1.5 Adiabatic representation for the exchange inelastic electron-atom amplitude

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Abstract

In order to eliminate the failures of the Born-Oppenheimer exchange inelastic electron -atom amplitude a unitary transformation is made of the standard adiabatic perturbational series. As the basis of the new representation are taken the adiabatical functions $\chi = A\Phi$, which at large distances lead to atomic eigenfunctions basis $\{\Phi\}$, $(A \to I)$. The unitary transformation matrix A is found in the two-state approximation. In this representation the Born-Oppenheimer amplitude does not violate the conservation laws. Expanding this amplitude in an asymptotic series the Ochkur amplitude is found in the adiabatical representation. It is shown that this amplitude is non-unique in respect to any unitary transformation satisfying the condition $A \to I$ at large distances.

1.6 Padé approximants in electron-atom scattering

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1. Introduction

In the elastic electron-atom scattering at high and intermediate energies the effects of nonadiabatic distortion of the atomic wave function by the incident electron are very important in order to describe correctly the angular distribution which is sharply peaked in the forward direction. For the elastic e^-—He scattering recent partial wave calculation have been performed by La Bahn and Callaway[1] using an "extended polarization potential". Their results agree with the absolute experimental data of Vrieus et al.[2] as normalized by Chamberlain et al.[3] in the energy range 100—300 eV. But when the energy increases their method does not work so well and an enormous computational work is demanded to obtain stable results.

Another approach is to describe the distortion effects through use of the second Born order f_2 (θ, E). In this paper first we compare various approximations for the cross section considering the elastic $e^{\pm}$—H scattering and the nwe extend the results obtained in a previous paper[4] using the Padé approximants method in the elastic e^--He scattering.

2. Cross sections with second order effects

Knowing $f_2(\theta, E)$ we can construct various approximations for the cross section:

$$\sigma_{B2}(\lambda;\theta,E)=|\lambda f_1(\theta,E)+\lambda^2 f_2(\theta,E)|^2,$$
$$\sigma_3(\lambda;\theta,E)=\lambda^2|f_1(\theta,E)|^2[1+2\lambda\,\mathrm{Re}\{f_2(\theta,E)/f_1(\theta,E)\}],$$
$$\sigma_P(\lambda;\theta,E)=|f_P(\lambda;\theta,E)|^2=|\lambda f_1(\theta,E)/[1-\lambda f_2(\theta,E)/f_1(\theta,E)]|^2,$$

where $\sigma_{B2}(\lambda;\theta,E)$ is the usual second Born approximation, $\sigma_3(\lambda;\theta,E)$ is the third order formula proposed by Kingston et al.[5] and $f_P(\lambda;\theta,E)$ is the [1,1] Padé approximant (c. f. r. Baker[6]) of the perturbative series for the scattering amplitude

$$f(\lambda,\theta,E)=\lambda f_1(\theta,E)+\lambda^2 f_2(\theta,E)+\dots$$

The second Born order can be expressed as an infinite summation

$$f_2(\theta,E)=\sum_n f_2^{(n)}(\theta,E)=\frac{1}{32\pi^4}\left(\frac{2\mu}{\hbar^2}\right)^2\lim_{\varepsilon\to 0}\sum_n\int \mathrm{d}\boldsymbol{q}\,\frac{\langle k_f,f|V|q,n\rangle\langle q,n|V|k_i,i\rangle}{q^2-k_n^2-i\varepsilon},$$

where V is the interaction potential between the incident particle and the atom, $k_n^2=\frac{2\mu}{\hbar^2}(E-E_n)$, being E_n a discrete or continuous eigenenergy of the atom, and E the total energy of the process. From this sum we extract a set of intermediate atomic states which can be calculated exactly

$$f_2(\theta,E)=\sum_{n=1}^{N} f_2^{(n)}(\theta,E)+g(\theta,E).$$

Then the function $g(\theta,E)$ is approximated in some way as follows:

a) Elastic e± — H scattering. — In the case of elastic e± — H scattering we assume $g(\theta,E)=0$, $N=1,2$. As we show in tables 1 and 2, the results obtained with the Padé method for $N=1$ agree quite well at intermediate energies with the values obtained by Smith et al.[7] with partial wave calculations in the static approximation, and for $N=2$ they agree with the results of Damburg and Peterkop[8] in the close coupling approximation.

On the other hand the results obtained using the third order approximation, which is not positive definite, agree with the partial wave calculations only in the e± — H scattering; in the e± — H scattering negative values are obtained for both the differential and total cross section.

TABLE 1

Elastic e± — H scattering — Total cross sections (in units of πa_0^2)

k	σ_{Born}	$\sigma_{B2}^{(1s)}$	$\sigma_3^{(1s)}$	$\sigma_P^{(1s)}$	σ_{Smith}	$\sigma_{B2}^{(1s+2s+2p)}$	$\sigma_3^{(1s+2s+2p)}$	$\sigma_P^{(1s+2s+2p)}$	$\sigma_{\mathrm{Damburg}}$
1	1.542	3.495	2.744	2.201	2.6	4.567	3.305	2.332	2.47
2	0.523	0.823	0.674	0.538	0.6	0.889	0.702	0.526	0.657

TABLE 2

Elastic e±—H scattering — Total cross sections (in units of πa_0^2)

k	σ_{Born}	$\sigma_{B2}^{(1s)}$	$\sigma_3^{(1s)}$	$\sigma_P^{(1s)}$	σ_{Smith}	$\sigma_{B2}^{(1s+2s+2p)}$	$\sigma_3^{(1s+2s+2p)}$	$\sigma_P^{(1s+2s+2p)}$	$\sigma_{Damburg}$
1	1.542	1.08	0.34	0.68	0.759	1.02	—0.221	0.521	0.589
2	0.523	0.508	0.372	0.332	0.349	0.52	0.344	0.308	0.310

b) Elastic e⁻ -He scattering — In the second kind of approximation we choose

$$g(\theta, E) = \frac{1}{32\pi^4}\left(\frac{2\mu}{\hbar^2}\right)^2 \lim_{\varepsilon\to 0} \int \frac{dq}{q^2 - p^2 - i\varepsilon} \sum_{n>N} \langle k_f, f | V | q, n\rangle \langle q, n | V | k_i, i\rangle,$$

where $p^2 = k^2 + w$ is an average parametrized excitation, and then we evaluate the sum using the closure relation for a complete system of atomic wave functions

$$\sum_n |n\rangle\langle n| = I_A.$$

For high energy processes in which the forward amplitude is important and the exchange effects can be neglected, we can fix the average excitation p^2 requiring the stationarity of $|f_P(\lambda;\, 0,\, E)|$. This quantity differs from the Schwinger functional by a phase factor physically meaningless when exchange effects are absent. In such a way using the Padé method we have calculated the angular distribution for the elastic e⁻— He scattering with $N = 1$ taking the variational form of the atomic ground state

$$\Phi_1(r_1, r_2) = \frac{Z^3}{\pi a_o^3} \exp[-Z(r_1 + r_2)/a_0], \quad Z = 27/16.$$

In the energy range 350—700 eV our theoretical values[4] agree very well with the absolute experimental results of Bromberg[9] and with those of Hughes et al.[10] normalized by Bromberg.

For energies lower than 300 eV we have not stationarity points for $|f_P(\lambda;\, 0,\, E)|$ and we can fix fenomenologically the average excitation p^2. In the energy range 75—400 eV we have a good agreement with the absolute experimental data of Vriens et al.[2] renormalized by Chamberlain et al.[3] and with those of Hughes et al.[10] normalized by Bromberg[9] (see Fig. 1 and 2). We also report the angular distributions obtained using the third order formula and approximating the higher intermediate states as suggested by Holt and Moiseiwitsch[11]; we can see that when the energy increases this approximation becomes more and more inaccurate.

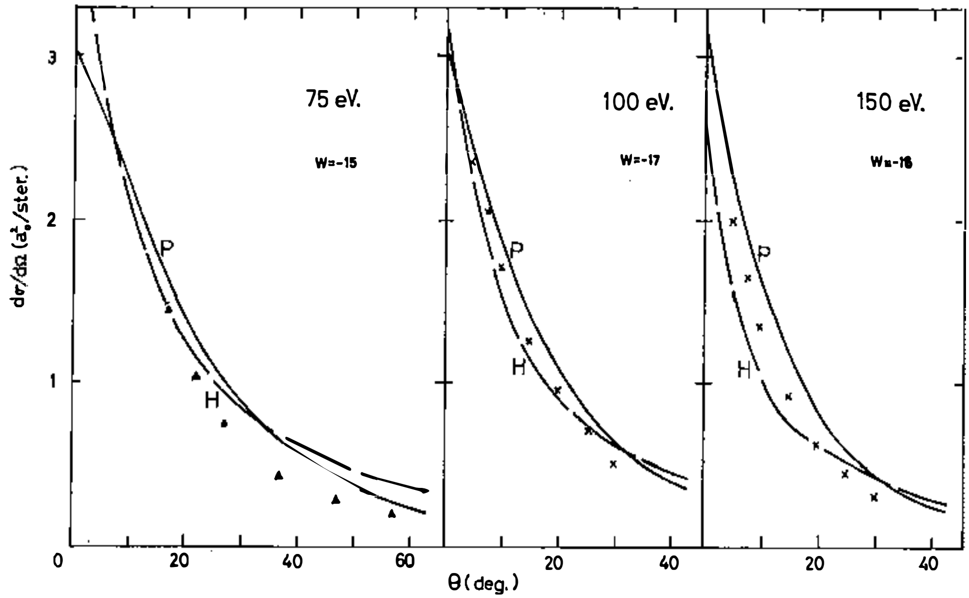

Fig. 1 — Differential cross sections for the elastic scattering of electrons by helium atoms. Curves P, results obtained in this work by the Padé approximants method; curves H, results obtained by the method of Holt and Moiseiwitsch; ▲ experimental points of Hughes et al. (1932) as normalized by Bromberg (1969); × experimental points of Vriens et al. (1968) as normalized by Chamberlain et al. (1969).

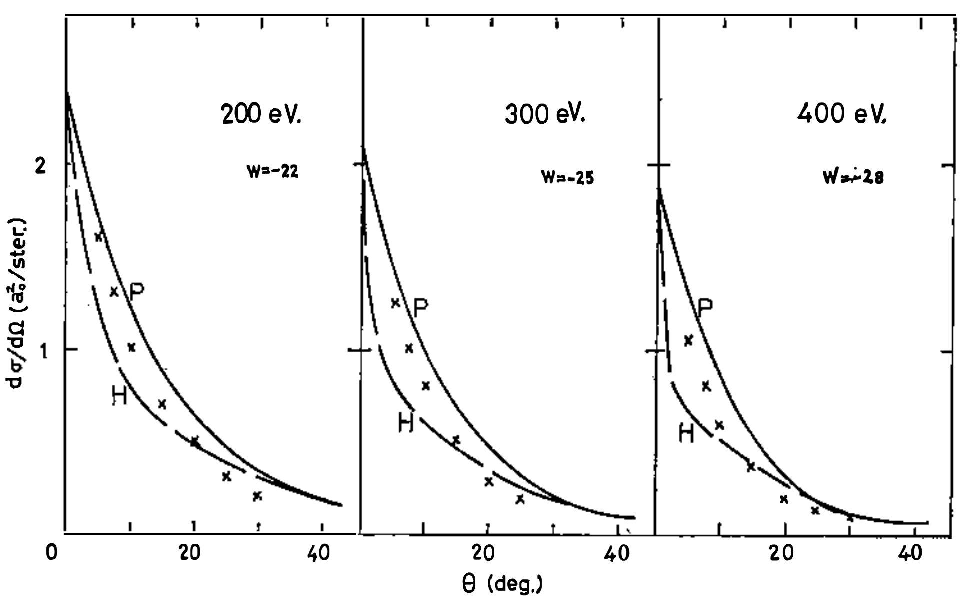

Fig. 2 — Differential cross sections for the elastic scattering of electrons by helium atoms. Curves P, results obtained in this work by the Padé approximants method; curves H, results obtained by the method of Holt and Moiseiwitsch; × experimental points of Vriens et al. (1968) as normalized by Chamberlain et al. (1969).

References

1) R. W. La Bahn and J. Callaway, Phys. Rev. **18** (1969) 179;
2) L. Vriens, C. Kuyatt and S. Mielczarek, Phys. Rev. **170** (1968) 163;
3) G. E. Chamberlain, S. Mielczareck and C. Kuyatt, Proc. of 6. Conf. on Atomic Collisions MIT (1969);
4) C. R. Garibotti and P. A. Massaro, to be published;
5) A. E. Kingston, B. L. Moiseiwitsch and G. B. Skinner, Proc. Roy. Soc. A **258** (1960) 237;
6) G. Baker, Advances in Theoretical Physics, Vol. **1** (1965);
7) K. Smith, W. F. Miller and A. J. P. Mumford, Proc. Phys. Soc. **76** (1960) 559;
8) R. Damburg, Ya, and R. K. Peterkop, Atomic Collisions (edited by V. Veldre, Ya), (1966);
9) J. P. Bromberg, J. Chem. Phys. **50** (1969) 3906;
10) A. L. Hughes, J. H. Mc Millen and G. M. Webb, Phys. Rev. **41** (1932) 154;
11) A. R. Holt and B. L. Moiseiwitsch, J. Phys. **B 1** (1968) 36.

1.7 Adiabatic representation calculations of the H (1s) —H (2 s) exchange excitation by electrons

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Abstract

In the adiabatical representation calculations are made on exchange excitation of hydrogen atom by electron impact. The differential and total exchange excitation of 2s state are calculated in Ochkur approximation using the proper adiabatical two-state basis and the quasi-adiabatical one. The difference in the two total exchange cross sections is negligible except for the part in the region about the cross section maximum. The total exchange cross section lies below the experimental one and is in better agreement with it than the cross section of the three-state close-coupling approximation.

1.8 Reaction rate coefficient for radiative attachment of electrons on H and alkali atoms

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Abstract

The radiative electron attachment process $e + A(^2S_{1/2}) \rightarrow A^-(^1S_0) + h\nu$ is studied in the electric-dipol transition approximation. The transition matrix element $\langle \psi_b \mid z \mid \psi_E \rangle$ is calculated using various representations for the bound- and free-state electron wave functions ψ_b and ψ_E. The averaging of the cross section of reaction (1) is taken over a Maxwellian distribution function in order to get the reaction rate coefficent. All integrations can be carried out analytically. The reaction rate coefficents in all representations are expressed in terms of confluent hypergeometric functions.