Alignment of the $1s2p$ vacancy states of Ne doubly ionized by 700–2000-keV proton impact

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The angular distribution of KL_{23}-LLL_{23} Auger electrons emitted from the decay of $1s2p$ vacancy states of Ne doubly ionized by 700–2000-keV protons has been measured. From the measured anisotropy of the Auger lines the alignment of the double-vacancy states has been deduced. Our data compared with different theories indicate that the shake-off plays an important role in the double-ionization process at these energies.

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I. INTRODUCTION

In the ionization of atoms by a directed beam of charged particles, the ions with vacancies in subshells with total angular momentum $j > \frac{1}{2}$ can be aligned with respect to the beam direction [1]. The alignment, which characterizes the spatial anisotropy of the ionized state, manifests itself in the nonisotropic angular distribution and polarization of x-rays and Auger electrons emitted from the aligned ions.

The alignment of an atom ionized in its inner shell by particle impact has been extensively studied in the past two decades. There are several papers devoted to the investigation of the alignment in single ionization, a case in which the existing theories in general describe the experimental data (for references see, e.g., [2]).

The alignment of double-vacancy states has been much less investigated. The first studies of the alignment in double ionization were reported by Jamison *et al.* [3,4], who measured the polarization of KL^1 X-ray satellite lines ($K\alpha'$, $K\alpha_3$, and $K\alpha_4$) of Al emitted after simultaneous K and L_{23} shell ionization. From the point of view of the alignment of the resulting states, the KL_{23} ionization is the simplest case of double ionization, because the spherical symmetric $1s$ shell, which cannot be aligned, is ionized simultaneously with the spatially asymmetric $2p$ subshell, which can be aligned. Jamison and Richard [3] proposed a qualitative explanation for the observed large polarization values. The basic idea is that the ionization of the $2p$ subshell occurs practically at zero impact parameters due to the simultaneous $1s$ ionization. The charge distribution of the $M=0$ substate of the $2p$ state is concentrated along the beam axis, which corresponds to small impact parameters, whereas the $M=\pm 1$ substate charge distribution is distributed over large impact parameters. In the case of zero impact-parameter collisions, the ionization of the $M=0$ substate is therefore more probable than that of the $M=\pm 1$ substate, leading to a nonstatistical population of the magnetic substates, and consequently to the alignment of the doubly ionized atom. The paper of Jamison and Richard [3] induced two independent theoretical works within the framework of the first-order perturbation treatment [5,6]. These theories will be outlined in Sec. IV. Up to now, there have been only a few further experimental works on the alignment of doubly (KL) ionized atoms, measured by x-ray spectroscopy [7–11] and the experimental results are only in qualitative agreement with the above-mentioned theories. (See the analysis in a review paper by Cleff [8].)

The study of the alignment by the nonisotropic angular distribution of Auger electrons has some advantages compared to the x-ray spectroscopy. For low atomic number elements the Auger yield is larger than the x-ray yield. Furthermore, with the help of high-resolution electron spectroscopy, the lines corresponding to different final states can be well separated. Albiez *et al.* [12] used 1.5–50-keV electrons to doubly ionize Ne and measured the angular distributions of Auger electrons to study the $(1s2p)^{-1}$ alignment. They found practically no alignment in their case. The alignment of the Ne $(1s2p)^{-1}$ state in ion impact ionization has also been investigated by Ricz and co-workers [13–15]. In one of their works [15] the $2p$ subshell alignment was investigated by 5.5-MeV/amu projectiles. A strong dependence on the projectile charge was obtained. This result could hardly be described by first-order theories, because in these theories, the alignment is almost independent of the projectile charge [16,17]. Furthermore, in the same work Ricz *et al.* [15] got practically zero alignment for 5.5-MeV proton bombardment. This observation is in strong disagreement with first-order perturbation theories, although it is generally accepted that in this case the first-order perturbation theories satisfactorily describe the ionization process.

To clarify this unexpected discrepancy, we have carried out the present investigation measuring the projectile energy dependence of the alignment in the ionization of the K and L shells of Ne. The energy range of the proton projectiles was between 700 and 2000 keV. In Sec. II we describe the background of the experimental method for studying the alignment of the Ne KL_{23} subshell through the angular distribution of satellite Auger electrons. Sec-

tion III is devoted to the experimental apparatus and the data evaluation procedure. In Sec. IV the theoretical calculations within the framework of the two-step ionization model are described and the results of the measurement and the calculations are compared. In Sec. V the role of the electron shake-off process is discussed. It will be shown also in Sec. V that by considering two possible ways of double KL vacancy production (double Coulomb ionization and single ionization followed by electron shake-off) and calculating an effective alignment, we obtain better agreement with the experimental results.

II. METHOD OF INVESTIGATION

Our basic experimental goal is to study the alignment of Ne atoms ionized by proton impact on their $1s$ and $2p$ subshells. If one assumes that the ionization and the subsequent decay are independent processes, the alignment of an ionized atom can be obtained from the anisotropy of the angular distribution of x rays and Auger electrons resulting from the decay of the state under study (see, e.g., [18]). In the case of doubly ionized Ne one can use Auger electrons to measure the alignment since the decay is dominated by the Auger channel (98%), and with electron spectrometers one can obtain high enough energy resolution to separate the satellite lines of the double-vacancy states. The angular distribution of Auger electrons depends on the alignment of the initial state and on the coefficients of the angular anisotropy of the particular Auger transition [18]. Generally, the angular distribution can be expressed as

$$I(\theta)=I_0\left[1+\sum_{n=2,\text{even}} A_n P_n(\cos\theta)\right] . \quad (1)$$

I_0 is the total intensity ejected into a unit solid angle and θ is the angle between the direction of the bombarding beam and that of the ejected Auger electron. P_n is the nth order Legendre polynomial. The anisotropy parameter A_n can be written as

$$A_n=\alpha_n \mathcal{A}_{n0} . \quad (2)$$

In Eq. (2), $\mathcal{A}_{n0}$ are the alignment parameters of the initial state of the Auger decay and α_n are the angular anisotropy coefficients. The α_n decay parameters generally depend on the Auger transition amplitude. The $\mathcal{A}_{n0}$ alignment parameters can be expressed in terms of the statistical tensors (or state multipoles) of the state [18].

In our particular case of doubly ionized Ne atoms, the $1s2s^22p^5$ configuration has the ^1P and ^3P multiplets. (In the following we use the LS coupling scheme which is assumed to be a good approximation for low-Z atoms like Ne.) From the selection rules of the Auger process it follows that the above initial states can decay into the

$$1s^22p^5(^2P) ,$$

$$1s^22s2p^4(^2S,^2P,^2D,^4P) ,$$

and

$$1s^22s^22p^3(^2P,^2D)$$

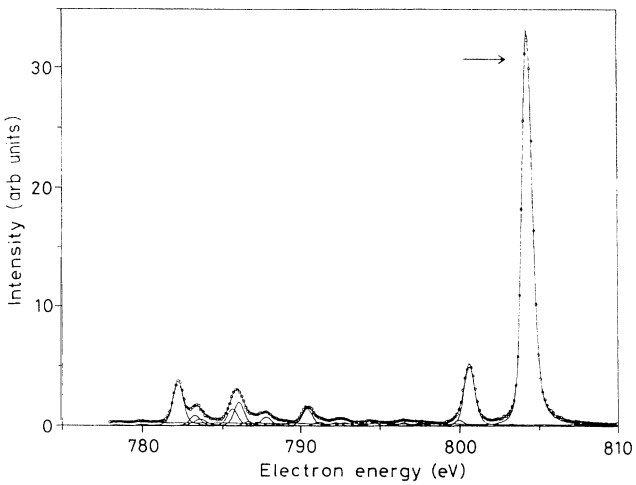

FIG. 1. Part of the Ne KL_{23}-LLL_{23} Auger spectrum. The spectrum was taken at 105° relative to the proton beam direction. The projectile energy was 1500 keV. The arrow points to the $1s2s^22p^6(^2S_{1/2})$-$1s^22s^22p^4(^1D_2)$ diagram line used for normalization. For lists of the identified Auger lines see, e.g., Refs. [12,20,21].

final states, resulting in 13 different KL_{23}-LLL_{23} Auger satellite lines in the spectrum [19].

Figures 1 and 2 show parts of our measured Ne KL_{23}-LLL_{23} Auger spectrum, recorded at a 105° angle with respect to the direction of the proton beam. The projectile energy was 1500 keV in this particular case. For a list of Auger lines of Ne in the measured energy region, see, e.g., [12,20,21]. These references contain fairly complete identifications of the Ne KL_{23}-LLL_{23} Auger lines. The most intense lines from the $1s2s^22p^5(^{1,3}P)$ initial states are those which lead to the $1s^22s^22p^3(^2P)$ and $1s^22s^22p^3(^2D)$ final states. For the $^{1,3}P$ initial states only one alignment parameter ($\mathcal{A}_{20}$) is nonzero; therefore, the angular distribution of the above lines is assumed to be

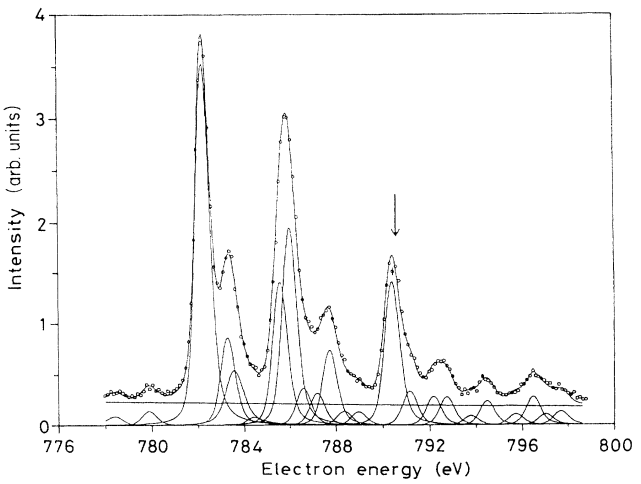

FIG. 2. Detailed view of the low-intensity KL_{23} satellite group region of Fig. 1. The arrow points to the $1s2s^22p^5(^1P)$-$1s^22s^22p^3(^2D)$ satellite line.

$$I(\theta)=I_0[1+\mathcal{A}_2P_2(\cos\theta)] . \quad (3)$$

We have investigated the angular distribution of the

$$1s2s^22p^5(^1P)\text{-}1s^22s^22p^3(^2D)$$

line to obtain the alignment parameter of the $1s2s^22p^5$ state. One has to note here that $\mathcal{A}_{20}$ should be the same for the two multiplets ^1P and ^3P if the ionization is spin independent, which is a generally accepted assumption. The

$$1s2s^22p^5(^1P)\text{-}1s^22s^22p^3(^2D)$$

line has been chosen because it is the most isolated among the satellite lines, and the α_2 parameter for this line in pure LS coupling has the exact value of $\sqrt{2}/2$ [12,15,22]. The α_2 value is also $\sqrt{2}/2$ for the

$$1s2s^22p^5(^3P)\text{-}1s^22s^22p^3(^2D)$$

line, but for the

$$1s2s^22p^5(^3P)\text{-}1s^22s^22p^3(^2P)$$

and

$$1s2s^22p^5(^1P)\text{-}1s^22s^22p^3(^2P)$$

lines, it depends on the Auger transition amplitude, i.e., on the type of wave functions used for its determination [12,22,23].

III. EXPERIMENTAL SETUP AND DATA EVALUATION

The measurements were performed using the ESA-21 triple pass electrostatic electron spectrometer [24]. The spectrometer made it possible to record the electron spectra at 13 different angles simultaneously, in the angular range of 0°–180° (relative to the projectile beam direction) with spacing of 15°. The electrons passing through the spectrometer were detected by channel electron multipliers. The Ne beam from an effusion target was crossed by the bombarding proton beam obtained from the 5-MV Van de Graaf accelerator of ATOMKI. The projectile energy range was between 700 and 2000 keV. The typical vacuum was about 4.0×10^{-5} mbar in the target chamber and 4.0×10^{-6} to 5.0×10^{-6} mbar in the spectrometer. The pressure in the buffer container before the jet inlet was 40 mbar. This produced a gas target dense enough to obtain good electron intensity while maintaining single-collision conditions.

The spectra have been analyzed using the EWA computer code developed by one of the authors (J.V.) [25]. We have shown earlier in Ref. [26] that the effect of the post-collision interaction (PCI) is not negligible even at these high projectile energies. In the fitting program we have used a five-parameter PCI line shape obtained from Refs. [27] and [28], as described in detail in Ref. [26]. A typical line shape used is shown in Fig. 3. In the fitting procedure the energy differences of the lines were fixed to the value given in Ref. [20]. The Lorentzian width (0.27 eV) and the asymmetry parameter for all the lines were also fixed and an energy-dependent Gaussian width was

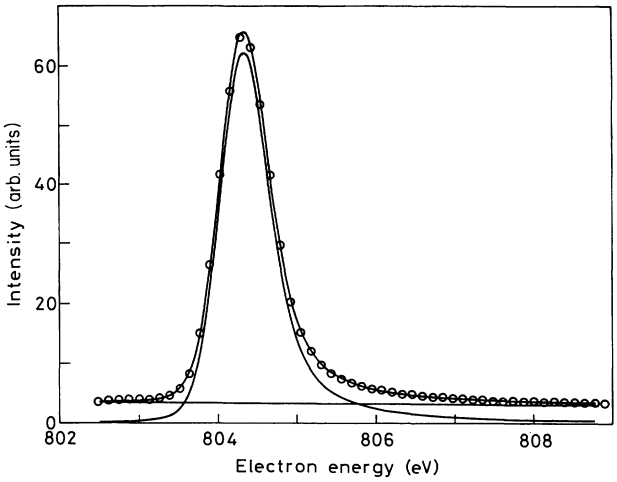

FIG. 3. An example for the post-collision-interaction distorted Auger line shape fitted to the Ne $1s2s^22p^6(^2S_{1/2})\text{-}1s^22s^22p^4(^1D_2)$ diagram line. (Projectile energy, 1500 keV; observation angle, 15° relative to the beam direction.) The line-shape asymmetry parameter is −0.46 (for a detailed explanation of the line shape used see, e.g., Ref. [26]).

used. The intensity (the area under the PCI shaped curve) of the Auger lines were obtained from the fits at different observation angles. In the next step they were normalized to the isotropic

$$1s2s^22p^6(^2S_{1/2})\text{-}1s^22s^22p^4(^1D_2)$$

diagram line. This normalization removed the possible detection efficiency differences between the different observation angles. Figure 4 shows a typical angular distribution after the normalization. To obtain the A_2 anisotropy parameter of the $1s2p$ vacancy state, the angular distribution of the normalized intensity of the

$$1s2s^22p^5(^1P)\text{-}1s^22s^22p^3(^2D)$$

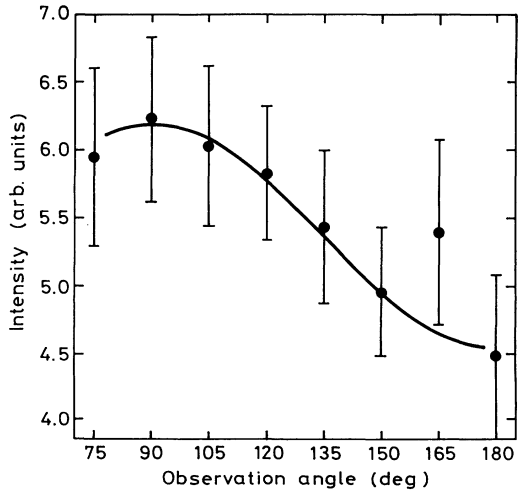

FIG. 4. The angular distribution of the $1s2s^22p^{5(1}P)\text{-}1s^22s^22p^3(^2D)$ satellite line at 700 keV projectile energy.

line was fitted by Eq. (3). To minimize the uncertainty of the fitting, only the spectra taken at backward angles (75°–180°) were used. The high continuous electron background in the forward direction made the fitting less accurate for the 0°–60° observation angles. In the evaluation of the alignment we have also omitted the 165° angular channel because we have found inconsistently high intensity values in this direction of observation and we have a strong indication that this behavior is due to an experimental mistake. From the A_2 asymmetry parameter the $\mathcal{A}_{20}$ alignment parameter was calculated by simply dividing A_2 by the value of the α_2 for the

$$1s2s^22p^5(^1P)\text{-}1s^22s^22p^3(^2D)$$

line ($\sqrt{2}/2$). In the calculation of the error bars of the alignment parameter, we have assumed that the errors have purely statistical origin. (See Table I.)

TABLE I. The experimental and theoretical alignment parameter values. The experimental errors are purely of statistical origin. HL, semiclassical approximation with hydrogenlike wave functions; HS, semiclassical approximation with Hartree-Slater wave functions; HS(corr). HS corrected for shake-off.

Energies (keV)	Experiment	HL	HS	HS(corr)
700	−0.29(11)	−0.571	−0.414	−0.294
1000	−0.23(7)	−0.560	−0.382	−0.243
1250	−0.24(8)	−0.553	−0.365	−0.212
1477	−0.20(5)	−0.548	−0.355	−0.190
1500	−0.20(1)	−0.547	−0.354	−0.188
1600	−0.19(13)	−0.546	−0.348	−0.182
2000	−0.09(14)	−0.541	−0.334	−0.154

IV. THEORETICAL DESCRIPTION OF THE SIMULTANEOUS K AND L_{23} COULOMB IONIZATION BY THE PROJECTILE

The alignment of the $2p$ state in simultaneous K and L_{23} Coulomb ionization has been calculated by Kocbach and Tauljberg [5] and by Merzbacher and Wu [6] within the framework of the semiclassical approximation. In their specific case they have investigated the proton and He impact on Al. The common basis of these calculations was the idea, primarily suggested by Jamison and Richard [3], that the alignment of the doubly KL_{23} ionized atom is practically the same as that of one which is singly ionized on its $2p$ shell by a zero impact-parameter collision. The reasons for this are the following: The first is that the ionization of the spherically symmetric $1s$ shell does not contribute to the alignment of the atom. The second reason is that the mean radius of the $1s$ shell is much smaller than that of the $2p$ shell and therefore the range of impact parameters is determined by the $1s$ ionization. The ionization probability of the $2p$ state is practically constant in this range of impact parameters, and can be approximated by its zero impact-parameter value.

Based on the above idea, Merzbacher and Wu have calculated the alignment of the $2p$ state using an oscillator model for the atom and assuming a straight-line trajectory for the projectile [6]. They have evaluated the $2p_m$ magnetic subshell ionization probability at zero impact-parameter ionization as a function of the projectile energy using first-order perturbation theory. The results obtained are in good agreement with the experimental results of Ref. [3] in the case of proton projectiles. Kocbach and Tauljberg performed similar calculations within the framework of the straight-line semiclassical approximation and independent electron model with hydrogenlike wave functions [5].

In the following we will briefly describe our calculations which are based essentially on the same model as developed by Kocbach and Tauljberg [5] except for the wave functions used. (See Table I.) In the present model we have assumed that (i) the ionization and relaxation takes place in two steps, (ii) the independent-particle model is valid for the ionization of the atom, (iii) the ionization can be described within the framework of the semiclassical approximation (SCA) with a straight-line trajectory of the projectile. The consequence of the second approximation is that the $P_m(b)$ double-ionization probability for a certain impact parameter b can be written as

$$P_m(b)=P_{1s}(b)P_{2p_m}(b) , \tag{4}$$

where $P_{1s}(b)$ and $P_{2p_m}(b)$ are probabilities of ionization of the $1s$ and $2p_m$ subshells, respectively [assuming that $P_{1s}(b)$ and $P_{2p_m}(b)\ll 1$]. Neglecting the spin-orbit interaction and using the LS coupling scheme, we can write the alignment of a state with total orbital momentum equal to 1 as [12]

$$\mathcal{A}_{20}=\sqrt{2}\frac{\sigma_1-\sigma_0}{2\sigma_1+\sigma_0} , \tag{5}$$

where σ_m is $(m=0,1)$

$$\sigma_m=2\pi\int P_{1s}(b)P_{2p_m}(b)b\,db . \tag{6}$$

Using the above arguments about the ranges of impact parameters, we find

$$\sigma_m\approx P_{2p_m}(b=0)\sigma_{1s} , \tag{7}$$

where $m=0,1$. In Eq. (7), $P_{2p_m}(b=0)$ is the probability of ionization of the $2p_m$ shell by zero impact-parameter collision and σ_{1s} is the cross section of ionization of the $1s$ shell. From Eqs. (5) and (7) it follows that the $\mathcal{A}_{20}$ alignment parameter for the $1s2p$ double ionization can be calculated as

$$\mathcal{A}_{20}=\sqrt{2}\frac{P_{2p_1}(b=0)-P_{2p_0}(b=0)}{2P_{2p_1}(b=0)+P_{2p_0}(b=0)} . \tag{8}$$

We have evaluated the $P_{2p_m}(b)$ single-ionization probability in the time-dependent perturbation theory (atomic units are used):

$$P_{2p_m}(b)=\int dE\left|i\int_0^\infty e^{i\omega t}\langle f|V(b,t)|i\rangle dt\right|^2 , \tag{9}$$

where $\omega=E_{\text{thr}}+E$, E is the ionized electron energy, E_{thr}

is the threshold energy, and the perturbing potential in the semiclassical approximation is

$$V(b,t)=-\frac{Z}{|\mathbf{r}-\mathbf{R}(b,t)|} . \quad (10)$$

If we assume straight-line trajectory for the projectile, then $\mathbf{R}(b,t)=\{0,b,vt\}$, where v is the velocity of the projectile. For the initial and the final states (denoted by i and f, respectively), we have used the Hartree-Slater wave functions, calculated with a Hermann-Skillman potential [29]. We have applied the frozen-core approximation, i.e., we used the same potential for the ionized atom as for the neutral one.

The computer code developed by one of the authors (N.M.K.) was tested using screened hydrogenlike wave functions and comparing the results with the calculations of Kocbach, Hansteen, and Gundersen [30]. The comparison gave an agreement within the limits of numerical errors ($\sim$2–3%). The results of the present calculation with Hartree-Slater wave functions are shown in Fig. 5 by a dashed line. The data presented by the dot-dashed line are the results obtained using hydrogenlike wave functions. In Fig. 5 the present experimental results (open circles) and that of Ref. [15] (solid circle) are also given. (See also Table I.)

We can conclude that (i) the results obtained with screened hydrogenlike wave functions and those obtained with Hartree-Slater wave functions are significantly different from each other and that (ii) both models describe the tendency of the experimental data, but the agreement is much closer with the Hartree-Slater wave functions. However, even this calculation does not describe the observations.

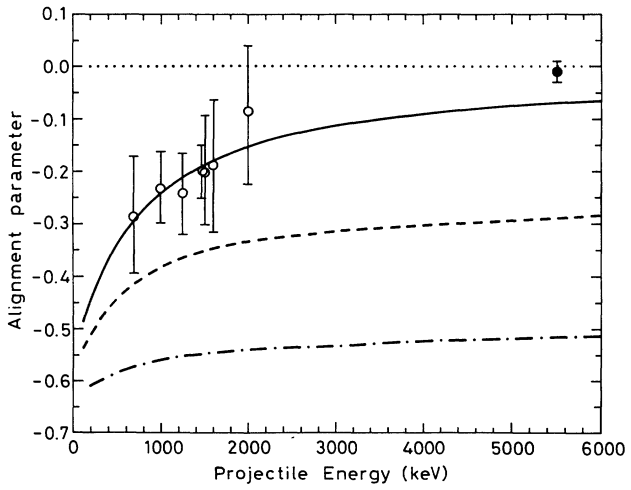

FIG. 5. The projectile energy dependence of the $\mathcal{A}_{20}$ alignment parameter of the Ne $(1s2p)^{-1}$ states. Dot-dashed line, the results of the calculations within the framework of the straight-line semiclassical approximation and independent electron model with hydrogenlike wave functions; dashed line, the same calculation as for the dotted line except that Hartree-Slater wave functions were used; solid line, the $\mathcal{A}_{20}^{\text{eff}}$ effective alignment parameter [shake-off corrected according to Eq. (13)] using the Hartree-Slater data for the P_{TS} and the 16.07% shake-off probability value of Ref. [32] for the P_{SO}. Dotted line, alignment due to electron shake-off ionization only. Open circles, experimental results of the present measurement; solid circle, experimental data of Ref. [15].

V. THE ROLE OF THE ELECTRON SHAKE-OFF

Besides the double Coulomb ionization of both the $1s$ and the $2p$ electrons, another mechanism which can produce KL_{23} double-hole configuration is the shake-off of the $2p$ electron after single $1s$ ionization. The shake-off process occurs when a primary ionization takes place in an inner shell and an outer-shell electron is ionized by the sudden change of the effective charge due to the loss of the inner-shell electron. Because the ionized $1s$ state cannot be aligned ($j<1$) and the shake-off process is assumed to produce no alignment, the alignment of the shake-off-produced $1s2p$ vacancy states will be zero.

Carlson and Nestor calculated the shake-off probabilities for different noble gases [32], and in the case of Ne obtained 16.07% for the probability of shake-off of a $2p$ electron after $1s$ ionization. Mehlhorn in Ref. [19] compared the satellite to diagram Auger transition probability ratio for Ne ionized by different projectiles (photon, electron, proton). He concluded that (i) the double-ionization satellites in photon bombardment are produced by shake-off and (ii) the similarity between the photon and the electron bombardment results is an indication that the shake-off is also important in the case of electron impact. The importance of the shake-off contribution to the electron-impact double ionization as well as the much smaller alignment in single ionization by electron impact as compared with proton impact might be the explanation of the result of Albiez *et al.* [12], who found practically zero Ne KL_{23} alignment in electron bombardment.

In the case of high-energy proton bombardment, Ricz *et al.* [15] have found that the alignment due to the double (K and L_{23}) ionization of neon is very small, contrary to the theoretical predictions of Refs. [6,5]. This observation can be an indication that the shake-off also plays a role in high-energy proton bombardment measurements. A further indication of the importance of the shake-off process can be given based on a work by McGuire [31], who studied theoretically the probability ratios of double to single ionization by high-energy protons and electrons.

According to McGuire [31], the shake-off transition amplitude (a_{so}) describing the single ionization of the first electron from the φ_1^i initial state into the φ_1^f final state, followed by a transition of the second electron from the φ_2^i initial state to the φ_2^f final state due to shake-off, is given by

$$a_{\text{so}}=\left[i\int_0^{\infty} e^{i(E_1^f-E_1^i)t}\langle\varphi_1^f|V|\varphi_1^i\rangle dt\right]\langle\varphi_2^f\varphi_2^i\rangle . \quad (11)$$

The alternative direct double Coulomb ionization was considered by McGuire [31] as a two-step second-order process, and its probability amplitude (a_{TS}) was given as:

$$a_{\mathrm{TS}}=\left[i\int_0^\infty e^{i(E_1^f-E_1^i)t}\langle\varphi_1^f|V|\varphi_1^i\rangle dt\right]\times\left[i\int_0^\infty e^{i(E_2^f-E_2^i)t}\langle\varphi_2^f|V|\varphi_2^i\rangle dt\right]. \quad (12)$$

In our particular case the first part of the above expressions describes the $1s$ ionization and the second part describes the $2p$ ionization. Let us consider the projectile energy dependence of the double (K and L_{23}) to single (K) ionization probability ratio (R). In the shake-off process, R is independent of the projectile energy, while in the two-step mechanism, R depends on it, because the $2p$ ionization cross section depends on the projectile energy.

To clarify the role of the shake-off in our measurements, we have obtained the ratio of intensities of the double (KL_{23}) hole Auger satellites to the intensities of the diagram (K) Auger lines. This ratio is assumed to be proportional to R. The projectile energy dependence of this ratio is shown in Fig. 6. From the above arguments it follows that the ratio R is proportional to the ionization probability of the $2p$ shell. In Fig. 6 our calculated probability for direct Coulomb ionization of a $2p$ electron during $1s$ ionization P_{TS} [$P_{2p}(b=0)$], the P_{SO} shake-off probability from Carlson and Nestor [32], and the sum of these two quantities are shown. Note that we have ignored the interference between the processes although they lead to the same final state. This is justified by the roughness of the models describing both processes, which we consider suitable for the first estimation. In more elaborate theory the interference between the shake-off and the two-step processes should be taken into account. In Fig. 6 it is difficult to distinguish whether the energy dependence of our measured satellites to diagram ratio

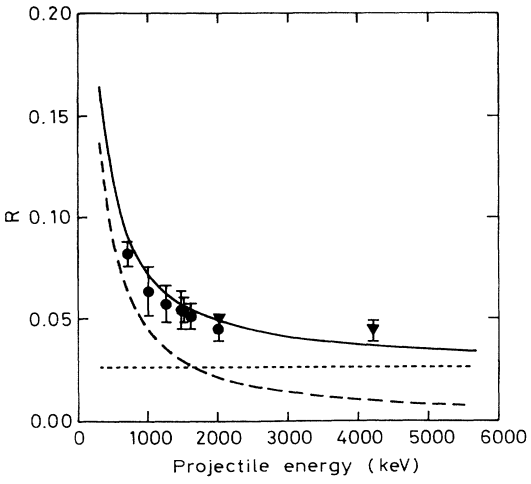

FIG. 6. Ratio R of the double ($1s2p$) to single ($1s$) ionization probabilities, as a function of the projectile energy. Dashed curves, $P_{2p}(b=0)$ $2p$ Coulomb ionization probability in zero impact-parameter collision, calculated with Hartree-Slater wave functions; dotted curve, probability of a $2p$ electron shake-off after $1s$ single ionization [32]; solid curve, sum of the preceding two quantities. Experimental data: circles, present measurement, KL_{23} satellite Auger intensity to K diagram Auger intensity ratio (R); solid triangles, data from Stolterfoht, Gabler, and Leithäuser [33].

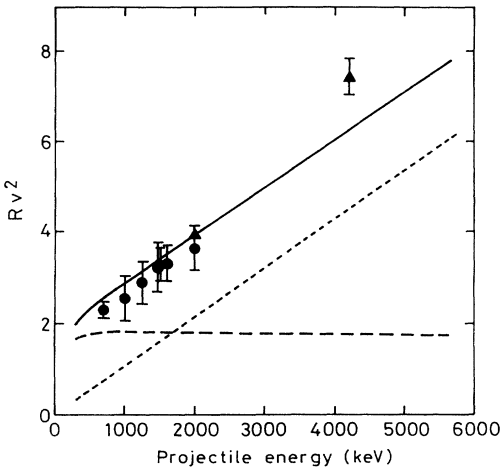

FIG. 7. The same as Fig. 6 except that all the quantities have been multiplied by the square of the velocity of the projectile in atomic units.

follows the dependence of the sum or the two-step ionization only. We have obtained Fig. 7 by multiplying all the data of Fig. 6 with the square of the velocity of the projectile in atomic units. In Figs. 7 and 6 we have also plotted the experimental ratio according to the *measurement* of Stolterfoht, Gabler, and Leithäuser [33]. In their measurement Stolterfoht, Gabler and Leithäuser obtained the satellite intensity to total intensity ratio. From this ratio one can determine R, assuming that the satellite intensity is dominated mainly by the KL_{23} satellite lines. It is seen from Fig. 7 that the energy dependence of the measured satellite to diagram ratio is close to that of the sum of the two-step and the shake-off ionization probabilities. This result gives evidence for the presence of the shake-off process in our measurements.

Tanis, DuBois, and Schlachter [34] and Berg *et al.* [35] in the case of a He target argued that for the two competing double-ionization processes, one has to distinguish at least three different projectile energy regions. The first region is where the two-step process is dominant, the second where the two-step and the shake-off processes are comparable, and the third where the shake-off is dominant over the two-step process. This argument can be applied for the double ionization in general. We can conclude from Figs. 6 and 7 that we made our measurements in the second region where one has to take into account both two-step and shake-off processes.

Based on the above arguments, one has to consider the presence of the shake-off process also in the calculation of the alignment in double (K and L_{23}) ionization. If the two mechanisms are producing different alignments, $\mathcal{A}_{20}^{\mathrm{TS}}$ and $\mathcal{A}_{20}^{\mathrm{SO}}$, then the resulting effective alignment which can be observed in the measurement is

$$\mathcal{A}_{20}^{\mathrm{eff}}=\frac{\sigma_{\mathrm{TS}}\mathcal{A}_{20}^{\mathrm{TS}}+\sigma_{\mathrm{SO}}\mathcal{A}_{20}^{\mathrm{SO}}}{\sigma_{\mathrm{TS}}+\sigma_{\mathrm{SO}}}=\frac{P_{\mathrm{TS}}\mathcal{A}_{20}^{\mathrm{TS}}}{P_{\mathrm{TS}}+P_{\mathrm{SO}}}, \quad (13)$$

because $\mathcal{A}_{20}^{\mathrm{SO}}=0$, $\sigma_{\mathrm{TS}}=\sigma_{1s}P_{\mathrm{TS}}$, and $\sigma_{\mathrm{SO}}=\sigma_{1s}P_{\mathrm{SO}}$. With

our computer code we have calculated $\mathcal{A}_{20}^{TS}$ and P_{TS}. For the P_{SO} we have used the value 0.1607 of Carlson and Nestor [32]. The results are shown in Fig. 5, where the solid curve shows the alignment values corrected for the shake-off process. As a result of our investigation, we can conclude that the shake-off plays an important role in the high-energy proton double $1s2p$ ionization.

VI. SUMMARY

We have measured the energy dependence of the alignment in simultaneous $1s$ and $2p$ ionization of Ne by protons, in the energy range 700–2000 keV. We have found that the absolute value of the alignment parameter increases as the energy of the projectile decreases, and that its sign is negative in the whole energy range. From the results of our SCA calculations we have seen that the results obtained with Hartree-Slater wave functions differ from the results obtained with hydrogenlike wave functions, and are closer to the experimental data. We have found indications that in addition to the direct Coulomb double ionization, we must consider another mechanism of double-vacancy production to explain our observations. Taking into account the shake-off process, and calculating an effective alignment, we have found much better agreement with our experimental results. In this way it became possible to explain the results of Ricz *et al.* [15] for high-energy proton collisions.

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