

# Shell-model picture of virtual detour transitions in $^{41}\text{Ca}$ radiative electron-capture decay

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(Received 17 November 1995)

For the first forbidden unique ( $1u$ ) radiative electron-capture  $\beta$  decay of  $^{41}\text{Ca}$ , a contribution of the  $\gamma/\beta$  detour transitions via virtual nuclear states to the bremsstrahlung spectrum has been considered in terms of the shell model. Calculations of the matrix elements for the virtual  $E1$   $\gamma$  and allowed Gamow-Teller  $\beta$  transitions have been performed with the use of the Warburton, Becker, Millener, and Brown interactions. For the effective charge, which describes the contribution of the detour transitions, an interval  $0.96 < e_{\text{eff}} < 1$  has been found. The model predictions are fairly close to the experimental value  $e_{\text{eff}} = 0.78$ . A possible origin of the small remaining deviation is discussed.

PACS number(s): 21.60.Cs, 23.40.Hc

## I. INTRODUCTION

The  $\beta$  decay via capture of an orbital electron, in which the emission of neutrino is accompanied by radiation of a photon, and both these particles statistically share the transition energy, is called the radiative electron capture (REC) process. This is a higher order process with a probability a few orders of magnitude lower than the probability of the nonradiative electron-capture decay, accompanied by the emission of the neutrino alone.

Total intensities and spectral distributions of photons were studied experimentally for a number of allowed electron-capture transitions and found to agree well with the theory of internal-bremsstrahlung (IB) [1]. In contrast to this, experiments on the forbidden REC in  $^{41}\text{Ca}$  and  $^{59}\text{Ni}$ , performed by the Aarhus-Warsaw Collaboration [2–4], revealed a striking disagreement with predictions of the IB theory [5–7] (for the first indication of this disagreement see Ref. [8]). The shape of energy spectra of photons was found to be quite different from the theoretical one, and the total number of photons per nonradiative decay appeared to be significantly higher than calculated.

To explain this disagreement, Kalinowski *et al.* [9–11] proposed to take into account detour  $\beta/\gamma$  or  $\gamma/\beta$  transitions via virtual nuclear states. They followed ideas developed by Ford and Martin [12] in connection with the analogous problem of an excess of photons observed for IB accompanying forbidden  $\beta^-$  decay.

Estimates show that for a direct decay of allowed type,

the role of detour transitions is negligible, while for a forbidden decay these transitions may compete. For forbidden decays with spin change by two units, like in the case of  $^{41}\text{Ca}$ , the detour transitions are presumably composed predominantly of a dipole  $\gamma$  transition followed by an allowed Gamow-Teller (GT)  $\beta$  transition, or vice versa.

The contribution of detour transitions to the IB spectrum is given by an effective charge  $e_{\text{eff}}$ . In the theory presented in Refs. [10,11], the value of this charge is considered as a free parameter. It can be derived from fitting the theoretical spectrum to the experimental one. There is, however, an obvious interest in reproducing the results through microscopic calculations. Until now such calculations have been performed only for the radiative capture decay of  $^{204}\text{Tl}$  [13].

The present paper provides a shell-model analysis of the radiative-electron-capture data for  $^{41}\text{Ca}$ . Matrix elements of the  $\gamma(E1)$  and  $\beta$  (GT) virtual transitions were calculated based on the shell-model approach which uses interactions developed by Warburton, Becker, Millener, and Brown (WBMB) [14].

## II. FIRST-FORBIDDEN UNIQUE RADIATIVE K CAPTURE IN $^{41}\text{Ca}$

The decay of  $^{41}\text{Ca}$  [15] proceeds via a single electron-capture transition to the ground state of  $^{41}\text{K}$ . The spin and parity of the initial and final states is  $7/2^-$  and  $3/2^+$ , respectively. The transition is thus first-forbidden unique ( $1u$ ). The forbiddenness of the decay is reflected in the half-life which is as long as  $T_{1/2} = 1.04(5) \times 10^5$  yr [16], despite the appreciable decay energy  $Q_{\text{EC}} = 421.3(4)$  keV [15].

We focus our attention on the radiative capture of the K electron. The theory for the relevant  $1S$  component of the

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photon spectrum seems to be more exact than for the remaining components. Experimentally, the  $1S$  component was selected in a coincidence measurement by gating the photons with the 3.3 keV potassium K x rays [3]. The end-point energy of this component is  $k_0 = Q_{EC} - B_{1S} = 417.7$  keV. Here,  $B_{1S} = 3.6$  keV is the binding energy of electron in the K shell of a potassium atom.

The theory of the radiative K capture with inclusion of the detour transitions can be found in Ref. [11] and references quoted therein. In the following we recall the main formulas and definitions, specified for the  $1u$  transition.

For the  $1S$  component, the probability of emission of a photon with energy in the interval  $k$ ,  $k + dk$  relative to the probability  $w_K$  of the nonradiative K capture is given by

$$\frac{dw_{1S}(k)}{w_K} = \frac{\alpha}{\pi m_e^2} \frac{k(k_0 - k)^2}{k_0^2} R_{1S}(k) dk, \quad (1)$$

where  $\alpha$  is the fine structure constant,  $m_e$  the electron rest-mass energy, and  $R_{1S}$  the shape factor. The formula for the shape factor, which accounts for the detour transitions, reads

$$R_{1S}(k) = R_{1S}^{\text{IB}}(k) + 2 \left( \frac{e_{\text{eff}} m_e}{k_0} \right)^2 + A_{1S} \frac{e_{\text{eff}} m_e k}{k_0^2}, \quad (2)$$

where  $R_{1S}^{\text{IB}}(k)$  is the shape factor resulting from the pure IB theory [1,6,7] and  $A_{1S}(k)$  is one of the components of the  $R_{1S}^{\text{IB}}(k)$  function. Intensity of the detour transitions is described by the effective charge  $e_{\text{eff}}$  in units of the elementary charge  $e$ . The term proportional to  $e_{\text{eff}}$  accounts for the interference between the IB and the detour transitions.

For the radiative capture decay of  $^{41}\text{Ca}$  one finds (Refs. [3,9,10]) a comparison of the theoretical and experimental spectra of the  $1S$  component. For  $e_{\text{eff}} = 0$ , that is on the level of the IB theory, the slope of the experimentally determined shape factor clearly differs from predictions. The intensity summed above 95 keV amounts to  $2.5 \times 10^{-4}$  relative to the nonradiative K capture, and exceeds the relevant theoretical value by a factor of 6.6. This theoretical value does not depend on the nuclear matrix element of the  $1u$  transition. If detour transitions are included a quite satisfactory agreement with the experiment is found for  $e_{\text{eff}} = 0.78$ . In this case, however, the theory is not independent of nuclear structure.

### III. THE EFFECTIVE CHARGE IN TERMS OF THE SHELL MODEL

As derived in Ref. [11], the effective charge, expressed through reduced matrix elements of the transitions involved in radiative capture process in  $^{41}\text{Ca}$ , is given by

$$e_{\text{eff}} = e_{\text{eff}}^{(i)} - e_{\text{eff}}^{(f)}, \quad (3)$$

where

$$e_{\text{eff}}^{(i)} = \frac{1}{e} \sum_n \varepsilon_{i,n} \sqrt{\frac{4\pi}{2I_n + 1}} \frac{\langle f || T(\text{GT}) || n \rangle \langle n || T(E1) || i \rangle}{\langle f || T(1u) || i \rangle}, \quad (4)$$

$$e_{\text{eff}}^{(f)} = \frac{1}{e} \sum_n \varepsilon_{f,n} \sqrt{\frac{4\pi}{2I_n + 1}} \frac{\langle f || T(E1) || n \rangle \langle n || T(\text{GT}) || i \rangle}{\langle f || T(1u) || i \rangle}. \quad (5)$$

The operators, related to a single nucleon, responsible for electric dipole  $\gamma$  transition and for Gamow-Teller and first forbidden unique  $\beta$  transition have the following form:

$$T(E1) = \left[ e_\pi \frac{1}{2} (1 - \tau_0) + e_\nu \frac{1}{2} (1 + \tau_0) \right] r Y_1,$$

$$T(\text{GT}) = \frac{\lambda}{\sqrt{4\pi}} \sigma \tau_+, \quad T(1u) = \lambda r (\sigma Y_1)_2 \tau_+,$$

where  $\sigma$  is the Pauli spin matrix vector,  $\tau_0$  and  $\tau_+$  are the diagonal and raising Pauli isospin matrices, respectively,  $Y_1$  are the spherical harmonics of rank one, and  $\lambda = |g_A/g_V|$ , where  $g_A/g_V$  is the ratio of the weak-interaction coupling constants. The proton and neutron effective charges,  $e_\pi$  and  $e_\nu$ , describing the electric dipole transitions may depend on the initial and final single-particle states involved [17]. The summations are performed over a complete set of nuclear states  $|n\rangle$  with angular momentum  $I_n$ . The correction of the nuclear  $E1$  transitions for the center-of-mass motion yields the effective charges  $e_\pi = (N/A)e$  and  $e_\nu = -(Z/A)e$ , where  $N, Z$ , and  $A$  are neutron, proton, and mass numbers, respectively [18].

The energy factors  $\varepsilon_{i,n}$  and  $\varepsilon_{f,n}$  are equal to

$$\varepsilon_{i,n} = \frac{E_n - E_i}{E_n - E_i + k}, \quad \varepsilon_{f,n} = \frac{E_n - E_f}{E_n - E_f + k},$$

where  $E_n$ ,  $E_i$ , and  $E_f$  are the energies of virtual, initial, and final states, respectively, and  $k$  is the energy of the photon. In a usual approximation of high excitations  $E_n - E_i \gg k$  one has  $\varepsilon_{i,n} = \varepsilon_{f,n} = 1$ . This approximation together with state-independent effective charges gives  $e_{\text{eff}} = (e_\pi - e_\nu)/e$ . When only the correction for the center-of-mass motion is taken into account, this gives  $e_{\text{eff}} = N/A + Z/A = 1$ . Any other choice for value of  $e_\pi$  on frequently used condition that  $e_\pi = e + \Delta e$  and  $e_\nu = \Delta e$  [17] always gives  $e_{\text{eff}} = 1$ , too.

If the spectrum of the virtual states is available, a reduction of  $e_{\text{eff}}$  due to the energy factors can be estimated.

#### A. Extreme single-particle shell model picture

Figure 1 presents single particle levels of  $^{41}\text{Ca}$  from the Woods-Saxon model with the universal set of parameters [19,20]. It also shows the  $1u$  transition between the  $|i\rangle = |v f_{7/2}, 7/2^-\rangle$  ground state of  $^{41}\text{Ca}$  and the  $|f\rangle = |(v f_{7/2})^2 \pi d_{3/2}^{-1}, 3/2^+\rangle$  ground state of  $^{41}\text{K}$ , as well as two possible  $\gamma(E1)/\beta(\text{GT})$  detour transitions via the virtual  $5/2^+$  excited states of  $^{41}\text{Ca}$ :

$$|1\rangle = |v f_{7/2} \pi f_{5/2} \pi d_{3/2}^{-1}, 5/2^+\rangle$$

and

$$|2\rangle = |(v f_{7/2})^2 \nu d_{5/2}^{-1}, 5/2^+\rangle.$$

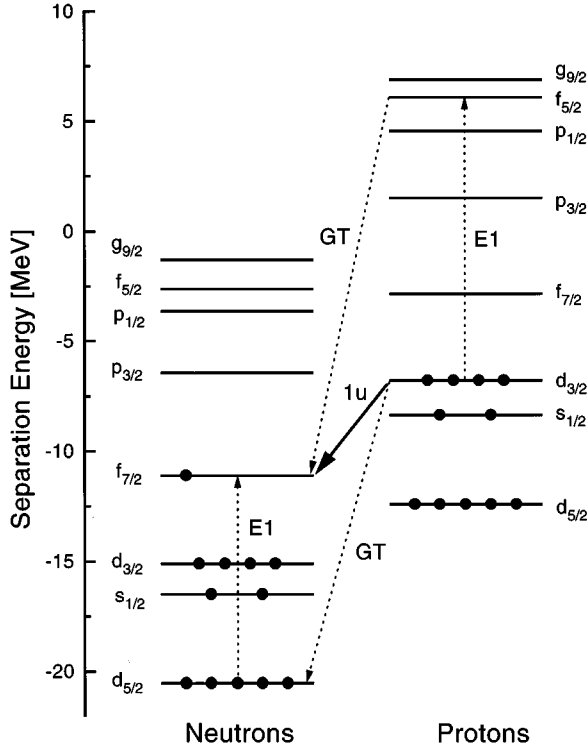


FIG. 1. Woods-Saxon model [19,20] predictions for the single-particle states of  $^{41}\text{Ca}$ , and for the single-particle transitions to be considered in the analysis of the radiative electron-capture  $^{41}\text{Ca} \rightarrow ^{41}\text{K}$  decay.

Any detour transitions with the opposite sequence,  $\beta(\text{GT})/\gamma(\text{E1})$ , are ruled out here by the Pauli principle. The complete set of intermediate states reduces here to the configurations  $|1\rangle$  and  $|2\rangle$ . Summing over these configurations can be performed with help of angular momentum algebra and yields  $e_{\text{eff}} = e_{\text{eff}}^{(i)} = [e_{\pi}(d_{3/2}, f_{5/2}) - e_{\nu}(d_{5/2}, f_{7/2})]/e$ , again equal to 1 for  $e_{\pi}/e$  and  $e_{\nu}/e$  equal to  $N/Z$  and  $-Z/A$ , respectively.

It is expected that in reality simple shell-model configurations, which presumably contribute to the detour transitions, are spread over many  $5/2^+$  levels due to residual interactions. A study of this effect will be presented in the following.

### B. The $sd$ - $pf$ model space with the WBMB interaction

A spectrum of the  $5/2^+$  excited states of  $^{41}\text{Ca}$ , and the relevant values of the  $E1$  and GT reduced matrix elements  $M_n(E1) = \langle n || T(E1) || i \rangle$  and  $M_n(\text{GT}) = \sqrt{4\pi} \langle f || T(\text{GT}) || n \rangle$  of importance for the detour transitions, have been obtained by shell-model calculations with the WBMB interaction. This interaction is described in detail by Warburton *et al.* [14]. It was originally developed to study mass systematics for  $A=29$ – $44$  nuclei.

Results of the present calculations are available for 100 states with isospin  $T=1/2$  and 63 states with  $T=3/2$ . They are shown in Figs. 2 and 3.

Figure 2 shows the distributions of the  $E1$  and GT transition strengths. To obtain these distributions, strength values of individual transitions, related to the matrix elements as follows:

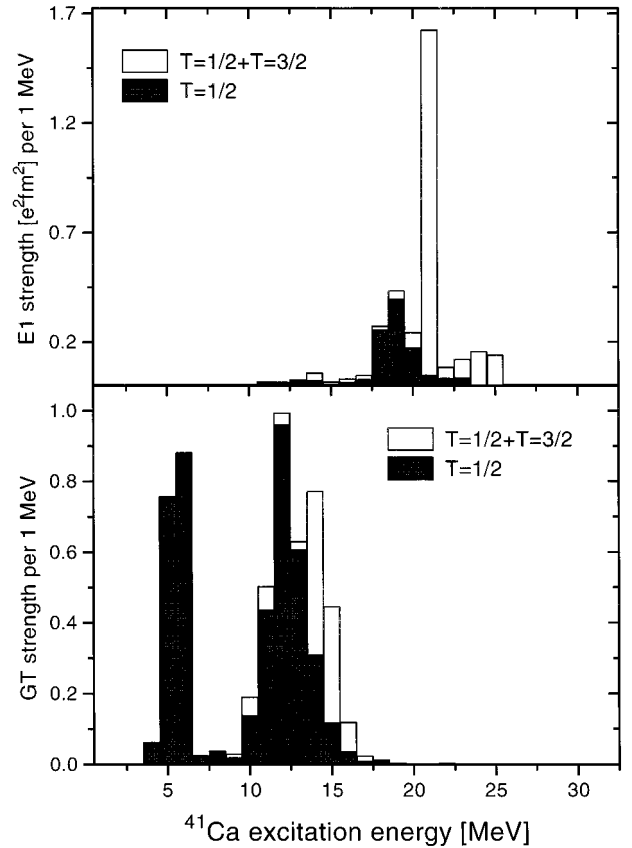


FIG. 2. Strength distributions versus the  $^{41}\text{Ca}$  excitation energy resulting from the shell-model calculations performed in the present work with the use of the WBMB interactions from [14]: the virtual  $E1$  transitions between the  $7/2^-$  ground state and  $5/2^+$  excited states of  $^{41}\text{Ca}$  (upper part), and the virtual Gamow-Teller  $\beta$  transitions between the  $5/2^+$  states of  $^{41}\text{Ca}$  and the  $3/2^+$  ground state of  $^{41}\text{K}$  (lower part). The position of IAS is 5.8 MeV.

$$B(E1) = \frac{1}{2I_i + 1} |M(E1)|^2 e^2 \text{fm}^2$$

and

$$B(\text{GT}) = \frac{1}{2I_n + 1} |M(\text{GT})|^2,$$

have been summed for 1 MeV intervals of excitation energy in  $^{41}\text{Ca}$ .

The calculated  $E1$  strength distribution is approximately centered around 20 MeV, which fits the systematics of the giant dipole resonances (see, e.g., [21]). As regards the calculated GT strength, its main part is observed around 12 MeV, that is about 6 MeV above the energy corresponding to the position of the isobaric analog (IAS) of the  $^{41}\text{K}$  ground state [22]. This agrees well with the systematics of the energy differences between GT resonances and IAS [23]. However, a non-negligible part of the GT strength is found below IAS.

The GT strength distribution is located on a tail of the  $E1$  distribution. From the broad excitation energy range, in which the two distributions overlap, one obtains a contribution to the numerator in the expression (4) for the effective

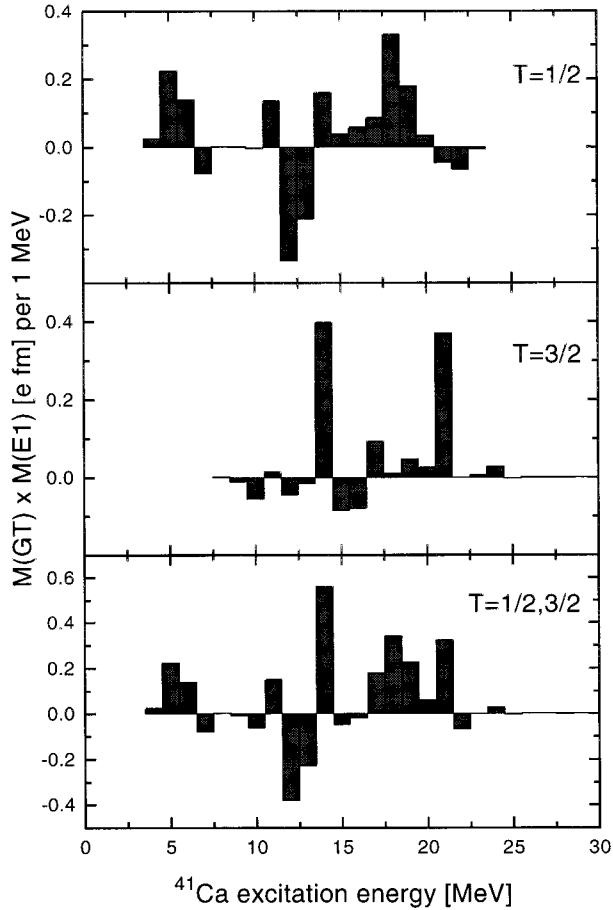


FIG. 3. Results of the shell-model calculations performed in the present work with the use of the WBMB interactions from Ref. [14]: products of the reduced matrix elements of the  $E1$  and Gamow-Teller virtual transitions which contribute to the detour transitions in the radiative electron-capture  $^{41}\text{Ca} \rightarrow ^{41}\text{K}$  decay.

charge. Obviously, the value of this numerator, and in consequence (for a given reduced  $1u$  matrix element) the effective charge is defined not only by absolute values of the reduced  $E1$  and GT matrix elements but also by their relative phase. This is illustrated in Fig. 3 through the products of these matrix elements summed for 1 MeV intervals of the  $^{41}\text{Ca}$  excitation energy.

Interval distributions of the matrix-element products are shown separately for the  $T=1/2$  and  $T=3/2$  virtual  $5/2^+$  states, and after adding the two isospin contributions. Summing the latter joint distribution over the entire excitation energy range yields

$$\sum_n M_n(\text{GT})M_n(E1) = 1.376 e \text{ fm.}$$

The role played by the neglected energy-dependent factor can be estimated by calculating the sum of the same product weighted by this factor with the value of the photon energy  $k$  replaced by the end-point value  $k_0$  what represents a lower limit of the sum:

$$\sum \frac{E_n - E_i}{E_n - E_i + k_0} M_n(\text{GT})M_n(E1) = 1.327 e \text{ fm.}$$

### C. Matrix element of the $1u$ transition

For the direct ground-state to ground-state  $1u$  transition, the relation between the matrix element and the relevant transition strength is

$$M(1u) = \langle f || T(1u) || i \rangle = \sqrt{(2I_i + 1)B(1u)} \text{ fm.} \quad (6)$$

For the decay of  $^{41}\text{Ca}$ , Warburton *et al.* [24] give the theoretical  $1u$ -transition strength based on the shell model with the WBMB interaction. The values  $B_1(\text{WBMB, free}) = 0.164 \text{ fm}^2$  and  $B_1(\text{WBMB, eff}) = 0.043 \text{ fm}^2$  correspond to omission and inclusion of an estimate of the ground-state correlations, respectively, where  $B_1$  is the strength according to the definition adopted in Ref. [24], which is related to  $B(1u)$  by  $B(1u) = (3/4\pi)B_1$ . It follows that the corresponding  $B(1u)$  values amount to  $0.0392$  and  $0.0103 \text{ fm}^2$ , respectively. As  $I_i = 7/2$ , the relevant  $M(1u)$  values are  $0.560$  and  $0.287 \text{ fm}$ .

The matrix element can also be derived from experimental data:

$$B(1u) = \frac{6.583 \times 10^8 \text{ s}}{(q_K/m_e)^2 (ft)} \text{ fm}^2. \quad (7)$$

The numerical value in the numerator corresponds to the relation  $B(\text{GT}) = 6166 \text{ s/ft}$  for a GT transition. For the  $^{41}\text{Ca}$ , the half-life equals  $t = 3.28(16) \times 10^{12} \text{ s}$ . The (allowed [25]) statistical-rate-function value amounts to  $f = 0.0150$ . With the K-capture neutrino energy  $q_K$  expressed in the electron rest-mass-energy units one obtains  $B(1u) = 0.020(1) \text{ fm}^2$  and  $M(1u) = 0.40(1) \text{ fm}$ .

### D. Limits for the effective charge

With  $M(1u) = 0.560 \text{ fm}$  and  $\sum M(\text{GT})M(E1) = 1.376 e \text{ fm}$  formula (4) leads again to  $e_{\text{eff}} = 1.00$ . If the sum of the products of the GT and  $E1$  matrix elements is taken with the  $(E_n - E_i)/(E_n - E_i + k_0)$  weight factor, the effective charge value is reduced by 4 percent. The interval for the effective charge is  $0.96 < e_{\text{eff}} < 1$ .

A replacement of  $M(1u) = 0.560$  with the other theoretical value,  $M(1u) = 0.287$ , would yield  $e_{\text{eff}} = 1.96$ . This result is rejected because of the obvious inconsistency between the two theoretical treatments of the  $1u$  and  $E1/\text{GT}$  transitions.

The experimental value of  $M(1u)$  occurs between the two theoretical matrix elements. In principle, to reproduce the experimental  $M(1u)$  value the theoretical approach could be improved by accounting for all inadequacies in the restricted shell-model calculations. However, if the same refined model were applied to calculate the GT and  $E1$  matrix elements, the upper limit for  $e_{\text{eff}}$  is expected to be again 1, while the lower limit would be close to that given above.

In the above considerations it is assumed that the effective charge is defined predominantly by the detour transitions in the  $E1/\text{GT}$  sequence — the contribution from formula (5) is consequently neglected. This assumption, justified in the case of the models discussed above, is likely to be invalid for

a more complete shell-model space. The GT/E1 detour transitions via intermediate virtual  $5/2^-$  states of  $^{41}\text{K}$  may have a non-negligible contribution to the theoretical  $e_{\text{eff}}$  value.

The results can be discussed in terms of the number of  $\hbar\omega$  excitations relative to the  $^{40}\text{Ca}$  closed-shell configuration. The present calculation assumes  $0\hbar\omega$  for the  $^{41}\text{Ca}$  ground state and  $1\hbar\omega$  for the  $^{41}\text{K}$  ground state. The Pauli allowed excited intermediate states are  $1\hbar\omega$  for  $^{41}\text{Ca}$  and  $2\hbar\omega$  for  $^{41}\text{K}$ . The detour transition [Eq. (4)] follows the path

$$^{41}\text{Ca}(0) \rightarrow E1 \rightarrow ^{41}\text{Ca}(1) \rightarrow \text{GT} \rightarrow ^{41}\text{K}(1),$$

where the number in parentheses indicates the assumed  $\hbar\omega$  value. The path of Eq. (5), given by

$$^{41}\text{Ca}(0) \rightarrow \text{GT} \rightarrow ^{41}\text{K}(2) \rightarrow E1 \rightarrow ^{41}\text{K}(1),$$

is zero because the GT operator cannot change  $\hbar\omega$ . Higher-order correlations will result, for example, in a  $(0+2)$   $\hbar\omega$  structure for the  $^{41}\text{Ca}$  ground state and a  $(1+3)$   $\hbar\omega$  structure for the  $^{41}\text{K}$  ground state. The complete set of intermediate states must include  $(1+3)$   $\hbar\omega$  for  $^{41}\text{Ca}$  and  $(2+4)$   $\hbar\omega$  for  $^{41}\text{K}$ . This leads to the additional routes for Eq. (4):

$$^{41}\text{Ca}(2) \rightarrow E1 \rightarrow ^{41}\text{Ca}(1) \rightarrow \text{GT} \rightarrow ^{41}\text{K}(1)$$

and

$$^{41}\text{Ca}(2) \rightarrow E1 \rightarrow ^{41}\text{Ca}(3) \rightarrow \text{GT} \rightarrow ^{41}\text{K}(3).$$

It also leads to nonzero routes for Eq. (5) of the form

$$^{41}\text{Ca}(2) \rightarrow \text{GT} \rightarrow ^{41}\text{K}(2) \rightarrow E1 \rightarrow ^{41}\text{K}(1)$$

and

$$^{41}\text{Ca}(2) \rightarrow \text{GT} \rightarrow ^{41}\text{K}(2) \rightarrow E1 \rightarrow ^{41}\text{K}(3).$$

We speculate that these last terms may give a value for  $e_{\text{eff}}^{(f)}$  which is out of phase with  $e_{\text{eff}}^{(i)}$ . Unfortunately, the shell-model dimensions of the intermediate  $(1+3)$   $\hbar\omega$  states are too large in order to carry out a calculation and this must be left to the future.

#### IV. SUMMARY AND CONCLUSIONS

The present work presents a shell-model treatment of the first forbidden unique radiative electron-capture decay of  $^{41}\text{Ca}$ . Following Kalinowski *et al.* [9–11], it takes into account a competition between two mechanisms of the photon

emission: the internal bremsstrahlung and the process of  $\gamma/\beta$  detour transitions via virtual nuclear states. The  $\gamma$  and  $\beta$  transitions are here of  $E1$  and allowed GT character, respectively.

In the general theory of the  $1u$  radiative electron-capture decay [9–11], a contribution of the detour transitions is expressed via the effective charge  $e_{\text{eff}}$ . A lower limit of  $e_{\text{eff}}$  resulting from the shell-model calculations performed in this work is 0.96. Although, the experimental value  $e_{\text{eff}}=0.78$  [10] is not far from it, and one may conclude that the detour transitions are indeed dominated by the  $E1/\text{GT}$  transitions, the deviation from the theoretical estimate seems significant. Indeed, a comparison of the experimental and theoretical shape factors given in Fig. 2 of Ref. [10] indicates that the uncertainty of the experimental  $e_{\text{eff}}$  value is below 0.10.

To clear up the origin of this small discrepancy between the experiment and theory one should calculate a contribution to  $e_{\text{eff}}$  from possible reversed sequence, GT/E1, virtual transitions. One may also consider such virtual detour processes as, e.g.,  $M1$  transitions followed by first forbidden nonunique transition, although in view of estimates performed already by Kalinowski [11] their contribution is expected to be negligible. Additionally, one could take into account that the axial current is only partly conserved. The coupling constant  $g_A$  may be different for the GT transitions between highly excited intermediate states and the final ground state than for the  $1u$  transition between the initial and the final ground states. In the present approach the weak-interaction coupling constant cancels out in the definition of  $e_{\text{eff}}$  [see Eqs. (3)–(5)]. If all that were not sufficient one could think about a contribution from nonnucleonic degrees of freedom.

As a by-product of this study, the distribution of the GT strength has been derived. It may be verified via a  $^{41}\text{K}(p,n)^{41}\text{Ca}$  reaction experiment which, to our knowledge, has not been performed earlier at energies and conditions suitable for the GT resonance identification.

#### ACKNOWLEDGMENTS

One of the authors (J.L.Ž.) thanks the Institute for Nuclear Science, Grenoble, for hospitality during his three months stay in France, where a part of this work was completed. This work was partially supported by the Polish Committee of Scientific Research under BST (J.L.Ž., M.P.) and Grant No. 2 P03B 034 08 (S.G.R.), and NSF Grant 94-03666 (B.A.B).

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