LEVEL DENSITIES AND THERMAL PROPERTIES OF ^{56,57}Fe

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Nuclear level densities for ^{56,57}Fe have been extracted from the primary γ-ray spectra using (^{3}He,^{3}He$'\gamma$) and (^{3}He,$\alpha\gamma$) reactions. Nuclear thermodynamic properties for ^{56}Fe and ^{57}Fe are investigated using the experimental level densities. These properties include entropy S, Helmholtz free energy F, caloric curves (i.e., the E-T relation), chemical potential μ, and heat capacity C_V.

I. INTRODUCTION

Nuclear thermodynamics has attracted considerable attention in recent years. Several temperature-dependent nuclear properties such as nuclear shapes and giant dipole resonance widths (and their fluctuation properties) have been investigated in the literature [1]. In this context one of the most interesting topics is that of phase transitions in atomic nuclei. One type of phase transition in atomic nuclei is the transition from a phase with strong pairing correlations to a phase with weak pairing correlations [2]. The onset of a discontinuity in thermodynamic variables and the evolution of zeros of the canonical and grand-canonical partition functions [3] in the complex plane have been discussed in terms of pairing transitions. Recently it has been shown using the static-path approximation (SPA) plus random-phase approximation (RPA) that the increase of moment of inertia with increasing temperature is correlated with the suppression of pairing correlations [4].

As a part of an ongoing effort, in the present work we extract several thermodynamic properties of ^{56}Fe and ^{57}Fe isotopes starting from nuclear level densities. The plan of this paper is as follows: The experiment, analysis tools, and the Oslo method are briefly presented in the next Section. Experimental level densities are given in Section III. Thermodynamical concepts are discussed in Section IV. Concluding remarks are given in Section V.

II. EXPERIMENTAL DETAILS AND DATA ANALYSIS

The self-supporting ^{57}Fe target was bombarded by a 2-nA beam of 45-MeV ^{3}He particles from the Oslo Cyclotron Laboratory at the University of Oslo. The target was

isotopically enriched to 94.7%, and had a thickness of 3.4 mg/cm^2. The outgoing charged particles were recorded by eight Si $\triangle$E-E telescopes, which were collimated and placed 5 cm away from the target at a ring 45° with respect to the beam direction. The particle telescopes covered 0.3% of the total solid angle. The thicknesses of the front and the end detectors were 140 and 3000μm, respectively, and the particle energy resolution was $\approx$ 0.3 MeV over the entire spectrum. The reaction γ rays were detected by 28 collimated 5″ x 5″ NaI(Tl) detectors with a total efficiency of $\approx$ 15% of 4π, and with 6% energy resolution at 1.3 MeV. In order to monitor the selectivity and populated spin distribution of the reactions, one 60% Ge(HP) detector was used. After an analysis procedure which is described in Ref. [5], a two-dimensional primary γ-ray matrix is extracted.

The primary γ-ray matrix is factorized using the Brink-Axel hypothesis [6, 7], according to which the probability of emitting a γ ray from an excited state is proportional to the γ-ray transmission coefficient $T(E_\gamma)$ and the level density at the final energy $\rho(E-E_\gamma)$. This factorization is determined by a least χ^2 method without assuming any functional form for the level density and the γ-ray transmission coefficient [8]. However, this method does not provide a unique solution. This factorization is invariant under the transformation [8]

$$\begin{aligned} \tilde{\rho}(E-E_\gamma) &= A\exp(\alpha(E-E_\gamma))\rho(E-E_\gamma) \\ \tilde{\mathcal{T}}(E_\gamma) &= B\exp(\alpha E_\gamma)\mathcal{T}(E_\gamma), \end{aligned} \tag{1}$$

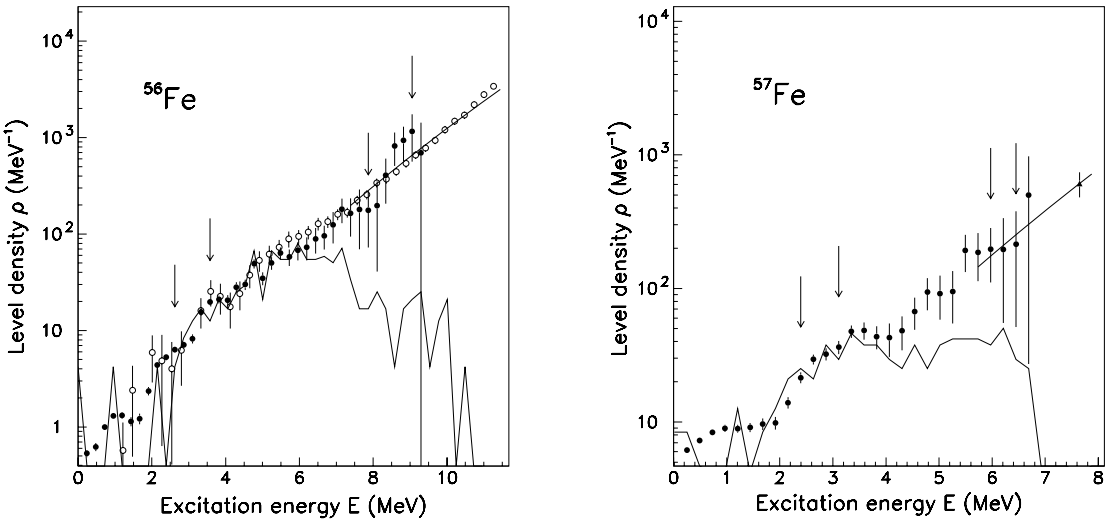
where A, B, and α are the free parameters of the transformation. Therefore it is very important to determine accurately the free parameters A, B, and α in order to find the physical solution. The parameters A and α are determined from the normalization of the level density to the discrete levels at low excitation energies and to the density of the neutron resonances at the neutron binding energy B_n. The parameter B is then determined using the average total radiative width of neutron resonances. Details of the normalization procedure are explained elsewhere [9].

III. NUCLEAR LEVEL DENSITIES

The normalized experimental level densities for ^{56,57}Fe using the Oslo method were reported earlier [10]. In the present paper, we investigate the thermodynamics of ^{56,57}Fe using the experimental level densities obtained from the Oslo method. However, before extracting the thermodynamic properties, we decided to re-normalize our experimental level densities. The reason for this renormalization is that during the past few years more data on the level densities of ^{56,57}Fe were obtained. Each of these data sets employed a different reaction: (i) The level density of ^{56}Fe was obtained from neutron evaporation spectra using the ^{55}Mn(d,n)^{56}Fe reaction [11]. (ii) The level density of ^{57}Fe was measured with both the ^{58}Fe(^{3}He,α)^{57}Fe and ^{59}Co$(d,\alpha)^{57}$Fe reactions recently [12]. Furthermore, new descriptions of the level density parameter a and backshift energy parameter E_1 suggested by von Egidy and Bucurescu [13] take into account shell corrections in the mass formula. Combining these recent experimental data with the new descriptions for the level density parameters provides a more reliable means for the normalization of the experimental level densities.

Figure 1 shows re-normalized level densities of ^{56,57}Fe from the ground state up to $E_x \sim B_n - 1$ MeV. The level density of ^{56}Fe obtained from the neutron evaporation data is also

shown. The agreement between the two methods is good. Individual levels are prominent in the ^{56}Fe data at $E_x = 847$ and 2084 keV excitation energies, these correspond to the first and the second excited states in ^{56}Fe. At around 2.6 MeV excitation energy for ^{56}Fe the increase in the level density data is interpreted as the first breaking of nucleon pairs. Similarly, the strong increase in the level density data of ^{57}Fe at $E_x \sim 1.8$ MeV that terminates $E_x \sim 2.8$ MeV reveals the first breaking of Cooper pairs in the underlying even-even core. These obvious anomalies in the level density data also appear in the thermodynamic quantities of the ^{56,57}Fe isotopes.



(a) (b)

FIG. 1: (a) Experimental level density of ^{56}Fe (full circles). The level density obtained from the ^{55}Mn(d,n)^{56}Fe reaction [11] is also shown (as open circles). The jagged solid lines represent the level density obtained from counting of discrete levels [14]. The smooth solid curve is the renormalized level density parametrization according to von Egidy and Bucurescu [13]. The data points between the arrows at low and high excitations are used for the normalization. (b) Experimental level density of ^{57}Fe (full circles). The level density obtained from the ^{58}Fe(^{3}He,α)^{57}Fe reaction [12] is also shown as a triangle at B_n.

IV. THERMODYNAMIC QUANTITIES

A Microcanonical Ensemble

The microcanonical ensemble is commonly accepted as an appropriate ensemble to use in investigating atomic nuclei, as the nuclear force has a short range and the nucleus does not share its excitation energy with its surroundings. The microcanonical entropy is closely related to the level density of the system at a given excitation energy. Several thermodynamic properties of the atomic nucleus can be derived from the entropy. The entropy is defined as the natural logarithm of the multiplicity Ω of accessible states within the energy interval E and $E + \delta E$:

$$S(E) = k_B \ln \Omega(E) \tag{2}$$

where k_B is the Boltzmann's constant. Here we set k_B to unity so that the entropy becomes dimensionless and thus the temperature T has the units of MeV.

However, one should note that the experimental level density is not the true multiplicity of states; i.e., it does not include $(2I + 1)$ degeneracy of magnetic substates. In order to obtain the state density, one needs to know the spin distribution as a function of excitation energy in order that multiplication of the spin dependent factor $(2\langle I(E)\rangle + 1)$ and the level density gives the state density. The spin distribution is usually assumed to be Gaussian with a mean of $\langle 2I + 1\rangle = \sqrt{2\pi}\sigma$ where σ is the spin cut-off parameter which depends very weakly ($\sigma \propto E^{1/4}$) on excitation energy:

$$\rho(E, I) = \rho(E)\frac{2I + 1}{2\sigma^2} \exp[-I(I + 1)/2\sigma^2] \tag{3}$$

where $\rho(E, I)$ is the level density for a given spin I. Thus the total level density (summed over all spins) is given by $\rho(E) = \sum_I \rho(E, I)$ and the total state density is given by $W(E) = \sum_I (2I + 1)\rho(E, I)$. The multiplicity of states could be obtained by simply multiplying a factor $\langle 2I + 1\rangle = \sqrt{2\pi}\sigma$ to the level density. There is little experimental data on the spin cut-off parameter. Theoretical calculations of the spin distribution of nuclear levels are difficult if correlations are assumed between individual spins.

Here we define a "pseudo" entropy based on the experimental level density, i.e., $\Omega(E) = \rho(E)/\rho_0$. The normalization constant ρ_0 is introduced and adjusted to the value $\rho_0 = 1$ MeV^{-1} such that the third law of thermodynamics is fulfilled as $S(T \to 0) = 0$.

Figure 2 shows the entropies of ^{56,57}Fe. The breaking of the first nucleon pair in the odd-mass system appears at a lower excitation energy than for the even system due to the reduced pairing gap Δ, which results from the odd valence neutron in the ^{57}Fe nucleus.

The entropies of ^{56,57}Fe appear fairly linear at high excitation energies. The slope of the entropy in the microcanonical ensemble is related to the temperature of the system by $T = (dS/dE_x)_V^{-1}$. The entropies of ^{56,57}Fe are fitted with a constant temperature model, shown as solid lines in Fig. 2. From this model, constant temperatures of $T = 1.50$ MeV and $T = 1.19$ MeV are obtained for ^{56}Fe and ^{57}Fe, respectively. These temperatures are interpreted as the critical temperatures T_c for the breaking of nucleon pairs.

The entropy difference between the even-odd and even-even nuclei is interpreted as the entropy of a single quasiparticle (particle or hole), assuming that the entropy is an extensive (additive) quantity. The entropy carried by the valence neutron particle in our case can be estimated by $\Delta S = S(^{57}\text{Fe}) - S(^{56}\text{Fe})$. The lower panel of Fig. 2 shows the single particle entropy as a function of excitation energy. The fluctuations at low excitation energies result from the lower pairing gap in the odd-mass system. At higher excitation energies above ~ 4 MeV, the entropy difference has a nearly constant value of $\Delta S = 0.82k_B$. This value is less than the value obtained for the rare-earth isotopes which is $\Delta S = 1.7k_B$ [15]. This is expected because ^{56}Fe and ^{57}Fe isotopes are in the vicinity of closed shells, and thus the entropy is less than that of the rare-earth isotopes.

Assuming a constant ΔS and a constant energy shift Δ between the two entropies, these two quantities are connected to the critical temperature T_c [15] by $T_c = \Delta/\Delta S$. From this relation, we can calculate the entropy difference $\Delta S = \Delta/T_c = 1.3/1.35 \sim 0.96k_B$ which is consistent with the present observations. Here the pairing gap parameter Δ is calculated using the three mass indicator of Dobaczewski *et al.* [16], and an average value

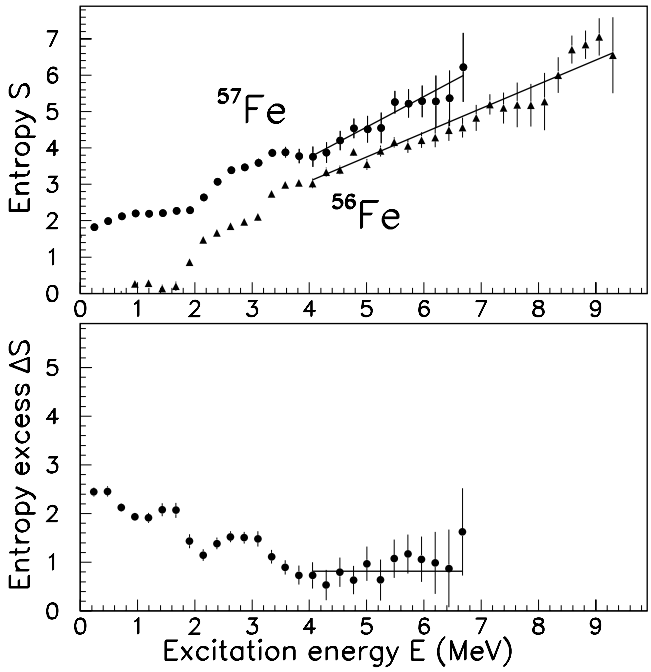


FIG. 2: Deduced entropies for ^{56,57}Fe (upper panel). The solid line is the constant temperature least square fit to the data. Lower panel: Deduced entropy excess for the single particle. The entropy excess $\Delta S = 0.82 k_B$.

is taken for the critical temperature.

B Canonical Ensemble

The partition function in the canonical ensemble for a given temperature is determined by

$$Z(T) = \sum_{E=0}^{\infty} \rho(E) \delta E e^{-E/T}, \tag{4}$$

where $\rho(E)$ is the measured level density, and δE is the energy bin used. The summation in $Z(T)$ goes to infinity and our level densities extend to $\sim B_n - 1$ MeV. Therefore we extrapolate the experimental level densities using the BSFG model parametrized by von Egidy and Bucurescu [13]. The Helmholtz free energy can be calculated from the partition function by

$$F(T) = -T \ln Z(T). \tag{5}$$

The entropy S, the average excitation energy $\langle E \rangle$, the heat capacity capacity C_V, and the chemical potential μ at a given temperature can be derived from $F(T)$ by

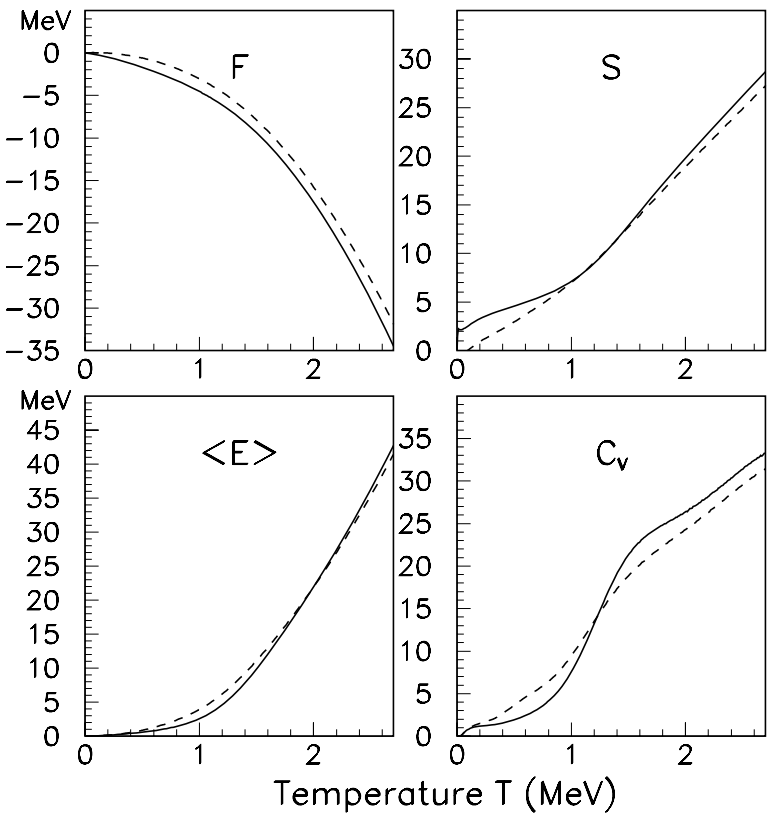


FIG. 3: The Helmholtz free energy F, average excitation energy $\langle E(T)\rangle$, entropy S, and heat capacity C_V for ^{56}Fe (dashed lines) and ^{57}Fe (solid lines), deduced in the canonical ensemble.

$$S(T) = -\left(\frac{\partial F}{\partial T}\right)_V, \tag{6}$$

$$\langle E(T)\rangle = F + TS, \tag{7}$$

$$C_V(T) = \left(\frac{\partial \langle E\rangle}{\partial T}\right)_V, \tag{8}$$

$$\mu(T) = \frac{\partial F}{\partial n}, \tag{9}$$

where n is the number of thermal particles. These thermal particles outside a core of Cooper pairs are responsible for the thermal properties of the nucleus at low excitations. At higher temperatures, pairing correlations are quenched, and the nucleus has a transition from a paired to unpaired phase.

Figure 3 shows the Helmholtz free energy F, average excitation energy $\langle E(T)\rangle$, entropy S, and heat capacity C_V for ^{56}Fe (dashed lines) and ^{57}Fe (solid lines). The Helmholtz free energy F and the average excitation energy $\langle E(T)\rangle$ behave smoothly as a function of

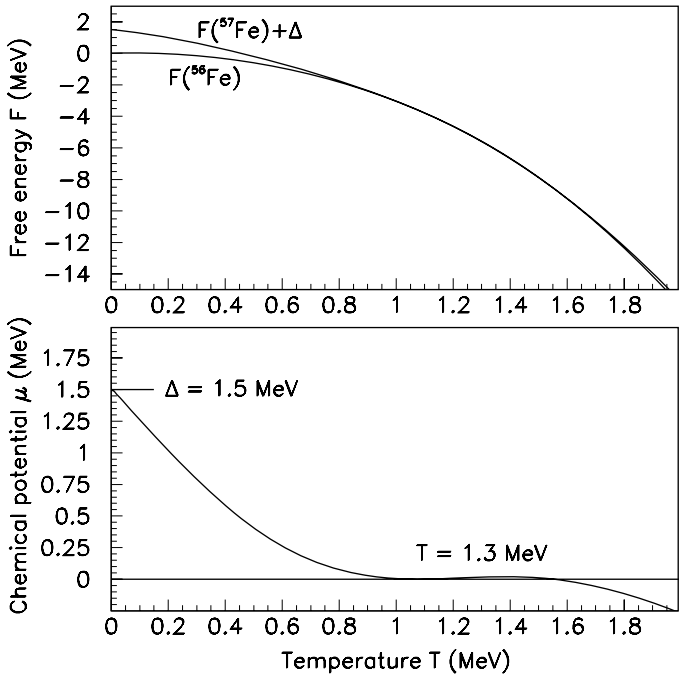


FIG. 4: The experimental Helmholtz free energies deduced in the canonical ensemble for ^{56}Fe and ^{57}Fe. The critical temperature for the quenching of pairing correlations lies between T_c ==1 - 1.5 MeV, where the chemical potential is $\mu \sim 0$.

temperature. At around $T \sim 1.3$ MeV, both isotopes are excited to energies comparable to their respective neutron binding energies. The average excitation energies for ^{56}Fe and ^{57}Fe coincide only at one point $T \sim 2$ MeV. Above this temperature the odd isotope has larger values as the temperature increases. The entropy S and heat capacity C_V are the first and second derivatives of F, respectively, and thus both reflect thermal variations. For temperatures below T =1 MeV, the entropy difference for ^{56}Fe and ^{57}Fe reaches ~ 2, the entropy of ^{57}Fe being larger. The entropies have the same values between T =1 and 1.5 MeV. Above T =1.5 MeV, the two entropies start to diverge. Both heat capacities have an S shape which is interpreted as a fingerprint for pairing transitions in nuclei. The structure in the heat capacity C_V for ^{57}Fe is more pronounced than C_V for ^{56}Fe. The contribution to the heat capacity from collective excitations is negligible, and has no influence on the S shape [17].

Figure 4 shows the chemical potential μ which is defined as the amount of energy required to excite a nucleon from the underlying core of paired nucleons, while the entropy and volume held fixed. The typical energy cost for creating a quasiparticle is $-\Delta$ which is also equal to the chemical potential. The chemical potential can be written as

$$\mu = \frac{\Delta F}{\Delta N} = \frac{F_{odd} - F_{even}}{1} = -\Delta. \tag{10}$$

thus giving $F_{even} = F_{odd} + \Delta$. The energy curve of ^{57}Fe can be interpreted as the free energy for an even-even system with one extra nucleon.

V. SUMMARY AND CONCLUSIONS

Nuclear level densities for ^{56,57}Fe are renormalized using the new level density parametrization suggested by von Egidy and Bucurescu. The level densities obtained with the Oslo method agree well with those obtained from other experiments. The experimental level densities are used to extract thermodynamic quantities. The entropies for ^{56,57}Fe obtained in the microcanonical ensemble reveal step structures indicating the breaking of nucleon Cooper pairs. The entropy carried by the single neutron is estimated to be $\Delta S = 0.82 k_B$ which is smaller than that of the rare-earth isotopes. Assuming a constant ΔS, a critical temperature for the depairing process was determined. In the canonical ensemble, several thermodynamical properties were also investigated.

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REFERENCES

[1] D. Kusnezov, Y. Alhassid, and K. A. Snover, Phys. Rev. Lett. **81**, 542 (1998).
[2] M. Sano and S. Yamasaki, Prog. Theor. Phys. **29**, 397 (1963).
[3] A. Schiller, M. Guttormsen, M. Hjorth-Jensen, J. Rekstad, and S. Siem, Phys. Rev. C **66**, 024322 (2002).
[4] K. Kaneko and A. Schiller, Phys. Rev. C **75**, 044304 (2007).
[5] E. Tavukcu, Ph.D. thesis, North Carolina State University (2002).
[6] D. M. Brink, Ph.D. thesis, Oxford University (1955).
[7] P. Axel, Phys. Rev. **126**, 671 (1962).
[8] A. Schiller, L. Bergholt, M. Guttormsen, E. Melby, J. Rekstad, and S. Siem, Nucl. Instrum. Methods Phys. Res. A **447**, 498 (2000).
[9] A. Voinov, M. Guttormsen, E. Melby, J. Rekstad, A. Schiller, and S. Siem, Phys. Rev. C **63**, 044313 (2001).
[10] A. Schiller *et al.*, Phys. Rev. C **68**, 054326 (2003).
[11] A. Voinov *et al.*, Phys. Rev. C **74**, 014314 (2006).
[12] A. Voinov, private communication.
[13] T. von Egidy and D. Bucurescu, Phys. Rev. C **72**, 044311 (2005).
[14] R. Firestone and V. S. Shirley, *Table of Isotopes* (Wiley, New York, 1996).
[15] M. Guttormsen, M. Hjorth-Jensen, E. Melby, J. Rekstad, A. Schiller, and S. Siem, Phys. Rev. C **63**, 044301 (2001).
[16] J. Dobaczewski, P. Magierski, W. Nazarewicz, W. Satuła, and Z. Szymański, Phys. Rev. C **63**, 24308 (2001).
[17] M. Guttormsen, M. Hjorth-Jensen, E. Melby, J. Rekstad, A. Schiller, and S. Siem, Phys. Rev. C **64**, 034319 (2001).