

LETTER TO THE EDITOR

Positron-neon elastic scattering

R I Câmpeanu† and J Dubau‡

† University of Cluj, Rumania

‡ DAPHE, Observatoire de Paris, 92190, Meudon, France

Received 5 July 1978

Abstract. A close-coupling calculation without the virtual positronium formation, but with correct account of the target polarisability is performed. The results are compared with the recent theoretical results of McEachran and colleagues and with both beam and swarm measurements. It is found that all the theoretical and experimental e^+ -Ne elastic cross sections to date are too low for very slow positrons.

The approximations used in slow positron-rare gases scattering calculations can now be tested against both beam and swarm experiments. For helium, where most of the theoretical effort was concentrated, a very good agreement was found between an elaborated variational calculation and the best beam and swarm results (Câmpeanu and Humberston 1975, 1977a,b). For neon and argon, there are only the adiabatic calculations of Massey *et al* (1966), Montgomery and LaBahn (1970) and McEachran *et al* (1978). The last of these calculations is the most elaborate one and, for argon, it agrees well with some of the beam and swarm experiments (Câmpeanu and Humberston 1978). However, for neon, the calculations of McEachran *et al* only agree with the beam measurements (figure 1) and give too large a shoulder in the lifetime spectrum (figure 2).

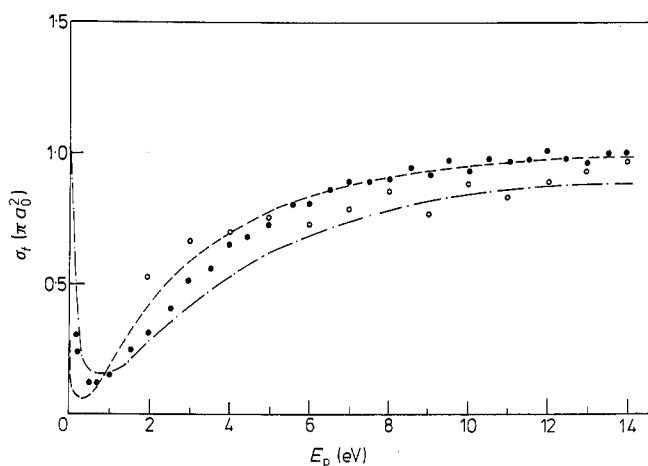


Figure 1. Positron-neon elastic cross sections. Theory: —, present calculations; ---, McEachran *et al* (1978). Experiment: ○, Canter *et al* (1973); ●, Kauppila *et al* (1976).

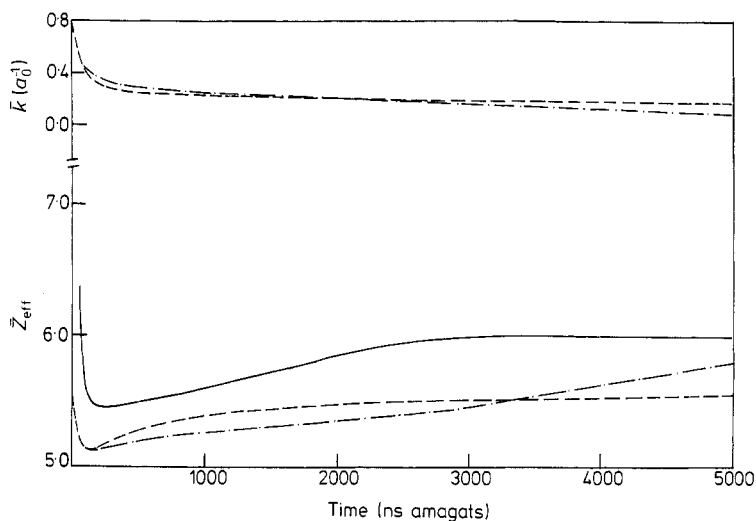
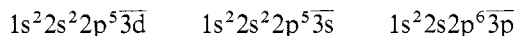


Figure 2. Time dependence of the annihilation effective charge averaged over the positron distribution. —, experiment of Killeen (1975); - - - calculated with our phaseshifts; - · - ·, calculated with the phaseshifts of McEachran *et al* (1978). Both calculations use the same $Z_{\text{eff}}(k)$ of McEachran *et al* and a k^2 initial velocity distribution.

In this paper, we shall present results obtained for $e^+ - \text{Ne}$ in the close-coupling approximation, without the virtual positronium formation included but with a correct representation of the target polarisability. This work is similar to the helium calculation of Cherepkov *et al* (1975). We have used the close-coupling program of Crees *et al* (1978), with target wavefunctions calculated with the program of Eissner and Nussbaumer (1969). The use of the Thomas-Fermi-Dirac-Amaldi potential (Gombás 1956) enabled us to obtain polarised pseudo-states by simply varying appropriate scaling parameters in the target wavefunctions. We have included in the scattering program the following virtual excited configurations:



where the bars indicate the pseudo-orbitals.

The target dipole-polarisability is given in this case by:

$$\alpha = \sum_{i=1}^3 \frac{\left| \langle \psi_0 | \sum_{j=1}^{10} Z_j | \psi_i \rangle \right|^2}{E_i - E_0}$$

where ψ_0 is the ground state wavefunction and ψ_i the $^1P^o$ term wavefunction in the three former configurations. E_0 and E_i are the corresponding eigen-energies and Z_j are the projections of the electron vectors on the positron-nucleus axis. The scaling parameters of the Eissner-Nussbaumer program were obtained by minimisation of the ground state energy, ψ_0 : $\lambda_s = 1.089$ and $\lambda_p = 0.968$. The other scaling parameters, $\lambda_{\overline{3s}} = 1.45$ and $\lambda_{\overline{3d}} = 2.0$, were chosen to maximise the polarisability α . The inclusion of the third pseudo-state had an insignificant effect and therefore we dropped this configuration. Our maximum value for the polarisability $\alpha = 2.315$ is lower than the value $\alpha = 2.56$ obtained by Burke and Mitchell (1974) with the same configuration basis but with an elaborated variational technique which used Clementi-Hartree-Fock

target functions. In the positron scattering, where the polarisation potential and the effective static potential are of opposite signs the correct polarisability is particularly important (Houston and Drachman 1971, Ho and Fraser 1975). We introduced the difference between our polarisability and the experimental value $\alpha = 2.663$ of Dalgarno and Kingston (1960) in a parametric polarisation potential included in the open channel. The potential form was:

$$\frac{\alpha'}{r^4} \{1 - \exp[-(r/r_{\text{cut}})^6]\}$$

where we used $\alpha' = 0.348$ and $r_{\text{cut}} = 0.955$, equal to the effective range of the 2p orbital and, implicitly, of the atomic core. This choice for r_{cut} was suggested by the work of Black *et al* (1972) in which the polarisation of the atomic core in the valence electron field was accounted for with a similar parametric potential. The s,p and d wave phaseshifts obtained in this way are given in table 1. The p and d phaseshifts did not depend on the choice of r_{cut} . The corresponding elastic cross sections are plotted in figure 1 and except for very low positron energies they are in very good agreement with the experimental results of Kauppila *et al* (1976).

Another test on our phaseshifts was their use in the diffusion program of Câmpeanu and Humberston (1977b). The omission of the electron-positron short range correlation leads to very inaccurate values for the annihilation effective charge Z_{eff} . We have therefore used $Z_{\text{eff}}(k)$ calculated by McEachran *et al* (1978) without the inclusion of high multipoles in their adiabatic approximation. This calculation gives the thermal positron energy $Z_{\text{eff}} = 6.1$ in best agreement to date with the experimental value of 6.0 measured by Killeen (1975). We used a k^2 initial velocity distribution. The $k(t)$ dependence, plotted on top of figure 2, shows that the slowing down process calculated with our theoretical phaseshifts is not fast enough and consequently the shoulder length in $Z_{\text{eff}}(t)$ is much larger than the experimental shoulder of Killeen (1975). As the annihilation term in the diffusion equation is not important, it appears that only the values of $\sigma_{\text{mi}}(k)$ below $k = 0.3$ are responsible for the shoulder being too long. In this energy range too small values for $\sigma_{\text{mi}}(k)$ imply too low a $\sigma_i(k)$ as well. This observation is expected since the inclusion of the virtual positronium formation would most probably modify $\sigma_i(k)$ in the way shown by Amusia *et al* (1976) in their positron-helium work. Figure 1 suggests that the correct $\sigma_{\text{mi}}(k)$ (and explicitly $\sigma_i(k)$) for small k will be even higher than the prediction of McEachran *et al* (1978).

Table 1. Positron-neon phaseshift in the close-coupling approximation with full neon polarisability but without virtual positronium formation.

k	η_0	η_1	η_2
0.1	0.010	0.004	0.001
0.2	-0.016	0.012	0.003
0.3	-0.064	0.021	0.007
0.4	-0.123	0.028	0.012
0.5	-0.188	0.032	0.017
0.6	-0.254	0.032	0.024
0.7	-0.320	0.027	0.031
0.8	-0.384	0.018	0.039
0.9	-0.444	0.007	0.046
1.0	-0.508	-0.004	0.053

We want to thank Professor M J Seaton, Drs W Eissner and P Storey for their help in the use of the two programs and Professors A D Stauffer and R P McEachran for sending their results in advance of publication.

References

- Amusia M Ya, Cherepkov N A, Chernysheva L V and Shapiro S G 1976 *J. Phys. B: Atom. Molec. Phys.* **9** L531-4
- Black J H, Weisheit J C and Laviana E 1972 *Astrophys. J.* **177** 567-72
- Burke P G and Mitchell J F B 1974 *J. Phys. B: Atom. Molec. Phys.* **7** 665-73
- Câmpeanu R I and Humberston J W 1975 *J. Phys. B: Atom. Molec. Phys.* **8** L244-8
- 1977a *J. Phys. B: Atom. Molec. Phys.* **10** L153-7
- 1977b *J. Phys. B: Atom. Molec. Phys.* **10** 239-50
- 1978 *J. Phys. B: Atom. Molec. Phys.* submitted for publication
- Canter K F, Coleman P G, Griffith T C and Heyland G R 1973 *J. Phys. B: Atom. Molec. Phys.* **6** L201-3
- Cherepkov N A, Amusia M Ya, Chernysheva L V and Shapiro S G 1975 *Proc. 9th Int. Conf. on the Physics of Electronic and Atomic Collisions* (Seattle: University of Washington) Abstract pp 155-6
- Crees M A, Seaton M J and Wilson P M H 1978 *Comput. Phys. Commun.* in press
- Dalgarno A and Kingston A E 1960 *Proc. R. Soc. A* **259** 424-9
- Eissner W and Nussbaumer H 1969 *J. Phys. B: Atom. Molec. Phys.* **2** 1028-43
- Gombás P 1956 *Handb. Phys.* **36** 109-231 (Berlin: Springer-Verlag)
- Ho Y K and Fraser P A 1975 *J. Phys. B: Atom. Molec. Phys.* **8** L230-5
- Houston S K and Drachman R J 1971 *Phys. Rev. A* **3** 1335-42
- Kauppila W E, Stein T S, Pol V and Jesion G 1976 *Proc. 4th Int. Conf. on Positron Annihilation* (Helsingor) Abstract A5
- Killeen T L 1975 *PhD Thesis* University of London
- Massey H S W, Lawson J and Thompson D G 1966 *Quantum Theory of Atoms, Molecules and the Solid State* ed. P. Lowden (New York: Academic Press)
- McEachran R P, Ryman A G and Stauffer A D 1978 *J. Phys. B: Atom. Molec. Phys.* **11** 551
- Montgomery R E and LaBahn R W 1970 *Can. J. Phys.* **48** 1288-303