hartree-Fock equations

Below we shall briefly describe computational methods and the reader is referred to I for mathematical details.

The CDHF equations for closed-shell systems are given by equation (I.29). They constitute a set of coupled systems of two first-order linear inhomogeneous integro-differential equations of the form

$$\mathbb{D}F = \mathbb{I}F + Q^{(0)} + \sum_a \lambda_a P_a \tag{1}$$

where F is a two-component column, $\mathbb{D}$ is a 2×2 matrix linear operator containing a first derivative, $\mathbb{I}$ is a linear integral operator, $Q^{(0)}$ is an inhomogeneous term and $\{P_a\}$ is a set of given two-component functions (cf (I.29)). The role of the Lagrange multipliers $\{\lambda_a\}$ (which are to be determined) is to ensure the orthogonality of F to the subspace spanned by $\{P_a\}$. The solution F should also satisfy proper boundary conditions, i.e. it must vanish at the origin and at infinity.

Because of the presence of the integral operator $\mathbb{I}$ equation (1) has to be solved in an iterative way. Assuming that an approximate solution $F^{(i)}$ at the ith iteration step is known, $F^{(i+1)}$ will satisfy the following differential equation

$$\mathbb{D}F^{(i+1)} = Q^{(i)} + \sum_a \lambda_a P_a \tag{2}$$

where

$$Q^{(i)} = \mathbb{I}F^{(i)} + Q^{(0)} \tag{3}$$

is a known inhomogeneous term. It should be emphasized that the Lagrange multipliers $\{\lambda_a\}$ have to be determined at each iteration step.

McEachran *et al* (1980) presented an elegant method of solving equation (2). Following, them, let us assume that $F_0^{(i+1)}$ is a solution of the equation

$$\mathbb{D}F_0^{(i+1)} = Q^{(i)} \tag{4}$$

and that $\tilde{F}_a^{(i+1)}$ satisfies the equation

$$\mathbb{D}\tilde{F}_a^{(i+1)} = P_a. \tag{5}$$

They showed that the Lagrange multipliers $\{\lambda_a\}$ are solutions of the set of algebraic equations

$$\sum_b \lambda_b \langle P_a|\tilde{F}_b^{(i+1)}\rangle = -\langle P_a|F_0^{(i+1)}\rangle \tag{6}$$

where $\langle|\rangle$ denotes a scalar product, and that

$$F^{(i+1)} = F_0^{(i+1)} + \sum_a \lambda_a \tilde{F}_a^{(i+1)}. \tag{7}$$

In the result, the main computational effort is involved in solving the systems of the two first-order inhomogeneous linear differential equations (4) and (5) and it has been found that the Sienkiewicz-Baylis integration algorithm (Sienkiewicz and Baylis 1987) is excellent for this purpose.

The CDHF equations were solved by the program POLAR (Szmytkowski 1992). The unperturbed radial atomic orbitals which entered these equations were generated by the MCDF code of Grant *et al* (1980).

As a test of correctness and accuracy of the program POLAR we calculated static dipole and quadrupole polarizabilities for many closed-shell atoms and ions, both in the relativistic and non-relativistic cases (in the latter case the speed of light c was simply multiplied by 1000). In both cases calculations were performed in the fully coupled approach, i.e. all atomic orbitals were allowed to be distorted. Such relativistic calculations were also performed by Johnson and co-workers (Kolb *et al* 1982, Johnson *et al* 1983), while frozen-core non-relativistic calculations (in the coupled Hartree-Fock approximation) were carried out by McEachran, Stauffer and their group (Markiewicz *et al* 1981, McEachran *et al* 1977, 1979, 1982). Comparison between the present results and those of the authors cited above does not show any serious discrepancy. As an illustrative example in table 1 we present the values of dipole polarizabilities for Zn, Cd and Hg atoms.

Table 1. Calculated values of dipole polarizabilities for Zn, Cd and Hg atoms (in atomic units). In the Toronto calculations only $(n-1)$s $(n-1)$p $(n-1)$d ns subshells (with $n = 4$, 5, 6 for Zn, Cd and Hg, respectively) were allowed to be polarized. The present results (second and fourth columns) and the results of Kolb *et al* (1982) were obtained in the fully coupled approximation.

Atom	Present (non-relativistic)	Toronto (non-relativistic)	Present (relativistic)	Kolb *et al* (1982) (relativistic)
Zn	54.06	54.07[a,b]	50.81	50.8
Cd	76.02	75.99[b]	63.68	63.7
Hg	81.42	81.38[c]	44.84	44.9

[a] Markiewicz *et al* (1981).
[b] McEachran and Stauffer (1992).
[c] McEachran and Stauffer (1987).

2.2. Scattering calculations

In the polarized orbital approximation the elastic scattering of positrons from a closed-shell target is an example of potential scattering in a central field. We recall that the scattering equation has the form (cf (I.43))

$$\begin{pmatrix} mc^2 - E + V(r) & -c\hbar\left(\frac{\mathrm{d}}{\mathrm{d}r} - \frac{\kappa}{r}\right) \\ c\hbar\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\kappa}{r}\right) & -mc^2 - E + V(r) \end{pmatrix} \begin{pmatrix} P(r) \\ Q(r) \end{pmatrix} = 0 \tag{8}$$

where E is the total energy of the positron (including the rest energy mc^2) and $V(r)$ is the central potential which consists of two (static and polarization) parts. The above equation must be solved subject to the initial condition

$$P(0) = Q(0) = 0 \tag{9}$$

and the asymptotic condition

$$P(r) \xrightarrow[r\to\infty]{} A_\kappa \sin(Kr - \tfrac{1}{2}\pi L + \delta_\kappa) \tag{10}$$

where δ_κ is the scattering phaseshift,

$$L = \begin{cases} -\kappa - 1 & \text{if } \kappa < 0 \\ \kappa & \text{if } \kappa > 0 \end{cases} \tag{11}$$

and

$$K^2 = (E - mc^2)(E + mc^2)(c\hbar)^{-2}. \tag{12}$$

Then the total elastic (Q_T) and elastic momentum transfer (Q_M) cross sections can be expressed in terms of the phaseshifts δ_κ:

$$Q_T = \frac{4\pi}{K^2} \sum_{\kappa=-\infty}^{+\infty} |\kappa| \sin^2 \delta_\kappa \tag{13}$$

and

$$Q_M = \frac{4\pi}{K^2} \sum_{\kappa=-\infty}^{+\infty} \frac{\operatorname{sgn} \kappa}{2\kappa + 1} [\kappa(\kappa+1) \sin^2(\delta_\kappa - \delta_{\kappa+1}) + \tfrac{1}{4} \sin^2(\delta_\kappa - \delta_{-\kappa})]. \tag{14}$$

The phaseshifts can be found by numerical outward integration of equation (8) with the initial condition (9) and by comparing the numerical solution in the asymptotic region with the analytical formula (10). However, the variable phase method (Babikov 1988, Calogero 1967) is much more suitable for extracting phaseshifts. In the relativistic version of this method one introduces a so-called phase function $\delta_\kappa(r)$ which satisfies the first-order non-linear differential equation

$$\begin{aligned} \frac{d\delta_\kappa(r)}{dr} = {} & -\lambda^{-1} \frac{V(r)}{c\hbar} [\hat{j}_L(Kr) \cos \delta_\kappa(r) - \hat{n}_L(Kr) \sin \delta_\kappa(r)]^2 \\ & -\lambda \frac{V(r)}{c\hbar} [\hat{j}_{L\mp1}(Kr) \cos \delta_\kappa(r) - \hat{n}_{L\mp1}(Kr) \sin \delta_\kappa(r)]^2 \end{aligned} \tag{15}$$

where

$$\lambda = \left(\frac{E - mc^2}{E + mc^2}\right)^{1/2} \tag{16}$$

and $\hat{j}_L(Kr)$ and $\hat{n}_L(Kr)$ are the Riccati–Bessel functions. The upper sign (−) should be taken for $\kappa > 0$, and the lower one (+) for $\kappa < 0$. The equation (15) should be solved subject to the initial condition

$$\delta_\kappa(0) = 0. \tag{17}$$

The phase function $\delta_\kappa(r)$ is related to the corresponding phaseshift δ_κ in the following way

$$\delta_\kappa = \lim_{r\to\infty} \delta_\kappa(r). \tag{18}$$

Another important quantity is the scattering length a defined as

$$a = -\lim_{K\to 0} \frac{\tan \delta_{-1}}{K}. \tag{19}$$

The scattering length can also be calculated using the variable phase method. For this purpose let us introduce a function $a(r)$

$$a(r)=-\lim_{K\to 0}\frac{\tan\delta_{-1}(r)}{K} \tag{20}$$

which is obviously related to the scattering length a in the following way:

$$a=\lim_{r\to\infty} a(r). \tag{21}$$

It is easy to show that the function $a(r)$ satisfies the non-linear first-order differential equation

$$\frac{\mathrm{d}a(r)}{\mathrm{d}r}=\frac{2mV(r)}{\hbar^2}[r-a(r)]^2+\frac{V(r)}{2mc^2}\left[\frac{a(r)}{r}\right]^2 \tag{22}$$

with an initial condition

$$a(0)=0. \tag{23}$$

However, a method of calculation of a based on the numerical integration of equation (22) fails if bound states exist in the potential $V(r)$ because the function $a(r)$ is singular at some intermediate distance r_0:

$$\lim_{r\to r_0} a(r)=\mp\infty. \tag{24}$$

In such a case it is desirable to introduce a new function $b(r)$ such that

$$a(r)=a_0\tan b(r) \tag{25}$$

where a_0 denotes the Bohr radius. The latter function is finite everywhere and satisfies the differential equation

$$\frac{\mathrm{d}b(r)}{\mathrm{d}r}=\frac{2mV(r)}{a_0\hbar^2}[r\cos b(r)-a_0\sin b(r)]^2+\frac{V(r)}{2a_0mc^2}\left[\frac{a_0}{r}\sin b(r)\right]^2 \tag{26}$$

with an initial condition

$$b(0)=0. \tag{27}$$

As follows from equations (21) and (25), the function $b(r)$ is related to the scattering length a by the equation

$$a=a_0\tan b(\infty). \tag{28}$$

Equation (26) can be used for calculation of the scattering length irrespective of whether there exist bound states in the potential $V(r)$ or not.

The advantage of the variable phase method is that if the scattering potential $V(r)$ tends asymptotically to zero and has a constant sign in that region, both functions $\delta_\kappa(r)$ and $b(r)$ converge *monotonically* to their asymptotic limits which enables one to find the phaseshifts and the scattering length with a great accuracy.

We used the sixth-order Adams predictor-corrector algorithm (Rice 1983) because of its accuracy and stability for numerical solving of the equations (15) and (26). We found that the presence of a long-range tail in the polarization potential required an integration out to several hundred atomic units until the functions $\delta_\kappa(r)$ and $b(r)$ converged to their asymptotic limits within prescribed tolerance.

The latter disadvantage can be avoided in a case of calculation of the scattering length. The idea is to integrate equation (26) numerically only to r_s such that

$$V(r) \simeq -\frac{\alpha_1 e^2}{2r^4} \qquad \text{for } r \geqslant r_s. \tag{29}$$

Denoting

$$a_s = a_0 \tan b(r_s) \tag{30}$$

we can extrapolate the function $a(r)$ to infinity with the aid of the following *non-relativistic* formula (Szmytkowski 1990a, b)

$$a(\infty) = \beta \frac{1 + \beta(1/r_s - 1/a_s)\tan(\beta/r_s)}{\tan(\beta/r_s) - \beta(1/r_s - 1/a_s)} \tag{31}$$

where $\beta = (\alpha_1/a_0)^{1/2}$. The result obtained by the direct numerical integration of equation (26) to very large r indicates that the use of this *non-relativistic* expression practically does not influence the quality of the final result (the relative difference was about 10^{-5}).

3. Results and discussion

We performed calculations of the phaseshifts, total elastic and elastic momentum transfer cross sections in the energy region 0–100 eV employing relativistic and non-relativistic *ab initio* calculated polarization potentials as well as model potentials of Sin Fai Lam (1980) and Sienkiewicz and Baylis (1991). The static potentials were calculated in a standard way (Szmytkowski 1991, equation (I.44)) using the relativistic or non-relativistic radial atomic orbitals generated by the MCDF program of Grant *et al* (1980).

Before we proceed further and present results, a few comments on the reliability of the approximation used should be given. Describing the unperturbed target in its ground state we used a single DHF determinant. It is well known that such an approach is not the best one and that a significantly better description could be obtained using a multiconfigurational wavefunction. It would require, however, a formulation of the multi-configurational relativistic polarized orbital method. But in view of the fact that above the corresponding thresholds this method does not take into account inelastic or rearrangement (Ps formation) processes, it is clear that other *ab initio* methods, such as the relativistic R-matrix (Chang 1975, Wijesundera *et al* 1992, Thumm and Norcross 1992), should be favoured in future.

3.1. *Ab initio polarization potentials*

In the numerical calculations we retained only the dipole term in the polarization potential. The dropping of the monopole and higher-order terms is justified by the simultaneous neglect of the non-adiabatic dynamic distortion effects in the derivation of the scattering equation (I.8a). Far away from the atom the effective potential (omitting, however, the additional terms derived by Seaton and Steenman-Clark (1977)) is of the form

$$V_{\text{eff}}(r) = -\frac{\alpha_1 e^2}{2r^4} - \sum_{k=2}^{\infty} \frac{(\alpha_k - 6\beta_{k-1})e^2}{2r^{2k+2}} \tag{32}$$

where the coefficients α_k and $6\beta_{k-1}$ are both positive and comparable in magnitude. Therefore, neglecting the dynamic distortion effects (i.e. putting $\beta_{k-1} = 0$) we were also forced to drop other than dipole contributions to the polarization potential.

Like the test calculations of polarizabilities, calculations of the dipole ($k = 1$) polarization potentials were carried out in the fully coupled approach, i.e. all 22 mercury relativistic subshells were allowed to be polarized which required the solution of 56 radial integro-differential CDHF equations. The resulting potentials, both relativistic and non-relativistic, are presented in figure 1 along with the model potentials of Sin Fai Lam and Sienkiewicz and Baylis. It is seen that the *ab initio* polarization potentials are much deeper than both model ones. Far away from the origin the long-range tails of potentials fall off like the inverse fourth power of the distance (cf equation (32)) with the dipole polarizability α_1 equal to 44.84 a_0^3 and 81.42 a_0^3 for the relativistic and non-relativistic polarization potentials, respectively. Including the relativistic effects the value of the mercury polarizability was reduced almost twice but it is still higher than the value 34.42 a_0^3 recommended by Miller and Bederson (1977). Further reduction would require more advanced methods based on the multi-configurational coupled Dirac–Hartree–Fock equations.

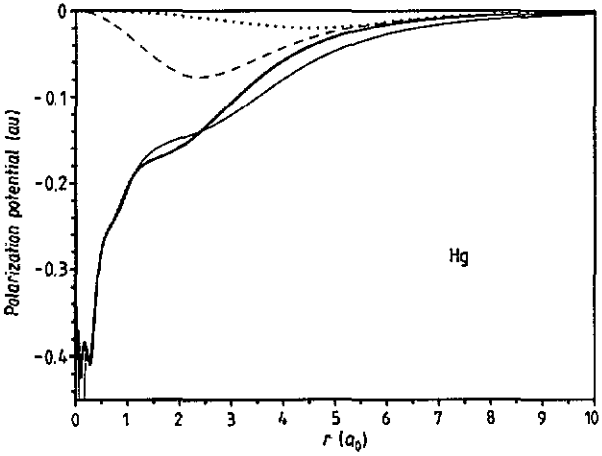

Figure 1. Dipole polarization potentials for mercury: ——, present relativistic; ——, present non-relativistic; · · · · ·, Sin Fai Lam (1980); – – –, Sienkiewicz and Baylis (1991). The non-relativistic *ab initio* potential reaches its minimum value −0.61 au at $r = 0.12\ a_0$.

3.2. *Scattering length*

In table 2 we present the calculated values of scattering lengths in the relativistic and non-relativistic cases. As is seen, the relativistic effects in static and polarization potentials changed the sign of the scattering length as compared with its non-relativistic value. The large positive value of the non-relativistic scattering length means that in the present model the non-relativistic mercury atom would be able to weakly bind a positron forming a compound Hge^+ with a binding energy about 0.01 eV. On the other hand, the large negative value of the relativistic scattering length means that a relativistic mercury atom is on the verge of supporting a bound state—one may speak of a virtual state with an energy of about 0.01 eV. Of course, these calculations, because of their

Table 2. Scattering length for positron scattering on mercury (in atomic units).

Present (non-relativistic)	Present (relativistic)	Sienkiewicz and Baylis (present)	Sin Fai Lam (present)	Sin Fai Lam (original)
40.73	−39.91	−14.10	−5.85	−6.5

approximate character, cannot definitely solve the problem whether the real mercury atom can bind a positron or not. Nevertheless, it is clear that the answer will depend on the relativistic effects in the target structure.

For comparison, in table 2 we also present the scattering lengths obtained with the polarization potentials of Sienkiewicz and Baylis and Sin Fai Lam. The fact that their absolute values are lower compared with the present relativistic result can be explained by the shallower polarization potentials used by these authors. Somewhat surprising is a relatively large difference between the present result ($-5.85\ a_0$) obtained using the Sin Fai Lam potential and his original result ($-6.5\ a_0$). It is, however, in accord with the observation of Sienkiewicz and Baylis that at very low energies the values of the total elastic cross section presented by Sin Fai Lam are too high.

3.3. Phaseshifts

The present results for the relativistic δ_{-1} and δ_{-2} phaseshifts are shown in figures 2(*a*) and (*b*) where they are also compared with the results of the calculations performed with the polarization potentials of Sin Fai Lam and Sienkiewicz and Baylis. In the low-energy range the agreement between these three relativistic sets of results is rather poor, although the general shape of the presented curves is the same. The S-wave phaseshift (δ_{-1}) of Sin Fai Lam goes through zero at an energy below 1 eV where

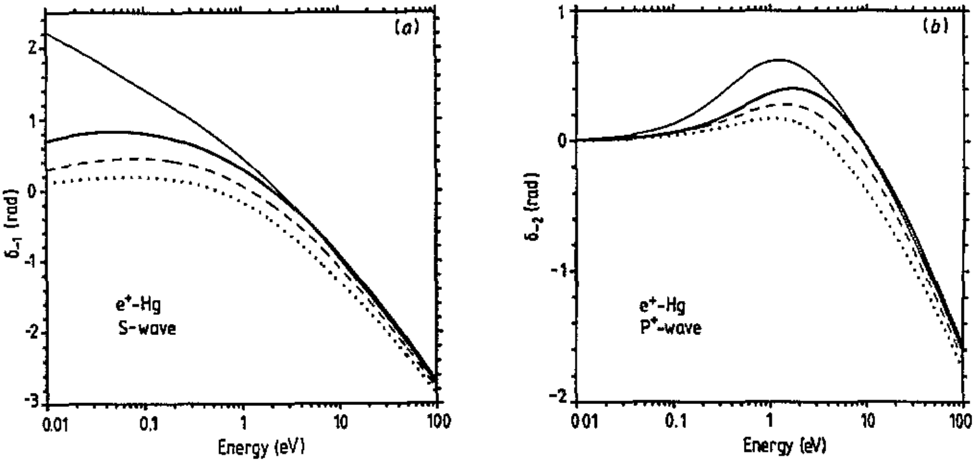

Figure 2. S-wave phaseshifts (δ_{-1}) (a) and P$^+$-wave phase shifts (δ_{-2}) (b) for elastic scattering of positrons from mercury: ——, present relativistic; ——, present non-relativistic; · · · · ·, present with the polarization potential of Sin Fai Lam (1980); – – –, present with the polarization potential of Sienkiewicz and Baylis (1991).

higher-order phaseshifts are still very small which should give rise to the Ramsauer–Townsend minimum in the total elastic and elastic momentum transfer cross sections, and indeed it is so (see section 3.4).

The comparison of the two sets of phaseshifts corresponding to a given quantum number of the orbital angular momentum L shows, in accord with the earlier conclusions of Hasenburg (1986) and Sienkiewicz and Baylis (1991) that differences between δ_L and δ_{-L-1} are negligible in the considered energy region. Consequently, the spin polarization of the scattered positrons due to the spin-orbit coupling is very small and its values are not presented here.

As an example of the importance of the relativistic effects in interaction potentials we have also plotted non-relativistic phaseshifts. Most striking is the quite different behaviour of the S-wave phaseshifts in the relativistic and non-relativistic cases (the non-relativistic value tends to π while the relativistic one tends to 0 when the energy decreases to zero). The conclusion is the same as in section 3.2—the non-relativistic mercury atom would be able to attach a positron whereas the relativistic atom could not.

3.4. *Total elastic and elastic momentum transfer cross sections*

Our results for the total elastic and elastic momentum transfer cross sections are shown in figures 3 and 4 where they are also compared with the results of calculations performed with the polarization potentials of Sin Fai Lam and Sienkiewicz and Baylis. The overall agreement between the three relativistic results is again rather poor and the respective curves differ not only in magnitude but even in shape. For the total elastic cross section only the results of Sin Fai Lam predict the existence of the Ramsauer–Townsend minimum in the vicinity of 0.5 eV and a broad maximum at higher energies while the other three sets of results decrease monotonically with increasing energy up to about 45–60 eV, where they start to grow very slowly. In the case of the elastic momentum transfer cross section the situation is somewhat different. Again the discrepancy between particular sets of the results is large, especially in the

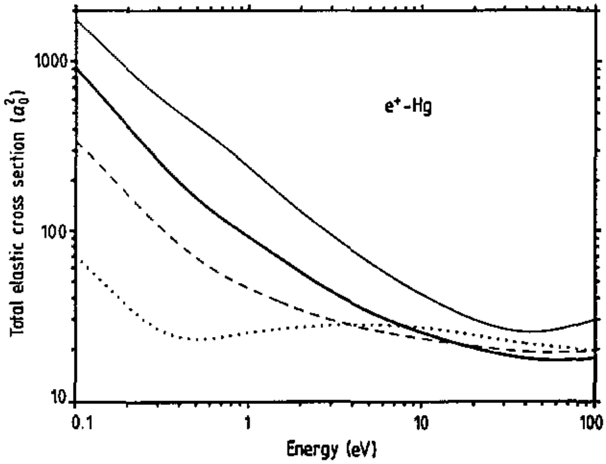

Figure 3. Total cross section for elastic scattering of positrons from mercury: ——, present relativistic; ——, present non-relativistic; · · · ·, present with the polarization potential of Sin Fai Lam (1980); – – –, present with the polarization potential of Sienkiewicz and Baylis (1991).

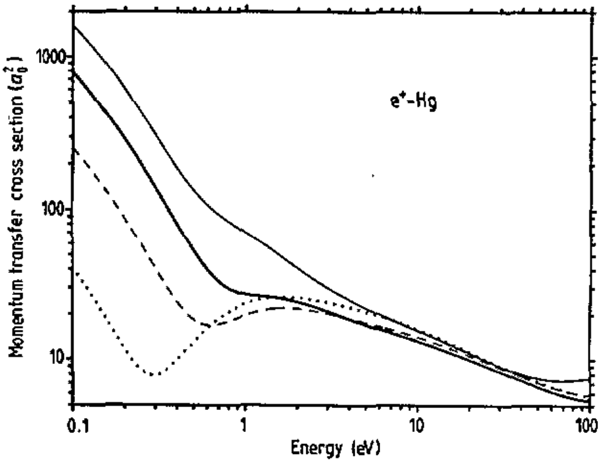

Figure 4. Momentum transfer cross section for elastic scattering of positrons from mercury: ——, present relativistic; ——, present non-relativistic; · · · · ·, present with the polarization potential of Sin Fai Lam (1980); – – –, present with the polarization potential of Sienkiewicz and Baylis (1991).

energy region below 30 eV, but now the results obtained with the potentials of Sin Fai Lam and Sienkiewicz and Baylis show the Ramsauer–Townsend minimum at energies of 0.3 eV and 0.6 eV, respectively. The relativistic and non-relativistic polarized orbital curves present only the change of slope in the region 0.5–2 eV, although this is hardly discernible in the latter case. The overall tendency of the non-relativistic cross sections to lie above corresponding relativistic curves is due to the much more attractive character of the non-relativistic polarization potential, especially in the asymptotic region, which results in enhanced forward scattering.

We also carried out a number of calculations of differential elastic cross sections at various energies, but in view of the lack of relevant experimental data we do not present results here.

The numerical values of the phaseshifts, differential, total elastic and elastic momentum transfer cross sections are available from the author upon request.

4. Conclusions

We performed relativistic calculations on the elastic scattering of low-energy positrons from mercury atoms. The relativistic polarization potential used in these calculations was obtained by solving the coupled Dirac–Hartree–Fock equations and the relativistic version of the variable phase method was employed for extracting phaseshifts and the scattering length. The results show that the relativistic effects in the e^+-Hg interaction potentials play a very important if not dominant role. In the low-energy region comparison with the previous model calculations of Sin Fai Lam (1980) and Sienkiewicz and Baylis (1991) shows an overall disagreement. In particular, the present calculations do not predict the existence of the Ramsauer–Townsend minimum in either the total elastic or the elastic momentum transfer cross section. In order to resolve these discrepancies experimental results are highly desirable.

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