

LETTER TO THE EDITOR

New calculations of $P(b)$ curves for $1s_\sigma$ excitation in low- Z ($Z \leq 10$) ion-atom scattering†

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Received 25 June 1986

Abstract. *Ab initio* fully relativistic SCF molecular calculations of energy eigenvalues as well as coupling-matrix elements are used to calculate the $1s_\sigma$ excitation differential cross section for Ne-Ne and Ne-O in ion-atom collisions. A relativistic perturbation treatment which allows a direct comparison with analogous non-relativistic calculations is also performed.

The dominant role of the $2p_\pi$ - $2p_\sigma$ rotational coupling in the K-shell vacancy production during ion-atom collision was established in a series of papers by Briggs, Macek, Taulbjerg and Vaaben (Briggs and Macek 1972, Briggs and Taulbjerg 1975, Taulbjerg and Briggs 1975, Taulbjerg *et al* 1976). This coupling arises in a scattering process as a result of the rotation of the internuclear axis, because angular momentum states referred to this axis are not eigenstates of the rotation operator. The K-shell vacancy is produced during the collision by a one-electron transition from the occupied $2p_\sigma$ orbital to an empty $2p_\pi$ orbital at small internuclear distances. The transition probability P is usually obtained as a function of the impact parameter b in the semiclassical approximation by integration of the coupled differential equations for the complex amplitudes, which represent the channels along a prescribed trajectory $R(t)$ between the two nuclei. This procedure is called a coupled-channel or strong-coupling calculation.

Taulbjerg *et al* (1976) have given a general scaling law for $P(b)$ which is widely used. As a basic ingredient in the coupled-channel calculation, one constant rotational matrix element is used between the two channels that represent the $2p_\pi$ and $2p_\sigma$ levels; the energy difference between these two levels is assumed to be proportional to R^2 . In their original paper Taulbjerg *et al* (1976) suggested that the results of such calculations be used to scale from some more accurate calculations, which at that time were non-relativistic *ab initio* calculations for the one-electron two-centre problem. The results of the scaling calculations are the dotted curves in figures 3 and 4, where we compare the experimental results of the $1s_\sigma$ excitation differential cross section with the various theoretical calculations. These dotted curves give a reasonable first approximation of the experiments for these light scattering systems if one considers the generality of the ansatz. On the other hand, it is not too surprising that the results are no longer good for scattering systems with $Z_1, Z_2 > 10$. It is expected that for heavier systems, many-body effects, spin-orbit splitting and other relativistic effects will lead to discrepancies.

† Supported by Gesellschaft für Schwerionenforschung (GSI), Darmstadt.

In addition, the difference between the results of this simple method and those from experiment (Luz *et al* 1979), even for these small- Z systems, shows definitely that more refined calculations are needed in order to understand the physical reason for the discrepancies.

We present here two theoretical procedures which both include relativistic effects. The first method is a perturbation calculation, which has been used in a similar form previously (Anholt *et al* 1977, Jakubassa and Taulbjerg 1980). The second method is a full-scale Dirac-Fock-Slater (DFS) calculation for the special systems Ne-Ne and Ne-O, which led to realistic *ab initio* energy eigenvalues of the levels as well as *ab initio* coupling-matrix elements. The details of the calculation procedure can be found in the paper by Sepp *et al* (1986).

The perturbation treatment has the great advantage of allowing a direct study of the transition from a non-relativistic to a relativistic treatment. The Hamiltonian of the system is taken as the sum

$$H = H_0 + H_{ls} + H_s$$

of the non-relativistic Hamiltonian H_0 at the internuclear distance $R = 0$, the spin-orbit Hamiltonian $H_{ls} = g_{ls}(R)(\mathbf{I} \cdot \mathbf{s})$ and the deviation H_s of the Coulomb potential from the united-atom value due to the internuclear separation R . The spin-orbit term $H_{ls}(R)$ was approximated by its value at $R = 0$ and the Stark term H_s by its quadrupole contribution. This Hamiltonian was then diagonalised in the subspace spanned by all six relativistic atomic $2p$ levels at $R = 0$. The resulting eigenstates were then used as molecular orbitals in the calculation of the dynamical matrix elements.

Figure 1 presents the energy levels in the vicinity of the united $n = 2$ levels from our DFS Ne-Ne calculation. The united $2p_{3/2}$ level splits into the $1(\frac{3}{2})_u$ and $2(\frac{1}{2})_u$ molecular levels (where the number in parentheses is the projection of the angular momentum onto the internuclear axis). The $2p_{1/2}$ level is the $1(\frac{1}{2})_u$ molecular level and the $2s$ is the $2(\frac{1}{2})_g$. As a result of the gerade and ungerade symmetry, only the u levels participate in the excitation process, because only the upper u levels carry a hole. Figure 2 presents the non-zero matrix elements resulting from the perturbation treatment for the Ne-Ne case as broken curves and the one from the *ab initio* calculations as full curves.

Using this information on the energy eigenvalues of the levels shown in figure 1, plus the information on the coupling-matrix elements, we have performed various

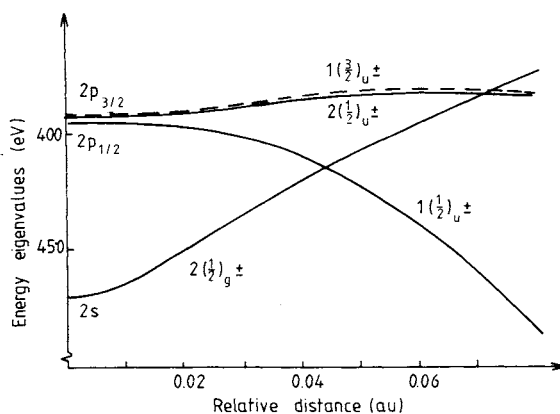


Figure 1. The energy eigenvalues of the system Ne^+-Ne at the united $n = 2$ levels.

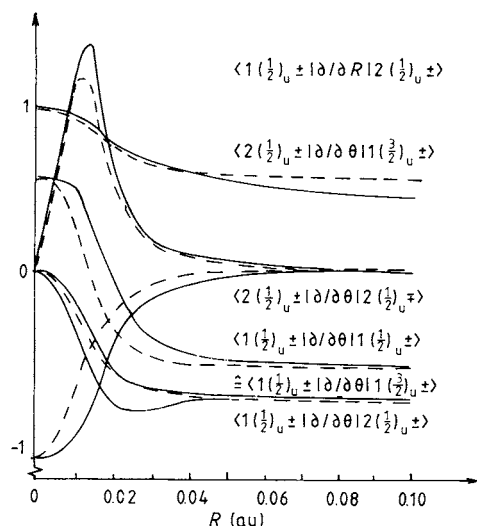


Figure 2. The relativistic coupling-matrix elements for the six sublevels of the united 2p levels for the Ne^+-Ne system. —, DFS results; ---, perturbation treatment.

coupled-channel calculations for the Ne-Ne system in order to determine the $1s_\sigma$ excitation, under the assumption that one hole is present in the non-relativistic 2p level. The actual calculation consists of two different calculations with holes in the $2p_{1/2}$ and $2p_{3/2}$ separated-atom levels respectively. The results of the various calculations are given in figure 3(a) for 363 keV impact energy, and in figure 3(b) for 700 keV impact energy. The full curve is a calculation in which the energy eigenvalues and the coupling-matrix elements of the *ab initio* calculations (full curves in figure 2) were used for all six levels that describe the relativistic 2p united levels. The broken curve, which leads to almost the same result, is a calculation in which we used the *ab initio* energy eigenvalues with the matrix elements from the perturbation calculation (broken curve in figure 2). The chain curve is a calculation in which both the energy eigenvalues and the matrix elements of the perturbation calculation were used. This result is almost identical to the non-relativistic calculation according to the general scaling law (dotted curve) given by Taulbjerg *et al* (1976). All these calculations show definitely that the information on realistic energy eigenvalues is the most important ingredient in such calculations. Both methods of calculation of the $P(b)$ curves with the good DFS energy eigenvalues are in very good agreement with the experimental results of Luz *et al* (1979).

As another low- Z system we have chosen Ne-O. The analogous calculations are presented in figure 4. The agreement between experiment and the results of these new calculations demonstrates three things.

(i) The quality of the differences of the energy eigenvalues, which determine the relative phases of the amplitudes in the coupled-channel calculations, is much more important than the quality of the coupling-matrix elements, at least in these small- Z systems. The two sets of matrix elements presented in figure 2, only lead to very small differences in the $P(b)$ curves as long as the energy eigenvalues are the same. The change to different energy eigenvalues alters the results drastically.

(ii) Relativistic influences in the $P(b)$ curves are non-negligible even for these small- Z systems. Of course, the relativistic influence is very indirect, manifesting itself via the good relativistic energy eigenvalues in the SCF process. In those small- Z systems

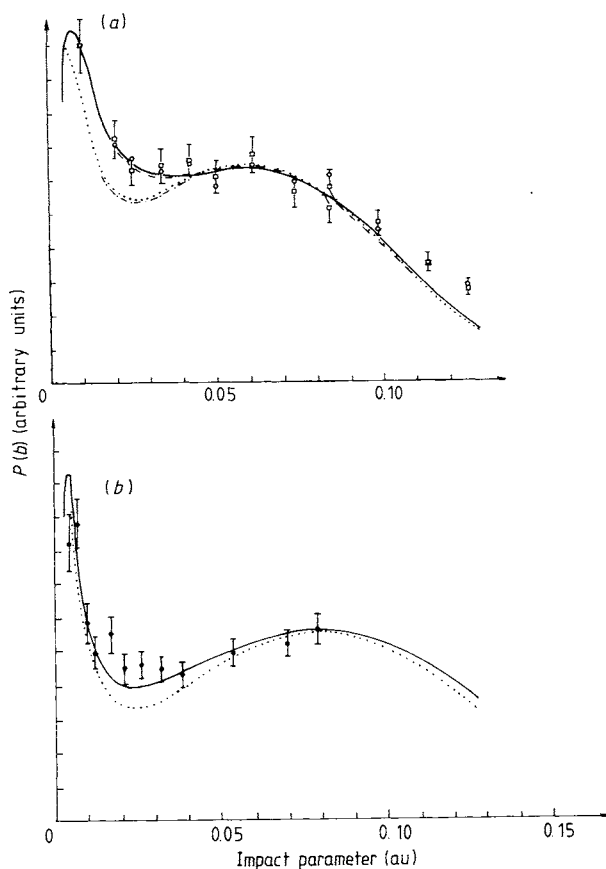


Figure 3. Experimental and theoretical $P(b)$ results for $1s_{\sigma}$ excitation for (a) $\text{Ne}^+ - \text{Ne}$ at 363 keV impact energy and (b) $\text{Ne}^{2+} - \text{Ne}$ at 700 keV impact energy. —, good matrix elements and good energy eigenvalues from the DFS calculation; ---, perturbation matrix elements and DFS energy eigenvalues; — · —, matrix elements and energy eigenvalues from the perturbation calculation; · · ·, according to the scaling law of Taulbjerg *et al* (1976). The experimental points are from Luz *et al* (1979). The theoretical curves are all fitted to the experimental results at the top of the adiabatic peak. Some of the curves are omitted in part (b) for simplicity.

the spin-orbit splitting is probably dominant, but the direct and indirect relativistic effects will become more and more important for heavier systems.

(iii) The good agreement between experiment and theory shows that it is indeed sufficient to perform a two-state (relativistically a six-state) coupled-channel calculation with realistic energy eigenvalues in order to obtain such good agreement for a wide range of impact parameters b .

In our opinion, the MO basis used in the above explanation, which involves only the 2p levels as originally suggested by Briggs, Macek, Taulbjerg and Vaaben (Briggs and Macek 1972, Briggs and Taulbjerg 1975, Taulbjerg and Briggs 1975, Taulbjerg *et al* 1976), is a much more physical explanation than the mathematically equivalent formulation in any other basis (like the AO basis) where many more basis states are needed to explain the same results, and where—from a physical viewpoint—it is not evident what is actually happening. In addition, it might be interesting to determine

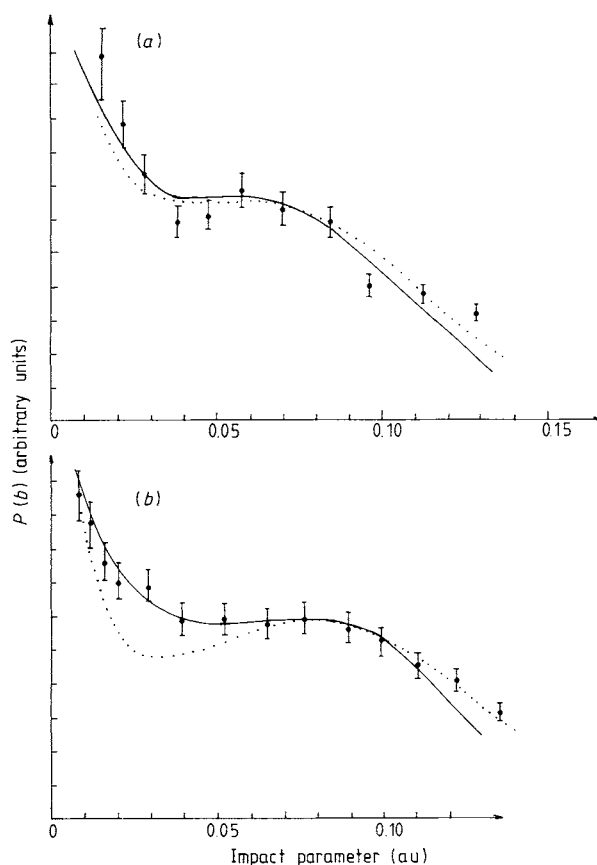


Figure 4. As figure 3 but for $\text{Ne}^+\text{-O}$ at (a) 250 keV impact energy and (b) 385 keV impact energy. The experimental points are from Luz *et al* (1979). Some of the curves are omitted for simplicity.

in a further analysis to what extent the non-relativistic scaling law of Taulbjerg *et al* (1976) is satisfied for the present relativistic calculations.

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