Shell-model calculation of ^{99}Tc beta decay in astrophysical environments

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Using the shell-model Lanczos method, we calculate the Gamow-Teller matrix elements for beta transitions of astrophysical interest from excited states of ^{99}Tc ($\frac{7}{2}^+$,141 keV; $\frac{5}{2}^+$,181 keV) to the ground and excited states of ^{99}Ru. The level schemes of low-lying positive-parity states in these nuclei and in the analogous isotonic nuclei ^{97}Nb-^{97}Mo are reproduced fairly well within a model space consisting of low-seniority excitations in the $1g\,2d$ shell, which are mixed via the Kallio-Kolltveit effective interaction. The calculations lead to a ^{99}Tc half-life of $\sim$20 yr at a stellar temperature of 3×10^8 K typical for the *s* process with a ^{22}Ne(α,n)^{25}Mg neutron source. Referring to recent studies of thermal-pulse *s*-process models, we stress that a substantial amount of ^{99}Tc can survive the *s* process in spite of its enormously enhanced decay rate. The factual observation of ^{99}Tc at the surface of certain stars, therefore, does not necessarily contradict an *s*-process scenario with ^{22}Ne as a neutron source.

I. INTRODUCTION

The very existence of Tc (most probably ^{99}Tc) at the surface of certain (e.g., type *S*) stars[1–3] is one of the strongest supports for the idea of nucleosynthesis of heavy elements by way of slow neutron capture (the *s* process).[4–8] On the other hand, empirical studies of the solar abundance curve for *s*-process nuclides (e.g., Refs. 9 and 10), as well as the existing astrophysical scenarios for the *s* process [e.g., the He-shell recurrent thermal pulses in intermediate-mass asymptotic-giant-branch stars with the ^{22}Ne(α,n)^{25}Mg neutron source[11–13]], suggest a typical temperature of $\sim 3\times10^8$ K at the *s*-process site.

A crucial question first raised by Cameron[14] is whether ^{99}Tc can survive such hot environments before it is dredged up to, and observed at, the surface of stars. Indeed, it is highly plausible[14–18] that the thermal population of the low-lying $\frac{7}{2}^+$ (141 keV) and $\frac{5}{2}^+$ (181 keV) levels shortens the beta-decay half-life drastically, since these states can undergo the Gamow-Teller allowed transitions, whereas the $\frac{9}{2}^+$ ground-state decay is second forbidden leading to the terrestrial half-life of 2.1×10^5 yr (Fig. 1). [The $\frac{1}{2}^-$ isomer (143 keV) decay is unique first forbidden and is, as expected, observed to be slow.[19]] If we limit, for explanatory convenience, the final ^{99}Ru states to the ground ($\frac{5}{2}^+$) and the first excited ($\frac{3}{2}^+$, 89 keV) states, the effective beta-decay rate of ^{99}Tc at the temperature T ($\le 5\times10^8$ K) is given by

$$\lambda_\beta^* \simeq \frac{\ln 2}{G}\left\{\frac{10}{t_{1/2}(\frac{9}{2}^+)}+\frac{8f(Q_{\rm g.s.}+141)}{ft(\frac{7}{2}^+\to\frac{5}{2}^+)}e^{-141/kT}+\frac{2}{t_{1/2}(\frac{1}{2}^-)}e^{-143/kT} +6\left[\frac{f(Q_{\rm g.s.}+181)}{ft(\frac{5}{2}^+\to\frac{5}{2}^+)}+\frac{f(Q_{\rm g.s.}+181-89)}{ft(\frac{5}{2}^+\to\frac{3}{2}^+)}\right]e^{-181/kT}\right\}\ \sec^{-1}, \quad (1)$$

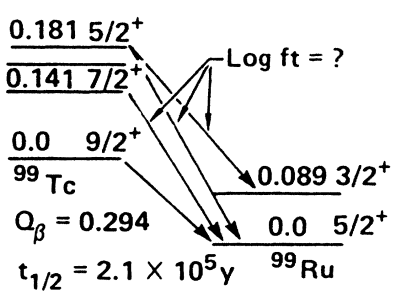

FIG. 1. ^{99}Tc β^- decays of astrophysical interest. Experimental data are taken from Ref. 19. Energies are in MeV.

where kT is the Boltzmann constant times the temperature and is expressed in keV [$kT=8.6166\times(T/10^8\ \mathrm{K})$], and

$$G\simeq 10+8e^{-141/kT}+2e^{-143/kT}+6e^{-181/kT}. \quad (2)$$

In Eq. (1), $t_{1/2}(\frac{9}{2}^+)$ ($=6.6\times10^{12}$ sec) and $t_{1/2}(\frac{1}{2}^-)$ ($\lesssim 2.4\times10^{10}$ sec) are the observed beta-decay half-lives of the ground and the isomeric states, and $Q_{\rm g.s.}$ ($=294$ keV) is the ground-state Q value. The $ft(J_i^+\to J_f^+)$ correspond to unmeasured transitions from excited states, where f is the integrated Fermi function for allowed transitions, and t is the partial half-life in sec. With $Z=44$: $\log f=0.06$, 0.19, and -0.12 for $Q_\beta=435$, 475, and 386 keV, respectively.[20] [In Eq. (1), the possible effects of ionization are excluded (see Sec. III).]

If we replace the unknown ft values in Eq. (1) by a "typical" value for known Gamow-Teller transitions in heavy nuclei, we have a ^{99}Tc half-life as short as the order of years[18] at $T=3\times10^8$ K. This time scale is shorter than the duration[11] of the thermal-pulse s-process environment which is $\simeq$10–100 yr. If most ^{99}Tc decays to ^{99}Ru, then it is in contradiction to the observations of substantial ^{99}Tc abundance at the surface of at least some red-giant stars. This seeming dilemma is the "^{99}Tc problem."

Any attempt to solve this ^{99}Tc problem faces a two-fold exercise: a reliable evaluation of λ_β^* (which requires a determination of the Gamow-Teller matrix elements of ft values for the excited-state transitions), and a detailed study of existing s-process models (such as the thermal-pulse model). The main emphasis of the present work is on the first aspect. To obtain better estimates of the beta-decay rate for ^{99}Tc, we have performed the large-basis shell-model calculations described in Sec. II. The resultant effective half-life of ^{99}Tc in stellar interiors, and their compatibility with observations of stellar surface abundances, are discussed in Sec. III from the viewpoint of the thermal-pulse model for the s process.

II. SHELL MODEL CALCULATION

In a simple shell model, the ground and low-lying positive-parity states in $^{99}_{43}$Tc$_{56}$ and $^{99}_{44}$Ru$_{55}$ may be described by $[(\pi 1g_{9/2})^3]_{J_i}$ and $[(\pi 1g_{9/2})^4(\nu 2d_{5/2})^{-1}]_{J_f}$ configurations, respectively, with a $^{90}_{40}$Zr$_{50}$ core (see Fig. 2). Between these configurations, the only possible beta transition is that of a $d_{5/2}$ neutron to a $g_{9/2}$ proton state which is strictly forbidden with respect to the Gamow-Teller operator. If this simplest model space were adequate, the ^{99}Tc beta-decay rate could not be enhanced in stellar interiors and the "problem" would be solved.

Let us, however, examine the analogous isotonic pair $^{97}_{41}$Nb$_{56}$-$^{97}_{42}$Mo$_{55}$. In adopting the above shell-model picture, we may expect $[(\pi 1g_{9/2})^1]$ and $[(\pi 1g_{9/2})^2(\nu 2d_{5/2})^{-1}]_{J_f}$ configurations for the ground state $(\frac{9}{2}^+)$ ^{97}Nb and the low-lying positive-parity states in ^{97}Mo, respectively. Again, the beta transition would be Gamow-Teller forbidden.

On the other hand, several Gamow-Teller transitions from the ground state of ^{97}Nb are observed, among which we pay special attention to that to the first-excited $\frac{7}{2}^+$ state in ^{97}Mo. The fact that this transition is relatively fast [$\log ft=5.4$ (Ref. 19)] contradicts the forbiddenness with respect to the Gamow-Teller operator described above. It is therefore apparent that the above simple model space is not sufficient for describing the ^{99}Tc Gamow-Teller decays of our concern.

With this background in mind, we have decided to study the properties of low-lying levels of the isotonic pairs, ^{97}Nb and ^{97}Mo, and ^{99}Tc and ^{99}Ru, on the same grounds in expanded model spaces. For this, we have performed a large-basis shell model calculation utilizing the Lanczos method.[21,22]

A. Hamiltonian

Our aim is to reproduce the properties of low-lying states of heavy nuclei with a minimum number of parameters. Therefore, we use the simplest of realistic, finite

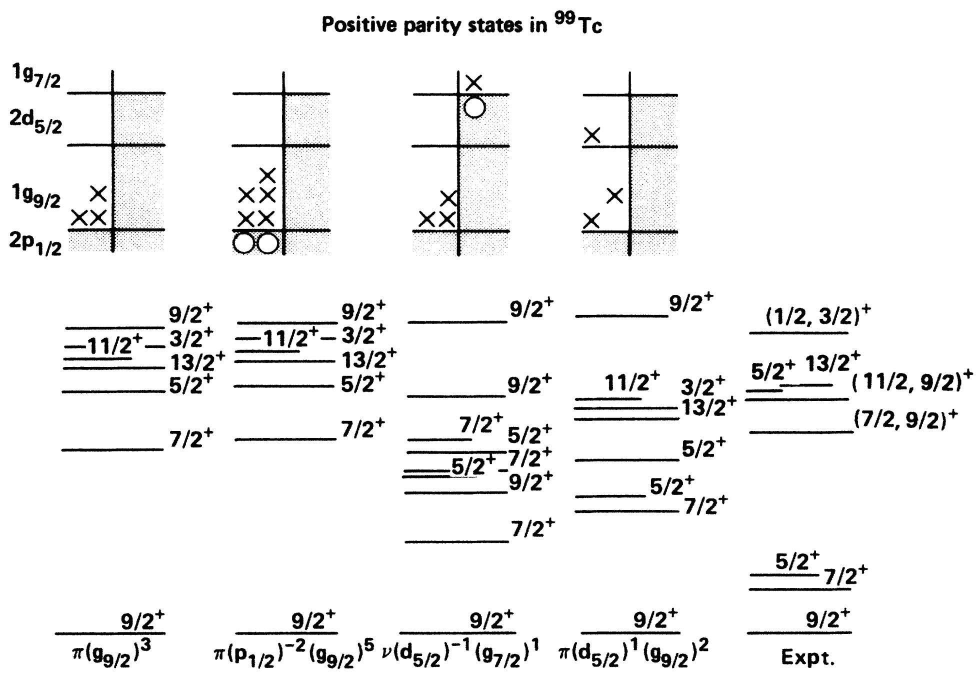

FIG. 2. ^{99}Tc low-lying positive-parity states calculated in Ref. 25. The results for the simplest model space are shown at the far left, while in others the respective configurations are added into the model space.

range two-body effective forces derived from nucleon-nucleon scattering, namely, the Kallio-Kolltveit force.[23] This force approximates a G-matrix effective interaction by applying the Scott-Moszkowski cutoff procedure[24] to the singlet-even and triplet-even components of an exponential-plus-hard-core nucleon-nucleon force:

$$V_{12}(r>1.025\ \text{fm})=\begin{cases}-864.7e^{-2.5214r}\ \text{MeV} & \text{for singlet-even}\\ -1302.3e^{-2.4021r}\ \text{MeV} & \text{for triplet-even}\end{cases} \quad (3)$$

and

$$V_{12}(r\leqq 1.025\ \text{fm})=0\ .$$

As for the one-body Hamiltonian, we start with the single-particle energies based on a Woods-Saxon calculation, and adjust them in a reasonable range to best reproduce the experimental energy spectra for low-lying positive-parity states.

B. Model space

As mentioned in the preceding discussion, the simplest model space of $(\pi 1g_{9/2})(\nu 2d_{5/2})$ is inappropriate. In addition, the existence of low-lying negative-parity states in ^{99}Tc and ^{97}Nb (the $\frac{1}{2}^-$ isomers in particular) suggest an admixture of proton excitations from the $1f2p$ shell. We have therefore tried many subspaces in the $(\pi 1f2p\,1g2d)(\nu 1g2d3s)$ shells but have found it difficult to reproduce the low-lying positive-parity spectra in ^{99}Tc and ^{97}Nb. Some of the ^{99}Tc results of our early trials[25] are reproduced in Fig. 2. It shows that, compared with experiment, either the lowest $\frac{7}{2}^+$ and $\frac{5}{2}^+$ states are much too high, or the level density at excitation energies below 700 keV is too high. It should also be noted that the three results in the middle part of Fig. 2 required rather drastic readjustments of the single-particle energies. Clearly, the $\frac{7}{2}^+$ and $\frac{5}{2}^+$ states correspond to the intruder states which are well known in this mass region. An adequate description of those levels, therefore, requires the introduction of configuration mixing which approximates the collective depression of these levels in the spectrum.

The low-lying positive-parity states of ^{99}Ru and ^{97}Mo turned out to be adequately reproduced if we allowed for two-neutron excitations from the $2d_{5/2}$ to the $1g_{7/2}$ or $3s_{1/2}$ orbital. The inclusion of configurations of this kind pushes the first $\frac{7}{2}^+$ level in ^{99}Tc down near to the ground state, although the first $\frac{5}{2}^+$ level remains too high and the overall density of low-lying levels is a bit too high. The fact that the observed Gamow-Teller decay of ^{97}Nb to the first $\frac{7}{2}^+$ level in ^{97}Mo is fast has led us to prefer the neutron excitation into the $1g_{7/2}$ orbital rather than the $3s_{1/2}$ orbital. Indeed, such an excitation is probably the most efficient way to have this fast transition since it opens a channel $\nu g_{7/2}\rightarrow\pi g_{9/2}$. Other Gamow-Teller channels, $\nu g_{9/2}\rightarrow\pi g_{9/2}$ and $\nu d_{5/2}\rightarrow\pi d_{5/2}$, will open if we permit neutron and proton excitations in ^{97}Mo from the $1g_{9/2}$ into $2d_{5/2}$ orbitals, respectively. The admixture of such transitions with those of current interest will be, however, relatively small since the energy necessary for such a promotion is expected to be large. This will probably be more true for transitions such as $\nu g_{9/2}\rightarrow\pi g_{7/2}$, $\nu d_{5/2}\rightarrow\pi d_{3/2}$, and $\nu g_{7/2}\rightarrow\pi g_{7/2}$. The proton excitations in the parent from the $1f2p$ shell do not open a channel favorable for Gamow-Teller transitions as long as we do not permit neutron excitations in the daughter from the $1f2p$ shell.

The introduction of a Gamow-Teller state into the basis for the diagonalization in the daughter nucleus requires a consistent inclusion of those states which will easily be mixed to it via nuclear forces. The inclusion of excitations of more than two particles also increases the size of the model space drastically. Because of computer space and time limitations, we have therefore decided to utilize the model space shown in Fig. 3. Since we are only interested in low lying states in the daughter nucleus, we ex-

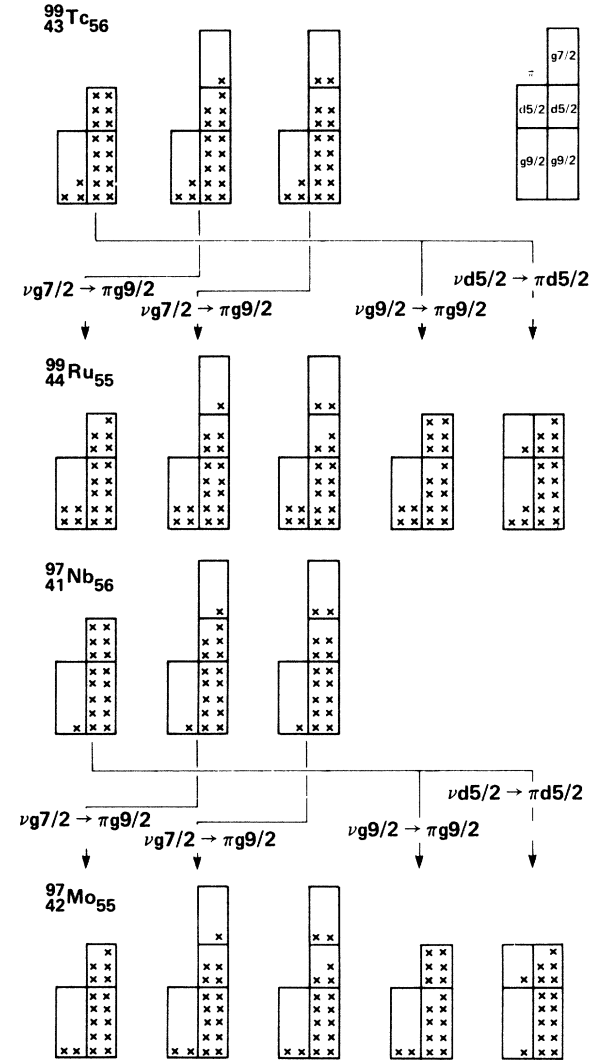

FIG. 3. Adopted model spaces for ^{99}Tc, ^{99}Ru, ^{97}Nb, and ^{97}Mo. The Gamow-Teller operator connects the parent and daughter configurations as shown by arrows.

clude those Gamow-Teller states which would lead to relatively high excitation energies. The total numbers of uncoupled Slater determinants with $j_z=\frac{1}{2}$ (we work in the m scheme) are 386, 2311, 3824, 9862 for ^{97}Nb, ^{97}Mo, ^{99}Tc, and ^{99}Ru, respectively. We obtain energy eigenvalues of low-lying states, which are converged to better than 1 keV, by applying as few as 30 Lanczos iterations.

C. Results

The level schemes calculated with the adopted model space (Fig. 3) are displayed in Fig. 4 and compared with experiments. The adopted single-particle energies for the $2d_{5/2}$ and $1g_{7/2}$ orbitals relative to the $1g_{9/2}$ orbital are 5.0 and 5.3 MeV, respectively. While the fits in ^{97}Nb and ^{99}Tc are fair, good agreements are obtained in ^{97}Mo and ^{99}Ru except for the first $\frac{9}{2}^+$ states which are too low in energy. (This is because we have permitted two neutron excitations into the $1g_{7/2}$ orbital in order to have the first $\frac{3}{2}^+$ states at low energy. As a result, the $\frac{9}{2}^+$ states go down in energy also.)

Having some confidence that the lowest positive-parity states in those nuclei are reasonably well described, we next proceeded to calculate the Gamow-Teller matrix elements for the ^{97}Nb ground state decays to the low-lying $\frac{7}{2}^+$ state in ^{97}Mo.

The resultant logft values are shown in Fig. 5 together with experimental values. It is seen that, compared with experiment, the calculated values for the transitions to the lower $\frac{7}{2}^+$ levels are much too high. One reason for this retardation is due to the fact that the main components of the initial and final wave functions are made of the configuration with two neutrons in the $1g_{7/2}$ orbital (see Fig. 3), and therefore the $\nu g_{7/2}\rightarrow\pi g_{9/2}$ transition is relatively weak. Indeed, if we lower the single-particle energy of the $2d_{5/2}$ orbital relative to that of the $1g_{7/2}$ orbital, a $\frac{7}{2}^+$ level appears at low energy in addition to those shown in Fig. 5. This new level has a strong single-particle character and the corresponding logft value is as small as 3.8. Accordingly, the transitions to the nearby $\frac{7}{2}^+$ levels become faster. The other possible cause for the relatively

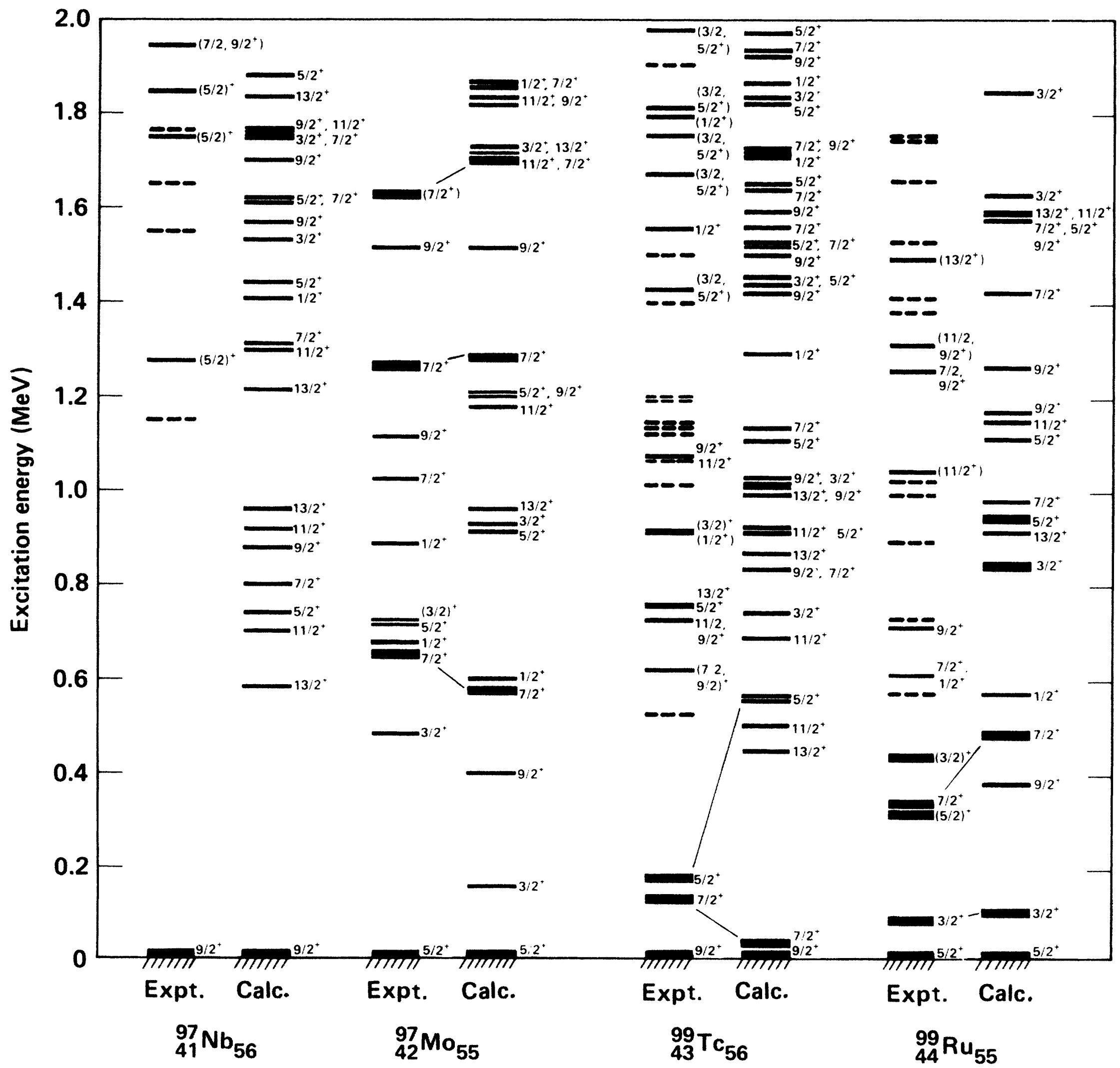

FIG. 4. Low-lying positive-parity states in ^{97}Nb, ^{97}Mo, ^{99}Tc, and ^{99}Ru, calculated with the adopted model spaces (Fig. 3) compared with experimental data taken from Ref. 19.

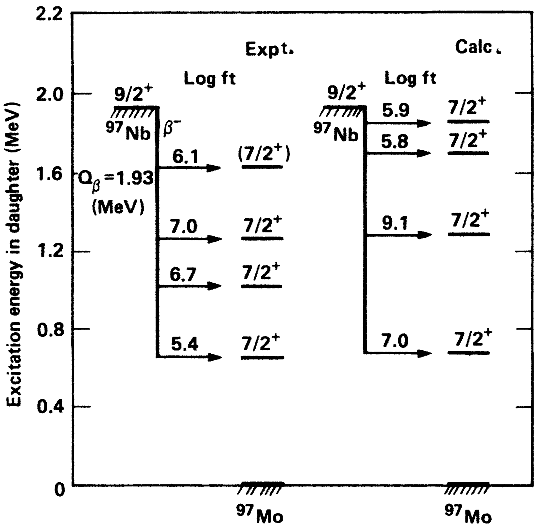

FIG. 5. $\log ft$ values for the ground-state ^{97}Nb decay to low-lying $\frac{7}{2}^+$ levels in ^{97}Mo. Experimental values are from Ref. 19.

high $\log ft$ values obtained in the present calculation may be related to our neglect of certain Gamow-Teller states in the basis for the daughter nucleus (Sec. II B).

For example, the admixture of the $\nu g_{9/2} \rightarrow \pi g_{7/2}$ strength into the low-lying transitions of current interest may not be negligible. On the other hand, the higher configuration mixing of n-particle, n-hole states ($n > 2$) will reduce the transition matrix elements, as is usually the case.

To continue the expansion of the model space in a consistent way is beyond the limitations of computer space and time now available to us. Nonetheless, we may expect that the introduction of higher-order correlations [including those configurations (like coupling to the Δ resonance) which produce Gamow-Teller quenching] will affect the Gamow-Teller transitions between the low-lying states of ^{97}Nb-^{97}Mo and ^{99}Tc-^{99}Ru pairs in a similar way. We therefore adopt in the following a mismatch factor of $\Delta \log ft = -1.6$ for the ^{97}Nb decay to the lowest $\frac{7}{2}^+$ level in ^{97}Mo, and use this same factor to renormalize all the calculated rates of the Gamow-Teller decays of the ^{99}Tc excited states. We believe that this is a consistent and useful procedure. The calculated $\log ft$ values for the ^{99}Tc decays of primary importance are shown in Fig. 6 with the renormalized values in brackets.

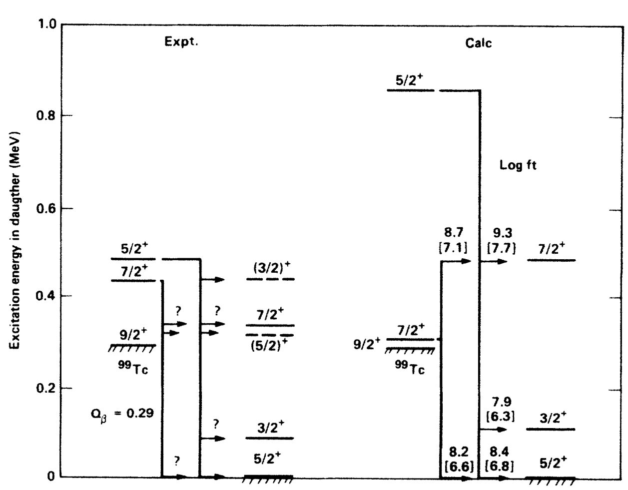

FIG. 6. Calculated $\log ft$ values for the ^{99}Tc transitions of astrophysical interest. The values renormalized to the ^{97}Nb ground-state decay to the lowest $\frac{7}{2}^+$ level in ^{97}Mo are shown in square brackets.

III. ^{99}Tc DECAY AND THE s PROCESS

Having obtained the ft values for the transitions between the low-lying states in ^{99}Tc and ^{99}Ru, and having renormalized them with the above mismatch factor, we now discuss the effective beta-decay rate of ^{99}Tc under stellar (primarily s-process) conditions. We have calculated the effective rate for the continuum- and bound-state beta decays by using the method given by Takahashi and Yokoi[26] in which the Saha ionization equation is solved with a simultaneous inclusion of the continuum depression due to surrounding electrons and ions. The results are shown in Fig. 7 as a function of temperature ($T \leq 5 \times 10^8$ K), while the density of the presumed He-dominant matter has been varied in the 10^3–10^4 g/cm^3 range. The results are essentially the same as those derived from Eq. (1) with our choice of $\log ft(\frac{7}{2}^+ \rightarrow \frac{5}{2}^+) = 6.6$, $\log ft(\frac{5}{2}^+ \rightarrow \frac{5}{2}^+) = 6.8$, and $\log ft(\frac{5}{2}^+ \rightarrow \frac{3}{2}^+) = 6.3$:

$$\lambda_\beta^* = (1.05 \times 10^{-13} + 1.6 \times 10^{-7} e^{-16.4/T_8} + 2.6 \times 10^{-7} e^{-21.0/T_8})/g \text{ sec}^{-1} , \quad (4)$$

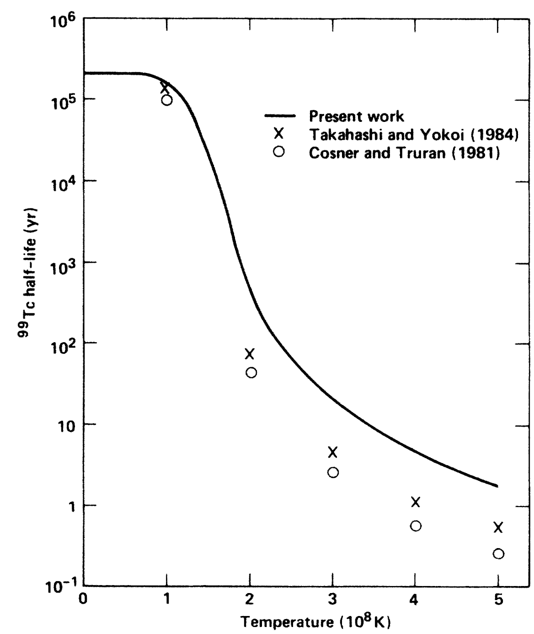

FIG. 7. Predicted β^- decay half-lives of ^{99}Tc in stellar interiors as a function of temperature in comparison with previous predictions from Refs. 15 and 17.

where T_8 is the temperature in units of 10^8 K, and $g=G/10$. (For the temperature range of interest, $g\simeq 1$.)

The reasons for this agreement are the following: (i) Because of the relatively high Q values, ionization effects on the continuum-state decay (mainly due to the changes of energetics) are minimal, and the bound-state decay contribution (for the typical s-process temperature, density, and composition) does not affect the total decay rate by more than 25%. (ii) The contribution from the transitions to ^{99}Ru levels other than its ground and first-excited states are negligible because of low Q values and $\log ft$ values which are not sufficiently small (the renormalized values are $\geqq 5.8$). The contributions from the decays of the excited states of ^{99}Tc higher than the first $\frac{5}{2}^+$ state are also negligible in the temperature range under consideration due to the Boltzmann factor. In Fig. 7, we compare our results with some previous calculations[15,17] to show that the effective half-life of ^{99}Tc under s-process conditions might be somewhat longer than previously thought. The deviation at high temperatures simply reflects the different choices of the $\log ft$ values for the unknown Gamow-Teller transitions. In Ref. 17, $\log ft(\frac{7}{2}^+\rightarrow\frac{5}{2}^+)=5.9$, $\log ft(\frac{5}{2}^+\rightarrow\frac{5}{2}^+)=6.6$, and $\log ft(\frac{5}{2}^+\rightarrow\frac{3}{2}^+)=6.2$ are adopted, while in Ref. 15 $\log ft=5.7$ is assumed for all the transitions. Allowing for a factor of 5 as a possible coherent error in our calculation of the ft values, we may conclude that the ^{99}Tc half-life at $T=3\times 10^8$ K lies somewhere in between 4 and 100 yr.

It has been occassionaly argued (e.g., Ref. 3) that such enormous enhancements of the ^{99}Tc decay rate at high temperatures might forbid its survival through the s process, and this has tempted some authors to reject the possibility that the neutron source is due to the ^{22}Ne(α,n)^{25}Mg reaction (which requires temperatures of $\sim 3\times 10^8$ K to be efficient). An alternative neutron source is the ^{13}C(α,n)^{16}O reaction, which starts to operate at lower temperatures of $\sim 10^8$ K. The corresponding astrophysical scenario has, however, its own inherent problems.[7]

Recently, those views have been challenged by Mathews *et al.*[27] Within the framework of schematized versions of the most well studied thermal pulse s-process model[11–13] combined with a detailed network of calculations, they demonstrated that, even with its effective half-life (at temperatures of $\sim 3\times 10^8$ K) as fast as a few years, the ^{99}Tc could indeed survive the s process. The reason is that the neutron production by the ^{22}Ne(α,n)^{25}Mg reaction, and hence the ^{99}Tc production, is even more enhanced at such temperatures and almost compensates for the destruction. In addition, they have resurrected the classical idea[28,29] that the observed abundance of ^{99}Tc in comparison with those of other species (such as Zr, Nb, and Mo) could be used as a good indicator of the lifetime of stellar mixing. A detailed s-process study based on He-shell thermal-pulse models, and of the models' compatibility with observations, is under way. The preliminary results,[30] however, support the above conclusions that the enhanced ^{99}Tc decay rate in stellar interiors does not necessarily contradict the fact that one sees ^{99}Tc at the surface of stars, nor preclude the ^{22}Ne(α,n)^{25}Mg reaction from remaining as the most promising candidate for the neutron source for the s process.

IV. CONCLUSIONS

We have performed a large-basis shell model calculation to estimate the Gamow-Teller matrix elements for the ^{99}Tc excited-state beta decays of astrophysical interest by utilizing the known ft values for the analogous isotonic nucleus, ^{97}Nb, as a guide. With a model space which consists of low-seniority particle-hole excitations within the $1g2d$ orbitals, the low-lying positive-parity states in ^{99}Tc, ^{99}Ru, as well as in ^{97}Nb and ^{97}Mo could be reproduced fairly well. The results imply that the effective half-lives of ^{99}Tc under typical s-process conditions might be slightly longer than previous predictions from pure systematics (~ 20 yr vs ~ 5 yr at $T=3\times 10^8$ K). Although much remains to be worked out to pin down the exact value for the ^{99}Tc decay rate in hot environments and the many uncertainties still underlie the currently accepted s-process scenarios, the present results make us confident that the observation of Tc at the surface of stars of certain types does not contradict the notion that the s-process neutron source is the ^{22}Ne(αn)^{25}Mg reaction at high temperatures of $\sim 3\times 10^8$ K.

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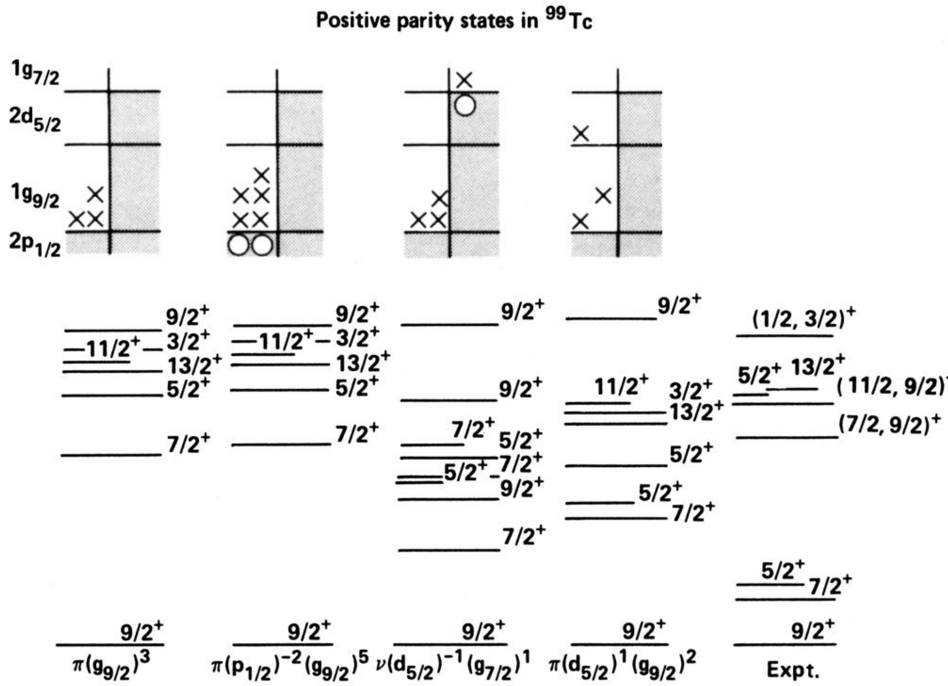

FIG. 2. ^{99}Tc low-lying positive-parity states calculated in Ref. 25. The results for the simplest model space are shown at the far left, while in others the respective configurations are added into the model space.