$0^+ \to 0^+$ radiative transitions

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(Submitted 3 August 1989; resubmitted 30 May 1990)
Zh. Eksp. Teor. Fiz. **98**, 1505–1513 (November 1990)

We studied experimentally and theoretically the one-photon $0^+ \to 0^+$ nuclear transition, which proceeds by involving the electron shell. We carried out measurements for the 1760 keV $0^+ \to 0^+$ transition in ^{90}Zr. We have established that the probability of one-photon transitions relative to internal conversion is $\eta = (5 \pm 2) \cdot 10^{-7}$ for the unshifted frequency, and $\eta_f \leqslant 10^{-8}$ for the frequency shifted by the binding energy of the K shell. We give a detailed theoretical analysis of the various processes that contribute to the one-photon $0^+ \to 0^+$ transition. The theoretical calculations are compared with the experimental data.

1. INTRODUCTION

The radiative decay of nuclei, proceeding with the involvement of the electron shell (electronic bridges), was studied theoretically in Refs. 1 and 2, and was observed experimentally for $M4$ transitions in the ^{93}Nb and ^{193}Ir nuclei in Refs. 3 and 4. It can be represented physically as multiple scattering of the conversion electron off the electrons of the atomic shell with subsequent radiative capture to a free state either below (elastic electronic bridge[5–9]) or above (inelastic electronic bridge[9–11]) the Fermi level. Nuclear decay via the electronic bridge is most probable for highly converted transitions, usually having high multipolarity L and low energy W. However, as was noted in Refs. 4, 8, and 11, in the experimental study of transitions with $L \neq 0$ there is always present the ambiguity related to the separation of the transitions via the electronic bridge from the direct radiative transitions in the nucleus. In that respect, $0^+ \to 0^+$ transitions for which the direct one-photon transitions are forbidden are "cleaner." In the present work we study the possibility of experimentally detecting the nuclear one-photon $0^+ \to 0^+$ transition, which proceeds with the involvement of the electronic shell of the atom, and we give a theoretical interpretation of such a process.

2. THE EXPERIMENT AND RESULTS OF THE MEASUREMENTS

For the object of study we have chosen the even-even ^{90}Zr nucleus, whose first excited state is an 0^+ state with energy $W = 1760$ keV. This state is populated by β^- decay of ^{90}Y. In addition to the 0^+ state the nearest 2^+ state is also populated (see Fig. 1). The probability of populating the 2^+ state is less by four orders of magnitude than to the 0^+ state. For this reason ^{90}Zr is an ideal object to study, since by comparing the probability for γ-discharge of the $0_2^+ \to 0_1^+$ and the $2_1^+ \to 0_1^+$ transitions it is easy to estimate the probability of the $0^+ \to 0^+$ γ transition via the electronic bridge. The experiments are made somewhat more complicated by the fact that the ^{90}Y decay proceeds with 99.99% probability to the ground state via β electrons with 2.2 MeV maximum energy. This means that measurements have to be carried out in the presence of a considerable bremsstrahlung γ background. From the ratio of radiative and ionization losses[12]

$$\frac{(dE/dx)_{\rm br}}{(dE/dx)_{\rm ion}} = \frac{Ez}{1600}, \qquad (1)$$

where E is the electron energy in units of the electron rest mass, it is easily estimated that if the electrons are stopped by an absorber made from hydrogen-containing polymers the bremsstrahlung yield will be no more than 0.5%. In addition, in the energy region up to 1 MeV the yield of the γ radiation was suppressed by approximately a factor of 10^3 with the help of a lead filter. At the same time the efficiency of detection of the photons in the region $w_\gamma \approx 1760$ keV was practically unchanged.

Owing to the need for carrying out measurements over a long time we used in the experiment a ^{90}Sr source in equilibrium with ^{90}Y (see Fig. 1). The ^{90}Sr source was uniformly spread over a 15×20 cm backing placed in the electron absorber of polysterene and in a lead shield (see above). Two different ^{90}Sr sources were used in the experiment. Their total activity was $(4 \text{ and } 6) \cdot 10^8$ Bq.

The measurements were carried out in a low-background setup using a semiconductor spectrometer with a ultrapure germanium detector of 230 cm^3 volume and a resolution of 1.8 keV on ^{60}Co γ lines. The measurements used a ^{90}Sr source, supplied by the "Izotop" facility and extracted from the decay products. In order to determine possible γ lines due to the presence in the sample of admixtures of radioactive nuclei, we performed preliminary careful measurements of the spectrum of the γ radiation of the given ^{90}Sr sample in the region 0–6 MeV. By comparing the obtained intensities and energies of the photons with tabulated data[13] we identified all nuclei with γ transitions in the region $E = 1742$ and 1760 keV (see Fig. 2) and analyzed the possibility of their formation in the decay products. It follows from these measurements that the contribution of all possible background γ lines with energies of 1742 and 1760 keV can amount to no more than 10^{-14} of the total activity of the utilized ^{90}Sr source.

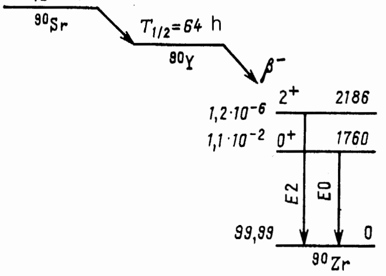

FIG. 1. The decay scheme of ^{90}Sr.

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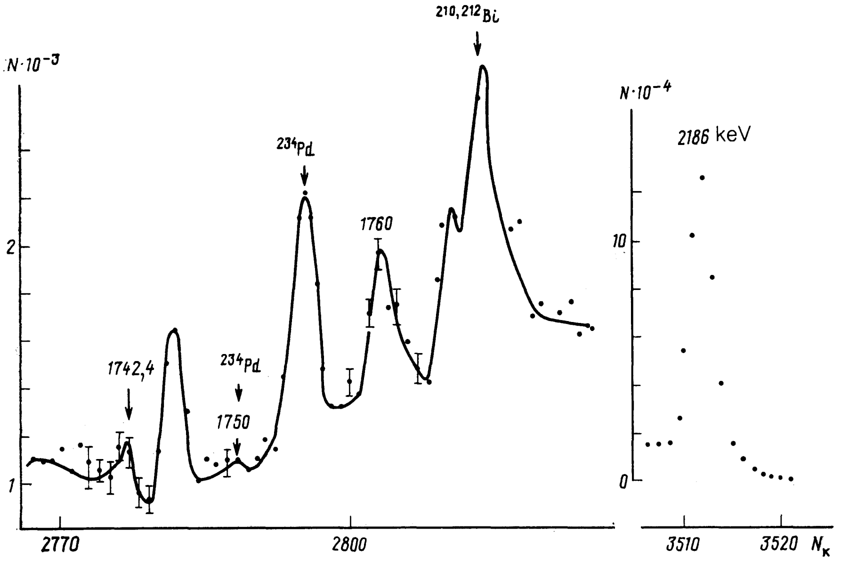


FIG. 2. Fragment of the photon spectrum in ^{90}Sr decay.

The principal measurements were carried out over a period of a month. A fragment of the γ spectrum of such a measurement is shown in Fig. 2 with the γ background due to bremsstrahlung subtracted out. As is evident from Fig. 2, γ lines with energy 1760 keV, equal to the energy W of the $0^+ \to 0^+$ transition (with ± 0.2 keV accuracy), are clearly observed. Such a γ line with unshifted energy $w_\gamma \approx W$ can be attributed to a transition via a quasi-elastic electronic bridge (see the next Section).

In the 1742 keV energy region of the spectrum there was also observed a γ line which can be identified as a transition due to an inelastic electronic bridge[9–11] that must be shifted by an amount corresponding to the binding energy in the K shell, $B_K = 18$ keV, from the energy of the $E0$ transition (see Fig. 2). However, there is present in this region the γ line of ^{234}Pa with energy 1741.7 keV. The intensity of this γ transition is low. It practically coincides with the intensity of the γ line with energy 1750 keV (see Fig. 2).[13] Moreover, since in this energy region the γ background due to bremsstrahlung is high, unambiguous conclusions on the probability of an inelastic electronic bridge are not possible. One can only point to the fact that the probability of the γ transition with the shifted energy (via the inelastic electronic bridge) is more than one order of magnitude less than the probability of the γ transition with "unshifted" energy.

It is convenient to determine the probability of the $0^+ \to 0^+$ transition by relying on the probability of the $2^+ \to 0^+$ transition. The 2^+ state is weakly populated in the β decay (see Fig. 1). At the beginning of our studies this transition was observed in only one experiment,[14] with the accuracy of its determination being 30%, since the number of counts in the γ peak with energy 2186 keV was at the level of 150–200. We have accumulated a total of about $3\cdot 10^5$ counts in γ 2186 keV. This permits the determination of the relative β-decay probability to the $2_1{}^+$ state with high precision, $(1.12 \pm 0.06)\cdot 10^{-6}$%. By making use of the data on the γ 2186 keV transition probability, as well as of the results of the study of the internal and pair conversion probability of the $E0$ transition in ^{90}Zr,[15] we find that the relative probability of the $0^+ \to 0^+$ transition with energy 1760 keV is equal to $(5 \pm 2)\cdot 10^{-7}$ per act of internal conversion of the $E0$ transition. The transition probability via the inelastic electronic bridge does not exceed 10^{-8} relative to internal conversion of the $E0$ transition.

As was discussed above, the appearance of the γ peak with energy 1760 keV due to admixtures of radioactive nuclei, with better than 10^{-14} accuracy relative to the total activity of the given source, is not possible. The obtained probability of the γ transition relative to the total probability of the ^{90}Sr decay is equal to $I_\gamma \approx (5 \pm 2)\cdot 10^{-7}\cdot 1.1\cdot 10^{-4} = 6\cdot 10^{-11}$. This means that the contribution of the admixtures to the probability of the quasi-elastic electronic bridge is no more than 1–2%, even if two standard deviations are taken into account.

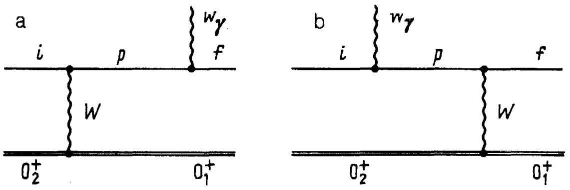
There exists one more channel for the formation of a false γ peak in the energy in $0^+ \to 0^+$ transitions. In $0^+ \to 0^+$ transitions a two-quantum decay is possible, whose probability in the case of the ^{90}Zr nucleus is equal to (see Ref. 16) $2\cdot 10^{-4}$ of the total decay probability of the 0^+ state. Here a continuous γ spectrum should be observed with energy from 0 to 1760 keV with a maximum in approximately the 900 keV region. A certain probability always exists that as a result of accidental summation a false peak will appear at the energy of the $E0$ transition. With the aim of taking this effect into account we have carried out measurements of the absolute efficiency of detection of photons in the 0.2–1760 keV energy region. It turned out to be, for the given geometry of the experiment, equal to 0.2% on the average for that energy region. For such a detection efficiency the probability of the summation peak relative to the total probability of the ^{90}Zr decay, with the weakening factor of the low-energy region of the γ spectrum taken into account, amounts to $I_{\gamma\gamma} \approx 1.1\cdot 10^{-4}\cdot 2\cdot 10^{-4}\cdot 2\cdot 10^{-4}\cdot 10^{-3} = 4\cdot 10^{-14}$, i.e., its contribution to the total γ 1760 keV intensity (see above I_γ) is no more than 0.5%.

In addition we have performed two measurements with different geometries and with sources differing in activity. In the case of the summation peak the relative γ 1760 keV yield should change by several factors. However in the experiment we obtained $I_\gamma(1760)/I_e(E0) = (5 \pm 2)\cdot 10^{-7}$ and $(6 \pm 3)\cdot 10^{-7}$ respectively, i.e., the different measurements are in good agreement.

Based on the above we conclude that the observed γ line with energy $w_\gamma \approx 1760$ keV corresponds to the one-photon $E0$ transition.

3. THEORETICAL ESTIMATES

Several channels of γ decay, differing in the values of energy and angular momentum transferred to the electron shell of the atom, contribute to the one-photon amplitude of the $0^+ \to 0^+$ transition via the electronic bridge. In lowest, third order of perturbation theory the process of interest is described by the diagrams



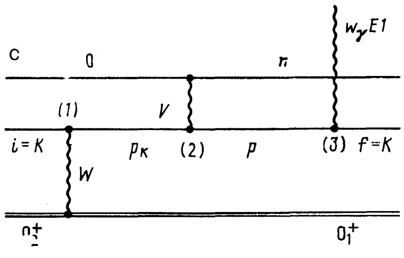
where the double lines correspond to the initial $0_2{}^+$ and final $0_1{}^+$ states of the nucleus, where *i, p,* and *f* refer to the electron in the atomic shell in the initial, intermediate and final states respectively, and where the wavy lines refer to the virtual and emitted photons with energy W and w_γ.

For $i = f$ the electronic bridge is elastic.[2] It is easy to see from the selection rules that for $0^+ \to 0^+$ transitions the contribution from the elastic electronic bridge vanishes. In the case of the inelastic electronic bridge ($i \neq f$) there are two possibilities of $0^+ \to 0^+$ transitions.

First, if the electron in the initial state with energy $\varepsilon_i \leqslant \varepsilon_F$ (ε_F is the Fermi energy) goes into the final state with energy $\varepsilon_f > \varepsilon_F$, then such a transition has the shifted frequency $w_\gamma = W - E_{\rm ex}$ ($E_{\rm ex} = \varepsilon_f - \varepsilon_i$ is the excitation energy of the atom).[3,4,9–11] In view of the finite resolving power of the detector $\Delta w_\gamma \approx 0.2$ keV, such transitions contribute to the total intensity of the 1760 keV γ line provided $E_{\rm ex} \leqslant \Delta w_\gamma$. This is satisfied for subshells whose binding energy is less than 200 eV. Estimates[17] show that the contribution of this channel to the relative probability of the $E0$ transition does not exceed 10^{-10}.

Second, if the electron level i is not completely filled then a $0^+ \to 0^+$ transition is possible at the unshifted frequency $w_\gamma = W$. Such a transition is possible for a neutral atom only with the participation of electrons from the valence shell. Estimates[17] show that in this case the relative probability does not exceed 10^{-16}.

In both cases these small values are due mainly to the small probability of virtual internal conversion [see diagram (a)] for electrons having low binding energy.[18] Since for $E0$ transitions the probability of internal conversion is to a high precision accounted for by K-electron conversion, it is natural to investigate the possibility that conversion on the K shell contributes to the probability of the process that we are interested in. The process depicted in the following diagram may serve as an example:



Here the virtual photon W takes the K-shell electron into the state p_K in the continuum. Thereafter that electron scatters inelastically on the electrons of the atom and after emission of the photon w_γ ends up in the initial state in the K shell. As a result the atom is left in the excited state $|n\rangle$. Here electrons near the Fermi level are excited with highest probability, and the excitation energy $E_{\rm ex} = \varepsilon_n - \varepsilon_0$ that is transferred to the electron shell is small (~ 10 eV).[19] Therefore experimentally, due to the finite energy resolution of the photons $\Delta w_\gamma \leqslant 200$ eV, such a transition will be identified as a transition at the unshifted frequency (quasi-elastic electronic bridge).

This process is small of higher order than those shown in the diagrams *a* and *b*. However, since conversion proceeds in this case on electrons from the K shell and that for the corresponding quantum numbers p and n the radiative $E1$ transition is possible, the contribution of this diagram can exceed the contribution of the processes of diagrams *a* and *b* for unshifted energy. We illustrate this by a numerical calculation. The transition amplitude $A_{0,n}$ corresponding to the diagram *c* has the form

$$A_{0,n} = \sum_{\substack{pljm\\ p_K m_K}} \frac{\langle 1S_{1/2} m_K | \hat{H}_\gamma^*(w_\gamma \lambda LM) | pljm\rangle \langle n, pljm | \hat{V} | 0, p_K S_{1/2} m_K\rangle}{(p^2 - p_0^2 + i0)} \times \frac{\langle p_K S_{1/2} m_K, 0_1{}^+ | \hat{H}_c | 1S_{1/2} m_K, 0_2{}^+\rangle}{(p_K{}^2 - p_{K0}{}^2 + i0)}, \qquad (2)$$

where $p_{K0}{}^2 = (1 + W - B_K)^2 - 1$, $p_0{}^2 = (1 + w_\gamma - B_K)^2 - 1$, and $\hat{H}_c$ and $\hat{H}_\gamma$ are the interaction Hamiltonians of the nucleus and the electromagnetic field with the electrons, with the latter normalized to one photon per unit volume.[1] For the interaction of the conversion electron with the bound electrons of the atom $\hat{V} = \Sigma_e \hat{V}(\mathbf{r}, \mathbf{r}_e)$ we choose the Coulomb interaction, ignoring retardation and exchange effects. Here and below the electron wave functions in the continuum are normalized to a δ-function in energy and we use the system of units in which $\hbar = c = m_e = 1$.

In the following we shall take as valid the inequality $p_0 \gg \alpha Z$ (α is the fine structure constant), which is satisfied in our case. Then the main contribution to the amplitude (2) comes from the poles of the Green's function corresponding to the virtual states $|pljm\rangle$ and $|p_K S_{1/2} m_K\rangle$ (resonance approximation).[19,20] Then the probability P_γ of the process under consideration is proportional to the conversion probability P_e, and we obtain for the differential in energy $w = W - w_\gamma$ ratio of these probabilities, after the necessary summations, averagings and integrations,

$$d\eta = \frac{dP_\gamma}{P_e} = 4\pi^3 \sum_{n\lambda LM} (2L+1)^{-2} \Big| \sum_{j=L\pm 1/2} \langle 1S_{1/2} \| \hat{H}_\gamma^*(w_\gamma \lambda L) \| p_0 Lj\rangle \times (-1)^{j-1/2} \Delta_{LM}{}^n(p_{K0}, p_0) \Big|^2 \delta(w - (\varepsilon_n - \varepsilon_0))\, dw, \qquad (3)$$

$$\Delta_{LM}{}^n(p_K, p) = \alpha \int_0^\infty \frac{dq}{q^2} \Big\langle n \Big| \sum_e \exp\{i\mathbf{q}\mathbf{r}_e\} \Big| 0 \Big\rangle \times \langle pLj \| j_L(qr) Y_L \| p_K S_{1/2}\rangle Y_{LM}(\Omega_q). \qquad (4)$$

We confine ourselves to the contribution to (3) from the λL-$E1$ transition. In the plane-wave approximation for the high-lying states in the continuum the reduced matrix elements in (4) can be evaluated analytically (see Appendix 1). Taking (A1) and (A3) into account and neglecting the change in the momentum of the conversion electron in the calculation of the reduced matrix elements of the radiative decay in (3) we can write for $d\eta$ the following factorized expression:

$$d\eta \approx Q_r G(w)\,dw, \tag{5}$$

where the factor $G(w)dw$ stands for the differential in energy w relative probability of excitation of the bound atomic electrons, accompanying internal conversion and caused by the dipole electron interaction

$$G(w) = \frac{\pi^2}{96}\left(\frac{\alpha}{W-B_K}\right)^2 \sum_n \int_{-\infty}^{\infty} dt \exp\{-iwt\} \int \frac{d\mathbf{q}\, d\mathbf{q}'}{q^2\, q'^2} \times \left\langle 0 \left| \sum_e \exp\{i\mathbf{q}\mathbf{r}_e\} \right| n \right\rangle \left\langle n \right| \times \exp\{i\hat{H}_A t\} \sum_e \exp\{-i\mathbf{q}'\mathbf{r}_e\} \exp\{-i\hat{H}_A t\} \left| 0 \right\rangle \times \left(1-2(1+W-B_K)\frac{w}{q^2}\right)\left(1-2(1+W-B_K)\frac{w}{q'^2}\right)\frac{\mathbf{q}'\mathbf{q}}{q'q}, \tag{6}$$

and the factor Q_r stands for the relative probability of the radiative $E1$ transition into the $1S_{1/2}$ state from a state in the continuum with angular momentum 1, prepared in the excitation process:

$$Q_r = |2^{1/2}\langle 1S_{1/2} \| \hat{H}_\gamma(WE1) \| p_{K0} P_{3/2}\rangle + \langle 1S_{1/2} \| \hat{H}_\gamma(WE1) \| p_{K0} P_{1/2}\rangle|^2. \tag{7}$$

In expression (6)

$$\hat{H}_A = \sum_e (\hat{V}_A(\mathbf{r}_e) + \hat{\mathbf{p}}_e^2/2)$$

is the unperturbed Hamiltonian of the atom.

We have calculated the reduced matrix elements of the $E1$ transition that enter (7) in the Dirac-Hartree-Fock-Slater model (DHFS).[21] As a result in the case of ^{90}Zr for $W = 1760$ keV we obtain

$$Q_r \approx 1{,}38 \cdot 10^{-5}. \tag{8}$$

To calculate the factor $G(w)$ we make use of the completeness property of the states $|n\rangle$ and take into account the equality (A4). Then after integrating in (6) over t and the angular variables of the vectors $\mathbf{q}$ and $\mathbf{q}'$ we obtain the following expression:

$$G(w) = \frac{\pi^3}{6}\left(\frac{\alpha}{W-B_K}\right)^2 \int_{q_{min}}^{q_{max}} dq \int_{2w/q}^{q_{max}} dq' \rho([q^2+q'^2+4w]^{1/2}) \times \left\{4(1+W-B_K)\frac{w^2}{q^4 q'^2} - \left(1+4(1+W-B_K)^2\frac{w^2}{q^2q'^2}\right)\frac{w}{q^2q'^2}\right\}, \tag{9}$$

where $\rho(q) = \langle 0|\Sigma_e \exp(i\mathbf{q}\cdot\mathbf{r}_e)|0\rangle$ is the Fourier transform of the electron density of the atom. The limits of integration over q and q' are restricted by the inequalities in (A3):

$$q_{max} \approx 2p_{K0}, \qquad q_{min} = p_{K0} - p_0 \approx \frac{(1+W-B_K)\,w}{(W-B_K)(1+2/(W-B_K))}$$

and the relation $qq' > 2w$.

It is evident from this expression that the main contribution to the integral comes from small q and $q' \ll 1/\alpha Z$, which corresponds to "soft" excitations of the atom. For such q and for small w the Fourier transform of the electron density $\rho(q)$ is given by the normalization to the electron number $[\rho(q \ll 1/\alpha Z) \approx Z]$. Further, for the dipole excitation factor G_{tot} integrated over the w spectrum we obtain in the case of ^{90}Zr

$$G_{tot} = \int_{w_{min}}^{W} dw G(w) \approx 1{,}7 \cdot 10^{-2}. \tag{10}$$

Here w_{min} is the minimum excitation energy in the ^{90}Zr atom, for which we have chosen the transition energy of the O_1-electron to the state O_2, calculated in the DHFS model:[21] $w_{min} = B_{O2} - B_{O1} \approx 0.44 \cdot 10^{-8}$ in units of the electron rest mass. We note that taking into account the realistic electron density of the atom[22] changes the result (10) by no more than 30%. Such a precision is quite acceptable since it is no worse than the experimental errors.

As a result, with the equalities (5), (8), and (10) taken into account, we obtain for the integrated over w relative probability of the $0^+ \to 0^+$ γ transition in ^{90}Zr

$$\eta_{tot} \approx 2{,}3 \cdot 10^{-7}. \tag{11}$$

4. CONCLUSION

The theoretical estimate (11) obtained here agrees with the corresponding experimental quantity for the $0^+ \to 0^+$ γ transition with unshifted energy in ^{90}Zr. Although in the present case the diagram c corresponds to a $0^+ \to 0^+$ transition through an inelastic electronic bridge, the energy transferred to the electron shell is connected with the excitation of electrons in the valence shell and is therefore small [see (9)]. This permits the identification of such a transition with transition with unshifted energy. We note the relatively large, compared to the diagrams a and b, contribution of the diagram c, which is small of higher order in the fine structure constant. This happens because taking this diagram into account makes possible the virtual conversion transition on the K shell with subsequent emission of an $E1$ photon, whose probabilities are usually large. The possibility of a relatively large contribution of the diagram c should also be considered in the general case of nuclear transitions with the participation of the atomic electron shell, for example for the $M4$ transitions in ^{193}Ir (Ref. 11) or the $E3$ transition in ^{235}U (Refs. 5–7).

The process depicted in the diagram c leads to the presence of an admixture of radiation of different multipolarity than that due to the radiative decay corresponding to the direct nuclear transition of the "bare" nucleus. Further, the relative contribution of this admixture is of the same order of magnitude as parity-nonconservation effects in electromagnetic nuclear transitions. In perspective it would be interesting to study the form of the γ lines for nuclear transitions with $L \neq 0$ with the help of crystal diffraction spectrometers.[23] Here, a satellite γ peak would be expected in the energy region shifted by roughly tens of electron volts from the main line. Its detection would provide direct confirmation of the validity of the interpretation proposed in this paper.

The authors are grateful to I. N. Vishnevskiĭ, A. V. Davydov, M. A. Listengarten, V. A. Krutov, and E. G. Drukarev for useful discussion of the results obtained here.

APPENDIX 1

We consider the reduced matrix element for the dipole transition between states in the continuum:

$$\langle p'Pj\|j_1(qr)Y_1\|pS_{1/2}\rangle=(-1)^{j-1/2}\left(\frac{2j+1}{4\pi}\right)^{1/2}R_j, \qquad \text{(A1)}$$

$$R_j=\int_0^\infty r^2\,dr\,(f_{p'Pj}(r)f_{pS_{1/2}}(r)+g_{p'Pj}(r)g_{pS_{1/2}}(r))\,j_1(qr), \qquad \text{(A2)}$$

where f_{plj} and g_{plj} are the large and small components of the electron wave functions in the continuum. We make use of the plane-wave approximation for these high-lying states[12]

$$f_{plj}=\left(\frac{(E+I)p}{\pi}\right)^{1/2} j_l(pr),$$

(where $E^2=p^2+1$ the proper energy of the state) and neglect the small components g_{plj}. Then the integration in (A2) can be performed analytically.[24] As a result we obtain, accurate up to terms of order $(p^2-p'^2)/p^2$,

$$R_{1/2}=R_{3/2}\approx\begin{cases}\dfrac{1}{8(E-1)}(1-2Ew/q^2), & |p-p'|<q<p+p',\\ 0, & q<|p-p'|,\quad q>p+p'.\end{cases} \qquad \text{(A3)}$$

Here we have taken into account the equality $|p^2-p'^2|=|E-E'|(E+E')\approx 2E|E-E'|$, which is valid for small energy transfers $w=|E-E'|\ll E$.

APPENDIX 2

By making use of properties of the function $\exp(-i\mathbf{q}'\cdot\mathbf{r}_e)$ it can be shown that

$$\sum_e \exp(i\mathbf{q}\mathbf{r}_e)\exp(i\{\hat{V}(\mathbf{r}_e)+\hat{\mathbf{p}}_e^2/2\}t)\exp(-i\mathbf{q}'\mathbf{r}_e)$$

$$=\sum_e \exp(i(\mathbf{q}-\mathbf{q}')\mathbf{r}_e)\exp(it\{\hat{V}(\mathbf{r}_e)+{}^1/_2(\hat{\mathbf{p}}_e-\mathbf{q}')^2\})$$

$$\approx\sum_e \exp(i(\mathbf{q}-\mathbf{q}')\mathbf{r}_e+i\mathbf{q}\mathbf{q}'t/2)\exp(i\{\hat{V}(\mathbf{r}_e)+\hat{\mathbf{p}}_e^2/2\}t). \qquad \text{(A4)}$$

In deriving the last equality we made use of the Baker-Hausdorff identity[25] and neglected gradients of the potentials $\hat{V}(\mathbf{r}_e)$.

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Translated by Adam M. Bincer