Anomalies in nuclear excitation by atomic-shell electron transitions

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The effect of the dynamic penetration of electron current into the nucleus on the nuclear-excitation process during electron transitions in the atomic shell is analyzed. Anomalies which are an order of magnitude stronger than corresponding anomalies in internal conversion coefficients may be seen in the course of this process.

The excitation of nuclei in the course of atomic transitions has been studied theoretically and experimentally over the past few years in the nuclei ^{189}Os, ^{197}Au, ^{237}Np, and ^{181}Ta. The process is known as "nuclear excitation by electron transition" (NEET). The effect can be summarized by saying that the nucleus is excited upon the upward transition of a vacancy from a low-lying atomic shell when the energy and multipolarity of a nuclear transition coincide with those of the atomic transition. Theoretical and experimental research on NEET is reviewed in Refs. 1 and 2.

Although the list of studies on the topic is fairly long, there has not yet been a study of the dynamic effect of the nuclear volume in NEET. In all the nuclei listed above, the electron transition in the NEET process occurs between $nS_{1/2}$ and $mP_{1/2}$ (m, $n=1$, 2,...) atomic states, for which the electron wave function $\psi(\mathbf{r})$ has a large amplitude at the origin. Because of this large amplitude, the electron current $j^{\mu}_{fi}(\mathbf{r}) = -e\bar{\psi}_f(\mathbf{r})\gamma^{\mu}\psi_i(\mathbf{r})$ (e is the charge of a proton, and γ^{μ} are the Dirac matrices) effectively penetrates into the nucleus in the course of $nS_{1/2} \leftrightarrow mP_{1/2}$ transitions, with the result that an "intranuclear" NEET becomes possible.

The static effect of the finite dimensions of a nucleus has already been taken into account in Refs. 1 and 2. In that case the electron wave functions are calculated in the Coulomb field of a nucleus of radius R_0 with a uniform charge distribution, while the coordinates of the electron current $j^{\mu}_{fi}(\mathbf{r})$ and of the nuclear current $J^{\mu}_{IF}(\mathbf{R}) = e\Psi^{+}_{F}(\mathbf{R})\hat{J}^{\mu}\Psi_I(\mathbf{R})$ (Ψ is the wave function, and $\hat{J}^{\mu}$ is the electromagnetic-current operator of the nucleus) satisfy the usual condition $R<r$, as in the case of a point nucleus.

However, the restriction to the region $R<r$, which is valid in a calculation of the probability for NEET in the case of, for example,[3] ^{189}Os, in which an $M1$ intraband transition occurs, is totally unjustified for nuclei with l-forbidden $M1$ transitions or with $E1$ transitions which are forbidden by the asymptotic quantum numbers of the Nilsson model. In such cases the region $R>r$ may, if there is a significant attenuation of nuclear transitions, contribute substantially to (or even dominate) the NEET probability.[3] This effect is analogous to the dynamic nuclear-volume effect in the process of internal conversion,[4] which has been recognized since the mid-1950s.

However, NEET is not just one more process in which it is possible to measure the same nuclear parameters as in anomalous conversion (although this is not a trivial matter, since measurements of anomalies in internal-conversion coefficients are still the only way to determine several characteristics of nuclei[5]). In some cases, a dynamic effect will be seen much more vividly in NEET than in internal conversion. The reason is as follows: The energies of transitions in NEET do not exceed the binding energy of K-shell electrons. In this case a conversion is possible in L and higher-lying shells, from which the electron goes "up" into states of the continuum. In NEET, everything is just the opposite. The electron goes "down" to a deeper shell (which may be the K shell), in which the amplitudes of the electron wave functions in the nucleus may be considerably larger than those for the conversion states of the continuum. As a result, when we switch from internal conversion to NEET, we find that the relative contribution from the nuclear region to the probability for the process is greater, since the overall radial integral of the electron matrix element is dominated in both processes by the region outside the nucleus and is not as sensitive to the amplitudes of the electron wave function at the origin.

Let us examine this mechanism in more detail. The energy of the interaction of electron and nuclear currents which causes the transition is

$$H_{\rm int}=\int_0^\infty d^3R\int_0^\infty d^3r j^\mu_{if}(\mathbf{r})D_{\mu\nu}(\omega_N;\mathbf{r}-\mathbf{R})J^\nu_{IF}(\mathbf{R}),\tag{1}$$

where $D_{\mu\nu}(\omega_N;\mathbf{r}-\mathbf{R})=-g_{\mu\nu}\exp(i\omega_N|\mathbf{r}-\mathbf{R}|)/|\mathbf{r}-\mathbf{R}|$ is the photon propagator. Writing its multipole expansion in the regions $R<r$ and $R>r$, making use of the standard set of scalar $[A_{LM}(\mathbf{r};\omega)$ and $B_{LM}(\mathbf{r};\omega)]$ and vector $[\mathbf{A}^{E,M,Y}_{LM}(\mathbf{r};\omega)$ and $\mathbf{B}^{E,M,Y}_{LM}(\mathbf{r};\omega)]$ electromagnetic potentials from Ref. 6 (Y is the longitudinal potential, and E and M are the electric and magnetic potentials in the Coulomb gauge), we can write $H_{\rm int}$ as the sum of two terms:

$$H_{\rm int}=H^R_{\rm int}+\Delta H_{\rm int}.\tag{2}$$

The first of these terms is the interaction energy in the Rose model (or in the "penetration-free" model[7]) and is given by

$$H^R_{\rm int}=4\pi i\omega_N\sum_{L,M}\left\{\int_0^\infty d^3RJ_0(\mathbf{R})A^*_{LM}(\mathbf{R};\omega_N)\int_0^\infty d^3rB_{LM}(\mathbf{r};\omega_N)j_0(\mathbf{r})\right.$$
$$\left.-\sum_{a=E,M,Y,}\int_0^\infty d^3R\mathbf{J}(\mathbf{R})\mathbf{A}^{a*}_{LM}(\mathbf{R};\omega_N)\int_0^\infty d^3r\mathbf{B}^a_{LM}(\mathbf{r};\omega_N)\mathbf{j}(\mathbf{r})\right\}.\tag{3}$$

The second term is an "additional" interaction energy which arises because of the dynamic penetration of the electron current into the nucleus:

$$\Delta H_{\rm int}=4\pi i\omega_N\sum_{L,M}\left\{\int_0^\infty d^3RJ_0(\mathbf{R})\left(B^*_{LM}(\mathbf{R};\omega_N)\int_0^R d^3rA_{LM}(\mathbf{r};\omega_N)j_0(\mathbf{r})\right.\right.$$

$$-A^{*}_{LM}(\mathbf{R};\omega_N)\int_0^R d^3r B_{LM}(\mathbf{r};\omega_N)j_0(\mathbf{r})\Bigg)-\sum_{a=E,M,Y,}\int_0^\infty d^3R\mathbf{J}(\mathbf{R})$$

$$\times\Bigg[\mathbf{B}^{a*}_{LM}(\mathbf{R};\omega_N)\int_0^R d^3r\mathbf{A}^{a}_{LM}(\mathbf{r};\omega_N)\cdot\mathbf{j}(\mathbf{r})$$

$$-\mathbf{A}^{a*}_{LM}(\mathbf{R};\omega_N)\int_0^R d^3r\mathbf{B}^{a}_{LM}(\mathbf{r};\omega_N)\cdot\mathbf{j}(\mathbf{r})\Bigg]\Bigg\}. \tag{4}$$

When the dimensions of the nucleus are taken into account systematically in Eqs. (3) and (4), we find the following expression for the energy of the electron–nucleus interaction in the case of EL transitions:

$$H_{\rm int}(EL)=4\pi i\omega_N\sum_{L,M}\frac{ie\Lambda'}{\sqrt{L(L+1)}}N^E_{LM}(\omega_N)\Bigg\{m^E_L(\omega_N)+i\delta_{E1}(nS_{1/2}\leftrightarrow mP_{1/2})$$

$$\times\frac{c_i c_f}{4\pi^2}\frac{R_0}{a_B}\left(\frac{\lambda_N}{a_B}\right)^2\left[\lambda^{(2)}\frac{1}{MR_0}\frac{n}{\sqrt{2}}+\lambda^{(1)}\frac{R_0}{a_B}\left(\frac{3}{10}(g^0_{P_{1/2}}+f^0_{S_{1/2}})-\eta\frac{\omega_N a_B}{10}\right)\right]\Bigg\}. \tag{5}$$

Here we have introduced the nuclear matrix element

$$N^E_{LM}(\omega_N)=\int_0^\infty d^3R\mathbf{J}(\mathbf{R})\mathbf{A}^{E*}_{LM}(\mathbf{R};\omega_N)$$

and the radial atomic matrix element

$$m^E_L(\omega_N)=\int_0^\infty dr r^2[Lh^{(1)}_L(r\omega_N)(g g_f+f_i f_f)-h^{(1)}_{L-1}(r\omega_N)((\kappa_i-\kappa_f-L)g_i f_f$$

$$+(\kappa_i-\kappa_f+L)f_i g_f)].$$

We have also introduced Voĭkhanskiĭ–Listengarten nucleus-penetration parameters for the electric multipoles,[8]

$$\lambda^{(1)}=\langle\Psi_F(\mathbf{R})|\hat{\mathscr{M}}_1|\Psi_I(\mathbf{R})\rangle/\langle U_\gamma\rangle,\quad \lambda^{(2)}=\langle\Psi_F(\mathbf{R})|\hat{\mathscr{M}}_2|\Psi_I(\mathbf{R})\rangle/\langle U_\gamma\rangle,$$

in which the nuclear matrix element for γ-ray emission of electric multipolarity $\langle U_\gamma\rangle$ is, by definition,

$$\int_0^\infty d^3RJ_0(\mathbf{R})(R/R_0)^L Y^*_{LM}(\mathbf{n}_R),$$

and the nuclear penetration operators are

$$\hat{\mathscr{M}}_1=\left(\frac{R}{R_0}\right)^3 Y^*_{LM}(\mathbf{n}_R),\quad \frac{\hat{\mathscr{M}}_2}{MR_0}=\left(\frac{R}{R_0}\right)^2\hat{\mathbf{J}}\cdot[\mathbf{n}_R\times\mathbf{Y}_{LL;M}(\mathbf{n}_R)]$$

[M is the mass of the proton, $Y_{LM}(\mathbf{n}_R)$ are the spherical harmonics, and $\mathbf{Y}_{LL;M}(\mathbf{n}_R)$ are the vector spherical harmonics[6]]. The δ-function $\delta_{E1}(nS_{1/2}\leftrightarrow mP_{1/2})$ stresses the point that the second term in braces (curly brackets)

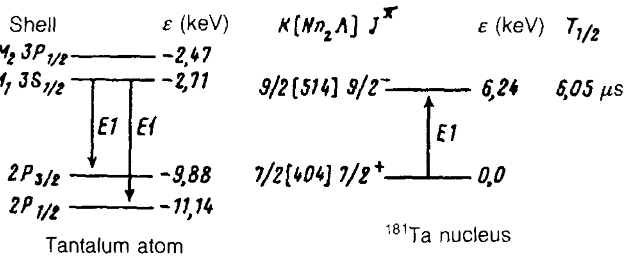

FIG. 1.

in (5), which is the actual contribution of the anomaly, is nonvanishing only for $E1$ transitions between the electron states $nS_{1/2}$ and $mP_{1/2}$. For the latter we can use the following expansions[7] in the region of the nucleus:

$$g(r)\approx a_B^{-3/2}c, \quad f(r)\approx a_B^{-3/2}cf^0 r/a_B$$

for $nS_{1/2}$ and

$$g(r)\approx a_B^{-3/2}cg^0 r/a_B, \quad f(r)\approx a_B^{-3/2}c$$

for $mP_{1/2}$, where c, f^0, and g^0 are constants, different for the two functions. In (5) we have also used the notation $\lambda_N=2\pi/\omega_N$ for the wavelength of the nuclear transition, Λ' for the angular electron matrix element from Ref. 7, and a factor $\eta=1$ for the $P_{1/2}\rightarrow S_{1/2}$ transition or $\eta=-1$ for the inverse transition.

As in the case of anomalies in the internal conversion coefficients, the term containing the nuclear charge parameter $\lambda^{(1)}$ in (5) plays a minor role in comparison with that played by the second term, which contains the parameter of the transition spin currents, $\lambda^{(2)}$. This is not merely an additional small factor resulting from the extra factor of R_0/a_B but in fact the familiar difference in selection rules in terms of the asymptotic quantum numbers of the Nilsson model for the matrix elements $\langle\hat{\mathcal{M}}_2\rangle$ and $\langle U_\gamma\rangle$ (Ref. 8).

There should be a very strong dynamic effect of the nuclear volume in NEET in the case of ^{181}Ta. Part of its level scheme is shown in Fig. 1. Measurements of the coefficient for internal conversion in the $3S_{1/2}$ shell in a nuclear transition with an energy 6.24 keV have shown that the partial coefficient for internal conversion to the $P_{1/2}$ state is increased by a factor of 13 by the anomaly (Ref. 9). This value leads to a value of 620 for the penetration parameter $\lambda^{(2)}$ (Ref. 5). Using this value of $\lambda^{(2)}$ in (5), we find that the probability for excitation of the $9/2^-$ level (6.24 keV) in the electron transition $3S_{1/2}\rightarrow 2P_{1/2}$ in NEET is increased by a factor of 170 when the anomaly is taken into account, from $P_{\rm NEET}=4.0\times10^{-16}$ to 6.8×10^{-14}. This difference between NEET and internal conversion is explained on the basis that the amplitude of the $2P_{1/2}$ state at the origin is much larger than that of the $P_{1/2}$ continuum wave function: $c2P_{1/2}\approx 244.7$ versus $cP_{1/2}\approx 55.6$. For the total radial matrix elements, which are governed primarily by the volume outside the nucleus, on the other hand, the increase upon the switch from conversion to NEET is very slight: $\mathrm{Im}[\mathrm{m}_1^E(\omega_N)\mathrm{NEET}]=-5.18$ versus $\mathrm{Im}[\mathrm{m}_1^E(\omega_N)_{\rm conv}]=-3.50$. In fact, these values are much smaller than the "anomalous" term in (5). [The asymptotic expression for the large component of the continuum wave function is $g_{lj}(r\to\infty)=\sin(pr+\pi\cdot l/2+\delta_{lj})$, where p is the electron momentum, δ_{lj} is a phase shift, and the wave functions of the bound states are normalized by the condition $\int_0^\infty drr^2(g^2(r)+f^2(r))=1$.]

An interesting situation has arisen in connection with the determination of the anomalies in internal conversion in the nucleus ^{237}Np. In the lower part of the spectrum, for the two $E1$ transitions from the $5/2^-$ level (59.5 keV) (the rotational band $K^\pi[Nn_z\Lambda]=5/2^-[523]$) to the $7/2^+$ state (33.2 keV) and the $5/2^+$ state (0,0) (both of these states belong to the $5/2^+[642]$ band), there are anomalies in the internal conversion coefficient (although this result is at odds with the selection rules in terms of the asymptotic quantum numbers of the Nilsson model[8]). For the $E1$ transition $7/2^-$ (102.96 keV) $\to$ $5/2^+$ (0,0) between the same rotational bands, no anomaly has so far been observed in the internal conversion coefficient. Accordingly, studies of NEET might yield an independent answer to the question of whether there is an anomaly in the $E1$ transition with an energy of 103 keV in ^{237}Np. The total probabilities for the process, for the case in which the penetration parameter $\lambda^{(2)}$ is -165 (Ref. 5), the same for the three nuclear transitions under consideration, are 3.2×10^{-12} without the anomaly and 4.6×10^{-12} with it.

We wish to stress that NEET might prove most useful for studying the dynamic nuclear-volume effect in low-energy nuclear transitions (with ω_N up to a few keV), in which the conversion occurs in the M and N shells, and measurements of anomalies in internal conversion coefficients are hindered by the relatively small amplitudes of the electron wave functions at the origin.

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