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LETTER TO THE EDITOR

Reduced close-coupling calculations for electron capture processes in collisions of multiply charged ions with atoms

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Abstract. A propensity rule has been found for the magnetic substate distribution of excited states populated in collisions between multiply charged ions with atoms. It is observed that the $m=-l$ substates are predominantly populated if the quantization axis is chosen to be perpendicular to the scattering plane. The result implies that it is possible to carry out reduced close-coupling calculations where only the $m=-l$ substates for each l are included in the basis expansion. Such reduced close-coupling calculations are desirable for treating electron capture to high-n excited states. The range of applicability of the propensity rule is examined for C^{6+}–H collisions.

For direct excitation in ion–atom collisions, Nielsen and Andersen (1987) have derived a propensity rule for the orientation of the excited states which has been confirmed in several experiments (Panev *et al* 1987, Andersen *et al* 1988). In their formulation, the quantization axis is chosen to be perpendicular to the scattering plane, and the propensity rule states that

$$\frac{\Delta E a}{v_{\mathrm{M}}}+\pi\,\Delta m=0 \tag{1}$$

where ΔE is the change in energy, a is the range of interaction and Δm is the change in magnetic quantum number. This relation applies to excitation processes (positive ΔE) or to de-excitation processes (ΔE negative), and the relation holds for collision energies where the velocity satisfies the Massey criterion ($v \simeq v_{\mathrm{M}}$). If the initial state is an s state, this propensity rule states that the $m=-1$ excited state is more likely populated than the $m=+1$ excited state. For the de-excitation process, the opposite is true. This propensity rule has been tested in a number of experiments and can be derived from a simple theoretical argument based on the distorted-wave approximation (Nielsen and Andersen 1987).

In the last few years, there have been several theoretical papers (Lin *et al* 1989, Dubois *et al* 1989, 1991, Hansen *et al* 1990, Nielsen *et al* 1990) examining the possibility of similar propensity rules for electron capture processes. While there exist few experimental data for the orientation parameters for collisions except at low energies (Roncin *et al* 1990), more sophisticated calculations appear to indicate that certain magnetic substates are predominantly populated. However, these calculations have been limited to collisions using light ions and only p states have been examined so far.

In this letter we examine the magnetic substate distribution for electron capture processes in collisions between multiply charged ions and simple target atoms. We adopt the standard semiclassical impact parameter formulation (Fritsch and Lin 1991) but the quantization axis is chosen to be perpendicular to the scattering plane. (The beam axis is the $+x$ direction, and the positive impact parameter is along the $+y$ direction. The right-hand rule thus defines the direction of the z axis). We will show that for each nl level, the $m=-l$ substate is the predominant electron capture channel, and that electron capture probability decreases rapidly with increasing m within each nl. This propensity rule implies the possibility of carrying out coupled-channel calculations by including only a small subset of magnetic substates in the basis expansion. Thus instead of including all the $n(n+1)/2$ channels for each given n manifold, one can carry out a reduced coupled-channel calculation by including only the dominant m substates. For example, if a single $m=-l$ substate is included for each l, then there will only be n basis functions for each n manifold. The need for such a reduced close-coupling calculation is obvious when one has to deal with electron capture to high-n states.

To illustrate the propensity rule for the m distribution, we carried out close-coupling calculations for the collision of C^{6+} on H in the velocity range of $v=0.1$–1.0 au. In this energy range, electron capture ends up predominantly at the $n=4$ states of C^{5+}. Including the initial state H(1s) and all the states of the $n=4$ manifold of C^{5+}, there are eleven basis functions in such a close-coupling calculation.

We first show in figure 1 the m distribution for electron capture to 4d and 4f states at $v=0.4$ au, by choosing the quantization axis either (a) perpendicular to the scattering plane, or (b) along the direction of the incident projectile. Since the initial state is an

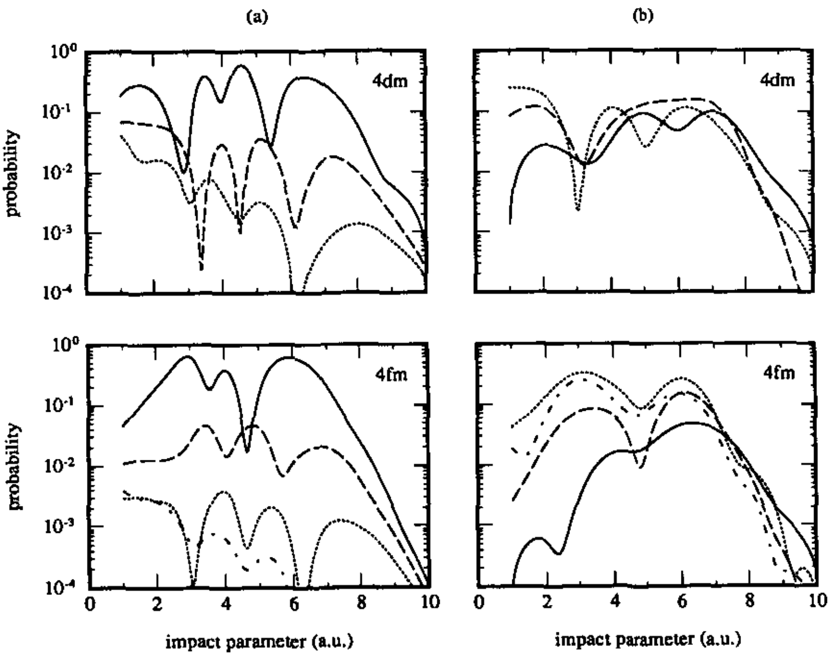

Figure 1. The probability distributions for electron capture to 4d and 4f substates in collisions between C^{6+} on H at $v=0.4$ au. (a) The quantization axis is chosen to be perpendicular to the scattering plane; (b) The quantization axis is chosen to be along the direction of the ion beam. Symbols in (a): full curves, $m=-l$; broken curves, $m=-l+2$; dotted curves, $m=-l+4$; chain curves, $m=+3$. Symbols in (b): full curves, $|m'|=l$; broken curves, $|m'|=l-1$; dotted curves, $|m'|=l-2$; chain curves, $|m'|=l-3$.

s state which is symmetric with respect to the scattering plane, in (*a*) the value of m has to satisfy $(-1)^{l-m}=1$ and thus m changes in steps of 2 for each l. In (*b*), it is understood that each m basis function is a linear combination of $+m$ and $-m$ spherical harmonics and thus only positive m or 0 are used to label the states.

From figure 1 it is clear that if the quantization axis is chosen to be perpendicular to the scattering plane (column (*a*)), the $m=-l$ substate is populated predominantly. The probability decreases by almost an order of magnitude for each step of increase of $\Delta m=2$. This is not the case if the quantization axis is chosen the traditional way which is along the direction of the beam axis. Although small values of m are preferred in the latter, the decrease of electron capture probability with increasing m is not dramatic. Thus the propensity rule for the m distribution is observed only if the quantization axis is chosen to be perpendicular to the scattering plane which will be the quantization axis adopted in the rest of this letter.

Since large-m substates are hardly populated, it is desirable to test if such basis functions can be discarded in a coupled-channel calculation. For this purpose, we perform (*a*) an 11-channel calculation including all states of the $n=4$ manifold of C^{5+}, (*b*) a seven-state calculation including only $m\leqslant 0$ states of $n=4$, and (*c*) a five-state calculation including only the $m=-l$ states of $n=4$. In each of the calculations above, only one state, H(1s), is included on the target. The calculated electron capture probabilities for $4lm(m=-l)$ substates are shown for $v=0.8$ in figure 2. It is clear that the probabilities for each $4lm$ $(m=-l)$ substate from all three calculations are practically identical.

The propensity rule works less satisfactorily for smaller collision velocities, but the results are still quite acceptable for the dominant channels. We show in figure 3 the

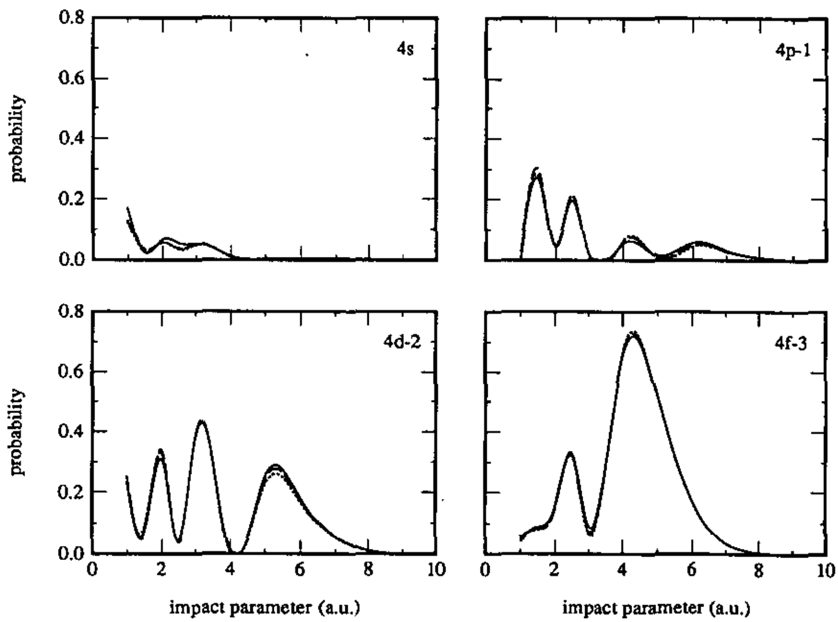

Figure 2. Comparison of electron capture probabilities to $4lm$ $(m=-l)$ substates of C^{5+} for C^{6+} on H at $v=0.8$ au. Full curves, from the full 11-state calculation; broken curves, from the seven-state calculation by including only the negative m in the basis set; dotted curves, from the five-state calculation by including only $m=-l$ substates in each l.

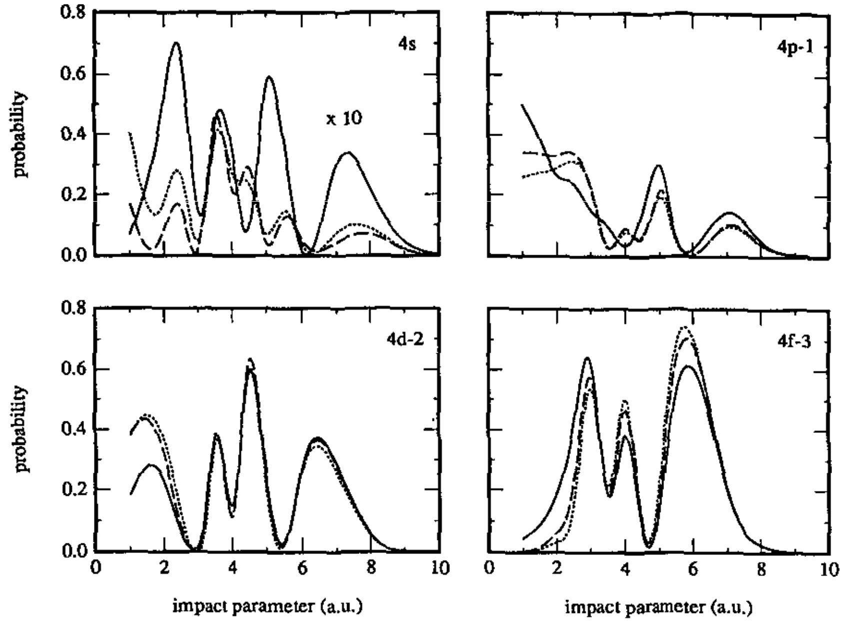

Figure 3. The same as figure 2 except for $v = 0.4$ au. Full curves, from the full 11-state calculation; broken curves, from the seven-state calculation by including only the negative m in the basis set; dotted curves, from the five-state calculaton by including only $m = -l$ substates in each l. Note that the 4s probabilities are magnified by a factor of ten.

same comparison at $v = 0.4$. Except for 4s, where the probability is much smaller, the results for $4f_{-3}$, $4d_{-2}$ and $4p_{-1}$ states from the three calculations are all in quite good agreement, both in magnitude and in the oscillations. At still lower energies, at $v = 0.2$, as shown in figure 4, the results from the reduced calculations become less satisfactory, but they are still acceptable for the dominant $4f_{-3}$ and $4d_{-2}$ states.

We next examine the total electron capture cross sections for the dominant $n = 4$ and the weaker $n = 5$ channels. In a reduced close-coupling calculation, only the $4lm(m = -l)$ and $5lm(m = -l)$ states of C^{5+}, and H(1s) are included, totalling 10 states. This is to be compared with the 26-state calculation if all the $n = 4$ and $n = 5$ states of C^{5+} and H(1s) are included. The total capture cross sections to the $n = 4$ and $n = 5$ shells from the reduced calculation are compared to those from the full close-coupling calculations carried out by Fritsh and Lin (1984), as shown in figure 5. We note that the agreement is quite good for $n = 4$ at all energies. For the weak $n = 5$ channels the agreement is good only at the higher energy region where the $n = 5$ cross section is also large.

The existence of a propensity rule for populating $m = -l$ substates is not too surprising. Obviously electrons that are closer to the scattering plane are more easily captured. With the quantization axis chosen to be perpendicular to the scattering plane, this means that $|m| = l$ substates are populated predominantly. Furthermore, from the classical viewpoint, one can expect that the electron tends to follow the rotation of the internuclear axis. This would give a state with negative m in the quantal description. Classical trajectory calculations are being carried out to confirm this interpretation.

An interpretation of the present propensity rule for populating the $m = -l$ substate in terms of quantal theory is less obvious. Note that the present result does not agree

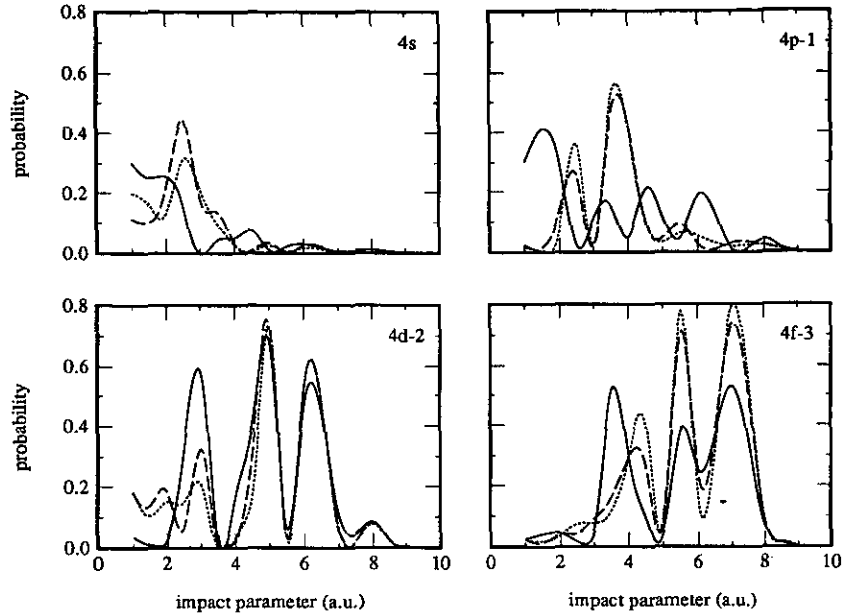

Figure 4. The same as figure 2 except for $v=0.2$ au. Full curves, from the full 11-state calculation; broken curves, from the seven-state calculation by including only the negative m in the basis set; dotted curves, from the five-state calculation by including only $m=-l$ substates in each l.

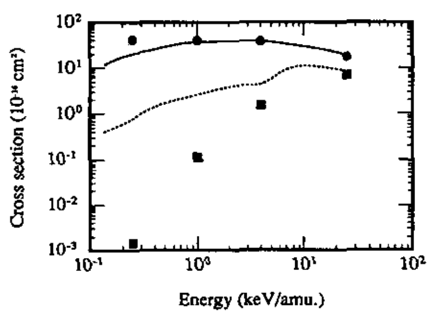

Figure 5. Total electron capture cross sections to $n=4$ and $n=5$ states for C^{6+} on H plotted against scattering energies. The full curve and the broken curve are from the calculation of Fritsch and Lin using a large basis set. The symbols are from the reduced calculations where only the $m=-l$ substates are included in the close-coupling expansion.

with equation (1) since both ΔE and Δm are negative for the example presented in this article. On the other hand, the present result is in agreement with a generalized propensity rule where the distortion of the Coulomb potential for both the initial and the final states is included (see Hansen *et al* 1990). We further remark that all these propensity rules are derived by using the perturbation theory which is of questionable validity for the present system where the electron capture probabilities are not small.

In summary, we have shown that by choosing the quantization axis to be perpendicular to the scattering plane, the dominant magnetic substate populated in electron capture processes is $m=-l$ for collisions between multiply charged ions with atoms.

This propensity rule can be used to reduce the number of basis functions in the close-coupling calculation when electrons are captured to high-n excited states.

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Note added in proof. After this paper had been accepted, it came to our attention that a similar magnetic substate distribution was postulated by Posthumus *et al* (1992). In the extended classical overbarrier model, these authors assumed that only the $M = L$ substate is populated in the collision if the quantization axis is chosen to be perpendicular to the collision plane. Note that in the present paper we showed that it is the $M = -L$ state which is populated.

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