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## Multiple ionization cross-sections of rare gas atoms by impact of highly charged particles at 35 MeV/a.m.u.

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**Résumé.** — La production d'ions de recul multichargés obtenus par impact d'ions lourds rapides et très chargés est étudiée. L'approximation de l'onde plane de Born au premier ordre, employée dans le cadre du modèle à électrons indépendants, fournit des sections efficaces d'ionisation multiple raisonnables pour des gaz rares, bombardés par du  $\text{Kr}^{q+}$  ( $q \sim 30$ ) à 35 MeV/u.m.a., qui est un faisceau typique disponible sur LISE <sup>(1)</sup> à GANIL. La contribution de la capture a été estimée dans le cas d'une cible d'hélium.

**Abstract.** — Production of multiply charged recoil ions by impact of swift highly charged projectiles is investigated. The first Born Plane Wave Approximation employed in the framework of the independent electron model (IEM) provides reasonable cross-sections for multiple ionization of rare gases by  $\text{Kr}^{q+}$  ( $q \sim 30$ ) at 35 MeV/amu, which is a typical ion beam on the LISE <sup>(1)</sup> line at GANIL. Contribution of capture is investigated in the case of helium target.

### 1. Introduction.

Much effort has been made, in the last few years, to obtain intense enough beams of very slow, highly charged ions [1]. Indeed, accurate spectroscopic data on multicharged ions require to get rid of the Doppler effect [2]. Further more, such beams are very welcome to investigate collisions between multicharged ions and neutral atoms under conditions similar to those of the interstellar medium [3]. They could be interesting to observe long life transient molecular states as well [4].

The fast ion beams of GANIL are good candidates to produce, in a gas-cell, highly charged recoil ions of very small velocity. The present paper is a first estimation of the efficiency to produce recoil ions of a given charge when 35 MeV/a.m.u. beams of  $\text{Kr}^{q+}$ ,  $q \approx 30$  (typical beams delivered at GANIL) are impinging on He, Ne or Ar gas targets.

The impact velocity  $v$  under consideration lies in

the high collision velocity range [11]. It is worth recalling that the latter is met when both ratios (hereafter referred to as collision parameters)  $v_{e,T}/v$  and  $v_{e,P}/v$  are less than 1, where  $v_{e,T}$  and  $v_{e,P}$  are typical orbital velocities of an « active » electron [11], in the target and in the projectile, respectively. In this case, molecular features of the collision vanish which results in a capture process of negligible importance compared to the direct ionization process. Presently,  $v$  is 36.40 a.u. including relativistic corrections (see paragraph 5 hereafter). In order to show that high impact velocity conditions are fulfilled, we consider the worst situations that might be met. On the one hand, the highest typical orbital velocity  $v_{e,T}$  is found for the  $K$ -shell of argon; it is less than 18 a.u. (a number obtained for an unscreened hydrogen-like  $K$  orbital). On the other hand, the highest typical orbital velocity  $v_{e,P}$  in  $\text{Kr}^{30+}$  may be estimated to about 17 a.u. This value is evaluated as follows: a  $\text{Kr}^{30+}$  ion has two vacancies in the  $L$ -shell. If one considers that the screening of the nuclear charge is only due to the  $K$ -shell electrons, the  $L$ -shell ones experience an effective charge  $Z_p \sim 34$ . Since a typical hydrogen-

<sup>(1)</sup> LISE is the « Ligne d'Ions Super Epluchés » (Super Stripped Ion Line) at GANIL (Grand Accélérateur National d'Ions Lourds) in Caen (France).

like orbital velocity is  $Z_P/n$ ,  $v_{e,P}$  is less than 17 a.u. in the case of the  $L$ -shell of  $Kr^{29+}$ . Thus, the worst imaginable values of the ratios are  $v_{e,T}/v \approx 18/36.40 = 0.49$  and  $v_{e,P}/v = 17/36.40 = 0.47$ .

The fact that, presently, the contribution of electron capture by the projectile is always negligible is illustrated in the case of helium targets, where capture probabilities have been calculated in the Continuum Distorted Wave (CDW) formalism using a code derived from one of Belkić *et al.* [5]. Thus, multiply charged ion production may be considered as a result of direct ionization processes only, i.e., as due to the simultaneous ejection of several electrons from the target. Then, the direct ionization process is estimated by means of the Plane Wave Born Approximation (PWBA) since collision parameters are relevant. Indeed, in a recent letter, Gayet and Salin [6] showed that PWBA is still valid to cope with single ionization of helium by  $He^{2+}$  impacts at 0.75 MeV/a.m.u., even for small impact parameters.

In the latter case,  $\frac{v_{e,T}}{v} \approx 0.31$  and  $\frac{v_{e,P}}{v} \approx 0.37$  values close enough to the above mentioned values to prevent us from using here methods more sophisticated than PWBA. This statement is also supported by the comparison made by McGuire [19] between PWBA calculations and measurements in the case of ionization of H by  $He^{2+}$ : both data appear to disagree clearly under 100 keV/a.m.u., i.e. for  $v_{e,T}/v \approx 0.5$ .

From the above values of the collision parameters, it is clear that PWBA would not stay a relevant approximation at lower impact energies, where the capture process shows up very rapidly [17, 20], while calculations at higher impact energies would require a relativistic model. Thus, the present impact velocity enables us to make realistic predictions as to recoil ion production. Actually, we are in a position to indicate how it depends on the projectile charge  $Z_P$  and on the target atom, as long as the collision parameters are  $\leq 0.5$ .

Then, an independent electron model (IEM) is employed to figure out multiple ionization probabilities. Such a model is known to be efficient for fast collisions [6, 7]. It requires the knowledge of the PWBA probability  $P_i(\rho)$  for ejecting one electron initially in the state  $i$  of the target, as a function of the impact parameter  $\rho$ . The calculation of  $P_i(\rho)$  is made consistently by assuming that each ejected electron experiences the same potential from the target in the initial and final states. Such an assumption is reasonable since a multiple ionization collision is a sudden process at such high impact velocities. Further, model potentials [8, 9, 10] are used to feature the target potentials seen by electrons in various target orbitals.

Atomic units are used throughout unless otherwise stated.

## 2. Multiple ionization cross-sections.

**2.1 PROBABILITY FOR EJECTION OF ONE ELECTRON.** — Consider a charged particle P (mass  $M_P$ , charge  $Z_P$ ) incident on a multi-electron neutral target which we represent as an ion T (mass  $M_T$ , charge  $+1$ ) bound to an « extra » electron  $e$  (mass 1, charge  $-1$ ) (see Fig. 1). During the collision, the « extra » electron (called active electron [11]) is ejected into the continuum while T recoils at about  $90^\circ$ . The total Hamiltonian of the system in the centre-of-mass frame is :

$$H = \left( -\frac{1}{2\mu} \nabla_R^2 - \frac{1}{2\mu_e} \nabla_r^2 + V(r) \right) + \left( \frac{Z_P}{R} - \frac{Z_P}{|\mathbf{R} - \mathbf{r}|} \right) \quad (1)$$

$$\text{where : } \mu = \frac{M_P M_T}{M_P + M_T + 1} \quad \text{and} \quad \mu_e = \frac{M_T}{M_T + 1} \approx 1.$$

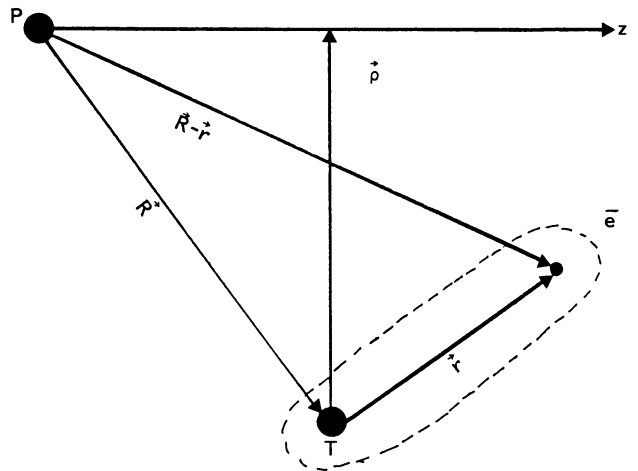


Fig. 1. — Coordinate system.

The principal term  $H_C$  in the first brackets of equation (1) is composed of three terms : the first one corresponds to the nuclear kinetic energy, the second one to the kinetic energy of the active electron and the third one represents the screening potential due to the ion T seen by the active electron. The perturbative term  $V_C$  in the second brackets of equation (1) corresponds to the Coulomb interactions between the projectile P and both components of the target, T and  $e$ , respectively. The first Born amplitude of ionization  $T_{i,f}$  is given by McDowell and Coleman [12] :

$$T_{i,f} = \langle e^{ik_f \cdot \mathbf{R}} \Phi_f(\mathbf{r}) | V_C | e^{ik_i \cdot \mathbf{R}} \Phi_i(\mathbf{r}) \rangle \quad (2)$$

where  $e^{ik_i \cdot \mathbf{R}}$  and  $e^{ik_f \cdot \mathbf{R}}$  are plane wave functions for the nuclear motion in the initial and final states respectively,  $\Phi_i(\mathbf{r})$  the initial wave function of an active electron characterized by quantum numbers

$(n_i, \ell_i, m_i, m_s)$  and  $\Phi_f(\mathbf{r})$  the final wave function of the electron ejected with the kinetic energy  $\frac{k^2}{2}$ .

$$\Phi_i(\mathbf{r}) = R_{n_i, \ell_i}(r) Y_{\ell_i}^{m_i}(\hat{r}) \tag{3}$$

$$\Phi_f(\mathbf{r}) = \frac{1}{k} \sum_{\ell_f=0}^{+\infty} \sum_{m_f=-\ell_f}^{+\ell_f} i^{\ell_f} e^{-i\sigma_f} \times R_{k, \ell_f}(r) Y_{\ell_f}^{m_f*}(\hat{k}) Y_{\ell_f}^{m_f}(\hat{r}). \tag{4}$$

Since the spins are unchanged in the present formalism, spinors are omitted in all wave functions.  $R_{n_i, \ell_i}$  is a real function.  $R_{k, \ell_f}$  is made as well through a suitable value of the phase shift  $\sigma_{\ell_f}$ .

The orthonormalisation condition on  $R_{k\ell_f}$  is :

$$\int_0^{+\infty} R_{k' \ell_f} R_{k \ell_f} r^2 dr = \delta(k' - k). \tag{5}$$

In the framework of a sudden approximation, one can consider that the electronic wave functions do not depend on the internuclear distance, i.e. :

$$\left\langle \Phi_f(\mathbf{r}) \left| \frac{1}{R} \right| \Phi_i(\mathbf{r}) \right\rangle \approx \delta_{i, f}. \tag{6}$$

After integration over the internuclear coordinate, a standard partial wave expansion leads to :

$$T_{i, f} = -\frac{Z_p}{kq^2} (4\pi)^{3/2} \sum_{\ell=0}^{+\infty} \sum_{m=-\ell}^{+\ell} \sum_{\ell_f=0}^{+\infty} \sum_{m_f=-\ell_f}^{+\ell_f} \{ (2\ell_i + 1)(2\ell + 1)(2\ell_f + 1) \}^{1/2} \times \begin{pmatrix} \ell_i & \ell & \ell_f \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_i & \ell & \ell_f \\ m_i & m & -m_f \end{pmatrix} (-1)^{m_f} i^{\ell} e^{i\sigma_{\ell_f}} Y_{\ell_f}^{m_f}(\hat{k}) Y_{\ell_f}^{m_f*}(\hat{q}) (-i)^{\ell_f} \int j_{\ell}(qr) R_{k, \ell_f}(r) R_{n_i, \ell_i}(r) r^2 dr \tag{7}$$

where  $j_{\ell}$  is the spherical Bessel function of  $\ell$ th-order and  $q$  the momentum transfer.

$$\mathbf{q} = \mathbf{k}_i - \mathbf{k}_f \tag{8}$$

$$\mathbf{q} = \boldsymbol{\eta} + \boldsymbol{\eta}' \tag{9}$$

where  $\boldsymbol{\eta}$  is the transverse momentum transfer and  $\boldsymbol{\eta}'$  the longitudinal momentum transfer.

$$\eta' = \frac{\varepsilon}{v} = \frac{k^2/2 + I_s}{v} \tag{10}$$

where  $\varepsilon$  is the energy transferred to the electron,  $I_s > 0$  is the ionization potential of the subshell  $(n_i, \ell_i)$  and  $v$  is the impact velocity.

A standard double Fourier transform provides the probability amplitude as a function of the impact parameter  $\rho$ , for a given momentum  $k$  of the ejected electron (McDowell and Coleman [12])

$$a_{i, f}(\rho, v) = \frac{1}{(2\pi)^2} \frac{1}{v} \int d\boldsymbol{\eta} e^{i\boldsymbol{\eta}\boldsymbol{\rho}} T_{i, f}. \tag{11}$$

Then the probability to eject an electron from the orbital  $(n_i, \ell_i, m_i, m_s)$  is :

$$P_{n_i, \ell_i, m_i, m_s}(\rho) = \int k^2 dk \int d\hat{k} |a_{if}|^2. \tag{12}$$

More explicitly, it is :

$$P_{n_i, \ell_i, m_i, m_s}(\rho) = \frac{4 Z_p^2}{v^2} (2\ell_i + 1) \sum_{\ell_f=0}^{+\infty} (2\ell_f + 1) \sum_{m_f=-\ell_f}^{+\ell_f} \sum_{\ell_f'=\ell_f}^{+\ell_f} (-1)^{\frac{\ell_f - \ell_f'}{2}} (2 - \delta_{\ell_f, \ell_f'}) \times (2\ell + 1)(2\ell' + 1) \begin{pmatrix} \ell_i & \ell & \ell_f \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \ell_i & \ell' & \ell_f \\ 0 & 0 & 0 \end{pmatrix} \left\{ \frac{(\ell - |m|)! (\ell' - |m|)!}{(\ell + |m|)! (\ell' + |m|)!} \right\}^{1/2} \times \begin{pmatrix} \ell_i & \ell' & \ell_f \\ m_i & m & -m_f \end{pmatrix} \begin{pmatrix} \ell_i & \ell & \ell_f \\ m_i & m & -m_f \end{pmatrix} \int_0^{+\infty} dk \times \int_0^{+\infty} d\boldsymbol{\eta} \frac{\eta}{\eta^2 + \varepsilon^2/v^2} J_m(\eta\rho) P_{\ell}^{|m|} \left( \frac{1}{\sqrt{1 + \eta^2 \frac{v^2}{\varepsilon^2}}} \right) \xi_{\ell_f}^{\ell_f}(q) \times \int_0^{+\infty} d\boldsymbol{\eta} \frac{\eta}{\eta^2 + \varepsilon^2/v^2} J_m(\eta\rho) P_{\ell'}^{|m|} \left( \frac{1}{\sqrt{1 + \eta^2 \frac{v^2}{\varepsilon^2}}} \right) \xi_{\ell_f'}^{\ell_f'}(q) \tag{13}$$

where :

$$m = m_f - m_i$$

$$\left\{ \begin{aligned} \xi_{\ell}^{\ell_f}(q) &= \int j_{\ell}(qr) R_{n_i, \ell_i}(r) R_{k, \ell_f}(r) r^2 dr \\ |\ell_i - \ell_f| &\leq \left\{ \begin{aligned} \ell \\ \ell_f \end{aligned} \right\} \leq |\ell_i + \ell_f| \end{aligned} \right. \quad (14)$$

$J_m$  is the Bessel function of  $m$ th-order,  $P_{\ell}^m$  the Legendre polynomial.

Indeed, the probability is independent of  $m_s = \pm 1/2$ . Furthermore, it depends only upon the absolute value of  $m_i$ , i.e. :

$$P_{n_i, \ell_i, -m_i} = P_{n_i, \ell_i, m_i} \quad (15)$$

**2.2 MULTIPLE IONIZATION CROSS-SECTIONS.** — According to the IEM developed by Hansteen and Mosebekk [13], the multiple ionization probability is deduced from the ionization probabilities calculated in a one active electron framework, i.e. probabilities introduced in section 2.1.

In what follows, we are interested in multiple ionization of rare gases, i.e. species made of complete subshells. A subshell  $n_i p$  contains 6 electrons, four of which have the same ejection probability  $P_{n_i, 1, 1}$  while both others are associated with the probability  $P_{n_i, 1, 0}$ . The probability  $P_{n_i, 0, 0}$  is related to a subshell  $n_i s$  which contains 2 electrons. More generally, a set  $i$  made of the two complete sublevels  $(n_i, \ell_i, m_i)$  and  $(n_i, \ell_i, -m_i)$  contains 4 electrons whereas there are only 2 in a set made of the unique complete sublevel  $(n_i, \ell_i, 0)$ . Thus one finds  $2(2 - \delta_{m_i, 0})$  electrons in such a set  $i$ . In the IEM, the probability  $\mathcal{F}_{j_i}$  to remove  $j_i$  electrons from the set  $i$  is :

$$\mathcal{F}_{j_i} = \binom{2(2 - \delta_{m_i, 0})}{j_i} (P_i)^{j_i} (1 - P_i)^{2(2 - \delta_{m_i, 0}) - j_i} \quad (16)$$

where the first factor of the r.h.s. of equation (16) is the binomial coefficient. Obviously, one has :

$$0 \leq j_i \leq 2(2 - \delta_{m_i, 0}) \quad (17)$$

Now, the probability  $\mathcal{F}_J$  to eject  $J$  electrons from the target atom is :

$$\mathcal{F}_J = \prod_i \sum_{\substack{j_i \\ \sum j_i = J}} \mathcal{F}_{j_i} \quad (18)$$

In this picture, the total cross-section for the simultaneous ejection of  $J$  electrons is :

$$\sigma_J = 2 \pi \int_0^\infty \rho d\rho \mathcal{F}_J(\rho) \quad (19)$$

**3. Electronic radial wave functions.**

**3.1 TARGET POTENTIALS.** — As indicated in the introduction, our IEM is consistently defined by assuming that an active electron experiences the same central potential in both entrance and exit channels. As a first step, present calculations are made with a model potential  $V(r)$  (Klapisch [8]).

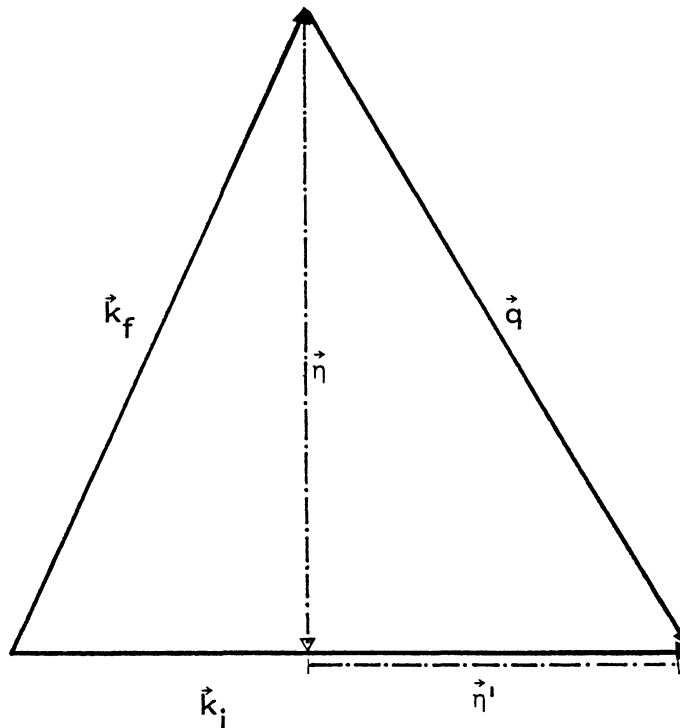


Fig. 2. — Momentum diagram.

For neon and argon targets, we used the potential of M. Aymar [10], corresponding to the case of an electron in the field of a singly ionized atom.

neon :

$$\begin{aligned} V(r) &= -\frac{1}{r} \{2 g_0(\delta_1 r) + 2 g_0(\delta_2 r) + 5 g_1(\delta_3 r) + 1\} \\ g_0(\delta r) &= e^{-\delta r} (1 + 1/2 \delta r) \\ g_1(\delta r) &= e^{-\delta r} \{1 + 3/4 \delta r + 1/4 (\delta r)^2 + 1/24 (\delta r)^3\} \\ \delta_1 &= 12.10807 \quad \delta_2 = 8.55326 \quad \delta_3 = 3.51927 \end{aligned} \quad (20)$$

argon :

$$V(r) = -\frac{1}{r} \{2 g_0(\delta_1 r) + 2 g_0(\delta_2 r) + 6 g_1(\delta_3 r) + 2 g_0(\delta_4 r) + 5 g_1(\delta_5 r) + 1\}$$

$$\begin{array}{lll} \delta_1 = 24.65853 & \delta_2 = 5.59555 & \delta_3 = 11.9054 \\ \delta_4 = 3.1237 & \delta_5 = 2.30707 & \end{array} \quad (21)$$

It is clear that the choices made above introduce a slight inconsistency since the model potentials are calculated in order to fit spectroscopic data for the excited levels of the atoms. By doing so, one gets the potential experienced by outer p electrons. However, wave functions of inner shell electrons obtained with this potential are accurate enough for present calculations, as stated by the comparison to the orbitals given by Clementi and Roetti [14] (see Figs. 3a, b).

For helium, we used a model potential issued from Bottcher [9].

$$V(r) = \frac{1}{r} \{e^{-4r}(1 + 4r) + 1\}. \quad (22)$$

All these three potentials become Coulomb potentials at large distances ; they describe the screening effect of the electronic cloud at small distances. Now, the bound and continuum radial wave functions  $R_{n_i, \ell_i}(r)$  and  $R_{k, \ell_f}(r)$  are solutions of the same radial Schrödinger equation :

$$\left\{ -\frac{1}{2} \frac{d^2}{dr^2} + \ell \frac{(\ell + 1)}{2r^2} + V(r) - E \right\} U(r) = 0 \quad (23)$$

$$U(r) = rR_{n_i, \ell_i}(r) \quad \text{respectively} \quad rR_{k, \ell_f}(r)$$

$$\begin{cases} \ell = \ell_i & \text{respectively} \quad \ell_f \\ E = -I_s & \text{respectively} \quad \frac{k^2}{2} \end{cases}$$

**3.2 RADIAL WAVE FUNCTION OF THE INITIAL ORBITAL  $U_{n_i, \ell_i}$ .** — In order to save computer time, we expand  $U_{n_i, \ell_i}$  on a basis of Slater orbitals which is optimized by comparison to the numerical solution obtained step by step by M. Aymar. This expansion was achieved by means of a code of Valiron [15].

**3.3 RADIAL WAVE FUNCTION OF THE FINAL ORBITAL  $U_{k, \ell_f}$ .** — The radial Schrödinger equation (23) can be modified to :

$$\frac{d^2}{dr^2} U_{k, \ell_f}(r) = g(r) U_{k, \ell_f}(r) \quad (24)$$

$$g(r) = 2(V(r) - E) + \ell_f \left( \ell_f + \frac{1}{2} \right) / r^2. \quad (25)$$

The Numerov algorithm is known to be particularly adapted to resolve this type of differential equations.

For a linear step  $h$ , it is written as :

$$U_{k, \ell_f}(r+h) = \{U_{k, \ell_f}(r-h)(g(r-h) - 12/h^2) + U_{k, \ell_f}(r)(10g(r) + 24/h^2)\} / \{12/h^2 - g(r+h)\}. \quad (26)$$

For all our calculations, we chose a constant step  $h$  of 0.01 a.u. The behaviour of regular solutions of equation (24) is employed to start the procedure, i.e. :

$$\begin{aligned} U_{k, \ell_f}(0) &= 0 \\ U_{k, \ell_f}(h) &= h^{\ell_f+1}. \end{aligned} \quad (27)$$

However the solutions are still to be normalized. The normalisation factor  $N$  is defined as follows :

$$NU_{k, \ell_f} = rR_{k, \ell_f}. \quad (28)$$

Since  $V(r)$  is purely coulombic at large distances, one has (Landau and Lifshitz [16]) :

$$NU_{k, \ell_f}(r) \xrightarrow{r \rightarrow \infty} \sqrt{\frac{2}{\pi}} \times \{F_{\ell_f}(kr) \cos \delta_{\ell_f} + G_{\ell_f}(kr) \sin \delta_{\ell_f}\} \quad (29)$$

where  $F_{\ell}$  and  $G_{\ell}$  are the regular and irregular Coulomb wave functions. Then  $N$  and  $\delta_{\ell_f}$  are known by identifying  $NU_{k, \ell_f}$  to the r.h.s. of equation (29) at two distances  $r_1$  and  $r_2$  which must be large enough to ensure a purely coulombic behaviour of  $V(r)$ . However it is worth noting that  $r_1$  and  $r_2$  should be not too large, not only to save computer time, but mainly in order to make it sure that the numerical solution  $U_{k, \ell_f}(r)$  does not exhibit a pathological behaviour due to the unavoidable numerical pollution by the irregular solution at the origin. Practically we have taken  $r_1 = 9$  a.u. and  $r_2 = 10$  a.u. in all cases.

$$\text{tg } \delta_{\ell_f} = \frac{U_{k\ell_f}(r_2) F_{\ell_f}(kr_1) - U_{k\ell_f}(r_1) F_{\ell_f}(kr_2)}{U_{k\ell_f}(r_1) G_{\ell_f}(kr_2) - U_{k\ell_f}(r_2) G_{\ell_f}(kr_1)} \quad (30)$$

$$N = \sqrt{\frac{2}{\pi}} \frac{\cos \delta_{\ell_f} F_{\ell_f}(kr_1) + \sin \delta_{\ell_f} G_{\ell_f}(kr_1)}{U_{k\ell_f}(r_1)}. \quad (31)$$

#### 4. Kinetic energy distribution of recoil ions.

In the present section, it is shown that, at high impact velocities :

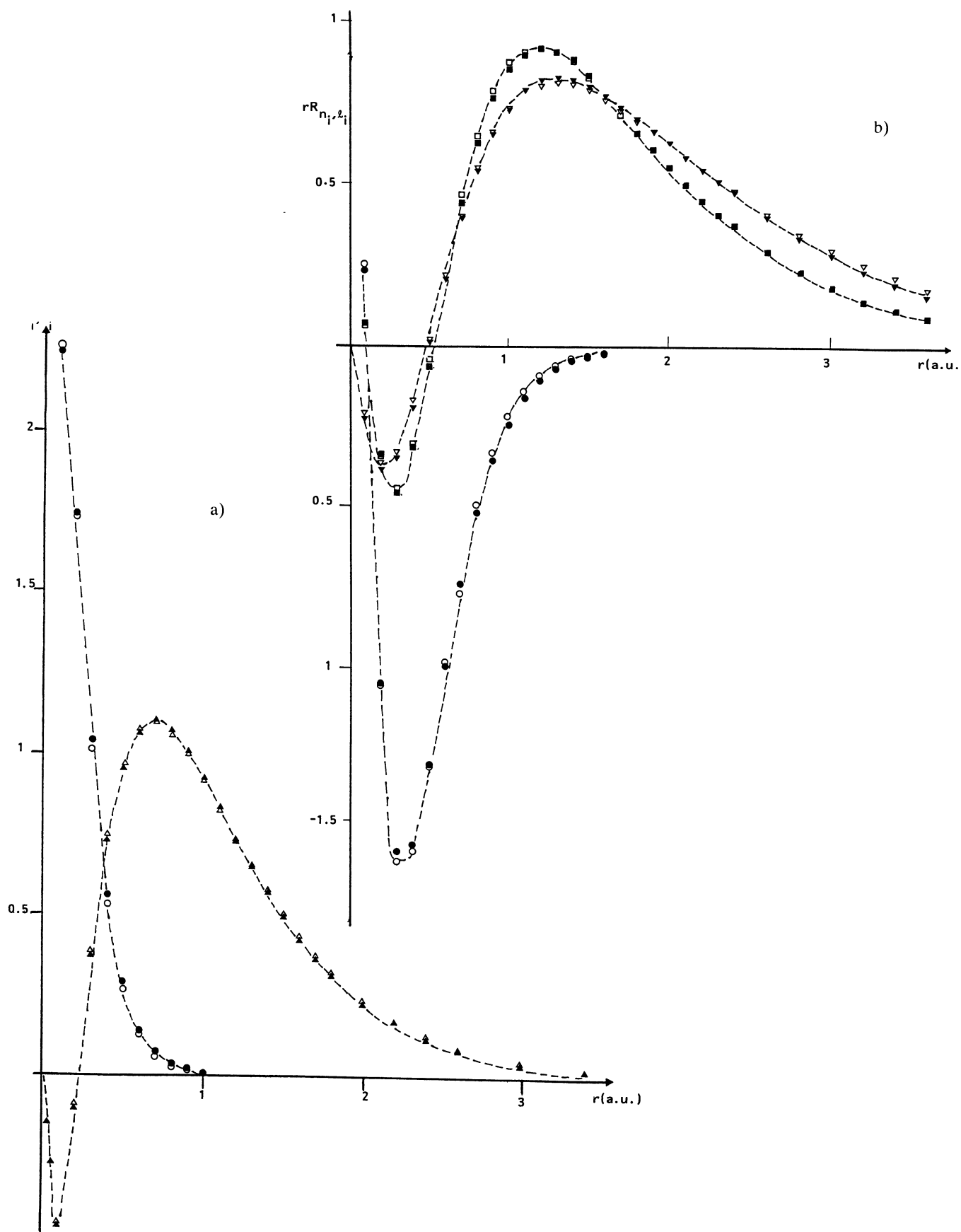


Fig. 3. — Radial wave functions  $rR_{n_i, \ell_i}(r)$ : (a) of neon ( $\circ$ )  $rR_{1s}$ , ( $\Delta$ )  $rR_{2s}$  calculated from Clementi and Roetti tables, ( $\bullet$ )  $rR_{1s}$ , ( $\blacktriangle$ )  $rR_{2s}$  calculated in this work; (b) of argon ( $\circ$ )  $rR_{1s}$ , ( $\square$ )  $rR_{2p}$ , ( $\nabla$ )  $rR_{3s}$  calculated from Clementi and Roetti tables, ( $\bullet$ )  $rR_{2s}$ , ( $\blacksquare$ )  $rR_{2p}$ , ( $\blacktriangledown$ )  $rR_{3s}$  calculated in this work; lines are drawn as a guide for the eye.

(i) target recoil occurs at  $90^\circ$  to the direction of the incident beam ;

(ii) the kinetic energy of recoil ions depends only upon the impact parameter  $\rho$  (not upon their final charge  $J$ ) ;

and (iii) the energy distribution of recoil ions of charge  $J$  is determined by the probability  $P_J(\rho)$  of creating them.

The demonstration is made in the laboratory frame by means of 4 reasonable assumptions :

(1) the projectile trajectory is a quasi straight line ;

(2) the projectile is considered as a point charge  $Z_P$  eventhough it could be a non-bare nucleus ;

(3) the projectile-target interaction takes place through the Hartree-Fock potential of the neutral target in its ground state ;

and (4) the displacement of the target during the collision is neglected.

Hypothesis (1) is known to be excellent. Hypothesis (4) is checked consistently at the end of the calculations : it is excellent too. As to assumption (2), it is good enough as long as the radius of the projectile ion is roughly smaller than the impact parameter. The radius of  $\text{Kr}^{30+}$  ions is about 0.18 a.u. Then, one expects the results to be reliable for  $\rho \cong 0.2$  a.u. Finally hypothesis 3 appears reasonable since total ionization cross-sections are dominated by momenta of the ejected electrons much smaller than the impact velocity. Hence, the electronic density of charge on the target is almost unchanged at the end of the collision whatsoever the number of ejected electrons.

Now the force experienced by the target is opposed to that sustained by the projectile, i.e. :

$$\mathbf{F}_T = Z_P \nabla_{\mathbf{R}} V_{\text{HF}}(R) = Z_P \frac{dV_{\text{HF}}(R)}{dR} \frac{\mathbf{R}}{R} \quad (32)$$

where  $V_{\text{HF}}(R)$  is a Hartree-Fock potential built in a standard way [8] with Clementi and Roetti's wave functions [14].  $\mathbf{R}$  is the internuclear distance which reads (see Fig. 1) :

$$\mathbf{R} = \rho + \mathbf{v}t = \rho + \mathbf{z}. \quad (33)$$

The momentum transferred to the target is

$$\begin{aligned} \mathbf{p}_T(\rho) &= \int_{-\infty}^{+\infty} \mathbf{F}_T(\mathbf{R}) dt \\ &= \frac{Z_P}{v} \int_{-\infty}^{+\infty} \frac{dV_{\text{HF}}(R)}{dR} \frac{\rho + \mathbf{z}}{R} dz. \end{aligned} \quad (34)$$

Since  $V_{\text{HF}}(R)$  depends only on  $R = |\mathbf{R}|$ , it is easy to show that

$$\int_{-\infty}^{+\infty} \frac{dV_{\text{HF}}(R)}{dR} \frac{\mathbf{z}}{R} dz = 0 \quad (35a)$$

$$\int_{-\infty}^{+\infty} \frac{dV_{\text{HF}}(R)}{dR} \frac{\rho}{R} dz = 2 \int_0^{+\infty} \frac{dV_{\text{HF}}(R)}{dR} \frac{\rho}{R} dz \quad (35b)$$

by changing  $z$  in  $-z$ . Therefore, the recoil momentum is :

$$\mathbf{p}_T(\rho) = 2 \frac{Z_P}{v} \rho \int_0^{+\infty} \frac{dV_{\text{HF}}(R)}{dR} \frac{dz}{R}. \quad (36)$$

It is oriented along the  $\rho$  axis, i.e. perpendicular to the projectile trajectory. For a given target, one has  $p_T(\rho) \propto Z_P v^{-1}$  as long as the four above mentioned assumptions are acceptable. Now, the number of recoil ions of charge  $J$  created per second is (see appendix 1).

$$N_J = n_P n_T v \ell s \sigma_J \quad (37)$$

where  $\sigma_J$  is given by equation (19). In the area  $2 \pi \rho d\rho$  it is :

$$dn_J = n_P n_T v \ell s P_J(\rho) 2 \pi \rho d\rho. \quad (38)$$

Hence the distribution function, to produce ions of a given charge state  $J$ , as a function of  $\rho$  is :

$$D_J(\rho) = \frac{1}{N_J} \frac{dn_J}{d\rho} = \frac{2 \pi}{\sigma_J} \rho P_J(\rho). \quad (39)$$

All ions created for this impact parameter  $\rho$  have the same recoil energy  $\varepsilon$

$$\varepsilon = \frac{P_T^2(\rho)}{2 M_T} = f(\rho) \quad (40)$$

the distribution function of recoil ions of charge  $J$  as a function of the recoil energy  $\mathcal{D}_J(\varepsilon)$  is such that

$$\int_0^{+\infty} \mathcal{D}_J(\varepsilon) d\varepsilon = 1. \quad (41)$$

Now one has :

$$\int_0^{+\infty} D_J(\rho) d\rho = \int_{-\infty}^0 D_J[\rho(\varepsilon)] \rho'(\varepsilon) d\varepsilon = 1. \quad (42)$$

From expressions (40), (41) and (42) it is readily shown that :

$$\mathcal{D}_J(\varepsilon) = - D_J(\rho) \rho'(\varepsilon) = - \frac{D_J(\rho)}{f'(\rho)} \quad (43)$$

where :

$$f'(\rho) = \frac{d\varepsilon}{d\rho}. \quad (44)$$

The integrals in expression (36) have been performed numerically up to a value  $z_0$  of  $z$  where we made it sure that the contribution of the interval  $[z_0, +\infty[$  is less than  $10^{-4}$ . Then, we figured out an upper limit  $\Delta_u$  of what the displacement  $\Delta$  of the target could be

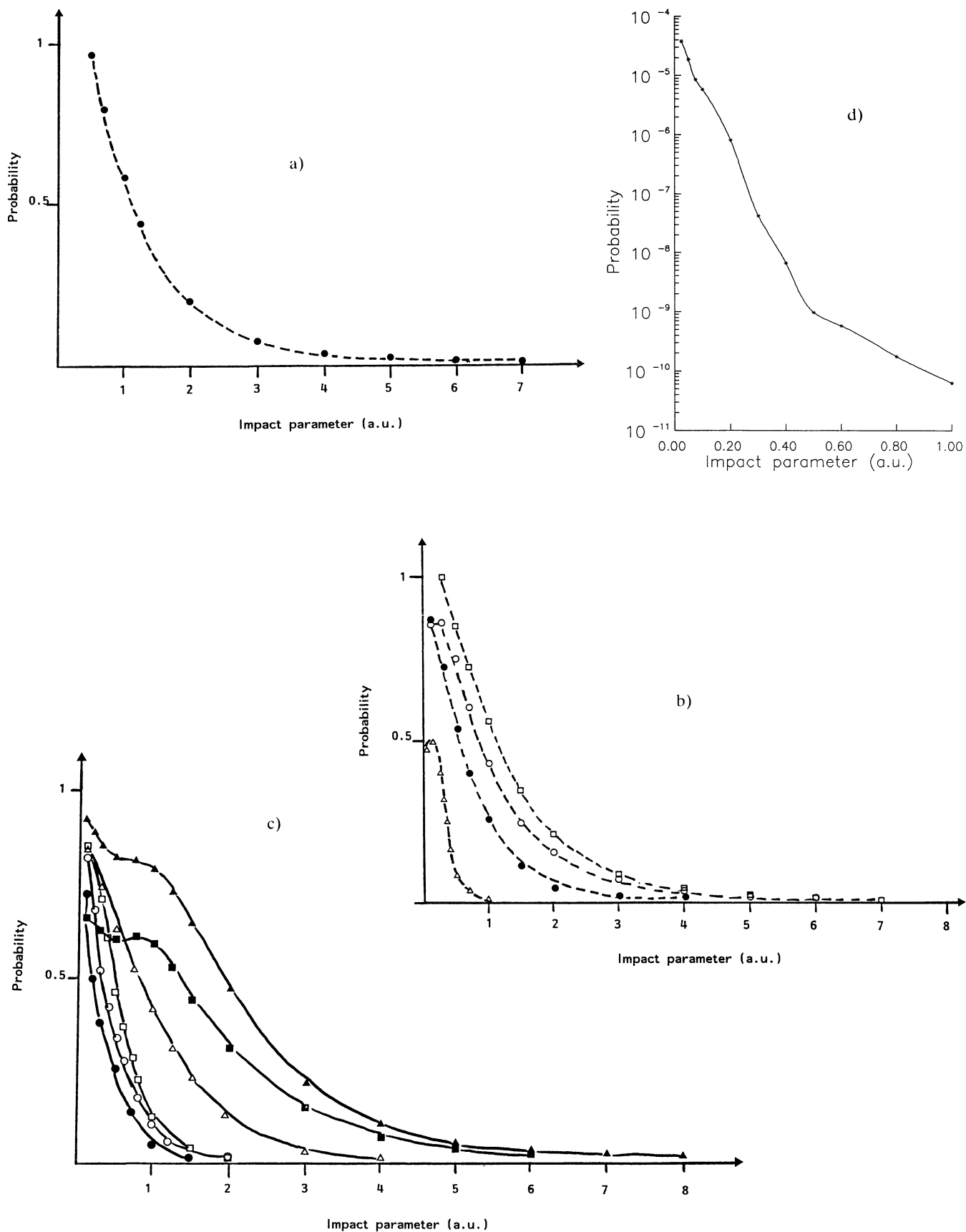


Fig. 4. — Probabilities of ejection of one electron  $P_{n_i, \ell_i, |m_i|}(\rho)$  of (4a) helium, (4b) neon, (4c) argon, by collision with 35 MeV/a.m.u. ions of charge 30. 4a: ( $\bullet$ )  $P_{100}$ ; 4b: ( $\Delta$ )  $P_{100}$ , ( $\bullet$ )  $P_{200}$ , ( $\circ$ )  $P_{210}$ , ( $\square$ )  $P_{211}$ ; 4c: ( $\bullet$ )  $P_{200}$ , ( $\circ$ )  $P_{210}$ , ( $\square$ )  $P_{211}$ , ( $\Delta$ )  $P_{300}$ , ( $\blacksquare$ )  $P_{310}$ , ( $\blacktriangle$ )  $P_{311}$ ; 4d: probability of capture  $P_C(\rho)$  of one electron from helium by 35 MeV/a.m.u.  $\text{Kr}^{34+}$  (see text).

during the lapse of time for the projectile to cover the distance  $[-z_0, +z_0]$ . Obviously one has :

$$|\Delta| < \Delta_u = \frac{p_T(\rho) 2 z_0}{M_T v}.$$

Down to values of  $\rho$  as small as 0.05 a.u.,  $\Delta_u$  is found to be much less than 0.01  $\rho$  for  $Z_p = 30$ . Hence hypothesis 4 is shown to be excellent.

**5. Results and discussion.**

The efficiency to produce highly charged recoil ions by typical swift ion beams of GANIL has been investigated for an actual beam of 35 MeV a.m.u.<sup>-1</sup> Kr<sup>30+</sup> ions. Although the collision treatment for ionization is not relativistic, the lab-impact energy is high enough to require a relativistic correction to evaluate the relative impact velocity  $v$ , i.e. :

$$v = c \sqrt{1 - \left( \frac{m_0 c^2}{T + m_0 c^2} \right)^2} \tag{45}$$

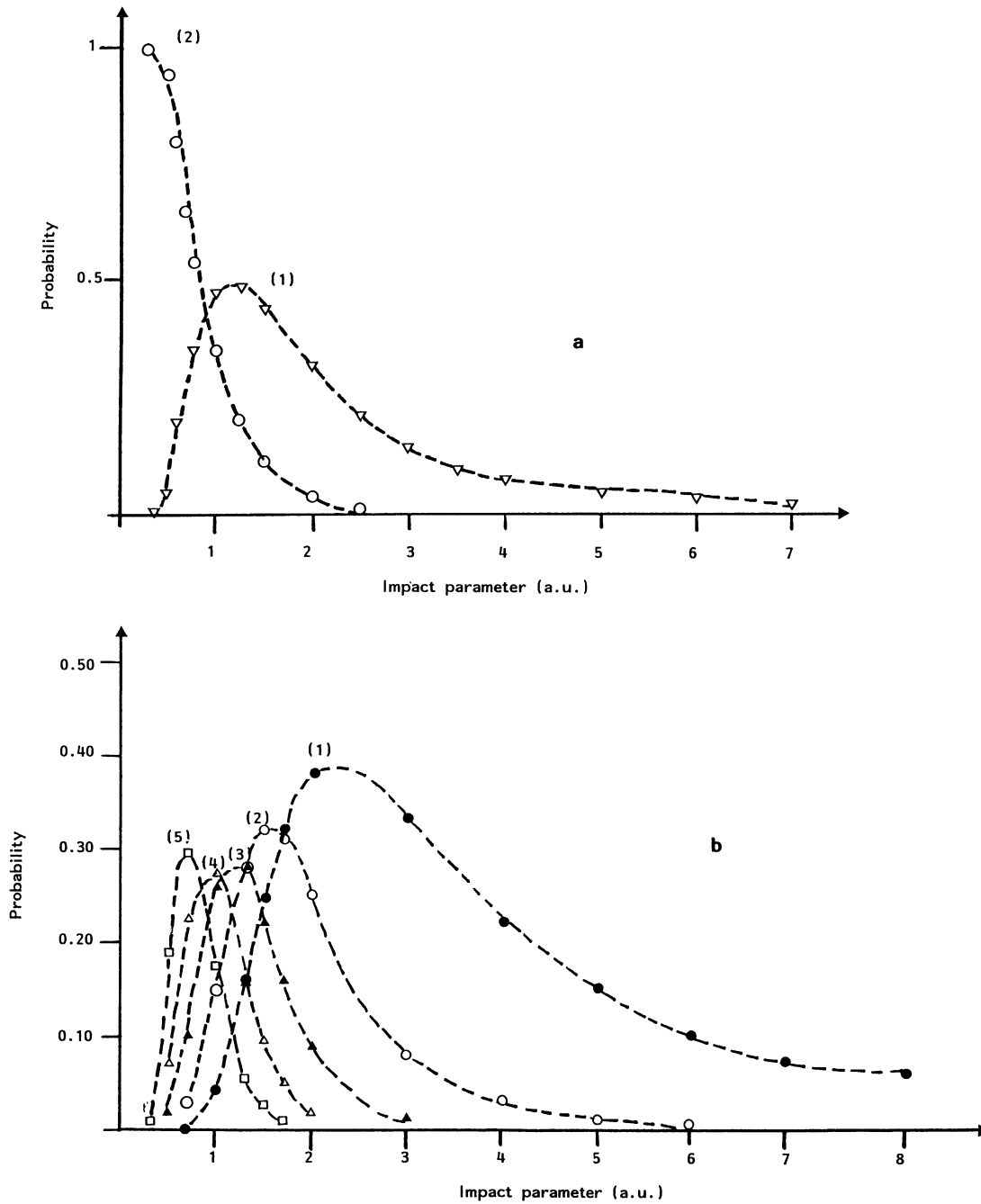


Fig. 5. — Probabilities  $\mathcal{P}_J(\rho)$  to remove  $J$  electrons from helium (5a), neon (5b, c) and argon (5d, e, f). The value of  $J$  is indicated in brackets.

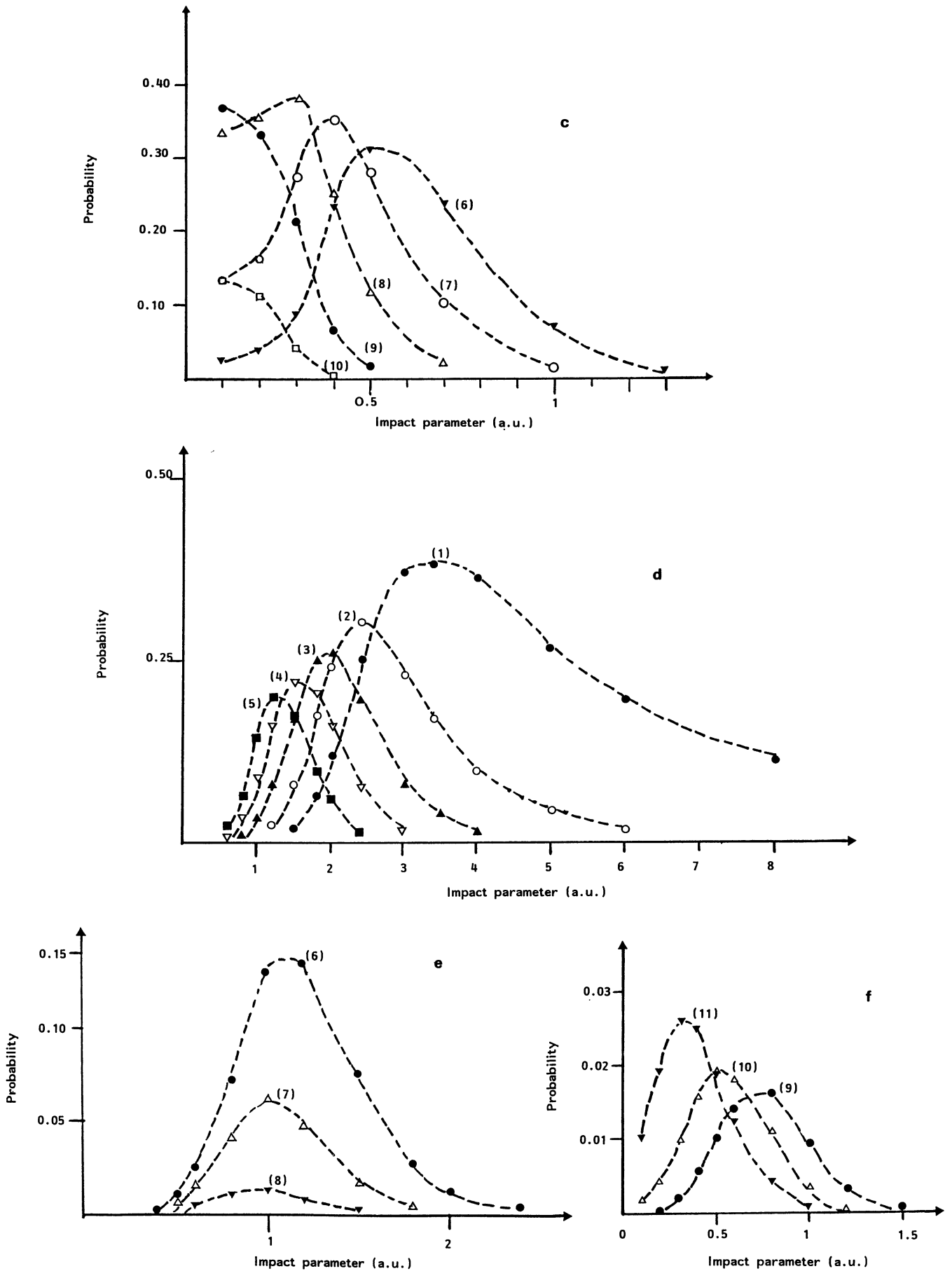


Fig. 5 (continued)

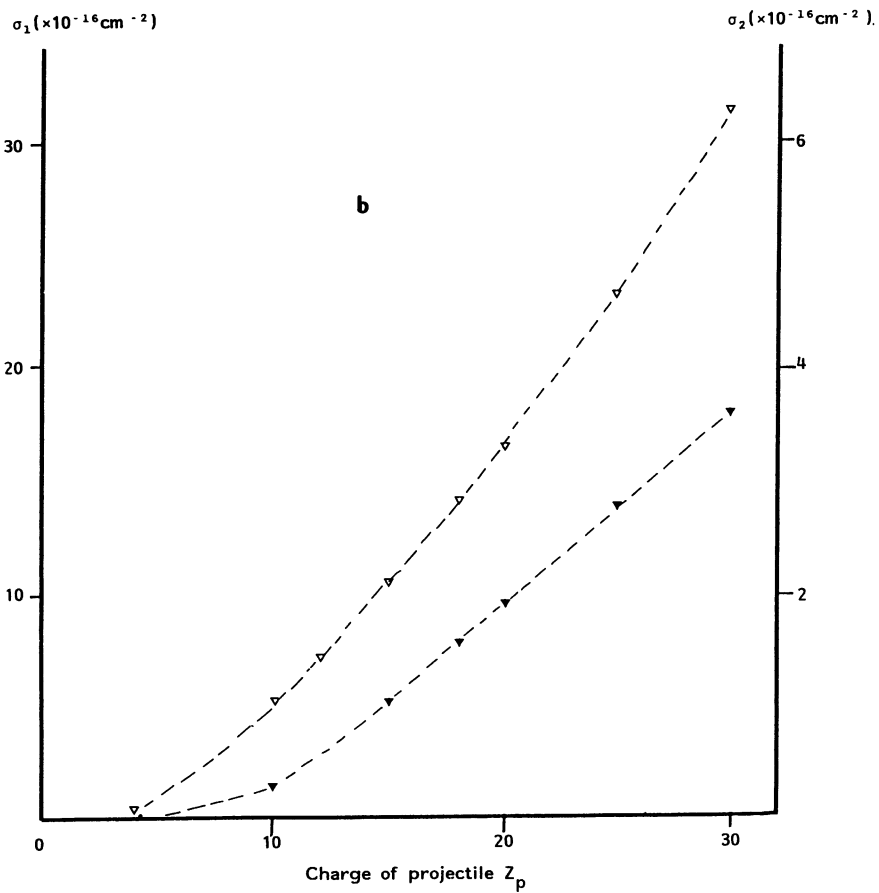
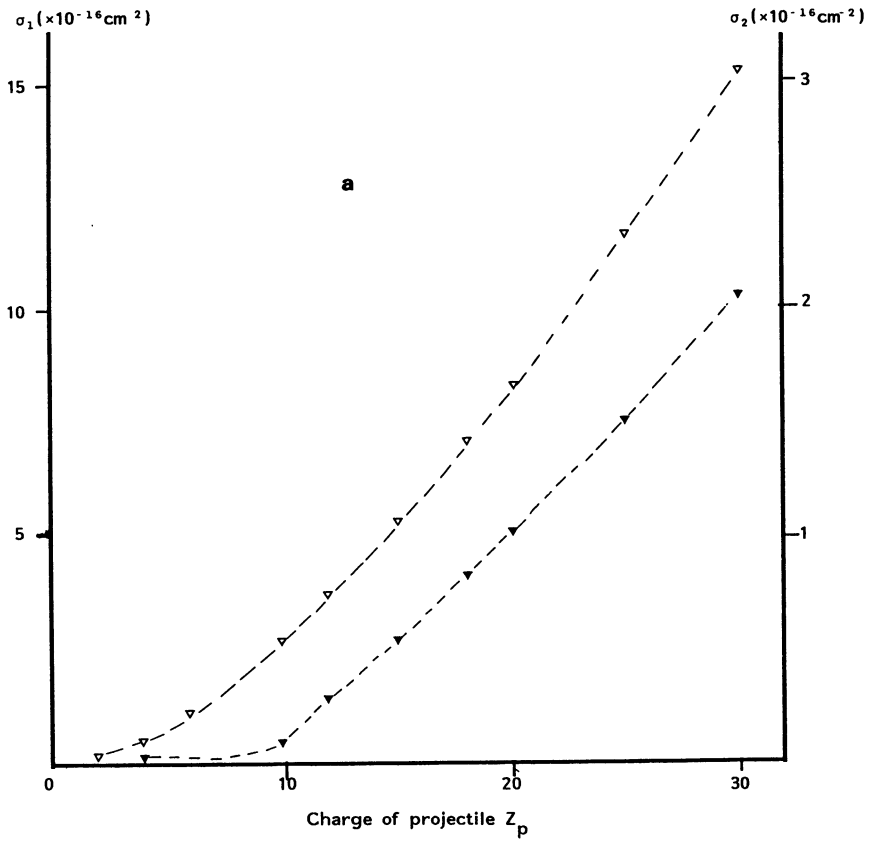


Fig. 6. — Total multiple ionization cross-sections  $\sigma_J(Z_p)$  of : 6a : neon, 6b : argon by collision with 35 MeV/a.m.u. ions of charge  $Z_p \leq 30$  : ( $\nabla$ )  $J = 1$ , ( $\blacktriangle$ )  $J = 2$ .

where  $c$  is the velocity of light,  $m_0 c^2$  is the average mass energy of a nucleon in a nucleus ( $m_0 c^2 \approx 931.48$  MeV) and  $T$  is the kinetic energy/a.m.u. of the projectile measured in the laboratory frame. For  $T = 35$  MeV/a.m.u., one has  $v = 36.40$  a.u. In figures 4a, b and c the probabilities  $P_i$  to eject an electron from the orbital  $i$  of helium, neon and argon respectively, are plotted as functions of the impact parameter  $\rho$  (see Eq. (13)).

The eventual contribution of the capture process to the stripping of the target is easily discarded. An insight of what this contribution could be, is given in figure 4d where the probability of capture  $P_c(\rho)$  by 35 MeV/a.m.u.  $\text{Kr}^{34+}$  in helium is drawn. It has been evaluated in the CDW approximation (Belkić *et al.* [17, 5]). The ion  $\text{Kr}^{34+}$  has a complete  $K$ -shell. Capture occurs onto shells beginning at the  $L$ -shell. The choice of this ion enables us to give an upper limit of the capture contribution. The probability of electron transfer  $P_c(\rho)$  appears to be much less than  $10^{-4} P_i(\rho)$  everywhere. A similar situation is expected with neon and argon targets. Indeed, figure 26 of the paper of Belkić *et al.* [17], gives a total cross-section  $\sigma_c^{\text{H}^+}$  for capture by 35 MeV protons from argon of the order of  $10^{-25}$  cm<sup>2</sup>. According to the OBK approximation (Brinkman and Kramers [18])  $\sigma_c^{\text{Kr}^{34+}}$  would be  $(34)^5 \sigma_c^{\text{H}^+}$ , i.e.,  $\sigma_c^{\text{Kr}^{34+}} \approx 4.5 \times 10^{-18}$  cm<sup>2</sup>. This number includes the capture onto the  $K$ -shell of the projectile, a process which cannot occur presently. Hence, a rough application of the  $n_f^{-3}$  law for the capture onto an orbital of principal quantum number  $n_f$  (see Belkić *et al.* [17]) shows that the above value of  $\sigma_c^{\text{Kr}^{34+}}$  must be affected by a factor 0.168 i.e. :

$$\sigma_c^{\text{Kr}^{34+}} \approx 7.6 \times 10^{-19} \text{ cm}^2.$$

This value is negligible compared to the single ionization total cross-section ; furthermore the range of impact parameters important for capture is so narrow that the contribution of charge transfer to multiple ionization is made even more negligible.

Hence, multiple ionization probabilities  $\mathcal{P}_J(\rho)$  plotted in figures 5a, b, c, d, e, f are obtained from equations (16) and (18).

The total multiple ionization cross-sections are displayed in table I. In the case of argon, the efficiency to make an  $\text{Ar}^{16+}$  ion is only  $10^{-4}$  that of making a singly ionized atom.

These calculations can be extended to other charge states of the projectile, using the fact that  $P_{n_i, \ell_i, |m_i|}(\rho)$  is proportional to  $Z_p^2$  (see Eq. (13)).

— For helium, it is not necessary to use again the binomial statistics ; indeed, total multiple ionization cross-sections  $\sigma_J$  ( $J = 1, 2$ ) are proportional to  $Z_p^{2J}$  because only one probability  $P_{1,0,0}$  occurs.

Table I. — Multiple ionization cross-section  $\sigma_J$  in units of cm<sup>2</sup> for 35 MeV/a.m.u.  $\text{Kr}^{30+}$  impinging on helium, neon and argon targets.

$J \backslash \sigma_J$	He	Ne	Ar
1	6.66 (− 16)	1.52 (− 15)	3.13 (− 15)
2	1.03 (− 16)	2.06 (− 16)	3.61 (− 16)
3		8.19 (− 17)	1.53 (− 16)
4		4.51 (− 17)	8.46 (− 17)
5		2.79 (− 17)	4.75 (− 17)
6		1.83 (− 17)	2.25 (− 17)
7		1.22 (− 17)	7.20 (− 18)
8		7.71 (− 18)	1.13 (− 18)
9		3.61 (− 18)	1.19 (− 18)
10		8.96 (− 19)	9.84 (− 19)
11			8.00 (− 19)
12			6.80 (− 19)
13			5.91 (− 19)
14			4.87 (− 19)
15			3.26 (− 19)
16			1.22 (− 19)

— For neon and argon, total multiple ionization cross-sections  $\sigma_J$  ( $J = 1, 2$ ) are plotted in figures 6a and b for  $Z_p \leq 30$ .

Typical ion productions per second in a 1 cm long gas cell that can be expected with 35 MeV/a.m.u.  $\text{Kr}^{30+}$  beams are indicated in table II where the intensity of the primary beam is that of GANIL, i.e.  $7 \times 10^{10}$  ions s<sup>−1</sup>. The pressure in the cell is set to  $10^{-3}$  mbar. The intensities of recoil ion beam have been calculated as indicated in appendix 1.

Then, the distribution functions of recoil ions of charge  $J$  versus the recoil energy, drawn in figures 8a, b, c and d for various targets and various charge states of the projectile are deduced from equations (39) and (43). One can see that these distributions  $\mathcal{D}_J(\varepsilon)$  are generally peaked for values of  $\varepsilon$  comparable to the mean energy of target atoms at room temperature.

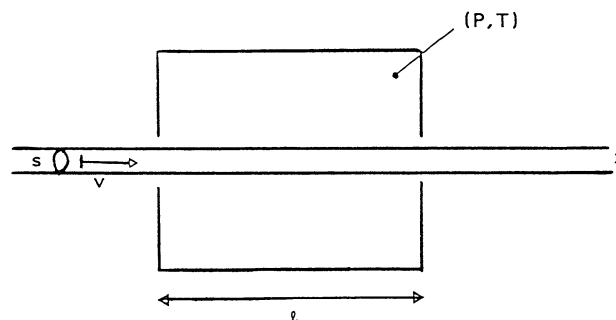


Fig. 7. — Gas cell and beam interaction diagram.

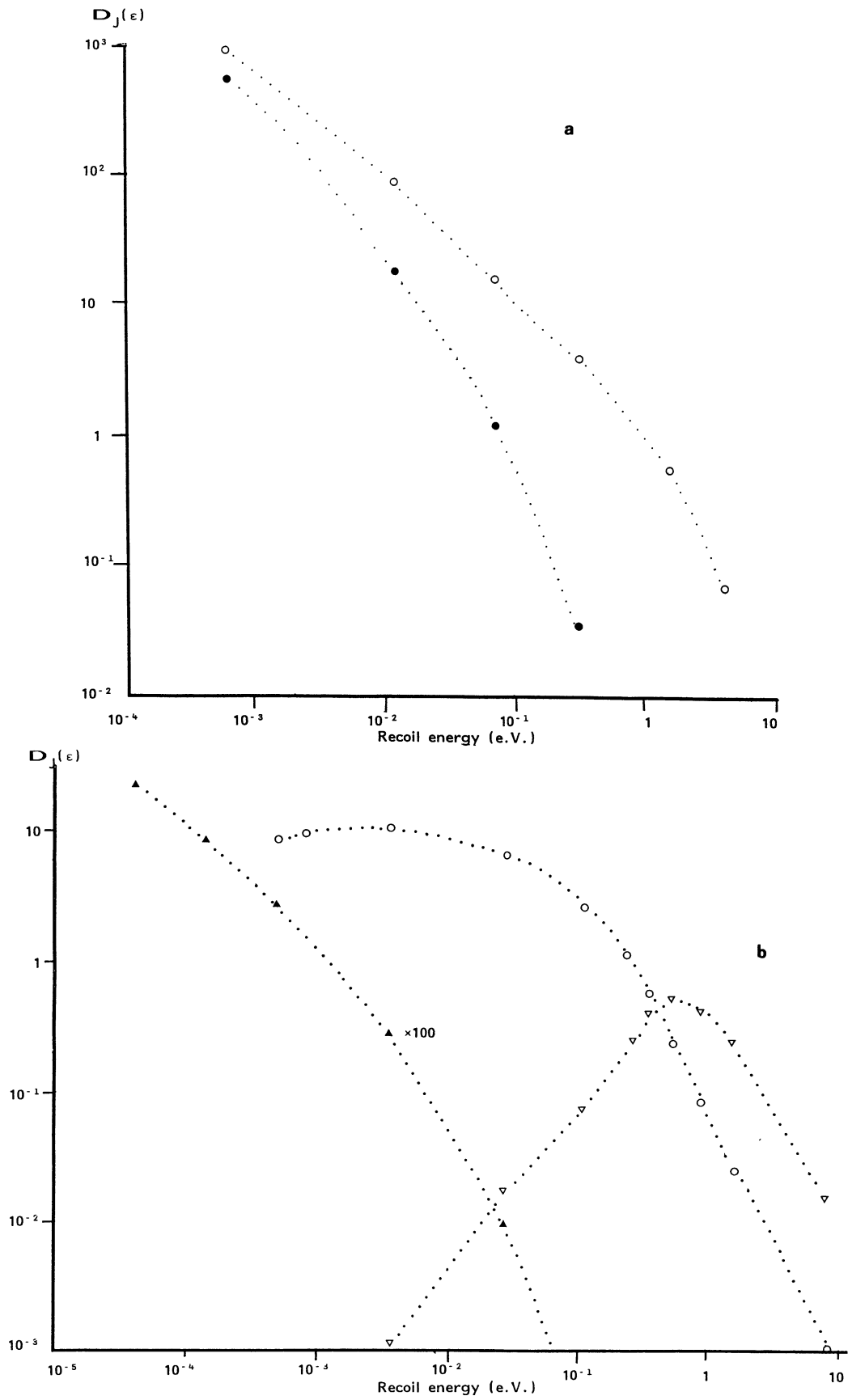


Fig. 8. — Distribution functions of recoil ions of charge  $J$ ,  $\mathcal{D}_J(\epsilon)$  obtained by collision with 35 MeV/a.m.u. ions of charge  $Z_p = 30$ : 8a: helium; 8b: neon; 8c: argon. 8a: ( $\bullet$ )  $J = 1$ , ( $\circ$ )  $J = 2$ ; 8b: ( $\blacktriangle$ )  $J = 3$ , ( $\circ$ )  $J = 7$ , ( $\nabla$ )  $J = 10$ ; 8c: ( $\nabla$ )  $J = 6$ , ( $\bullet$ )  $J = 8$ , ( $\circ$ )  $J = 11$ ; 8d:  $\mathcal{D}_{10}(\epsilon)$  in case of argon for various  $Z_p \leq 30$ , ( $\blacksquare$ )  $Z_p = 4$ , ( $\blacktriangledown$ )  $Z_p = 10$ , ( $\bullet$ )  $Z_p = 15$ , ( $\circ$ )  $Z_p = 25$ , ( $\square$ )  $Z_p = 30$ .

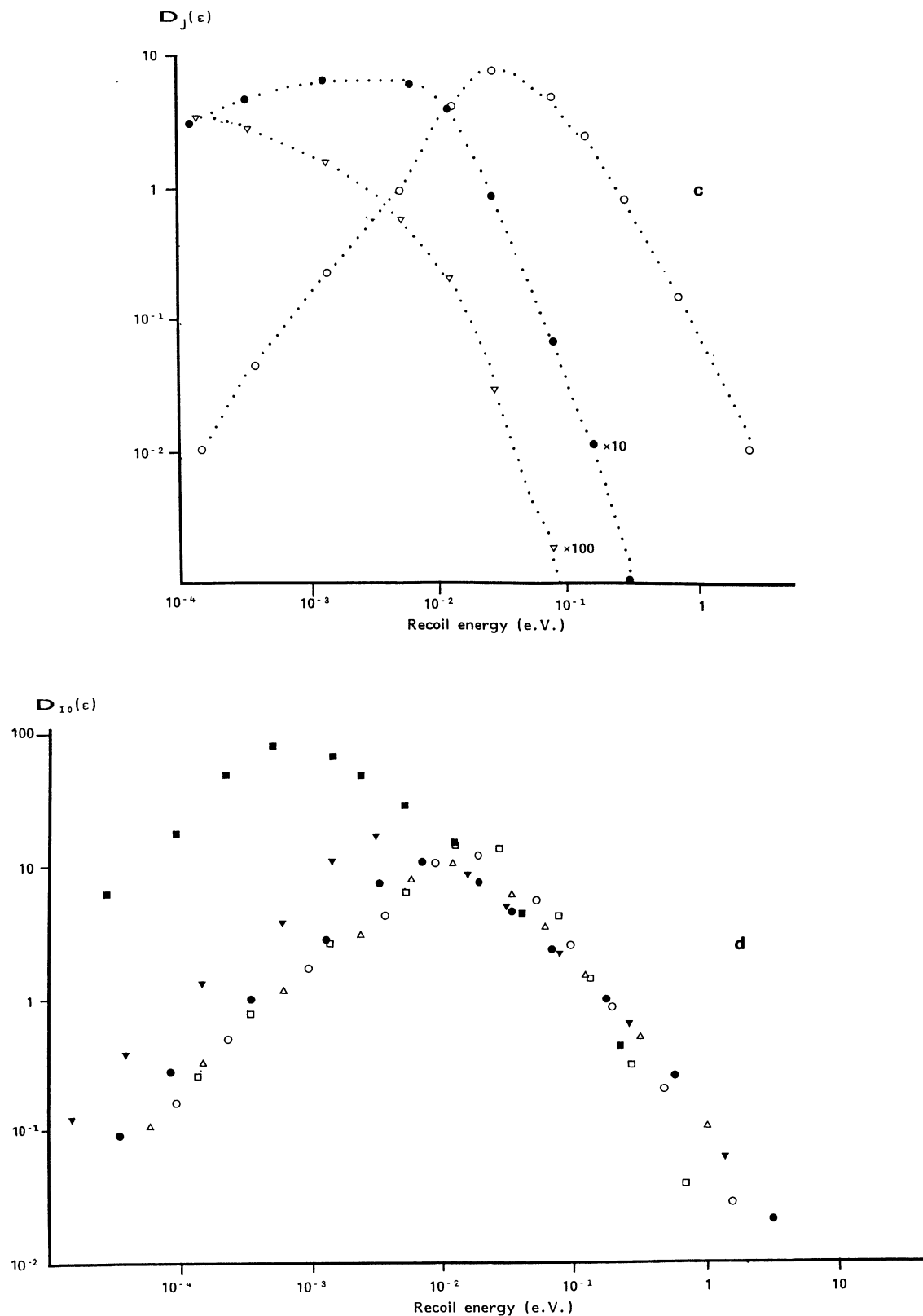


Fig. 8 (continued)

Table II. — Intensity  $N_J$ , in units of ions per second, of secondary beams of recoil ions of helium, neon and argon which can be expected using a primary beam of  $\text{Kr}^{30+}$  at 35 MeV/a.m.u. (see text).

$J \backslash N_J$	He	Ne	Ar
1	1.15 (9)	2.63 (9)	5.41 (9)
2	1.78 (8)	3.56 (8)	6.25 (8)
3		1.42 (8)	2.65 (8)
4		7.80 (8)	1.46 (8)
5		4.83 (7)	8.22 (7)
6		3.17 (7)	3.89 (7)
7		2.11 (7)	1.25 (7)
8		1.33 (7)	2.06 (6)
9		6.25 (6)	1.95 (6)
10		1.55 (6)	1.70 (6)
11			1.38 (6)
12			1.17 (6)
13			1.02 (6)
14			8.43 (5)
15			5.64 (5)
16			2.11 (5)

### Conclusion.

GANIL is a facility which delivers ion beams that provide us with ideal conditions to predict the characteristics of recoil ion beams by means of theoretical tools as simple as the PWBA and the IEM. It is worth noting that more sophisticated and much more costly methods must be employed to make similar predictions in different conditions [20].

### Acknowledgments.

We would like to thank A. Salin for useful discussions and suggestions.

### Appendix 1.

INTENSITY OF A SECONDARY BEAM  $N_2$  OF RECOIL IONS DEDUCED FROM THE MULTIPLE IONIZATION CROSS-SECTION  $\sigma$ . — Consider a cell of length  $\ell$ , containing a gaseous target at pressure  $P$ , on which a projectile beam of section  $s$ , impringes at the impact velocity  $v$ .

$n_p$  and  $n_T$  are the number of projectiles and targets per unit volume respectively and  $\sigma$  is the multiple ionization cross-section.

The number of recoil ions created per second is :

$$N_2 = n_p \times n_T \times v \times \sigma \times \ell \times s. \quad (1)$$

Using the ideal gas law, one obtains easily :

$$n_T = \frac{P}{RT} \mathcal{N} \quad (2)$$

where  $\mathcal{N}$  is the Avogadro number,  $T$  the cell temperature and  $R$  the ideal gas constant.

The intensity of the primary beam  $N_1$  is usually given in units of ions per second. Obviously, one has :

$$n_p = \frac{N_1}{v \cdot s}. \quad (3)$$

Equation (1) becomes :

$$N_2 = N_1 \frac{P}{RT} \mathcal{N} \sigma \ell. \quad (4)$$

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