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On low-energy nuclear electron capture

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Abstract

The atomic states formed in electron-capture beta decay (EC) have a finite width, so that decays can take place even with energies far from the resonance energies. Here, the lineshape deviates considerably from the normally assumed Breit-Wigner form. The lineshapes far from resonance are discussed and are shown to be important in calculations of total decay rates when the Q-value is low or the emitted atomic radiation is of low energy. The implications for neutrino mass searches employing electron capture decays are also discussed.

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1. Introduction

In the standard treatment of nuclear electron capture (see e.g. ref. [1]) the main role of the atom is to deliver an electron with a well defined energy; one disregards that the atom after the capture is in an excited state. The lifetime of the final state leads to a natural width of 1 – 20 eV, for the K shell up to 50 eV. The resulting energy spread is small compared to typical nuclear decay energies and is in general neglected. In this approximation the decay gives discrete neutrino energies, $E_\nu = Q - B_i$, where B_i is the atomic binding energy of a captured electron with quantum numbers i , and the corresponding transition rates are for allowed beta decay

$$\lambda_i = c\psi_i^2(Q - B_i)^2, \quad (1)$$

where the constant c contains the weak coupling constant and the nuclear matrix element, and ψ_i is the atomic wavefunction of the electron i evaluated at the nucleus. Experimentally one has of course always studied electron capture (EC) by means of the atomic decays, i.e. by measuring the x-rays, the Auger electrons or the complete atomic decay cascade following the capture.

The atom is, however, not a passive spectator to a nuclear decay. The incomplete overlap between the initial and final state atomic wavefunctions and effects of exchange will change the decay rates, as already discussed by Bahcall [2]. The aim of the present paper is to go even further from the description of electron capture as a "nucleus-only" event towards a description where the atom is included completely. Two obvious consequences of the electron capture are the change in nuclear charge and the disappearance of an inner shell electron. The adaption to the change in nuclear charge was treated by Bahcall, the atomic decays that follow EC will here be shown also to affect the total transition rate. The latter effects are normally small so that crude estimates can be given for when these atomic decays must be considered.

Even though not widely appreciated, a detailed theory of x-ray emission after EC exists: the theory of internal bremsstrahlung (IB) [3]. Photons that accompany EC are normally thought of as belonging to two types: at low energy x-rays and at high energy internal bremsstrahlung; but they cannot be so separated in a proper theoretical treatment. The x-rays lie at low energies in the p-IB spectrum (after the capture and the photon emission an electron is missing, in p-IB this electron comes from a p-state), and one can conversely regard the high energy IB as being simply the tails of the x-rays. The fact that the photon spectrum contain x-rays as resonances at low energy can, as pointed out by De Rújula [4], for nuclei with low Q -value be used to put limits on the electron neutrino mass. The limits obtained so far are an order of magnitude higher than the ones on the electron anti-neutrino mass.

The corresponding theory of electron emission after EC, i.e. internal ionization (II), is more complicated and was only recently [5] rephrased in terms of Auger and Coster-Kronig transitions. A theory of total absorption measurements, where all of

the atomic cascade after EC is detected, has also been given [6]. Here a Breit-Wigner shape, with the width Γ taken from experimental data, is ascribed to every atomic state, so that the intensity stemming from the state i at an excitation energy E is given by:

$$\lambda_i = c \frac{\Gamma_i}{2\pi} \frac{\psi_i^2}{(E - B_i)^2 + \frac{1}{4}\Gamma_i^2} (Q - E)^2 dE. \quad (2)$$

The total spectrum is obtained as a sum over all i (a similar expression is the basis of the calculations in ref. [5]). The resulting line shape is shown as the full line in Figure 1.

The expression (2) is a simple generalisation of equation (1) and is a first step away from the narrow line approximation. The inclusion of the neutrino phase space (the factor $(Q - E)^2$) makes the line shape deviate from a Breit-Wigner one; other energy dependent factors stemming from the atomic decay has to be added to equation (2) and will modify the shape even further. The basic observation of this paper is that not only will the intensity far from the resonance change, the total intensity – and therefore the total decay rate – will also change, in special cases up to several per cent.

Figure 1: The lineshapes in a total absorption experiment according to equation (2) [6], solid line, and equation (4), dashed line. The parameters used are $Q = 3$ keV, $B_i = 2$ keV, $E_i = 1$ keV, $\Gamma_i = 10$ eV, $P = 1$. The spectrum represented by the dashed line vanishes below E_i , this energy remains as atomic excitation energy after the first step in the atomic cascade. The total intensity according to equation (4) is only 0.6 % smaller than the total intensity according to equation (1). The intensity at the endpoint is, however, enhanced by a factor 2.

2. Qualitative arguments

It might be instructive to look in some detail at the atomic cascade (from now on called AC) following the electron capture. The first step, emission of an x-ray or an Auger or Coster-Kronig electron, is already treated as IB- or II-radiation, respectively. Virtually no attempt has been made theoretically to go beyond this first step (work has been done on double internal bremsstrahlung [7], but not with both photons being in the x-ray region). It is also an open question how many steps it would be possible to include, as the decaying atom in many experimental set-ups will interact with neighbouring atoms before the cascade is through. Assuming that the influence of the secondary steps is small the AC-spectrum can be obtained as the sum of all IB- and II-spectra, each spectrum being moved upward in energy by the amount remaining in the atom after the first step (this amount is being released later in the detector). All the endpoints will thus coincide; this greatly enhances the sensitivity for m_ν , which was one of the points of ref. [6].

Such a calculation has still to be performed, the main problem being the lack of reliable calculations of II. Some features of the AC-spectra can, nevertheless, be extracted from such a procedure. First, it is possible that interference effects might show up. They are known to be prominent in IB-spectra (for an illustrative example using ^{163}Ho , see ref. [8]), will also exist in II-spectra and could still be visible when all partial spectra has been added. The assumption of incoherence that underlies equation (2) might therefore not be true. Second, as the IB- and II-spectra explicitly contain energy dependent factors, coming from the matrix elements and the phase space factors for the photon and the electron, respectively, these "correction" factors will also appear in the AC-spectrum. They are different for each partial spectrum so that explicit expressions are complex.

These factors (to keep the nomenclature short they will be called "atomic phase space factors" in the following) are automatically included when the cascade is looked at in detail. They will be approximated here by including in the simpler equation (2) an energy-dependent factor, $a(E)$. Let E_i be the energy of the atom after emission of the first x-ray or Auger electron, so that the energy of the emitted radiation is $B_i - E_i$; $a(B_i - E_i)$ should then be one. The energy-dependence will here be assumed to be a power of $E - E_i$, this will in the next section be shown to be the case for the x-ray spectrum but is only a first approximation for Auger spectra. The correction factor is zero for $E < E_i$ (where the spectrum vanishes) and is for $E \geq E_i$ given by

$$a(E) = \left(\frac{E - E_i}{B_i - E_i} \right)^P, \quad (3)$$

so that the decay rates now read:

$$\lambda'_i = c \frac{\Gamma_i}{2\pi} \frac{\psi_i^2}{(E - B_i)^2 + \frac{1}{4}\Gamma_i^2} \left(\frac{E - E_i}{B_i - E_i} \right)^P (Q - E)^2 dE \quad (4)$$

for $E \geq E_i$ and $\lambda'_i = 0$ for $E < E_i$. The energy dependence is discussed in detail in the following two sections for x-ray and Auger electron emission, respectively. The effects of such a factor on neutrino mass searches and on EC decay rates are discussed in sections 5 and 6, respectively.

3. X-ray cascades

In discussing the energy dependence coming from x-rays we can start either from the theory of internal bremsstrahlung or from detailed accounts of x-ray emission. In the first approach the interference effects will also be included; but as the IB-spectra at low energy has been treated extensively [3, 4, 8] the discussion here will start instead from the work on x-ray cascades of Weisskopf and Wigner [9]. This gives the possibility of looking at the effect of the later steps in the atomic cascade. The factor $c\psi_i^2(Q - E)^2$ from the electron capture is then added by hand. To include also the interference effects the electron capture and the atomic decays should be treated simultaneously.

The starting point is equation (29a) of ref. [9] giving the intensity λ for a cascade from state A through state B to state C where the two photons emitted have energies k and k' respectively:

$$\lambda = c \frac{k}{E_{AB}} \frac{k'}{E_{BC}} \frac{\Gamma_{AB} dk}{(E_{AC} - k - k')^2 + \frac{1}{4}\Gamma_A^2} \frac{\Gamma_{BC} dk'}{(E_{BC} - k')^2 + \frac{1}{4}\Gamma_B^2} \quad (5)$$

Here c is a constant and the rest of the notation should be selfexplaining. By integrating over k' one will get the lineshape for the transition A to B. As is well known this will have a width of $\Gamma_A + \Gamma_B$. The energy of the following x-ray will, as pointed out by Weisskopf and Wigner, be statistically coupled to the energy of the first x-ray, so that the summed energy $k + k'$ will have a distribution with width Γ_A , i.e. a smaller width than the first step in the cascade taken alone. This is easily seen from the formula above by introducing the variable $E = k + k'$ in stead of k ; the two Breit-Wigners then decouple.

The "phase space" factors k/E_{AB} and k'/E_{BC} give the extra energy dependence coming from the x-ray transitions. The prescence of the factor k' means that the integration over k' will not give exactly Γ_{BC}/Γ_B as would be the case for a pure Breit-Wigner. Even more important: the value of the integral depends of the value of k (or equivalently, E) so that we after integrating k' out get an extra energy de-

pendence on top of the factor k . The resulting change is largest for small E and becomes negligible as E approaches Q . The behaviour at the spectral endpoint is therefore not affected, although the total intensity will change. The further complications from the later steps in the cascade will be neglected at the moment and the approximation (3) used with $P = 1$. This suffices for the discussion of the neutrino mass experiments; the uncertainty introduced in the total decay rate will be discussed in section 6.

4. The Auger processes

In discussing the Auger processes — “Auger” is here meant to include also Coster-Kronig transitions — we can similarly start either from the theory of internal ionization or from the atomic theory of Auger decays. Several approaches exist to the calculation of II-spectra [1], not all of them exhibiting the close connection that exists with Auger processes. Work on II has been concentrated on K-ionization in K-capture where no resonances are present in the spectrum, so the relationship with the Auger processes was only pointed out [5] a few years ago. The connection is seen most directly in the independent electron approach of ref. [10], where the matrix element for electron ejection have two components, one from shake-off due to the change in charge distribution in the capture and one from the interaction between the electrons. The last term contains the Auger processes.

The formulas for the KK-process [1] contain a matrix element and a phase space factor $kW = k(E + mc^2)$, W being the total energy of the outgoing electron and E being the kinetic energy. This is corrected for the influence of the potentials the outgoing electron feels (the penetration factors): The Coulomb potential gives the Fermi-factor which at low energies goes as $1/k$, so the variations from the phase space and the Fermi-factor cancel for non-relativistic electrons. For higher angular momenta the centrifugal barrier must be included as it is of the same order of magnitude as the atomic binding energies and therefore will be important at the lowest energies. The matrix elements themselves are also energy dependent. The rather complicated dependence [1] reduces for low electron energies ($k \ll \alpha Zmc$) to a constant as a function of E . In the detailed calculations strong deviations from this appear at energies above $8 \cdot (Z/50)^2$ keV.

More work has been done on Auger processes, but the finite width of the line has normally been neglected. As these processes involve two electrons — compared with one in x-ray transitions — they have turned out to be much more difficult to treat theoretically. The line shape of an Auger peak can be given analytically in the hydrogenic approximation, as done in Appendix A, but due to the complicated nature of the processes only general trends of these results should be trusted. As an illustration the spectrum has been calculated numerically for the M_1 - M_3N_7 transition in Dy using the formulas in the Appendix. The nucleus ^{163}Ho , which is the presently best candidate for m_ν searches by means of electron capture, decays mainly by M_1 - and N_1 -capture. The Coster-Kronig transition to M_3N_7 is one of the major de-

cay modes [11] of the resulting M_1 -hole in Dy, so that this transition will give an appreciable contribution to the AC-spectrum of ^{163}Ho . Figure 2a shows the factors modifying the Breit-Wigner shape, the full line is the factor $(Q - E)^2$ and the dashed line the combination $a(E) \cdot (Q - E)^2$. The energy-dependence of $a(E)$ is seen to be mild, giving a reduction of close to a factor 2 at the endpoint.

Figure 2: Energy dependences from phase spaces and matrix elements in the M_1 - M_3N_7 transition in Dy following M_1 -capture from ^{163}Ho . The Q -value has here been set to 2.68 keV corresponding to an endpoint in this spectrum at 1000 eV. Figure 2a shows the spectral shape with the Breit-Wigner divided out. The full line includes only effects of the neutrino phase space, the dashed line also the factors coming from the atomic transition. Figure 2b shows the spectrum including interference divided by the spectrum with no interference, the full line giving the effect in the direct matrix element and the dashed line the effect in the exchange matrix element. See the text for details. In all cases the spectra were normalized to one at the position of the Coster-Kronig peak, marked with an arrow.

The interference effects were serious for the corresponding x-ray transitions [8]. To get an estimate of their importance here a calculation was done including the

virtual L_1 -capture followed by a L_1 - M_3N_7 transition and the N_1 -capture followed by a virtual N_1 - M_3N_7 transition. Figure 2b shows the resulting change: the spectra including interference effects are here divided by the spectra with only the M_1 - M_3N_7 process included. The direct matrix element and the exchange matrix element were calculated separately and are shown as the full and dashed line, respectively. No interference dips are seen in the vicinity of the peak in contrast to the situation for x-rays. This can be understood as the amplitude for an Auger-transition is largest for a transition within a shell. The dominant term in the direct matrix element is thus the term corresponding to M_1 - M_3N_7 and the background from the other amplitudes is so small that the effects of interference only are seen far from the peak. The effects are larger for the exchange term, where the N_1 - M_3N_7 transition also is important. The present estimate does not include contributions from the continuum (where first an M_3 and an N_7 electron scatter and go to two virtual states in the continuum and one of these electrons then is captured by the nucleus). The continuum contributions are important for the x-rays and might also alter the situation here. We should, however, expect much less effects of interference on the major Auger — or rather Coster-Kronig — transitions.

The energy dependence suggested in equation (3) is clearly only a first approximation here. As the general variation in the example is slightly decreasing with energy, the power $P = -1/2$ will be used later.

5. Effects of the altered shape

The scaling factor in equation (3) is valid for one channel only and will for a level with many decay channels be more complicated. In the following the energy dependence of the strongest decay channel is used as an approximation. The effect of such a scaling factor is shown in Figure 1 as the dashed curve. The phase space factors — both the one of the atomic radiation and the factor $(Q-E)^2$ from the neutrino phase space — make the lineshape for the atomic transitions deviate from the standard Breit-Wigner one. (Which is why one is sensitive to neutrino masses. Up to now m_ν has been taken to be zero, to include it, replace the $E_\nu^2 = (Q-E)^2$ in the neutrino phase space with $p_\nu c E_\nu$.) For normal x-ray emission these deviations are hardly measurable [12]. The deviations can, however, become large for Coster-Kronig transitions in the outer shells, where the width of the atomic level no longer is negligible compared to the energy of the emitted electron. As a somewhat extreme example one can also cite s-IB. The atomic transition is here a spin-flip inside the s-shell with emission of an M1-photon. The factor k from the photon here makes the "main" peak (at zero energy!) vanish, only the positive energy "tail" is visible at all with the shape being determined exclusively by the phase space factors.

At the endpoint the most important factor is of course the neutrino phase space, which makes the spectrum go to zero. The effect of the atomic phase space factors is mainly to change the absolute intensity. The signal of a massive neutrino is therefore still in the first approximation given by the form $c \cdot (Q-E)[(Q-E)^2 - m_\nu^2]^{1/2}$, where

c is a constant. The rate at the endpoint and thus the feasibility of an experiment is, however, affected by the atomic phase space factors. In x-ray spectra the rate (for a given Q-value) is increased due to the factor k, in Auger spectra the rate will rather decrease although, as argued in the previous section, no simple general result can be written down. The estimates of the rates from II-spectra of ^{163}Ho given in ref. [5] is therefore probably too high and should be lowered by a factor about 2 giving a "fraction of goodies" (to keep the terminology of ref. [3-5]) of $5 \cdot 10^{-11}$ for $Q \approx 2.6$ keV and $m_\nu = 30$ eV. The rates in the AC-spectra will also change. The major atomic transitions are included here – in IB and II one is normally only sensitive to the transitions of highest energy, which in general are the weakest –, these tend for Q-values below B_K , which all the candidates for m_ν -searches have, to be low-energy Coster-Kronig transitions, so a total decrease in the rate at the endpoint should be expected. The simple estimates above would yield a reduction of a factor 2 compared to ref. [6], e.g. a "fraction of goodies" of $3 \cdot 10^{-8}$ for $Q \approx 2.6$ keV and $m_\nu = 30$ eV.

6. Electron capture decay rates

6.1 General results

With a line of Breit-Wigner shape the integrated intensity is the same as given in equation (1). This no longer holds when the neutrino and atomic phase space factors are included as in equation (4). The tails of the line are weighted differently and the total decay rate will change. Only when the width of the atomic excited state created in the electron capture is small, can one forget that this "final state" is not stable. In decays to broad levels the subsequent decay of these levels must be included.

With the "Ansatz" (3) for the energy dependence of the atomic factors the change of rate relative to the rate when a pure Breit-Wigner shape is assumed is:

$$R_P = \int_{E_i}^Q \frac{(Q-E)^2}{(E-B_i)^2 + \frac{1}{4}\Gamma_i^2} \left(\frac{E-E_i}{B_i-E_i} \right)^P dE \left[\int_{-\infty}^{+\infty} \frac{(Q-B_i)^2}{(E-B_i)^2 + \frac{1}{4}\Gamma_i^2} dE \right]^{-1}. \quad (6)$$

Introducing the dimensionless quantities $q = 2(Q-B_i)/\Gamma_i$ and $b = 2(B_i-E_i)/\Gamma_i$ this can be rewritten:

$$R_P = \frac{1}{\pi} \int_{-b}^q \frac{1}{1+x^2} \left(\frac{q-x}{q} \right)^2 \left(\frac{x+b}{b} \right)^P dx. \quad (7)$$

Three values of P will be considered here. $P = 0$ to show the effects of the neutrino phase space alone, $P = 1$ as is appropriate for IB-spectra and $P = -1/2$ as an esti-

mate of the trend in II-spectra. The two first cases can be solved analytically and give:

$$\begin{aligned} R_0 &= \frac{1}{\pi q^2} \left[q + b + (q^2 - 1)(\tan^{-1} q + \tan^{-1} b) - q \ln \frac{1 + q^2}{1 + b^2} \right], \\ R_1 &= \frac{1}{\pi b q^2} \left[\frac{1}{2} b^2 - \frac{3}{2} q^2 - b q + \frac{1}{2} (q^2 - 2 b q - 1) \ln \frac{1 + q^2}{1 + b^2} + (b q^2 + 2 q - b)(\tan^{-1} q + \tan^{-1} b) \right]. \end{aligned} \quad (8)$$

For normal decays where $q \gg 1$ and $q \gg b$ this reduces to

$$\begin{aligned} R_0 &= \frac{1}{2} + \frac{1}{\pi} \tan^{-1} b, \\ R_1 &= \frac{1}{2} + \frac{1}{\pi} \tan^{-1} b + \frac{1}{2\pi b} \left(\ln \frac{q^2}{1 + b^2} - 3 \right). \end{aligned} \quad (9)$$

Even with a large Q and with $P = 0$ we will get changes on the level of 1 % as long as b is small. The cause is seen from equations (6)-(9) to be the "cutoff" of the integration below the resonance at b . Going to $P = 1$ the effects get even larger for large Q . The values of R_P are given as a contour plot in Figure 3 for the three values of P , the variation being traced as a function of b and q . In the case of $P = -1/2$ no appreciable effect is found for $q \geq 10^3$. As the true energy dependence of Coster-Kronig transitions is only approximately given by using $P = -1/2$ the limit of $\approx 10^{-3}$ from Figure 3a is not exact. However, for high q the effects for Coster-Kronig transitions are most likely less than for x-ray transitions. Even with this quite different behaviour for photons and electrons we can in general expect changes on the percent level in the decay rates independent of the Q -value when low-energy atomic transitions are involved. Note that R_P as expected goes to one in the limit of narrow levels, i.e. for b and q large.

6.2 Remarks on applicability

As shown in section 3 the later steps in the cascade will also affect the total decay rate, the point being that when a small total energy is given to the atom also later steps in the cascade will have a limited "energy window" so that the integration over these steps again is cut off. Only the atomic phase space factors enter here so that the resulting change will be smaller than that of equation (7). To get the order of magnitude of the change the simple model of equation (5) has been used with $\Gamma_B = \Gamma_A/5$ and $E_{BC} = (5/27) \cdot E_{AB}$ (appropriate for a K_α x-ray followed by an L x-ray). The change brought about by the second step in the cascade was here independent of q and gave a decrease in $R_1 - 1$ (Figure 3c) of 3 - 4 % for $b = 10$ and 0.3 - 0.4 % for $b = 100$, vanishing for higher b . The inevitable conclusion is that for both x-rays and Auger processes detailed atomic calculations must be performed

Figure 3: Contour plot of $R_p - 1$ in % for the values $P = -1/2, 0$ and 1 in Figure 3a, 3b and 3c, respectively. The ordinates are $q = 2(Q - B)/\Gamma$ and $b = 2(B - E)/\Gamma$. Typical values for b are $10^3 - 10^4$ for K x-rays and $\leq 10^2$ for M Coster-Kronig transitions. X-ray transitions are represented by $P = 1$, while Auger transitions will be in the range $-1/2$ to 0 . The cross in Figure 3c represents K capture in ^{139}Ce , while the crosses in Figure 3a and 3b represent (major Coster-Kronig transitions following) M and N capture in ^{163}Ho , the leftmost cross corresponding to M capture.

in order to get accurate values of the change in decay rate. Only the order of magnitudes obtained here can be used to estimate when such a calculation is needed.

Interference effects were not included in equations (6)-(9). As argued in section 4 they will be most important for weak decay branches and can therefore be neglected in a first treatment.

The effect of the line shape is in most cases lower than the exchange and overlap effects [1, 2] but is of the order of the difference in the exchange correction calculated in different approaches and should therefore be included in the analysis of precision experiments. This is most important where outer shells contribute appreciably to the total decay rate and can affect determinations of Q -values, nuclear matrix elements or fluorescence yields. As a special application, note that the suggested [13] method of using relative capture rates from different shells to determine the neutrino mass is basically unsound, because a more detailed treatment of the peak shape is needed whenever the Q -value is small enough for the method to be applied. One can then gain in sensitivity by using the shape of the spectrum instead of just the integrated number of counts.

The corrections mentioned here are a part of the radiative corrections for electron capture decays. The radiative corrections have been studied extensively for beta decays [14] and contain apart from the internal bremsstrahlung effects from Feynman-graphs with virtual photons. This latter contribution is not included here. The "real photon" part is here expressed in terms of atomic decays and should therefore include all electromagnetic interactions in the final atom.

6.3 Examples

For normal decays q will be around 10^6 for light nuclei decreasing to between 10^3 and 10^4 for heavy nuclei. For the K-shell b will decrease from 10^4 to 10^3 at the same time (for light nuclei Auger decays dominate, for heavier x-rays, but the b values are almost the same), from Figure 3 one then sees that the change of decay rate for K-capture normally is less than 10^{-3} . As an example K-capture in ^{139}Ce is marked in Figure 3c.

In the higher shells, L, M etc., Auger and Coster-Kronig decays dominate and the change of decay rate can only be estimated roughly. The q values are here around 10^5 , while b is smaller than 10^3 (often less than 10^2) and will differ for the different Auger and Coster-Kronig branches. The two values of $P = -1/2, 0$ can be used to bracket the range of the results. For $P = -1/2$ there will be small effects for very large q , e.g. in the decay of ^{22}Na , where the capture rate will decrease a few tenths per cent. This is seen experimentally in the EC/β^+ ratio that is known [1] to an accuracy of $3 \cdot 10^{-3}$. For $P = 0$ there will be changes on the per cent level for low b values, e.g. in ^{37}Ar , ^{51}Cr , ^{55}Fe and ^{71}Ge . This is felt in the L/K capture ratios that are known to better than 1 %. The effect is in both cases on the level of the quoted uncertainty in the theoretical values of ref. [1].

For decays with low Q -value we can get q lower than 10^3 and larger effects can occur. The best example is the N/M ratio of ^{163}Ho that, as illustrated in Figure 3, will decrease by a few percent increasing Q as deduced from the N/M ratio (or the M/total ratio) by around 20 eV. The Q -value is here about 500 eV above the M_1 binding energy. Another example is given by ^{157}Tb where an excited state transition has a Q -value of [15] 8.0 ± 0.5 keV and the relevant binding energies are 8.4 keV

for the L_1 shell and 7.9 keV for L_2 . Throughout the allowed range for the Q-value major effects are expected for L-capture, e.g., even for a Q as low as 8.0 keV (400 eV below the L_1 -resonance) due to the finite width there will be as much capture from L_1 as from L_2 . However, the effect on the total decay rate is small, as M-capture dominates. In the case of $P = 0$ per cent changes also occur for the M/L ratio of ^{193}Pt and for the excited state transition of ^{81}Kr .

To sum up, changes larger than 1 % are only expected for L, M etc. capture, especially for low Q-values. If greater accuracy is needed even K capture can be affected.

7. Conclusion

The atom must be taken into account in accurate descriptions of nuclear electron capture. It was shown that when the atomic levels from which electrons are captured are broad (broad here meaning relative to the energy of the atomic radiation and not relative to the nuclear Q-value), one must include effects of the atomic decay cascade. In this case a nonnegligible number of decays will take place far from the mean energy of the levels. The rate of these decays is influenced by the phase space factors of the emitted neutrino and the subsequent atomic radiation and by the energy-dependence of the atomic matrix elements. Two implications were given. First, the rate at the endpoint (which determines the countrate in a neutrino mass experiment) is altered. The effect is already included in the theory of IB, where the rates are enhanced. Its inclusion for II- and AC-spectra seems on the other hand to give a decrease of intensity. Second, the total decay rates can change up to several per cent for Q-values close to atomic binding energies and will also be affected noticeably when the atomic radiation is of low energy; an estimate of the order of magnitude of the change was given.

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APPENDIX A

THE AUGER LINE SHAPE

In the standard treatments of Auger processes [16, 17] one "hides" all factors multiplying the matrix element by including them in the normalization of the wavefunction of the outgoing electron. The k -dependence is therefore given exclusively by the matrix elements that can be calculated from the hydrogenic wavefunctions of ref. [16]. The detailed atomic structure is not included in the hydrogenic approximation, so that only the general trends of the solutions can be trusted. Other approaches to the calculation of Auger processes can be found in ref. [18].

The notation follows that of ref. [16], the hole in state $(n'l')$ is filled by an electron from the state (nl) while an electron in state $(n'l')$ is emitted with momentum k and angular momentum l_A . The Auger-peak corresponds to a momentum κ of the outgoing electron. The remaining variables are $c_1 = 2Z''/(n'a\kappa)$, $c_2 = 2Z/(na\kappa)$, $c_3 = 2Z'/(n'a\kappa)$, $\eta = Z^*/k$ and ν , where the Z 's are effective charges, a is the Bohr radius and ν is the multipolarity of the interaction between the electrons. In ref. [16] only the case of $k = \kappa$ is treated. Introducing k explicitly and rewriting slightly, the matrix element for the Auger transition is in atomic units:

$$\begin{aligned} & \{(n''l'')|(nl)(n'l'), \nu, l_A\} \left[G(l_A, \eta) \left(\frac{k}{\kappa} \right)^{l_A + \frac{1}{2}} \right]^{-1} = \quad (A1) \\ & A_{n''l''} A_{n'l'} A_{nl} \sum_{s''=0}^{n''-l''-1} \sum_{s'=0}^{n'-l'-1} \sum_{s=0}^{n-l-1} B_{n''l''s''} B_{n'l's'} B_{nl_s} \times \\ & \left[\frac{(l'' + s'' + l + s + 2 + \nu)!}{\left(\frac{c_1 + c_2}{2} \right)^{l'' + s'' + l + s + 3 + \nu}} \frac{(l' + s' + l_A + 1 - \nu)!}{\left(\frac{c_2}{2} + i \frac{k}{\kappa} \right)^{l' + s' + l_A + 2 - \nu}} {}_3F_1 \left\{ l_A + 1 + i\eta, l' + s' + l_A + 2 - \nu; 2l_A + 2; \frac{2i}{\frac{c_2}{2} \frac{\kappa}{k} + i} \right\} \right. \\ & - (l'' + s'' + l + s + 2 + \nu)! \sum_{j=1}^{l'' + s'' + l + s + 3 + \nu} \frac{(l'' + s'' + l' + s' + l + s + l_A + 4 - j)!}{(l'' + s'' + l + s + 3 + \nu - j)!} \\ & \times \left(\frac{c_1 + c_2}{2} \right)^{-j} \left(\frac{c_1 + c_2 + c_3}{2} + i \frac{k}{\kappa} \right)^{j - l'' - s'' - l' - s' - l - s - l_A - 5} \\ & \times {}_2F_1 \left\{ l_A + 1 + i\eta, l'' + s'' + l' + s' + l + s + l_A + 5 - j; 2l_A + 2; \frac{2i}{\frac{c_1 + c_2 + c_3}{2} \frac{\kappa}{k} + i} \right\} \\ & + (l'' + s'' + l + s + 1 - \nu)! \sum_{j=1}^{l'' + s'' + l + s + 2 - \nu} \frac{(l'' + s'' + l' + s' + l + s + l_A + 4 - j)!}{(l'' + s'' + l + s + 2 - \nu - j)!} \\ & \times \left(\frac{c_1 + c_2}{2} \right)^{-j} \left(\frac{c_1 + c_2 + c_3}{2} + i \frac{k}{\kappa} \right)^{j - l'' - s'' - l' - s' - l - s - l_A - 5} \\ & \left. \times {}_2F_1 \left\{ l_A + 1 + i\eta, l'' + s'' + l' + s' + l + s + l_A + 5 - j; 2l_A + 2; \frac{2i}{\frac{c_1 + c_2 + c_3}{2} \frac{\kappa}{k} + i} \right\} \right] \end{aligned}$$

$$\begin{aligned}
 &= \sum_{s'=0}^{n'-l'-1} C_{s'} \frac{(l' + s' + l_A + 1 - \nu)!}{\left(\frac{c_A}{2} + i\frac{k}{\kappa}\right)^{l'+s'+l_A+2-\nu}} {}_2F_1\{l_A + 1 + i\eta, l' + s' + l_A + 2 - \nu; 2l_A + 2; \frac{2i}{\frac{c_A}{2} \frac{k}{\kappa} + i}\} \\
 &+ \sum_{m=-l''-l-3-\nu}^{n''-l''+n'-l'+n-l-4} D_m \frac{(l'' + l' + l + m + l_A + 4)!}{\left(\frac{c_1+c_2+c_A}{2} + i\frac{k}{\kappa}\right)^{l''+l'+l+m+l_A+5}} \\
 &\quad \times {}_2F_1\{l_A + 1 + i\eta, l'' + l' + l + m + l_A + 5; 2l_A + 2; \frac{2i}{\frac{c_1+c_2+c_A}{2} \frac{k}{\kappa} + i}\},
 \end{aligned}$$

where the constants are

$$\begin{aligned}
 C_{s'} &= A_{n''l''} A_{n'l'} A_{nl} \sum_{s''=0}^{n''-l''-1} \sum_{s=0}^{n-l-1} B_{n''l''s''} B_{n'l's'} B_{nls} \frac{(l'' + s'' + l + s + 2 + \nu)!}{\left(\frac{c_1+c_2}{2}\right)^{l''+s''+l+s+3+\nu}} \\
 D_m &= A_{n''l''} A_{n'l'} A_{nl} \sum_{s''=0}^{n''-l''-1} \sum_{s'=0}^{n'-l'-1} \sum_{s=0}^{n-l-1} B_{n''l''s''} B_{n'l's'} B_{nls} \times \\
 &\quad \left[(l'' + s'' + l + s + 1 - \nu)! \sum_{j=1}^{l''+s''+l+s+2-\nu} \frac{1}{(l'' + s'' + l + s + 2 - \nu - j)!} \left(\frac{c_1 + c_2}{2}\right)^{-j} \delta_{m,s''+s'+s-j} \right. \\
 &\quad \left. - (l'' + s'' + l + s + 2 + \nu)! \sum_{j=1}^{l''+s''+l+s+3+\nu} \frac{1}{(l'' + s'' + l + s + 3 + \nu - j)!} \left(\frac{c_1 + c_2}{2}\right)^{-j} \delta_{m,s''+s'+s-j} \right],
 \end{aligned} \tag{A2}$$

the A and B coefficients are given in ref. [16] and

$$G(l_A, \eta) = \frac{2^{l_A+1}}{(2l_A + 1)!} \exp\left(\frac{\pi}{2}\eta\right) |\Gamma(l_A + 1 + i\eta)|. \tag{A3}$$

Here the factor $G(l_A, \eta)(k/\kappa)^{l_A+\frac{1}{2}}$ varies slowly with energy. For small k the imaginary parts can be neglected in the denominators in (A1). Furthermore, by using the series expansion for the hypergeometric function one sees that the k -dependence of the first and last argument cancels so that it can be rewritten as a confluent hypergeometric function independent of k . For low k the matrix elements are therefore constant. However, the approximations are only valid for $k \ll \kappa$, so that we in general must expect a k -dependence in the neighbourhood of the Auger-peak.

The numerical example in the text is for the M_1 - M_3N_7 transition in Dy. Only one component of the transition has been calculated, the one where the outgoing electron has $l_A = 2$ and $j_A = 5/2$ and the remaining two-hole configuration couple to an angular momentum $J = 3$. The matrix element is [16] $D/3 - E/7$, D and E being the direct and exchange matrix elements, which turn out to be of the same order of magnitude here. The effective charges were estimated from the mean radii given in [19]. Figure 2a shows the atomic phase space factor, i.e. the spectrum with the Breit-Wigner shape divided out, as a function of the energy of the outgoing electron. With the matrix elements set to a constant so that only the ν -phase space contribute the full line is obtained, when the matrix element is included the dashed line

is obtained; both curves are normalized to one at the peak-position (they thus correspond to the curves marked by full and dashed lines, respectively, in Figure 1).

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