Tendências em Matemática Aplicada e Computacional, **1**, No. 1 (2000), 169-173.
Sociedade Brasileira de Matemática Aplicada e Computacional.

Studies of Positron Collisions with He and H_2 using Second Born Approximation

J. L. S. LINO, Núcleo de Pesquisas em Matemática e Matemática Aplicada, Universidade Braz Cubas UBC, Campus I, 0877-380, Mogi das Cruzes, SP, Brazil.

Abstract. We discuss recent developments in the implementation of the second Born approximation for positron-molecule collision calculations. The evaluation of matrix elements involving the operator $VG_p^{(+)}V$ is done by direct numerical quadrature and designed to molecules of arbitrary geometry. Integral cross sections are obtained for e^+ - He and e^+ - H_2 collisions from 50 to 500 eV.

1. Introduction

Originally introduced many years ago in quantum scattering theory, the second Born level of approximation (SBA) has attracted a considerable amount of interest [1]. This approximation has been extensively used and with considerable success in the analysis of intermediate and high-energy scattering of positrons (electrons) against atomic targets [1]. For molecular targets the problem involving a non-spherical potential forces a laborious and large computational effort for the SBA, almost equivalent to more sophisticated theoretical treatments as the close coupling approximation [2], the R-matriz [3], the Kohn Variational Principle [4] and the Schwinger multichannel method [5]. These methods, specially designed for low-energy positron(and electron) scattering, involve several additional concepts and techniques strictly related to molecular features and quite frequently combine basis set approaches with numerical techniques. Although the SBA has been extensively used for atomic targets there exist no detailed study for molecular targets using the SBA (for molecular targets, there are practically no SBA data available in the literature). The motivation for the present work is twofold. Provide the literature with SBA cross sections, which can be quite useful in the development of new scattering methodologies [6]. In order to do this, we have to evaluate reliable (numerically stable) second Born type of terms, without restrictions on molecular geometries.

2. Procedure

As it is well known the SBA amplitude is obtained by adding to the first Born approximation (FBA) the following expression:

$$f_{B2}(\vec{k}_f, \vec{k}_i) = < S_{\vec{k}_f} \mid VG_P^{(+)}V \mid S_{\vec{k}_i} >, \tag{2.1}$$

where the $G_p^{(+)}$ is the projected outgoing-wave Green's function defined formally as $G_p^{(+)} = P(E - H_o + i\varepsilon)^{-1}$, and P is the target-space unit operator

$$P = \sum\!\!\!\!\!\!\int_{\ell} \mid \Phi_\ell >< \Phi_\ell \mid = 1. \tag{2.2}$$

In the present paper, P is truncated and carries only energetically open bound state channels. With the help of the linear momentum representation [7] of the one-particle unit operator the truncated f_{B2} can be rewritten as

$$< S_{\vec{k}_f} \mid V G_P^{(+)} V \mid S_{\vec{k}_i} >= \sum_{\ell}^{open} \int_o^{\infty} dk \frac{2k^2}{k_\ell^2 - k^2} g^{\ell}_{\vec{k}_f \vec{k}_i}(k), \tag{2.3}$$

where

$$g^{\ell}_{\vec{k}_f \vec{k}_i}(k) = \int d\Omega_{\vec{k}} < S_{\vec{k}_f} \mid V \mid \Phi_\ell \vec{k} >< \vec{k} \Phi_\ell \mid V \mid S_{\vec{k}_i} >, \tag{2.4}$$

and the function $g^{\ell}_{\vec{k}_f \vec{k}_i}(k)$ is essentially an angular integration of first Born terms with different magnitude of $\vec{k}$'s (off-shell terms). In the SBA, the difficulty in evaluating Eq. (3), associated with possible discontinuities, has been examined and treated in a similar way as in the subtraction method [7, 8]. Add and subtract the expression $\frac{2k^2}{k_\ell^2 - k^2} g^{\ell}_{\vec{k}_f \vec{k}_i}(k_\ell)$ to Eq. (3). The subtracted term makes the integration smoother (since the numerator and the denominator of the composed expression will vanish simultaneously for k's around k_ℓ) and the added term is evaluated analytically. When V is defined for the electron case, the SBA amplitude is given by

$$f_{SBA}(\vec{k}_f, \vec{k}_i) = \pm f_{FBA}(\vec{k}_f, \vec{k}_i) + f_{B2}(\vec{k}_f, \vec{k}_i), \tag{2.5}$$

where the upper and lower signs are for electrons and positrons, respectively. In the present implementation two different quadratures are used for $\vec{k}_i$ and $\vec{k}_f$ to avoid situations where $\mid \vec{k}_f - \vec{k}_i \mid$ are too small [9]. To obtain integral cross section we just evaluate the square modulus of this amplitude, summing over all $\vec{k}_f$ directions and averaging over the $\vec{k}_i$'s. To check the procedures to evaluate SBA and FBA cross sections we have considered tree tests: (a) the form factor given by $f_{FBA}(\theta = 0)$ which is a kind of blueprint of each target at the FBA level [1]; (b) the optical theorem for the SBA amplitude, which is a good test for the residue since numerically it should give

$$\sigma_{total}^{FBA} = \frac{4\pi}{k} Im \frac{1}{4\pi} \int d^3 k_i f_{SBA}(\vec{k}_i, \vec{k}_i), \tag{2.6}$$

where σ_{total}^{FBA} is the total cross section calculated on the FBA; and (c) the use of a known potential scattering problem to test the structure of our computer codes. We tested it by feeding our programs with scattering amplitudes for the Yukawa potential at the FBA and by comparing the outcoming SBA cross sections with the known analytical results. The numerical integrations were carried out using a

regular Gauss-Legendre method. They were tested with several quadratures until full convergence was achieved. The Eq.(3) involves a infinite summation over all the states, both discrete and continuous of the target and perform this infinite summation exactly is extremely difficult [1]. Its summation is greatly simplified by making the call simplified second Born approximation (SSBA)[10].

3. Results

He and H_2

These calculations, were carried out within the static approximation, *i.e.,* no polarization effects are taken into account (only the ground state is available for the He, and H_2 and not studing the SSBA). For the ground state of He and H_2 we used a self-consistent-field (SCF) wave function obtained with Cartesian Gaussian Functions, chosen as in Refs. [11] (See table 2.21.1) and [9], respectively. Table I shows our FBA and SBA integral cross sections for positron - He scattering along with results of Ref.[10]. As noted, our results agree very well with Ref.[10] for

Table I: Integral cross section (a_o^2): positron - He

Energy(eV)	FBA(our result)	SBA(our result)	SBA(Ref.[10])	Expt.[15]
50	2.230	1.996	1.410	3.707
100	1.289	1.336	0.892	2.104
150	0.904	0.972	0.670	
200	0.891	0.941	0.524	1.54
300	0.476	0.516	0.400	
400	0.362	0.391	0.311	0.596
500	0.292	0.316	0.299	

E $\geq$ 300 eV.

In Eq.(3) the appearance of summation makes an SBA calculation computationally prohibitive. The most usual form of calculating an approximation to (3) (used in Ref.[10]) is taking exactly only the terms corresponding to the N lowest energy intermediate states and substituting k_ℓ^2 for k^2 - $2w_c$ for all other states, where w_c is an average excitation energy. As only the ground state is available in our study (the only difference between the 2 methods is due to multichannel effects which is considered only in their calculation) we may conclude that these effects are not important for E $\geq$ 300 eV. Table II shows our FBA and SBA integral cross sections

for positron-H_2. For e^+ - H_2 there is unfortunately no SBA results with which these results can presently be compared.

Table II: Integral cross section (a_o^2): positron - H_2

Energy(eV)	FBA(our result)	SBA(our result)
50	3.215	3.366
100	1.715	1.801
150	1.173	1.234
200	0.891	0.941
250	0.719	0.770
300	0.603	0.654
400	0.453	0.479
500	0.365	0.356

4. Conclusions

We have calculated cross section for He and H_2 by the intermediate-energy positron impact. These elastic cross section were obtained within a second Born approximation (SBA). It would be of particular interest to apply the SBA to excitation electronic. Efforts in this direction are now in progress.

This research was supported by Fundação de Amparo à pesquisa do Estado de São Paulo (FAPESP), São Paulo, and Núcleo de Pesquisas em Matemática e Matemática Aplicada da UBC, São Paulo. These calculations were made at Centro Nacional de Processamento de Alto Desempenho do Nordeste, São Paulo e ITA-CTA.

References

[1] H.R.J. Walters, *Phys. Rep.*, **116** (1984).

[2] S. Chung and C.C. Lin, *Phys. Rev. A*, **17** (1987), 1874.

[3] C.J. Gillan, O. Nagy, P.G. Burke, L.A. Morgan and C.J. Noble, *J. Phys.B*, **20** (1987), 4585.

[4] B.I. Schneider and T.N. Rescigno, *Phy. Rev.A*, **37** (1988), 3749.

[5] J.L.S. Lino, J.S.E. Germano, E.P. Silva and M.A.P. Lima, *Phys. Rev. A*, **58** (1998),3502; E.P. da Silva, J.S.E. Germano, J.L.S. Lino, C.R.C. Carvalho, A.P.P. Natalense and M.A. P. Lima, *Nucl. Instrum. Methods Res. B,* **143** (1998), 140; J.L.S. Lino, *Resumos do XXII CNMAC*, (1999), 237; J.L.S. Lino, A.R. Farias, N.S. Araujo, *Resumos do XXII CNMAC*, (1999), 236.

[6] J.L.S. Lino, "Ph.D Thesis", ITA-CTA, São Jose dos Campos, São Paulo, Brazil, 1995; J.L.S. Lino and M.A.P. Lima, in "XX Cong. Int. on Phys. Collisions", Vienna, Austria, 1997.

[7] M.A.P. Lima, L.M. Brescansin, A.J.R. da Silva, C. Winstead and V. McKoy, *Phys. Rev.*, **41** (1990), 327.

[8] S.K. Adhikari and L. Tomio, *Phys. Rev. C*, **37** (1988),41.

[9] J.L.S. Lino, J.S.E. Germano and M.A.P. Lima, *J. Phys. B,* **27** (1994), 1881.

[10] B.D. Buckley and H.R.J. Walters, *J. Phys. B*, **7** (1974), 1380.

[11] R. Poirier, R. Kari and I.G. Csizmadia, "Handbook of Gaussian Basis Sets", 1985.

[12] D.K.Watson, R.R. Luchese, V. McKoy, and T.N. Rescigno, *Phys. Rev. A,* **21** (1980), 738.

[13] E. Clementi, em J. Chem. Phys. **40** (1964), 1944.

[14] B.H. Wells and S. Wilson, *J. Phys. B*, **22** (1989), 1285; W.C. Fon, K.A. Berrington and A. Hibbert, *J. Phys. B*, **14** (1981), 307.

[15] K.F. Canter, P.G. Coleman, T.C. Griffith and G.R. Heyland, *J. Phys.B* **6** (1973), L201.

[16] B. van Wingerden, E. Weigold, F.J. de Heer and K.J. Nygaard, *J. Phys. B*, **10** (1977), 1345.

[17] A. Deuring, K. Floeder, D. Fromme, W. Raith, A. Schwab, G. Sinapius, P.W. Zitzewitz and J. Krug, *J. Phys. B,* **16** (1983), 1633.