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Probability and selection rule for nuclear excitation by electron transition

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A quantum-mechanical formalism to calculate the nuclear excitation by electron transition (NEET) is presented. Emphasis is on the explicit calculations of the transition matrix elements for electric multiple and magnetic dipole NEET and discussions of the selection rules. One of the features of this formalism is that the part of the matrix element in connection with the nuclear partner is related to the nuclear partial radiative width, which is a measurable quantity. This makes it available to evaluate the NEET probability more reliably. The predicted results for NEET probabilities in ^{189}Os, ^{197}Au, and ^{237}Np are given along with the available measured data.

I. INTRODUCTION

An excited atomic state, e.g., a K-shell hole state, may decay through various processes. In addition to the known x-ray and Auger electron emissions, nuclear excitation by electron transition (NEET) has attracted much attention. In this process the excitation energy is transferred from the electron system to the nucleus via the near-field interaction. NEET is the inverse process of internal conversion. In the earlier stage of this study, it was recommended that NEET could be used to separate isotopes [1]. Recently, there are some suggestions that NEET perhaps is a useful technique in developing a gamma-ray laser, which is considered one of the major scientific and technological challenges in the next decade [2,3]. The idea is that [4] as the electron system has relatively larger electromagnetic multipole moments in comparison with that of the nucleus, it could effectively absorb energy from external irradiation fields. Then NEET or other techniques would be used to transfer the energy from the electron system to the nucleus to accomplish a fast nuclear interlevel transfer. In this process the electron system plays a role of an intermediate mechanism for transferring energy, angular momentum, or parity change from the irradiation field to the nucleus. The probability for a nuclear transition induced directly by an external laser field proves to be extremely small [5,6].

There are few experimental investigations on NEET [7–9]; all of these were made at Osaka University. As for theoretical studies, only preliminary calculations were published up to now [1,10]. There are no complete calculations for magnetic dipole NEET. Even for electric multipole NEET, the matrix elements in connection with the nuclear partner were treated improperly. The hindrance factors [11], which prove to be very important especially for electric dipole transitions, have never been discussed in any previous calculations. This ignorance might lead to a great overestimation of the predicted NEET probabilities.

A strict treatment of NEET requires the solution of the complete channel equations including all possible decay channels as well as intermediate states. As the main aim of this paper is put on the explicit calculations of NEET matrix elements and discussions of the NEET selection rule, we proceed with the following calculations based on the framework of nonrelativistic quantum mechanics. First, we present a simplified formula to evaluate NEET probabilities, which shows a Lorentzian resonance structure and the resonance width represents the effect of x-ray and Auger electron emissions. Then we give detailed calculations of the transition matrix elements for electric multipole and magnetic dipole NEET. One feature of these calculations is that the matrix element in connection with the nuclear partner is expressed in terms of the nuclear partial radiative width, which is a measurable quantity and has been systematically studied with collections of a large body of data. This treatment makes it possible to evaluate the NEET probability more reliably. All of those are contained in Sec. II. Section III gives the predicted results for NEET probabilities in ^{189}Os, ^{197}Au, and ^{237}Np along with the published data. Section IV is a brief conclusion.

II. PROBABILITY, MATRIX ELEMENT, AND SELECTION RULE

We first calculate the NEET probability. The initial- and final-state wave functions of the nucleus-electron system for a NEET process are written as $\Psi_i=\Psi(I_i\Pi_i n_i l_i j_i FM)$ and $\Psi_f=\Psi(I_f\Pi_f n_f l_f j_f FM)$, respectively. I is the nuclear state spin, Π is its parity, (n,l,j) designates a single-electron state in an atom, $\vec{F}=\vec{I}+\vec{j}$ is the total spin of the nucleus-electron (or hole) system, and M is its projection. In the NEET process, the nucleus is excited from the state $(I_i\Pi_i)$ to the state $(I_f\Pi_f)$, while the atom decays from its initial state $(n_i l_i j_i)$ to the state $(n_f l_f j_f)$. The unperturbated energy eigenvalues of Ψ_i and Ψ_f are E_i and E_f, respectively.

Provided only the lowest order of the NEET process is taken into account, the wave function of the whole system is

$$\Psi(t)=a_i(t)\Psi_i+a_f(t)\Psi_f \ . \tag{1}$$

The NEET probability is normally very small, and the excited electron state decays chiefly through the channels of x-ray or Auger electron emissions. Thus it is justified to assume

$$|a_i(t)|^2=e^{-\lambda_i t} , \tag{2}$$

where $\tau_i=1/\lambda_i$ is the lifetime of the initial electron (hole) state. Inserting Eq. (1) into the Schrödinger equation,

$$i\hbar\frac{\partial\Psi(t)}{\partial t}=(H_0+\mathcal{H}')\Psi(t) , \tag{3}$$

where $\mathcal{H}'$ is the nucleus-electron interaction. The equation for the NEET amplitude is

$$i\frac{da_f(t)}{dt}=E_f a_f(t)+\mathcal{H}'_{fi}a_i(t) , \tag{4}$$

and the initial condition $a_f(0)=0$. Noting that

$$a_i(t)=e^{-iE_i t/\hbar-\lambda_i t/2} ,$$

it then yields

$$a_f(t)=\frac{\mathcal{H}'_{fi}}{(E_f-E_i)+i\Gamma_i/2}\times e^{-iE_f t/\hbar}(1-e^{i(E_f-E_i)t/\hbar-\lambda_i t/2}) , \tag{5}$$

where $\Gamma_i=\hbar\lambda_i$ is the level width and $\mathcal{H}'_{fi}$ is the transition matrix element, which we will discuss shortly. The NEET probability is

$$P=|a_f(\infty)|^2=\frac{|\mathcal{H}'_{fi}|^2}{(E_f-E_i)^2+\Gamma_i^2/4} \ . \tag{6}$$

Equation (6) shows a Lorentzian resonance around $E_f=E_i$, and Γ_i is the resonance width. For inner-shell hole states of intermediate or heavy elements, the values of Γ_i can be of an order of several tens of electronvolts [12].

Now we turn to the calculation of the transition matrix element and study the transition-selection rule. Beginning with an electric 2^L-pole multipole transition, the interaction Hamiltonian can be written as a scalar product of two tensors of rank L:

$$\mathcal{H}'^{(EL)}=\overline{\mathcal{Y}}_L(N)\overline{\mathcal{Y}}_L(e)\equiv\sum_\mu(-1)^\mu\mathcal{Y}_{L\mu}(N)\mathcal{Y}_{L-\mu}(e) , \tag{7}$$

where

$$\mathcal{Y}_{L\mu}(N)=\sum_k e_k r_k^L Y_{L\mu}(\hat{r}_k) \tag{8}$$

is the known nuclear electric 2^L-pole multipole transition operator,

$$\mathcal{Y}_{L\mu}(e)=-\frac{4\pi e}{2L+1}\frac{1}{r_e^{L+1}}Y_{L\mu}(\hat{r}_e) \tag{9}$$

is related to the 2^L-pole multipole field at the origin produced by the electron, and $Y_{L\mu}(\hat{r})$ is the spherical harmonics. Then the transition matrix element is

$$\begin{aligned}\mathcal{H}'^{(EL)}_{fi}&=\langle I_f\Pi_f n_f l_f j_f FM|\overline{\mathcal{Y}}_L(N)\mathcal{Y}_L(e)|I_i\Pi_i n_i l_i j_i FM\rangle\\&=(-1)^{I_f-F-1/2+L-l_i}e\left[\left[\frac{4\pi(2I_f+1)(2j_f+1)(2l_i+1)(2j_i+1)}{(2L+1)}\right]^{1/2}\right]\\&\times\mathcal{W}(I_i j_i I_f j_f,FL)\mathcal{W}(l_i j_i l_f j_f,\tfrac{1}{2}L)\langle I_f\Pi_f|\mathcal{Y}_L(N)|I_i\Pi_i\rangle\int\mathcal{R}_f(r)r^{-(L-1)}\mathcal{R}_i(r)dr ,\end{aligned} \tag{10}$$

where the $\mathcal{W}$'s are Racah coefficients and $\mathcal{R}(r)\equiv\mathcal{R}_{nlj}(r)$ is the electron (or hole) radial wave function. $\langle I_f\Pi_f|\mathcal{Y}_L(N)|I_i\Pi_i\rangle$ is the nuclear reduced transition matrix element, which is related to the reduced transition probability by

$$\begin{aligned}\mathcal{B}^{(EL)}_{fi}&=\sum_{\mu_i\mu_f\mu}\frac{1}{2I_i+1}|\langle I_f\Pi_f\mu_f|\mathcal{Y}_{L\mu}(N)|I_i\Pi_i\mu_i\rangle|^2\\&=\frac{2I_f+1}{2I_i+1}|\langle I_f\Pi_f|\mathcal{Y}_L(N)|I_i\Pi_i\rangle|^2 .\end{aligned} \tag{11}$$

The connection between the reduced transition probability and the partial radiative width is straightforward. As we know well that the partial radiative widths have already been systematically investigated and a great deal of data have been collected, Eq. (11) provides a solid foundation for estimating the transition matrix elements. We note that Morita [1] evaluated the matrix element by a entirely coherent model $\langle I_f\Pi_f|\mathcal{Y}_L(N)|I_i\Pi_i\rangle=ZeR_N^L$, where Z is the nuclear charge and R_N is the nucleus radius. This is certainly severe overestimation, especially for an electric dipole transition in heavy nuclei. It is well established that most of the electric dipole transition strength is collected to the giant dipole resonance region. The $E1$ transition probability is even less than a single-particle value, the Weisskopf unit, by a hindrance factor [11], which is on the average of the order of 10^{-2}–10^{-4}. From Eqs. (7) and (8), it is clear that the transition-selection rules are analogous for both the nucleus and electron partners in an electric 2^L-pole NEET process.

Now we proceed to calculate the magnetic dipole NEET probability, which was never discussed in detail previously. The Hamiltonian for the interaction of a point nuclear magnetic moment $\bar{\mu}_I$ with magnetic field $\bar{B}_e$ produced by the electron at the nucleus is

$$\mathcal{H}'^{(M1)} = -\bar{\mu}_I \bar{B}_e \ , \tag{12}$$

where

$$\bar{\mu}_j = \mu_N \sum_k (g_{sk}\bar{\sigma}_k + g_{lk}\bar{l}) \ , \tag{13}$$

$\mu_N = e\hbar/2Mc$ is the nuclear magneton, $g_{sk} = 2.79$ for protons and -1.9 for neutrons, and $g_{lk} = 1$ for protons and 0 for neutrons. Writing the explicit expression of $\bar{B}_e$ (e.g., see Ref. [13]), it yields

$$\mathcal{H}'^{(M1)} = \bar{\mu}_L \bar{\mu}'_0 + \bar{\mu}_L \bar{\mu}'_l \ , \tag{14}$$

where

$$\bar{\mu}'_0 = \frac{4\mu_B}{3r_e^2}\delta(r_e)\bar{s} \ , \tag{15}$$

stemming from the fact that s electrons have nonzero probability densities at the origin. $\bar{s}$ is the electron-spin operator, and $\mu_B = e\hbar/2mc$ is the Bohr magneton. The first term in Eq. (14) is called the Fermi contact interaction.

$$\bar{\mu}'_l = \frac{2\mu_B}{r_e^3}\left[\bar{l} - \bar{s} + \frac{3(\bar{r}_e\bar{s})}{r_e^2}\bar{r}_e\right] \tag{16}$$

is the contribution from the electron probability density outside the nucleus. It is easy to verify that

$$-s_\nu + \frac{3(\bar{r}\,\bar{s})}{r^2}r_\nu = -\sqrt{8\pi}(Y_2 s)_{1\nu} \equiv -\sqrt{8\pi}\sum_\mu c^{1\ \nu}_{1\ -\mu\ 2\ \mu+\nu} Y_{2\ \mu+\nu}(\hat{r}) s_{-\mu} \ . \tag{17}$$

Note that $\bar{Y}_2(\hat{r}_e)$ is a spatial tensor of rank 2, which may change the orbital angular momentum by two units. Then the transition matrix element for a magnetic dipole NEET is

$$\begin{aligned}\mathcal{H}'^{(M1)}_{fi} &= \langle I_f \Pi_f n_f l_f j_f FM | \mathcal{H}'^{(M1)} | I_i \Pi_i n_i l_i j_i FM \rangle \\ &= (-1)^{j_i + I_f - F}\sqrt{(2j_f+1)(2I_f+1)}\,\mathcal{W}(I_i j_i I_f j_f, F1)\langle I_f \Pi_f | \mu_I | I_i \Pi_i \rangle \\ &\times \left\{ \delta_{l_i 0}\delta_{l_f 0}\frac{2}{\sqrt{3}}\mu_B \mathcal{R}_i(0)\mathcal{R}_f(0) + 2\mu_B \int \mathcal{R}_f(r)\frac{1}{r}\mathcal{R}_i(r)dr \right. \\ &\times \left[\delta_{l_i l_f}(-1)^{3/2 - l_i - j_i}\sqrt{l_i(l_i+1)(2l_i+1)(2j_i+1)}\,\mathcal{W}\left(l_i j_i l_f j_f, \frac{1}{2}1\right) \right. \\ &\left. \left. + 3\sqrt{5}\sqrt{(2l_i+1)(2j_i+1)}\,C^{l_f\ 0}_{l_i\ 0\ 2\ 0}\begin{bmatrix} l_f & 1/2 & j_f \\ l_i & 1/2 & j_i \\ 2 & 1 & 1 \end{bmatrix} \right] \right\} , \end{aligned} \tag{18}$$

where $\mathcal{R}(0)$ is the value of electron radial wave function at the origin, the C's are the Clebsch-Gordan coefficients.

$$\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & j \end{bmatrix}$$

is the Wigner $9j$ symbol [14], and $\langle I_f \Pi_f | \mu_I | I_i \Pi_i \rangle$ is the reduced matrix element of nuclear magnetic moment, which is related to the usually accepted magnetic dipole reduced transition probability by

$$\mathcal{B}^{(M1)}_{fi} = \frac{3}{4\pi}\frac{2I_f+1}{2I_i+1}|\langle I_f \Pi_f | \mu_I | I_i \Pi_i \rangle|^2 \ . \tag{19}$$

In total there are three terms on the right-hand side of

TABLE I. Theoretical values for NEET probabilities and measured data. E_i and E_f are the unperturbated energy eigenvalues of the initial and final states of the nucleus-electron system. Γ_i is the level width of the initial electron (hole) state [12]. Γ_{fi} is the nuclear partial radiative width, taken from Ref. [16] (^{189}Os), [17] (^{197}Au), and [18] (^{237}Np), respectively. F is the total spin of the nucleus-electron system. $\mathcal{H}^*_{fi}$ and P^* are the transition matrix element and NEET probability by assigning the nuclear reduced radiative partial width the single-particle value (the Weisskopf unit). $\mathcal{H}'_{fi}$ and P are the corresponding values calculated by using the published data for Γ_{fi}. P_{expt} are the measured NEET probabilities published in Refs. [7–9].

	$E_f - E_i$ (eV)	Γ_i (eV)	Γ_{fi} (μeV)	Type of transition	F	$\mathcal{H}'^*_{fi}$ (eV)	P^*	$\mathcal{H}'_{fi}$ (eV)	P	P_{expt}
^{189}Os	1261.5	34	0.40	$M1$	2	0.155	1.2×10^{-8}	3.7×10^{-2}	1.2×10^{-9}	$(1.7\pm0.2)\times10^{-7}$
^{197}Au	74.18	40	0.343	$M1$	1	0.225	1.2×10^{-5}	4.3×10^{-2}	4.2×10^{-7}	$(2.2\pm1.8)\times10^{-4}$
^{237}Np	1902.0	80	8.2	$E1$	3	3.1	3.6×10^{-6}	0.15	8.5×10^{-9}	$(2.1\pm0.6)\times10^{-4}$
					4	2.45	2.3×10^{-6}	0.122	5.6×10^{-9}	

Eq. (18). The first one comes from Eq. (15), which is of a nonvalishing value only for the *s-s* wave transition. The next is the contribution from the electron orbital angular momentum operator in Eq. (16), whereas the third one stems from Eq. (17). It should be noted that the selection rule for electrons in magnetic dipole NEET is different from that of the nucleus partner. The latter is still a spin-flip transition, but the former allows change of two units for single-particle orbital angular momentum.

III. NEET IN ^{189}OS, ^{197}AU, AND ^{237}PU

As an example, we calculate the NEET probabilities in ^{189}Os, ^{197}Au, and ^{237}Np in terms of the formalism given above. The nuclear and atomic level diagrams concerned are shown in Fig. 1. Table I lists the parameters used in the calculations and the calculated results along with the available measured data. For each NEET process, if there is more than one channel available (e.g., mixed $M1$-$E2$ transitions or different allowed values of the system total spin F), then the results for each channel are given. As indicated above, a crucial point in the calculations is the evaluation of the nuclear matrix elements, which are deduced from the measured radiative transition probabilities in the present project. In order to demonstrate the importance of this treatment, we present two sets of the predicted interaction matrix elements and NEET probabilities in Table I. One is that calculated with the published data of partial radiative widths, whereas the other set is obtained by assigning a single-particle value, the Weisskopf unit, to the reduced transition probabilities. The ratios of the two sets for NEET probabilities would just be the hindrance factors, which are 0.057 (^{189}Os, $M1$ transition), 0.0356 (^{197}Au, $M1$ transition), and 0.002 34 (^{237}Np, $E1$ transition), respectively. The predicted NEET probabilities would be still less than Morita's results [1], which were based on an entirely coherent model.

It can be seen from Table I that there is a great discrepancy between the presently predicted and published data. One should note that the experimental technique for NEET is very difficult. The useful signals should be extracted from very complicated spectra, and reliable results can be obtained only if careful corrections are made to eliminate the effects from all other possible nuclear excitation mechanisms. More accurate measurements are highly recommended. From the view of theoretical investigation, a complete calculation of NEET should be performed in the formalism of relativistic quantum mechanics.

IV. CONCLUSION

The results can be summarized as follows.

(1) Equation (6) is a simplified formula to calculate the NEET probability based upon nonrelativistic quantum

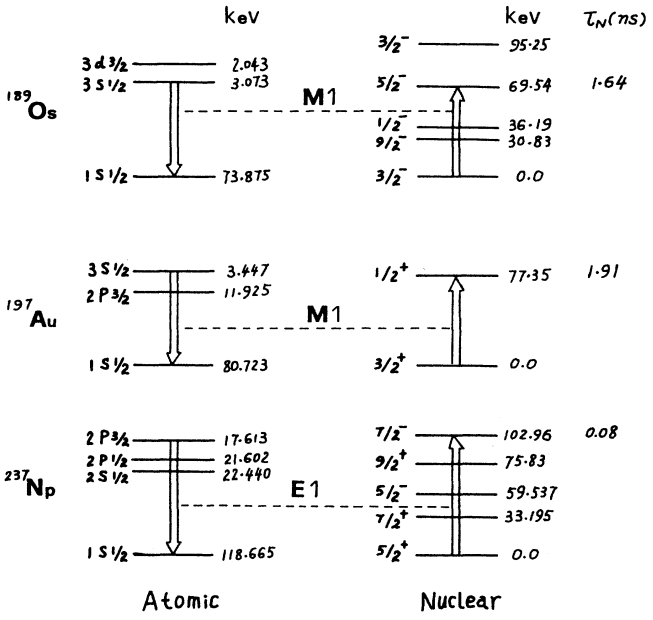

FIG. 1. NEET diagrams. The atomic levels are taken from Ref. [15]. The nuclear levels are taken from Ref. [16] (^{189}Os), [17] (^{197}Au), and [18] (^{237}Np), respectively. τ_N is the level lifetime.

mechanics. In this equation the effect on NEET from x-ray and Auger-electron emissions is attributed to the Lorentzian resonance width.

(2) The transition matrix element for electric 2^L-pole NEET is given in Eq. (10). In this case the nucleus and electron partners are of the same selection rule. The transition matrix element of the nucleus partner is just the reduced matrix element adopted usually in nuclear gamma decay, which may be deduced from the well-established database on radiative partial widths. This formalism makes the estimation of the NEET probability more reliable. It is indicated that the previous calculations using entirely coherent model or single-proton model would cause severe overestimations, especially for electric dipole transitions in heavy nuclei.

(3) Equation (18) gives detailed calculations of the transition matrix element for magnetic dipole NEET, which contains three terms stemming from the nonzero probability density of *s*-wave electrons inside the nucleus, the electron orbital angular momentum, and intrinsic magnetic moment outside the nucleus, respectively. One feature of the electron transition operator is that it contains a term with spatial tensor of rank 2. Thus the transition-selection rule for the electron partner is no longer a pure spin-flip. It allows a change of two units for electron orbital angular momentum. In contrast, the orbital angular momentum of a single nucleon remains unchanged during the transition.

(4) The NEET probabilities in ^{189}Os, ^{197}Au, and ^{237}Np were calculated in terms of the present formalism. In those calculations the experimentally identified hindrance factors for the concerned partial radiative widths were

taken into account. A great discrepancy has been found between the predicted and published data [19]. More accurate measurements are suggested to identify the origin of the discrepancy.

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[19] We have received a letter from Prof. M. Morita in June 1991, informing that he and his collaborators (M. Morita in June 1991, H. Ohtsubo, T. Sato, and K. Oka) performed a similar theoretical investigation on NEET using time-dependent perturbation theory. Their results were collected in 1990 in Osaka University as a Governmental Report for Grand-in-Aid for Scientific Research. This report was written in Japanese.