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Centroids of Gamow–Teller Transitions at Finite Temperature in fp-shell Neutron-rich Nuclei

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Abstract

The temperature dependences of the energy centroids and strength distributions for Gamow–Teller (GT) 1^+ excitations in several fp-shell nuclei are studied. The quasiparticle random phase approximations (QRPA) are extended to describe GT states at finite temperature. A shift to lower energies of the GT^+ strength is found, as compared to values obtained at zero temperature.

Weak-interaction mediated reactions on nuclei in the core of massive stars play an important role in the evolutionary states leading to a type II supernova. These reactions are also involved in r-process nucleosynthesis [1]. Nuclei in the fp-shell participate in these reactions in the post-silicon burning stage of a pre-supernova star [2]. The astrophysical scenarios, where these reactions can take place, depend upon various nuclear structure related quantities [3]. Among them, the energy centroids for GT and IAS transitions can determine the yield of electron and neutrino captures. The dependence of such nuclear observables upon the stellar temperature is a matter of interest [4]. In the present letter we are addressing the question about the temperature dependence of the energy-centroids of $GT^{\pm}$ transitions [5]. We have performed microscopic calculations of these centroids using the finite-temperature quasiparticle random phase approximation [6] and for temperatures (T) below critical values related with the collapse of pairing gaps ($T \leqslant 1$ MeV) [7]. These temperatures are near the values characteristic of the pre-supernova core [4]. The consistency of the approach has been tested by evaluating, at each temperature, the Ikeda Sum Rule and total GT^- and GT^+ strengths [8].

The starting Hamiltonian is

$$H = H_{\mathrm{sp}} + H_{\mathrm{pairing}} + H_{\mathrm{GT}} \tag{1}$$

where by the indexes (sp), (pairing) and (GT) we are denoting the single-particle, pairing and Gamow–Teller ($\sigma\tau \cdot \sigma\tau$) terms, respectively. For the pairing interaction, both for protons and neutrons, a separable monopole force is adopted with coupling constants G_{p} and G_{n} and for the residual proton–neutron Gamow–Teller interaction H_{GT} the form given by Kuzmin and Soloviev [9] is assumed. As shown in the context of nuclear double β decay studies [10] the Hamiltonian (1) reproduces the main features found in calculations performed with realistic interactions. The structure of the residual interaction-term can be defined as the sum of particle-hole ($\beta^{\pm}$) and particle–particle ($P^{\pm}$) terms of the $\sigma\tau^{\pm}$ operators, as shown in [9, 10], namely:

$$H_{\mathrm{GT}} = 2\chi(\beta^-\beta^+) - 2\kappa(P^-P^+) \tag{2}$$

in standard notation.

To generate the spectrum of 1^+ states associated with the Hamiltonian (1) we have transformed it to the quasiparticle basis, by performing BCS transformations for proton and neutron channels separately, and then diagonalized the residual interaction between pairs of quasiprotons (p) and quasineutrons (n) in the framework of the pn-QRPA [10, 12]. This procedure leads to the definition of phonon states in terms of which one can write both the wave functions and the transition matrix elements for $\sigma\tau^-$ and $\sigma\tau^+$ excitations of the mother nucleus. Since the procedure can be found in textbooks we shall omit further details about it and rather proceed to the description of the changes which are needed to account for finite temperature effects. Like before one has to treat pairing correlations first, to define the quasiparticle states at finite temperature, and afterwards transform the residual interaction into this basis to diagonalize the pn-QRPA matrix. The inclusion of thermal effects on the pairing Hamiltonian is performed by considering thermal averages in dealing with the BCS equations. Details of this procedure can be found in [7]. The most notable effect of thermal excitations on the pairing correlations is the collapse of the pairing gaps, at temperatures of the order of half the value of the gap at zero temperature. For a separable pairing force the finite temperature gap equation is written [7]

$$\Delta(T) = G \sum_{\nu} u_\nu v_\nu (1 - 2f_\nu(T)) \tag{3}$$

where the factors $f_\nu(T) = (1 + e^{E_\nu/T})^{-1}$ are the thermal occupation factors for single quasiparticle states. The quasiparticles energies $E_\nu = \sqrt{(e_\nu - \lambda)^2 + \Delta(T)^2}$ are now functions of temperature, as well as of the occupation factors u and v.

The thermal average procedure of [7] accounts for the inclusion of excited states in taking expectation values at finite temperature. It has also been used to describe two-quasiparticle excitations and QRPA states at finite temperature [6]. In the basis of unlike (proton–neutron)-two-

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quasiparticle states the thermal average gives, for the commutator between pairs, the expression:

$$\langle[\alpha_{\nu,n}\alpha_{\mu,p}, \alpha^{\dagger}_{\rho,p}\alpha^{\dagger}_{\gamma,n}]\rangle = \delta_{\nu,\gamma}\delta_{\mu,\rho}(1 - f_{\nu,n} - f_{\nu,p}). \quad (4)$$

These factors have to be included in the pn-QRPA equations [12] in taking the commutators which lead to the pn-QRPA matrix, as they have been considered in dealing with pairs of like-(neutrons or protons)-quasiparticles [6]. More details about this procedure, for the particular case of proton–neutron excitations, will be given in [16].

The single particle basis adopted for the present calculations consists of the complete f-p and s-d-g shells and the corresponding intruder state $0h_{11/2}$, both for protons and neutrons. In this single particle basis, with energies obtained from a fit of the observed one-particle spectra at the beginning of the fp-shell, and taking ^{40}Ca as an inert core we have solved temperature dependent BCS equations [7] for temperatures $0\,\text{MeV} \leqslant T \leqslant 0.8\,\text{MeV}$. The coupling constants G_p and G_n, of the proton and neutron monopole pairing channels of eq. (1), have been fixed to reproduce the experimental data on odd-even mass differences. In Table I the calculated neutron and proton pairing gaps at $T = 0\,\text{MeV}$ are compared to the experimental values extracted from [11]. Once the pairing coupling constants are determined one can calculate the standard zero temperature pn-QRPA [10, 12] equations of motion to reproduce the known systematics [5] of $GT^{\pm}$ energies and strengths. From the comparison between the calculated and experimental values of $GT^{\pm}$ energies and $B(GT^{\pm})$ strengths we have fixed the values of the coupling constants χ and κ of the Hamiltonian eq. (2).

The consistency of the pn-QRPA basis is also given by the ratios between the calculated and expected values of the Ikeda's sum rule $3(N–Z)$. The values of the above quantities are shown in Table II. The experimental values of the $B(GT^{+})$ strengths have been approximated by using the expression [13]

$$\frac{B(GT^{+})}{Z_{\text{valence}}(20 - N_{\text{valence}})} = a + b(20 - Z_{\text{valence}})N_{\text{valence}} \quad (5)$$

where $a = 3.48 \cdot 10^{-2}$ and $b = 1.0 \cdot 10^{-4}$ (see also [14]).

The overall agreement between calculated and experimentally determined values at zero temperature, both for pairing and GT observables, is rather good. We are now in a position to calculate these observables at finite temperature. At a given value of T we have solved the pairing gap equations and the pn-QRPA equations. With the resulting spectrum of 1^{+} states, both for GT^{-} and GT^{+} excitations, and the corresponding transition matrix elements of the $\sigma\tau^{+}$ operator we have obtained the values shown in Table III, where from the energy-centroids

$$E(T) = \frac{\sum_n E_n(1^{+})\,|\langle 1^{+}_n \|\sigma\tau^{+}\| \text{g.s}\rangle|^2}{\sum_n |\langle 1^{+}_n \|\sigma\tau^{+}\| \text{g.s}\rangle|^2} \quad (6)$$

we have extracted the temperature dependent shifts

$$\delta_E(T) = E(T = 0) - E(T). \quad (7)$$

Since the changes of the calculated centroids for GT^{-} excitations at different temperatures are minor we are showing only the quantities which correspond to GT^{+} transitions. Let us discuss some features shown by the result of the present calculations by taking the case of ^{56}Fe as an example. As known from previous studies [12], the repulsive effects due to the proton–neutron residual interactions affect both the GT^{-} and the GT^{+} unperturbed strength distributions, moving them up to higher energies. The large upwards-shift, as compared to the strength distribution of the unperturbed proton–neutron two-quasiparticle states, is exhibited by the GT^{-} distribution [12]. At finite temperatures two different effects become important, namely: the vanishing of the pairing gaps and the thermal blocking of the residual interactions. In order to distinguish between both effects we have computed GT-strength distributions for the case of the unperturbed proton–neutron two-quasiparticle basis. The pairing gaps, for protons and neutrons, collapse at temperatures $T \approx 0.80\,\text{MeV}$. At temperatures below these critical values ($T = 0.7\,\text{MeV}$) the neutron and pairing gaps decrease to about 50% and 40% of the corresponding values at $T = 0$, respectively. At this temperature ($T = 0.7\,\text{MeV}$) these changes amount to a lowering of the centroid for GT^{+} transitions of the order of

Table I. *Experimental and calculated pairing gap parameters at zero temperature. The experimental values, extracted from ref. [11], are listed in parenthesis. All values are given in units of MeV*

Nucleus	Neutron Gap	Proton Gap
^{54}Fe	1.647 (1.694)	1.560 (1.520)
^{56}Fe	1.359 (1.363)	1.593 (1.568)
^{58}Ni	1.262 (1.298)	1.752 (1.725)
^{60}Ni	1.469 (1.489)	1.743 (1.726)

Table II. *Experimental and calculated energy centroids and total strengths for $GT(^{\pm})$ transitions, at zero temperature. The available experimental values are listed in parenthesis. The energies (E) correspond to excitations from the ground state of the mother nucleus. The experimental values of the $B(GT^{-})$-strengths (third column, in parenthesis) are taken from ref. [17] and the experimental values of the $B(GT^{+})$-strengths (fourth column, in parenthesis) have been obtained by using eq. (5) (ref. [13]). The last column shows the ratio between calculated ($B(GT^{-})$-$B(GT^{+})$) and expected ($3(N$-$Z)$) values of the Ikeda Sum Rule*

Nucleus	$E(GT^{-})$ (MeV)	$B(GT^{-})$	$B(G^{+})$	Ratio
^{54}Fe	8.91 (8.90)	9.290 (7.8 ± 1.9)	3.306 (3.312)	0.997
^{56}Fe	9.31 (9.00)	14.630 (9.9 ± 2.4)	2.632 (2.928)	0.999
^{58}Ni	9.48 (9.40)	10.860 (7.4 ± 1.8)	4.836 (3.744)	1.000
^{60}Ni	9.22 (9.00)	14.890 (7.2 ± 1.8)	2.890 (3.148)	1.000

Table III. *Calculated values of the shift $\delta_E(T)$, eq. (7), of the energy centroid for GT^{+} excitations for different values of the temperature (T). The experimentally determined energy centroids, (E_{exp}), are taken from the compilation of data given in ref. [5]. All values are given in units of MeV*

Nucleus	E_{exp} (MeV)	$T = 0.4\,\text{MeV}$	$T = 0.6\,\text{MeV}$	$T = 0.8\,\text{MeV}$
^{54}Fe	3.5	0.179	0.745	1.483
^{56}Fe	6.0	0.216	0.807	2.038
^{58}Ni	3.7	0.071	0.342	0.955
^{60}Ni	5.4	0.118	0.450	0.932

1 MeV. When the residual interaction is turned on the resulting shift to lower energies is ≈ 1.20 MeV. From these results it can be seen that the total downward shift of the GT^+ centroid is not solely due to pairing effects but also due to the thermal blocking of the proton–neutron residual interactions. This result can be understood as follows. Since GT^+ transitions are naturally hindered by the so-called Pauli blocking effect the smearing out of the Fermi surface due to pairing correlations, at zero temperature, tends to favour them. When temperature dependent averages are considered, eq. (3), the pairing correlations are gradually washed-out as the temperature increases. This in turn leads to a sharpening of the Fermi surface thus decreasing the value of the energy of the unperturbed proton–neutron pairs. In addition, from the structure of the pn-QRPA equations at finite temperature, it can easily be seen that factors such as in eq. (4) will appear, screening the interaction terms. This additional softening of the repulsive GT interaction adds to the decrease of the unperturbed proton–neutron energies and the result is a larger shift of the GT^+ centroids. It should be noted that the position of the centroid of the GT^- transitions is less sensitive to these effects, as we have mentioned before. The calculated shifts for these centroids are of the order of (or smaller than) 0.5 MeV.

This result, concerning GT^- centroids, is understood by noting that the collapse of the proton pairing gap does not affect the BCS unoccupancy factor (u_p) for proton levels above the Fermi surface as well as the BCS occupancy factor (v_n) for neutron levels below the Fermi surface and the energy of the unperturbed proton–neutron pairs remains nearly the same. Table III shows similar features for the changes of the GT^+ energy-centroids in other cases.

To conclude, in this work we have presented the result of temperature dependent QRPA calculations of GT transitions in some neutron-rich nuclei in the fp-shell. The energy centroids of these transitions have been calculated at temperatures below the critical values associated with the collapse of the pairing correlations. The inclusion of thermal averages on the QRPA equations of motion leads to the softening of the repulsion induced by the Gamow–Teller interaction on proton–neutron pairs as well as to the sharpening of the proton and neutron Fermi surfaces. The combined effects of both mechanisms leads to a downwards-shift of the GT^+ strength while the GT^- centroids remain largely unaffected. We have observed the constancy of the total GT^+ strength, as a function of temperature, in agreement with previously reported results of the Monte Carlo Shell Model Method [15]. The shift of the GT^+ centroids at finite temperatures will effectively lower the energy thresholds for electron capture reactions in stellar environments leading to more neutronization at lower stellar densities during gravitational collapse. On the other hand the neutrino induced r-process reactions will remain relatively unaffected by the small ($\leqslant 0.5$ MeV) thermally induced shifts of GT^- centroids. Considering that the empirically determined energies of the GT^+ centroids are known with an accuracy of the order of 0.43 MeV [5] the temperature-dependent effects reported here may be significant for astrophysical rate calculations and their consequences for pre-supernova stellar evolution and gravitational collapse. Work is in progress to predict $GT^+(GT^-)$ centroids and strengths, by using the pn-QRPA method at finite T, for nuclei for which experimental data through charge-exchange (p,n)((n,p))-reactions in the opposite direction is available to constrain the former one [16].

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