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ON THE CHARGE
OF THE RECOIL ATOM IN THE
 β -DECAY OF HE^6

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1. Introduction.

The β -decay of a nucleus will often be accompanied by excitation or ionization processes in the atomic core. Partly, the β -particle may collide with an atomic electron during its passage through the atom, partly the sudden change of the nuclear charge from Z to $Z \pm 1$ will cause a rearrangement of the electrons as a consequence of which the atom may be excited or ionized. The importance of this latter effect is evident in case of positron emission, but also in β^- -decay there is an appreciable probability for secondary ionization processes.

The charge of the recoil atom may thus exceed one unit and the effect is therefore of importance for many types of measurements of the energy and momentum spectrum of the recoil atoms. Considerable interest attaches to these measurements which may yield detailed information regarding the mechanism of β -decay (KOFOD-HANSEN 1951).

The ionization accompanying β -decay has been investigated theoretically by FEINBERG (1941) and MIGDAL (1941). FEINBERG has shown that the dominating effect is due to the "shaking" of the atomic core due to the change of nuclear charge. This result follows also from a simple qualitative consideration: The time taken for a relativistic β -particle to leave a shell of electrons bound by a charge Ze is $t \approx \hbar^2/Zme^2c$. If now this time is short compared with the period of revolution for these electrons $1/\nu \approx \hbar^3Z^2/me^4$, that is, if $\nu t \approx Z\alpha$ is small compared with unity, the change in the potential for the atomic electrons takes place so rapidly that the wave function after the β -process is almost equal to the original wave function (ψ). The relative change $\Delta\psi/\psi$ in the wave function during the emission of the β -electron will just be of the order νt . The calculation of the resulting excitation and ionization processes thus amounts to the expansion of the ground state

wave function of the original atom on the stationary state wave functions of the new atom.

In the case of H transforming into He, this expansion can readily be performed, and one finds an ionization probability of 2.5 %. For heavier atoms the calculation becomes rather complicated due to the complex character of the wave functions. Estimates based on approximate wave functions were obtained by MIGDAL, but they only apply to the ionization probability of the K, L and M electrons in heavy atoms.

We have attempted a more detailed calculation in the case of He transforming into Li. The β -decay of He^6 is of particular interest for the β -recoil studies (ALLEN 1949).

The ground state of He has angular momentum 0 and positive parity. The only states of Li II of this character, which lie below the ionization limit, are the states usually designated as $1s\ ns\ ^1S_0$. The notation refers to the approximation in which the wave equation separates in the coordinates of the two electrons. All other $0+$ states, such as $2s\ ns$ ($n \geq 2$) or $2p\ np$ etc., which would be bound states if the interaction between the electrons could be replaced by a central potential, lie in the continuum. They are therefore virtual states which, on account of the interaction, decay by auto-ionization (Auger effect).

The ionization probability may thus be calculated by subtracting from unity the probabilities for transition to the bound states ($1s\ ns$). Since this difference is relatively small it is necessary to use rather accurate wave functions for the bound states. Still, this method is advantageous because it is difficult to obtain adequate wave functions for the continuous spectrum and since calculations with continuum wave functions are very laborious.

Accurate wave functions for the ground state of He and Li II have been given by HYLLERÅS. In section 2, we derive wave functions for the $1s\ ns$ ($n \geq 2$) states of Li II for which sufficiently accurate expressions have not previously been given. The expansion coefficients are evaluated in section 3, and the results obtained are compared in section 4 with approximate direct estimates of the transition to free states, including the virtual states. In section 5 we shall consider various minor effects neglected in previous sections. A few remarks will also be made concerning the ionization by β -decay in heavier atoms.

2. Wave functions for bound states.

In order to calculate the probabilities for transitions to bound states of Li we need wave functions for the ground state of He (ψ_{He}) and for the $1s ns^1S_0$ states of Li II ($\psi_{1s ns}$).

Ground state of He.

For ψ_{He} we have used the very exact wave function

$$\psi_{\text{He}}^{(1)} = 1.388 e^{-1.818s} (1 + .3534u + .1282t^2 - .1007s + .0331s^2 - .0317u^2).$$

In calculations where such great accuracy is not necessary we have used the wave functions

$$\begin{aligned} \psi_{\text{He}}^{(2)} &= 1.34 e^{-1.82s} (1 + .290u + .132t^2) \quad \text{and} \\ \psi_{\text{He}}^{(3)} &= 1.68^3/\pi e^{-1.68s}. \end{aligned}$$

Here as in the following we have used atomic units (BETHE 1933).

The variables u , s , and t are defined as follows

$$\begin{aligned} s &= \left| \vec{r}_1 \right| + \left| \vec{r}_2 \right| \\ t &= \left| \vec{r}_1 \right| - \left| \vec{r}_2 \right| \\ u &= \left| \vec{r}_1 - \vec{r}_2 \right|, \end{aligned}$$

where \vec{r}_1 and \vec{r}_2 are the radii vectors for the two electrons. The wave functions $\psi_{\text{He}}^{(1)}$ and $\psi_{\text{He}}^{(2)}$ have, with the exception of the normalizing factor, been calculated by HYLLERÅS (1929), and are cited by BETHE in Handbuch der Physik (p. 358). In our quotation, they are normalized for the whole configuration space of the two electrons according to the formula

$$2 \pi^2 \int_0^\infty ds \int_0^s du \int_0^u (\psi)^2 u (s^2 - t^2) dt = 1.$$

Ground state of Li II.

For $\psi_{1s 1s}$ we have used the very exact wave function given by HYLLERÅS (1930 a)

$$\begin{aligned} \psi_{1s 1s} &= 6.219 e^{-3s} (1 + .11475s + .37594u + .18468t^2 + 0.1412s^2 \\ &\quad - .17939u^2 + .05666us - .05506t^2u + .02918u^3) \end{aligned}$$

which is normalized according to the above formula. BETHE'S quotation in Handbuch der Physik (p. 362) seems to lack a factor $1/2$ on the coordinate dependent terms in the paranthesis.

$1s\ 2s\ ^1S_0$ state of Li II.

A sufficiently good approximation for the wave function of this state appears not to have been given previously. We have carried out a calculation according to the scheme used by HYLLEÅS (1930 b) for the calculation of the $1s\ 2s$ state wave function of He. Since the interaction between the electrons is relatively less important for Li II than for He, we can expect to get a rather good approximation to the wave function by means of the variational function

$$\psi = e^{-ks} [(a_1 + a_2 s) \cosh \beta t + a_3 t \sinh \beta t],$$

where k , β , a_1 , a_2 and a_3 are varied.

Rather long and tedious calculations, quite analogous to those performed by HYLLEÅS, lead to the normalized wave function

$$\psi_{1s\ 2s} = e^{-2.04s} [(1.334s - 2.172) \cosh 1.000t + 1.114 \sinh 1.000t].$$

The ionization energy corresponding to this wave function is

$$I_{\text{theor}} = 117900\ \text{cm}^{-1}$$

while the energy found experimentally is

$$I_{\text{exp}} = 118700\ \text{cm}^{-1}$$

(extrapolated value given by WERNER 1927; cf. also MOORE 1949). The difference amounts to .7 %.

$1s\ 3s\ ^1S_0$ state of Li II.

For this state we have used the following Hartree approximation. The motion of the inner electron is considered to be unperturbed, and the resultant potential for the second electron is found. Then, using the experimentally known term value, we get the following differential equation for the radial wave function (ψ_1) of the outer s -electron,

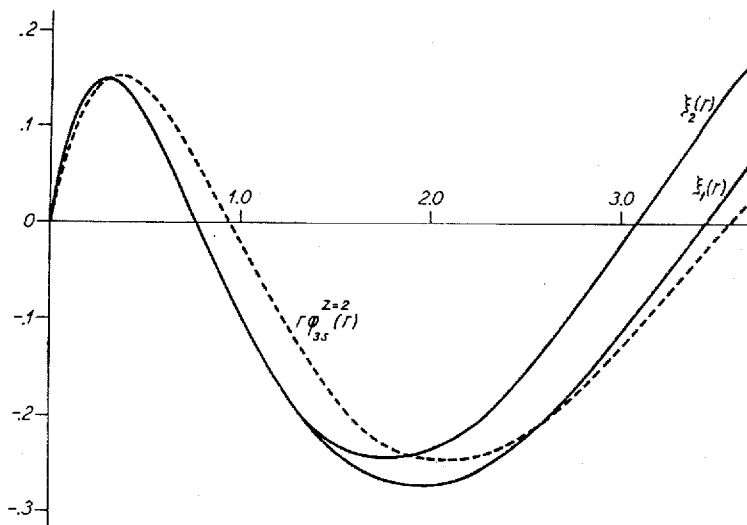


Fig. 1. Radial wave functions for the outer electron in the $1s3s$ state (ξ_1) and the $1s4s$ state (ξ_2) compared with the Coulomb wave function ($r\varphi_{3s}^{Z=2}(r)$) for the $3s$ state corresponding to complete screening ($Z = 2$).

$$d^2 \xi_1/dr^2 + [4/r + 2e^{-6r}(1/r + 3) - .46] \xi_1 = 0,$$

where $\xi_1 = r\psi_1$.

This differential equation is solved numerically for $r < 1.2$. For greater values of r , where the second term in the paranthesis is negligible, the solution which tends to 0 as $r \rightarrow \infty$ is a confluent hypergeometric function with the asymptotic expansion

$$\xi_1(r) = -e^{-y_1} y_1^{2.95} (1 - 2.874/y_1 + 1.257/y_1^2 + .0101/y_1^3 - .0007/y_1^4),$$

where $y_1 = .678r$. This solution turns out to fit rather well with the numerical solution at $r = 1.2$, as shown in fig. 1. The difference between logarithmic derivatives is about 10 per cent.

As a total normalized wave function for the $1s3s$ state we have used

$$\psi_{1s3s} = .659 (e^{-3r_2} \xi_1(r_1)/r_1 + e^{-3r_1} \xi_1(r_2)/r_2).$$

In order to obtain an estimate of the accuracy of this wave function we have calculated the scalar product to the two functions ψ_{1s2s} and ψ_{1s3s} which were derived by quite different methods. One finds

$$\iint \psi_{1s2s} \psi_{1s3s} d\tau_1 d\tau_2 = -.054.$$

1s 4s 1S_0 state of Li II.

For this state we use a similar treatment. The wave function for the outer electron is supposed to be a solution of the equation

$$d^2 \xi_2 / dr^2 + [4/r + 2e^{-3r}(1/r + 3) - .26] \xi_2 = 0,$$

where $\xi_2 = r\psi_2$.

For $r < 1.5$ the solution is almost identical to ξ_1 (cf. BETHE, loc. cit., p. 288). For $r > 1.5$ we use the asymptotic expansion

$$\xi_2(r) = -.83 e^{-y_2} y_2^{3.93} (1 - 5.74/y_2 + 8.09/y_2^2 - 2.41/y_2^3 - .021/y_2^4),$$

where $y_2 = .509r$. The factor .83 is chosen such as to make $\xi_2(r)$ coincide with $\xi_1(r)$ for r small (fig. 1).

The normalized wave function for the 1s 4s state is then

$$\psi_{1s4s} = .421 (e^{-3r_1} \xi_2(r_1)/r_1 + e^{-3r_2} \xi_2(r_2)/r_2).$$

The wave functions for the higher s states will, in nearly the whole region where $\psi_{\text{He}} \neq 0$, be similar to ψ_{1s4s} . The normalizing factor will be approximately proportional to $n_{\text{eff}}^{-3/2}$, where n_{eff} is the effective quantum number for the outer electron.

3. Expansion coefficients for transitions to bound states.

We denote the probability for transition to the $rs ns$ state by

$$P(r, n) = |a(r, n)|^2 = \left| \iiint \psi_{\text{He}} \psi_{rs ns} d\tau_1 d\tau_2 \right|^2$$

and from the wave functions given in the previous section we obtain the following results:

$$a(1.1) = \iint \psi_{\text{He}}^{(1)} \psi_{1s1s} d\tau_1 d\tau_2 = .8184$$

$$P(1.1) = .670$$

$$a(1.2) = \iint \psi_{\text{He}}^{(1)} \psi_{1s2s} d\tau_1 d\tau_2 = .408$$

$$P(1.2) = .166$$

$$a(1.3) = \iint \psi_{\text{He}}^{(2)} \psi_{1s3s} d\tau_1 d\tau_2 = .163$$

$$P(1.3) = .027$$

$$a(1.4) = \iint \psi_{\text{He}}^{(2)} \psi_{1s4s} d\tau_1 d\tau_2 = .088$$

$$P(1.4) = .008.$$

In view of the inaccuracy of ψ_{1s3s} and ψ_{1s4s} we have, in the last two cases, used the less accurate wave function $\psi_{\text{He}}^{(2)}$. Probably the most uncertain of the values quoted above are $a(1.2)$ and $a(1.3)$. To illustrate the strong dependence of these quantities on the wave functions, we quote two results for the expansion coefficients, obtained by means of less accurate helium wave functions

$$a^* (1.2) = \iint \psi_{\text{He}}^{(2)} \psi_{1s2s} d\tau_1 d\tau_2 = .399$$

$$P^* (1.2) = .159$$

$$a^* (1.3) = \iint \psi_{\text{He}}^{(3)} \psi_{1s3s} d\tau_1 d\tau_2 = .142$$

$$P^* (1.3) = .020.$$

It is to be emphasized that the difference between these results and the values given above provides no direct indication of the accuracy of the values since the essential sources of error probably are the lithium wave functions. The results exhibit a tendency of $P(1.n)$ ($n \geq 2$) to increase with increasing accuracy of the wave functions, a tendency which was found to be very characteristic of the whole calculation. It thus appears probable that the use of more accurate wave functions would lead to still higher values for $P(1.n)$.

According to section 2, we may assume the expansion coefficients of ψ_{He} on the higher s states to be proportional to $n_{\text{eff}}^{-3/2}$, that is

$$P(1.5) + P(1.6) + \dots =$$

$$(4 - .075)^3 P(1.4) [1/(5 - .075)^3 + 1/(6 - .075)^3 + \dots] = .012$$

since n_{eff} equals $n - .075$.

The total probability for transitions to bound states is found to be

$$P_{\text{bound}} = \sum_{n=1}^{\infty} P(1.n) = .883.$$

The uncertainty of P_{bound} has roughly been estimated on the basis of the scalar product of ψ_{1s2s} and ψ_{1s3s} (p. 7) to be of the order of one to two per cent.

According to the result for P_{bound} the probability for transitions to free states should be .117. However, in view of the indication that the use of more accurate wave functions would lead to a slightly larger value of P_{bound} , an indication which is supported by the estimates in the next section, we give as final estimate of the ionization probability

$$\underline{P_{\text{ion}} = (10.5 \pm 1.5) \text{ per cent.}}$$

This rather large value for P_{ion} may be of significance in recoil experiments. The corrections to be made to the results obtained by ALLEN (1949) in such experiments may easily be evaluated. They are found to be almost of the same order of magnitude as the difference between the curves for the different coupling cases. Still, with the present experimental uncertainties, the corrections hardly alter the conclusions which may be drawn from the measurements.

An experimental test of the value for P_{ion} may be possible by measurements of the motion of recoil atoms in combined electric and magnetic fields (KOFOED-HANSEN 1951). Measurements of the photons emitted from excited states of Li II might also give a valuable test of the theoretical calculations.

4. Transitions to free states.

In a discussion of free states we may use two different approaches.

1) The interaction between the electrons is represented by a screening of the nuclear potential; we thus write $1/r_{12} = V_1(r_1) + V_2(r_2) + W$ and neglect the potential W . In this approximation the states with energy greater than the ionization potential are of three different types: 1) States, where both electrons are free ($E_1 E_2$), 2) states, where one electron is bound the other free ($1sE, 2sE \dots$), 3) states, where both electrons are "bound" ($2s 2s, 2s 3s, \dots$). States of the last type are virtual; they decay by Auger effect (auto-ionization) into states of the second type.

The Auger transition is caused by the neglected potential W , and the decay time may be calculated by considering this potential as a perturbation (WENTZEL 1927).

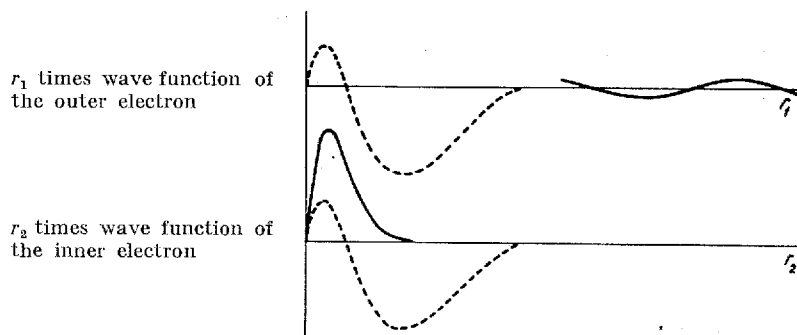


Fig. 2.

II) In a more rigorous treatment only states of the first two types in I) exist. For nearly all values of E we may in good approximation separate the wave equation in the two electrons as in I). For energy values close to the energy of the virtual states this approximation however breaks down and a sort of resonance phenomenon occurs. As illustrated in fig. 2, the wave function for the stationary states may be looked upon as a combination of a $1sE$ state with a $2s\ 2s$ state. This figure should be understood in the sense that for great distances of the outer electron the total wave function is the symmetrized product of the two full-drawn curves, that is of a Coulomb wave function for the continuous spectrum and a Coulomb wave function for the $1s$ state approximately. For smaller distances the amplitude of the total wave function grows up rapidly, and its dependence on both electron-coordinates is quite changed. For small values of r_1 and r_2 the wave function may be approximated by the $2s\ 2s$ wave function (dotted curves).

From the wave function described in this way, the decay time of the $2s\ 2s$ state may be calculated as the outgoing probability current.

An accurate computation of the expansion coefficients on the free states of Li II would be highly complicated. We shall attempt an approximate calculation in order to estimate the order of magnitude of the ionization probability and its distribution on the various types of free states.

For energies different from those of the virtual states the wave function for the free states may be approximated by the

product of $1s, 2s \dots$ Coulomb wave functions (with $Z = 3$) and Coulomb wave functions (with $Z = 2$) for the continuous spectrum. The total transition probability to these states is given by

$$P_{\text{cont}} = \int_0^{\infty} \{ |a(1.E)|^2 + |a(2.E)|^2 + \dots \} dE + \int_0^{\infty} \int_0^{\infty} |a(E_1.E_2)|^2 dE_1 dE_2.$$

Since the widths of the virtual states are small ($< 100 \text{ cm}^{-1}$) the contribution to P_{cont} from the energy regions of the virtual states is negligible.

In the neighbourhood of the energies of the virtual states, the amplitude of the wave functions for small r is much larger than the amplitude of simple Coulomb wave functions used above. An approximate estimate of the transition probability for this energy region may be obtained by using the normalized wave functions for the virtual states. If we write

$$P_{\text{virt}} = P(2.2) + P(2.3) + P(2.3) + \dots + P(3.3) + \dots$$

the sum

$$P_{\text{free}} = P_{\text{cont}} + P_{\text{virt}}$$

will give the total transition probability to free states.

The value of P_{cont} may be calculated by noting that

$$\begin{aligned} & \left| \int \varphi_{1s}^{z=2}(1) \int \psi_{\text{He}} \varphi_{\text{ns}}^{z=3}(2) d\tau_1 d\tau_2 \right|^2 + \left| \int \varphi_{2s}^{z=2}(1) \int \psi_{\text{He}} \varphi_{\text{ns}}^{z=3}(2) d\tau_2 d\tau_1 \right|^2 + \dots \\ & + \frac{1}{2} \int_0^{\infty} |a(n_1 E)|^2 dE = \left| \iint \varphi_{\text{ns}}^{z=3}(2) \psi_{\text{He}} d\tau_1 d\tau_2 \right|^2. \end{aligned}$$

$\varphi_{\text{ns}}^{z=m}(1)$ represents the normalized Coulomb wave function for electron 1 in the ns state with $Z = m$. The factor $1/2$ comes from the symmetrization.

In view of the approximate character of the free state wave functions used, we have calculated the transition probability by using $\psi_{\text{He}} = \psi_{\text{He}}^{(3)}$ and found

$$P_{\text{cont}} = .015.$$

The contribution to this result from the $E_1 E_2$ states is negligible ($< .001$).

The evaluation of P_{virt} can only be made with rather great uncertainty. Several authors have derived approximate wave functions for virtual states of He I (WU 1934, WILSON 1935). For Li II apparently no calculations exist. Since, however, it has not been possible with the wave functions so far constructed to account adequately for the properties of virtual states in light atoms (WU 1944, 1950), we shall here only attempt order of magnitude estimates based on simple Coulomb wave functions.

If we assume for the wave function of the $2s 2s$ state

$$\psi_{2s 2s} = \varphi_{2s}^z(1) \varphi_{2s}^z(2)$$

the most appropriate value of Z is expected to lie in the interval $2.7 < Z < 3$. The corresponding limit for $P(2.2)$ is $.011 < P(2.2) < .03$. In the same approximation we get a maximum value for $P(2.3)$ of $.007$ and for $P(3.3)$ of $.0002$.

Altogether we find

$$P_{\text{virt}} \lesssim .04 \quad \text{and} \quad P_{\text{free}} \lesssim .06.$$

There is a considerable discrepancy between this estimate and the result $P_{\text{bound}} = .883$ obtained in section 3, since the sum of P_{bound} and P_{free} should equal unity. This discrepancy may partly be due to the uncertainty in P_{bound} , but for the larger part must be ascribed to the very uncertain determination of P_{free} .

The estimates made in this section serve primarily to indicate the distribution on the free state transitions and to show the importance of transitions to virtual states. From the very small probability for double ionization ($E_1 E_2$ states) we may further conclude that the average charge on the lithium recoil is

$$\langle z \rangle = \underline{1.105 \pm .015},$$

provided we use the value for P_{ion} quoted on p. 10.

5. Discussion.

In the above treatment a number of minor effects have been neglected. Although, as we shall see, they are all negligible in case of He, some may become significant for heavier atoms.

I) As mentioned in section 1, the β -electron will have a chance, by direct interaction with the atomic electrons, to knock one of these out of the atom. The probability for this process (P_{dc}) as compared with the probability for ejection of this electron due to the effect of "shaking" (P_s), has been estimated by FEINBERG (1941).

For a relativistic β -particle he finds

$$P_{dc}/P_s \approx I/mc^2 \approx (Z\alpha)^2,$$

where I is the ionization energy of the electron and Z is the effective nuclear charge.

In the case of the He^s decay the contribution of direct collision thus amounts to

$$P_{dc} \approx .0001,$$

which obviously can be neglected. In heavier atoms P_{dc} and P_s may become of the same order of magnitude only for electrons in the inner shells. As P_s is small for these electrons (MIGDAL 1941) the contribution of P_{dc} to the total ionization probability will always be negligible. Since, however, the removal of one of the inner electrons will give rise to a cascade of Auger electrons (cf. section III) the direct collision may become important for that small fraction of the recoil atoms which are highly ionized.

II) Our results have to be corrected for the recoil motion of the nucleus, since the expansion of ψ_{He} on lithium wave functions must be carried out using wave functions referring to a lithium atom in motion.

The velocity (v) of the lithium recoil, corresponding to the maximum recoil energy ≈ 1500 eV, is of the order of $v_0/20$, where $v_0 = Z\alpha c$ (the velocity of the atomic electrons). In this case we would expect the correction for the transition probabilities to be of the order $(v/v_0)^2 \approx .003$.

We have also carried out a more exact calculation using lithium

wave functions corresponding to a moving atom and obtained substantially the same result.

The result shows that in general we may neglect the effect of the recoil motion when we have to do with free atoms. For atoms bound in molecules this effect will be of great importance, since the molecule may be disrupted.

III) In the calculations we have made the assumption that the lifetime of the virtual states against Auger effect (τ_{aug}) is small compared with the radiation lifetime (τ_{rad}). According to WENTZEL (1927), the ratio of the two lifetimes is of the order $\tau_{\text{aug}}/\tau_{\text{rad}} \approx 10^{-6} Z^4$ and thus very small for lithium. All states in which both electrons are excited therefore practically always lead to ionization.

According to the estimates in section 4 the Auger effect is actually responsible for the main part of the ionization. For heavier atoms we would expect the Auger effect to play a similar role. In earlier papers on the ionization of atoms by β -decay, the Auger effect has not been taken into account (FEINBERG 1941, MIGDAL 1941). MIGDAL thus calculates the ionization probability due to the "shaking" effect by expanding the wave functions for the original atom only on the wave functions for the continuous spectrum of the resulting atom.

If we take into account the Auger effect, the emission of an electron, from the K -shell say, would, as long as the condition $\tau_{\text{aug}}/\tau_{\text{rad}} < 1$ is fulfilled, give rise to a shower of Auger electrons, which would leave the atom several times ionized. (This would also be the case if the K -electron were only excited into some allowed bound state). As Z increases the Auger effect will be less probable, but only for the inner shells, where the screening is small.

For the most loosely bound electrons the situation is very similar to the case of $\text{He} \rightarrow \text{Li}$, and one has to take into account that only a small part of the ionization is due to direct transition to the continuous spectrum.

We have made some rough estimates on the average charge of heavier recoil atoms, using the results of MIGDAL and correcting them for the effects mentioned above. It appears that the average extra charge of the recoil from a β -process will increase with the

nuclear charge Z , so that for heavy atoms it may be quite considerable (of the order 0.5—1).

I wish to express my sincere thanks to Mr. AAGE BOHR for suggesting this problem and for many helpful discussions. My thanks are further due Professor NIELS BOHR for his continuous interest in my work.

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