Propensity rule for the magnetic substate distribution in electron capture at high impact energies

C. C. Montanari, M. S. Gravielle, and J. E. Miraglia
Instituto de Astronomía y Física del Espacio, Consejo Nacional de Investigaciones Científicas y Técnicas, Casilla de Correo 67, Sucursal 28, 1428 Buenos Aires, Argentina
(Received 19 September 1996)

We prove the validity of a propensity rule for populating magnetic substates by electron capture processes in the intermediate and high-energy range by using the eikonal impulse approximation. This rule says that if the quantization axis is chosen to be perpendicular to the scattering plane, the $M=-l$ final substates are predominantly populated. A scaling rule in terms of the projectile charge is used to display results of the eikonal impulse and the continuum distorted-wave methods. [S1050-2947(97)05510-8]

PACS number(s): 34.50.Fa

Lundsgaard and Lin [1] studied the magnetic-substate distributions of excited states populated by electron capture processes in collisions between multiply charged ions and atoms. They observed that if the quantization axis is chosen to be perpendicular to the scattering plane, the $M=-l$ final substates are predominantly populated, where l and M are the orbital and magnetic quantum numbers of the final state, respectively. In later works [2] it was shown that the dependence of electron capture probabilities with the orientation of the initial state follows a similar rule. The tendency to populate the $M=-l$ final magnetic substate was envisaged by Lin and collaborators [1,2] from a classical viewpoint. When the quantization axis is chosen to be perpendicular to the scattering plane (see Fig. 1) an electron with $M=-l$ follows the rotation of the internuclear axis staying mostly in the collision plane. Therefore, electron capture is more likely to a final state in which the sense of the electron rotation is identical to that of the internuclear axis. This propensity rule proved to be valid for transitions at large impact parameters and for projectile velocities near the orbital velocity of the target electron. At lower impact velocities the electron has enough time to oscillate between the two collision centers, and then the propensity rule works less satisfactory.

The purpose of this contribution is to examine the validity of the propensity rule in the intermediate- and high-energy range. We study the population of the final magnetic substates of bare multicharged ions colliding with H$(1s)$,

$$P^{Z_P+}+\mathrm{H}(1s)\rightarrow P^{(Z_P-1)+}(nlm)+\mathrm{H}^+. \tag{1}$$

Results are displayed employing a scaling rule that let us gather the data corresponding to different projectile charges within a universal band [3]. Atomic units are used.

We work in the nonrelativistic time-independent quantum formalism, and calculate the transition matrix element T_{nlm} for the reaction (1) by using the *usual* coordinate system (x,y,z), with the z quantization axis along the incident beam direction. From T_{nlm} we obtained the associated transition amplitude $a_{nlm}(\rho)$ (ρ being the impact parameter) through the well-known Fourier transform. The propensity rule requires the rotation of the *usual* coordinate system (x,y,z) into the *natural* coordinate system (x',y',z') shown in Fig. 1 [1,2]. In this system the x' axis is in the direction of the incident beam and the y' axis is in the collision plane, so that the projectile lies on the $+y'$ side. The z' quantization axis is perpendicular to the collision plane, forming a right-handed Cartesian system, (x',y',z'). In the natural system the transition amplitude $A_{nlM}(\rho)$, with M being the final magnetic quantum number with respect to the z' axis, can be obtained from $a_{nlm}(\rho)$ by using the following unitary transformation [4]:

$$A_{nlM}(\rho)=\sum_m D^l_{mM}(\omega)a_{nlm}(\rho). \tag{2}$$

In Eq. (2) $D^l_{mM}(\omega)$ is the Wigner coefficient [5] and $\omega=-90°$ indicates the rotation of the x axis into the z one around the y axis. Note that the nl quantum numbers do not change under the rotation of the coordinate system.

In the *usual* coordinate system the cylindrical symmetry with respect to the beam axis allows one to obtain the capture cross section σ_{nlm} as follows:

$$\sigma_{nlm}=2\pi\int \rho\, d\rho|a_{nlm}(\rho)|^2. \tag{3}$$

Although this symmetry is lost in the rotated frame, we can still define the quantity δ_{nlM} as

$$\delta_{nlM}=2\pi\int \rho\, d\rho|A_{nlM}(\rho)|^2, \tag{4}$$

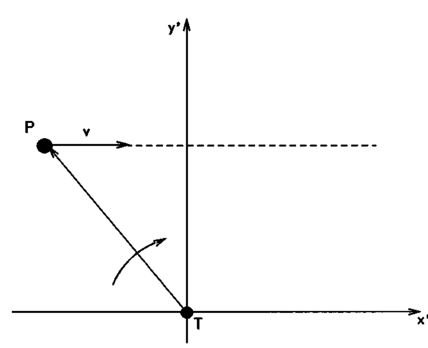

FIG. 1. Natural frame of reference for atomic collisions. The $+z'$ axis is pointing out the plane.

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which is not related to any experimental cross section but measures the total probability of populating the M substate over the whole range of ρ in the scattering plane. Both magnitudes are connected by the closure relation

$$\sigma_{nl}=\sum_{m} \sigma_{nlm}=\sum_{M} \delta_{nlM}, \tag{5}$$

where σ_{nl} is the capture cross section to the nl subshell. Notice that if δ_{nlM} corresponding to a particular value of M is the only dominant term in Eq. (5), this term gives a good estimate of σ_{nl}, which is a quantity liable to be experimentally measured. And this is the usefulness of the propensity rule. For example, to obtain σ_{nl} when l is very large, instead of calculating the contribution of the $2l+1$ magnetic substates we can estimate its value by only calculating δ_{nl-l}. The percentage of contribution from each δ_{nlM} to σ_{nl} is given by the so-called fractional distribution

$$\Delta_{nlM}=\frac{\delta_{nlM}}{\sigma_{nl}}\,100. \tag{6}$$

We calculate the fractional distributions for reaction (1) by using the eikonal impulse (EI) [6] and the continuum-distorted-wave (CDW) [7–9] approximations. Both methods have already proved to be successful to deal with a wide variety of atomic collision systems [3,10,11] in the intermediate- and high-energy regions. To display Δ_{nlM} we use as variable the scaled transfer momentum $\widetilde{W}_{P_z}$ defined as

$$\widetilde{W}_{P_z}=\frac{W_{P_z}}{\widetilde{Z}_P}=\frac{\widetilde{v}^2+\widetilde{Z}_T^2-1}{2\widetilde{v}}, \tag{7}$$

where W_{P_z} is the component of the usual transfer momentum of the projectile parallel to the impact velocity. The other scaled parameters are

$$\widetilde{Z}_P=\frac{Z_P}{n},\quad \widetilde{v}=\frac{v}{\widetilde{Z}_P},\quad \widetilde{Z}_T=\frac{Z_T}{\widetilde{Z}_P}, \tag{8}$$

with Z_T (Z_P) being the target (projectile) Coulomb charge, v the velocity of the incident ion, and in our case $Z_T=1$. This scaling rule was derived from the distorted-wave theory [3], and allows us to plot together results corresponding to different projectile charges. The scaling is valid in the high velocity region ($v>Z_P>Z_T$), and in the intermediate region ($Z_P\geqslant v>Z_T$) with the condition $Z_T<Z_P/n$.

In Figs. 2 and 3 we plot the fractional distributions calculated using the EI and CDW approximations, respectively. Impact velocities larger than the initial electronic velocity are considered, i.e., $v>Z_T$. Projectile charges range from 3 to 6 for $n=2$ and 3, and from 5 to 8 for $n=4$. As the initial $1s$ state is symmetric with respect to the scattering plane, only the amplitudes having even values of $l-M$ survive [1,2]. It implies that for each nl subshell, the magnetic quantum number M associated with the natural coordinate system changes in steps of 2.

From Figs. 2 and 3, it can be observed that in all the cases considered Δ_{nlM} with $M=-l$ is largely dominant, as it is predicted by the propensity rule. Further, the proposed scal-

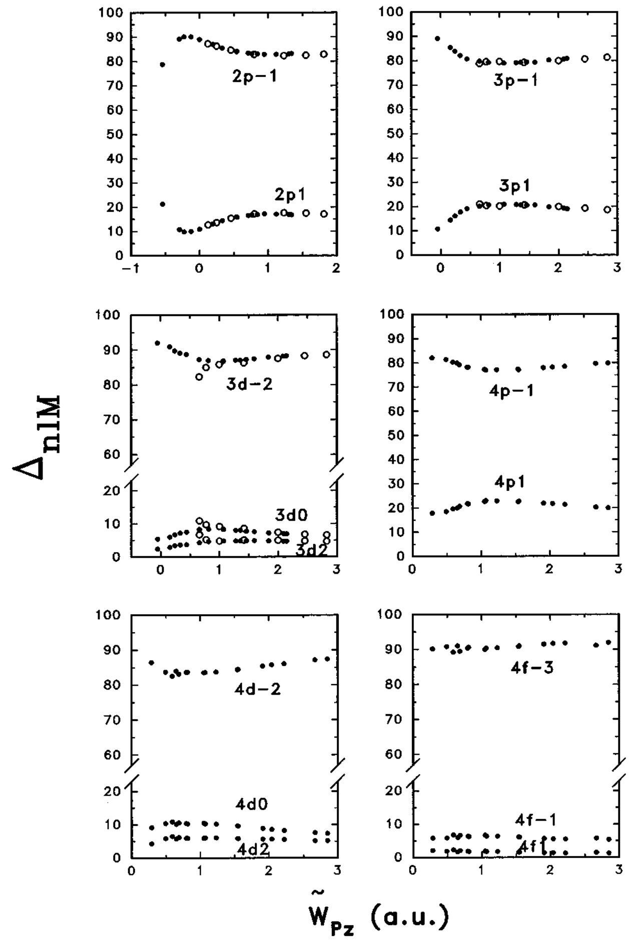

FIG. 2. Fractional distributions Δ_{nlM} of the magnetic substates in the EI approximation, for reaction (1), as functions of a scaled transfer momentum $\widetilde{W}_{P_z}$. Note that M is defined with respect to a quantization axis perpendicular to the scattering plane, as it is explained in the text. Symbols: filled circles, results corresponding to projectile charges $Z_P=5$, 6, and 8; hollow circles, $Z_P=3$.

ing shows a good performance allowing us to display the calculations for different projectile charges together. Results for $Z_P=3$ are distinguished from the rest to make clear that they lightly escape from the universal band in the intermediate velocities region. And it is so because for $Z_P=3$ and $n\geqslant 3$ the condition $Z_T<Z_P/n$ is not verified.

The EI and CDW results strongly verify the qualitative tendency given by propensity rule. However, by comparing Figs. 2 and 3 both theories show differences in the absolute values of the M distributions as l increases. For $l=1$ the EI and CDW fractional distributions tend to the same high-energy limit, though they present different structures at intermediate energies. For $l=2$ both approximations give values of Δ_{nlM} that disagree each other less than 20% for $\widetilde{W}_{P_z}>1$. The worst case corresponds to $l=3$; while the CDW approximation predicts that Δ_{4f-3} decreases with increasing energies (or equivalently with increasing $\widetilde{W}_{P_z}$), the EI one gives nearly a constant. Here the largest velocities considered approach to the limit where the Thomas mechanism (v^{-11} dependence) starts dominating [12]. Since the CDW theory gives the correct m distribution for the Thomas cross section one may expect it to be correct in the high-energy limit [13].

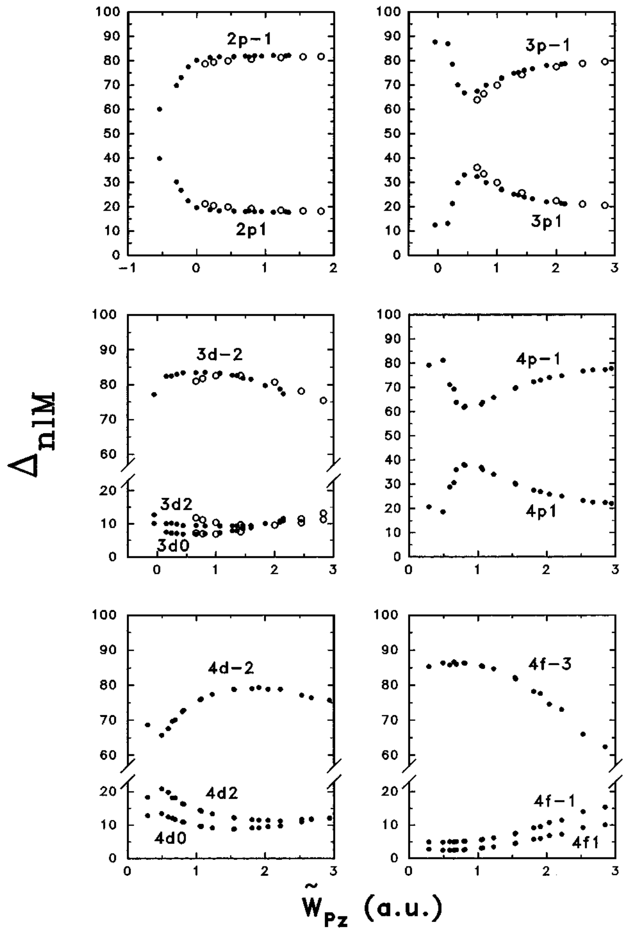

FIG. 3. Similar to Fig. 2 for the CDW approximation.

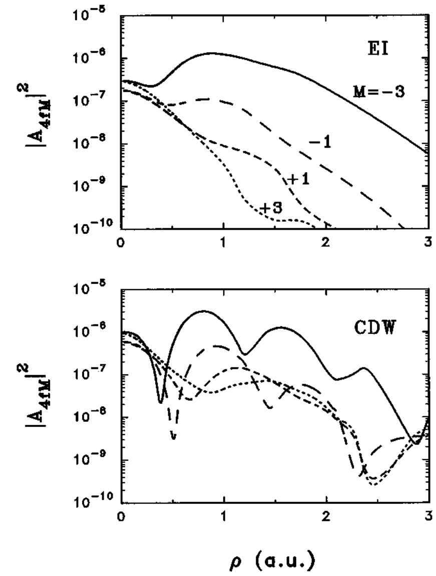

FIG. 4. Electron capture probabilities $|A_{4fM}(\rho)|^2$ as a function of the impact parameter ρ for collisions of C^{6+} on H(1s) at $v=6.36$. Calculations are made in the EI and CDW approximations. Notation: solid lines, $M=-3$; long dashed lines, $M=-1$; short dashed lines, $M=1$; and dotted lines, $M=3$.

The CDW and EI results of Δ_{nlM} decrease as M goes from $-l$ to l, in agreement with the findings of Lin and collaborators [1,2]. However, for $l=2$ the CDW results verify that $\Delta_{nd2}>\Delta_{nd0}$, showing a change of order in the distributions of less contribution to σ_{nl}. On the other side, the EI and CDW approximations give similar values of σ_{nl} for $\widetilde{W}_{P_z}>0$

For low velocities the propensity rule applies specially at large impact parameters [1,2]. To study this tendency we show in Fig. 4 capture probabilities $|A_{4fM}(\rho)|^2$ for collisions of C^{6+} on H(1s) at $v=6.36$. This is the same collision system studied by Lundsgaard and Lin at smaller velocities ($v=0.2-0.8$). Again we display results in both the EI and CDW approximations. Three regions can be recognized. As $\rho\to 0$ the probabilities of the different M substates are almost equal. At intermediate impact parameters ($\rho\sim 1$), which is the region of interest, probabilities for $M=-l$ are dominant. When $\rho\to\infty$, where the contribution to σ_{nl} is negligible, both theories largely disagree. In this region the EI approximation strongly verifies the propensity rule, while the CDW probabilities corresponding to different M substates get mixed up. This different behavior is an interesting point to study.

In conclusion, the propensity rule for populating the $M=-l$ final substates was expected to be valid in the region where the projectile velocity is near the orbital velocity of the target electron. However, the present work proves the validity of the propensity rule in the intermediate and high velocities range.

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