# Pairing correlations and thermodynamical quantities in $^{96,97}$Mo

Z. Kargar*
*Physics Department, Shiraz University, Shiraz, Iran 71454*
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The nuclear level densities of $^{96,97}$Mo are calculated in the framework of superconducting theory. The parameters of nuclear level density are so chosen that the saddle point conditions are satisfied and the best fit to the experimental data yields. Then, using these parameters the energy, the entropy and the spin cut-off factor are calculated as a function of temperature. The curves show structures, reflecting the phase transition from a correlated to an uncorrelated phase. The critical temperature for quenching of pairing correlations is found at $T_c \sim 0.7$–$0.9$ MeV.

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## I. INTRODUCTION

In atomic nuclei many of thermodynamical quantities are not measured directly in contrast with the case of superconducting metals. These properties are expected to manifest themselves in various aspects of nuclear reactions. The nuclear level density is the most characteristic quantity in this respect as it can be obtained from nuclear reactions experiments.

Experimentally, level densities are extracted at low excitation energies from counting discrete levels and from counting resonances at the neutron binding energy. The Oslo group has established a method to extract level densities at excitation energies up to the neutron binding energy from measured $\gamma$ spectra [1–5]. This method has been recently applied to extract level densities in $^{96}$Mo and $^{97}$Mo isotopes using pick up ($^3$He, $\alpha\gamma$) and inelastic scattering ($^3$He, $^3$He$'\gamma$) reactions on a $^{97}$Mo target [6].

The two residual interactions in nuclear physics are short-range or pairing [7,8] and long-range or quadrupole. The energy gap in the spectra of even-even nuclei and odd-even effect observed in the nuclear masses are manifestation of pairing effect in nuclei. Pairing correlations significantly influence all nuclear properties such as binding energy, $\beta$-decay probability, collective modes, moment of inertia, and level density [9].

In recent experimental and theoretical studies the S-shape of the heat capacity curves is known as a signature of the pairing transition from a strongly paired states at low temperature to unpaired at higher temperature [10–16]. In order to specify the characteristics of the temperature dependance of the thermodynamic functions resulting from pair correlations, we have studied the behavior of the energy, the entropy and the spin cut-off parameter of level density—characterizing the distribution of angular momentum of states. To compare our theoretical results with the experimental data, we have obtained the entropies of $^{96,97}$Mo nuclei from the heat capacities extracted from experimental level densities of $^{96,97}$Mo nuclei [17]. In Sec. II we carry out the BCS calculations. The calculation procedures and the results are given in Sec. III.

*kargar@susc.ac.ir

## II. THEORY

The standard theory of pairing as applied to excited states is based on the grand partition function obtained from the BCS Hamiltonian [18–24]:

$$\ln \mathcal{Z}(\alpha,\beta) = -\beta\sum_k(\epsilon_k-\lambda-E_k) + 2\sum_k Ln[1+\exp(-\beta E_k)] - \beta\frac{\Delta^2}{G}, \quad (1)$$

where $T=1/\beta$ is the statistical temperature, $\epsilon_k$ is the energy of single particle state, $\lambda=\alpha/\beta$ is the chemical potential, $E_k=[(\epsilon_k-\lambda)^2+\Delta^2]^{1/2}-\Delta$ is the quasiparticle energy, and $G$ is the pairing strength. The gap parameter $\Delta$ is defined by the gap equation:

$$\sum_k\frac{1}{E_k}\tanh\left(\frac{1}{2}\beta E_k\right)=\frac{2}{G}. \quad (2)$$

The quantities $\alpha$ and $\beta$ are so chosen that the saddle point conditions

$$N=\frac{\partial \ln\mathcal{Z}}{\partial\alpha} \quad (3)$$

and

$$E=-\frac{\partial \ln\mathcal{Z}}{\partial\beta} \quad (4)$$

are satisfied. $N$ represents the nucleon number and $E$ is the energy of the system.

For a system of two kinds of fermions, namely $N$ neutrons and $Z$ protons one makes use of the additive properties

$$E=E_n+E_p, \quad (5)$$
$$S=S_n+S_p, \quad (6)$$
$$\ln\mathcal{Z}(\alpha_n,\alpha_p,\beta)=\ln\mathcal{Z}(\alpha_n,\beta)+\ln\mathcal{Z}(\alpha_p,\beta). \quad (7)$$

Once the partition function is known, the state density can be expressed in terms of the grand partition function within the saddle point approximation

$$\omega(N,Z,E)=\frac{e^S}{(2\pi)^{3/2}D^{1/2}}, \quad (8)$$

 

where

$$S = \ln \mathcal{Z} - \alpha_n N - \alpha_p Z + \beta E \tag{9}$$

is the entropy, and $D$ is the determinant of $3\times3$ matrix defined by the elements

$$d_{ij} = \frac{\partial^2}{\partial x_i \partial x_j} Ln\mathcal{Z}, \tag{10}$$

where $x \equiv (\alpha_n, \alpha_p, \beta)$ and second derivatives are evaluated at the saddle point.

We can calculate the total level density for a system of $N$ neutrons and $Z$ protons at excitation energy $E^*$,

$$\rho(N, Z, E^*) = \frac{\omega(N, Z, E^*)}{(2\pi\sigma^2)^{1/2}}, \tag{11}$$

where $\sigma^2$ which determines the width of angular momentum distribution of states is referred to as the spin cut-off factor,

$$\sigma^2 = \sigma_p^2 + \sigma_n^2 \tag{12}$$

with

$$\sigma_n^2 = \frac{1}{2}\sum_k m_k^{n2} \text{sech}^2\left(\frac{1}{2}\beta E_k^n\right), \tag{13}$$

$m_k'$s are the magnetic quantum numbers and the same relation holds for $\sigma_p^2$.

## III. RESULTS AND DISCUSSION

In this section we shall present the results for $^{96}$Mo and $^{97}$Mo nuclei obtained using the BCS theory described in the previous section. To take into account the effect of quadrupole-quadrupole interaction, we used the deformed single particle levels of Nilsson *et al.* [25]. The basic input for numerical calculations is the ground state gap parameter, taken from [26,27]. In order to calculate energy, we need to know $E$ at $T = 0$. So we put $T = 0$ and solve Eqs. (2) and (3) to find $\lambda$ and $G$ for specified number of particles and $\Delta$. Then, by setting $\Delta = 0$ and solving the same equations, the critical temperature $T_c$ and the corresponding chemical potential $\lambda_c$ are evaluated. Finally, using the obtained value of $G$ the quantities $\lambda(T)$ and $\Delta(T)$ are evaluated for a given value of temperature. These values are then used to compute the other quantities such as the energy, the entropy, the spin cut-off factor, and the level density. The results are not sensitive to the number of levels as long as the adequate number is included so that the levels of largest "$k$" have very small occupational probabilities.

The excitation energy of the nuclear system with temperature $T$ is

$$E^* = E(T) - E(0), \tag{14}$$

where $E(0)$ is the ground state energy evaluated from the obtained values of $\lambda(0)$ and $G$. Also, $E(T)$ is the energy at temperature $T$ which is evaluated from the obtained values of $\lambda(T)$ and $\Delta(T)$. In effect the calculations are done for each kind of particles and the total energy is calculated using Eq. (5).

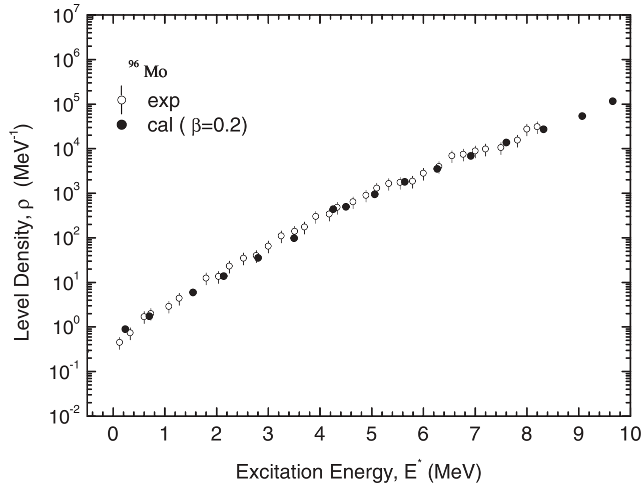


FIG. 1. The experimental [6] and the calculated level density as a function of excitation energy for the $^{96}$Mo nucleus. The deformation parameter is taken to be $\beta = 0.2$.

The odd neutron in $^{97}$Mo nucleus has the effect of reducing the gap parameter through blocking. We have taken into account this by reducing the ground state for nuclear pairing. For information on this procedure see [20,24].

The nuclear level density is evaluated from Eq. (11). The initial values of $\Delta_n$ and $\Delta_p$ are adjusted to improved the fit to the data. The resulting level densities are compared with the experimental values. Figures 1 and 2 show the logarithm of the level density as a function of excitation energy for $^{96}$Mo and $^{97}$Mo nuclei at deformation of $\beta = 0.2$. As can be seen from the figures the overall agreement between the experimental and theory with inclusion of pairing correlations is very good. The role of pairing effect is not apparent in the plots. To see the effect of pairing correlations, we investigate the thermodynamical properties of nuclear system.

The caloric curve for $^{96}$Mo and $^{97}$Mo nuclei are plotted in Fig. 3. The bump in the curves manifests the effect of pairing.

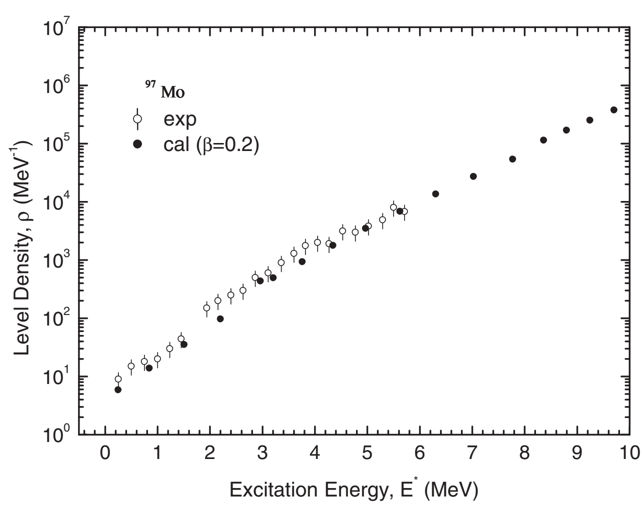


FIG. 2. The experimental [6] and the calculated level density as a function of excitation energy for the $^{97}$Mo nucleus. The deformation parameter is taken to be $\beta = 0.2$.

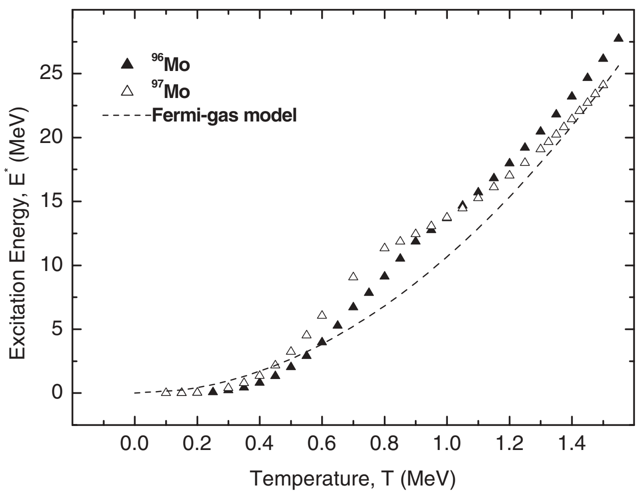


FIG. 3. Dependence of the excitation energy on temperature for $^{96,97}$Mo nuclei. The dotted line is the Fermi-gas values with he level density parameter $a = A/9$.

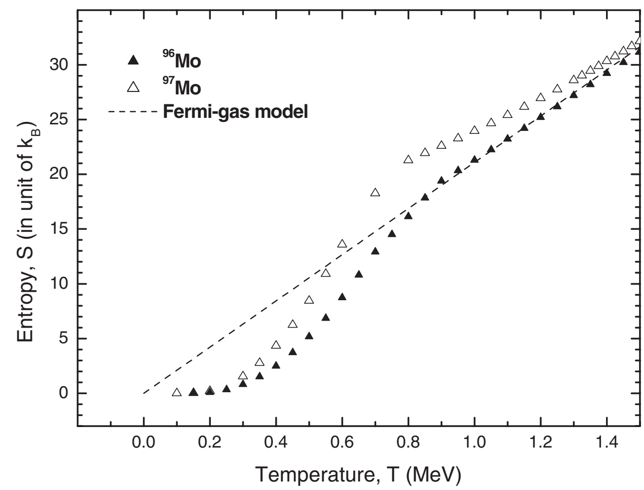


FIG. 5. The entropy versus temperature for $^{96,97}$Mo nuclei. The dotted line is the Fermi-gas values with he level density parameter $a = A/9$.

The critical temperature for quenching of pair correlations is found around $T_c \approx 0.7$–$0.9$ MeV. Below the critical temperature, the $^{97}$Mo nucleus has more excitation energy than the $^{96}$Mo nucleus at the same temperature. But, with increasing temperature the needed energy to heat the $^{96}$Mo nucleus to a given temperature $T$ is more. On the same figure the results from the Fermi-gas model [28] are also shown for comparison. The level density parameter is taken to be $a = A/9$, where $A$ is the mass number [24].

The entropy of the nuclear system is evaluated from Eq. (9) at temperature $T$ from the obtained values of $\lambda(T)$ and $\Delta(T)$ for neutron system and proton system. Then the total entropy is calculated from Eq. (6). The results are plotted for $^{96}$Mo and $^{97}$Mo nuclei as a function of excited energy in Fig. 4. The entropy of $^{97}$Mo nucleus is higher than of $^{96}$Mo nucleus due to the effect of unpaired neutron in odd system. Examination of the figure shows that the entropy difference between these nuclei is about 2.5 for excitation energy above 9 MeV. This is comparable with the value found for the rare-earth nuclei [29,30], but it is greater than the observed value of $\Delta S \gtrsim 1$ for deformed Mo isotopes [6]. The effect of pair-breaking process and phase transition is apparent from Fig. 5, which shows the variation of entropy versus temperature. The entropy curves exhibit structures. At higher temperature the vanishing of pairing interaction is apparent. The structural change in the entropy curves can be interpreted as a signature of the transition from strongly paired states at low temperature to unpaired at higher temperature. The dashed line on the figure represents the Fermi-gas values with the level density parameter $a = A/9$ [24]. Examination of Figs. 3 and 5 shows that above the critical temperature the energy and the entropy are approximated by the Bethe formulas, $E = aT^2$ and $S = 2aT$, respectively.

As we have regarded the nuclear system as two distinct systems, in Figs. 6 and 7 the contributions of the neutron

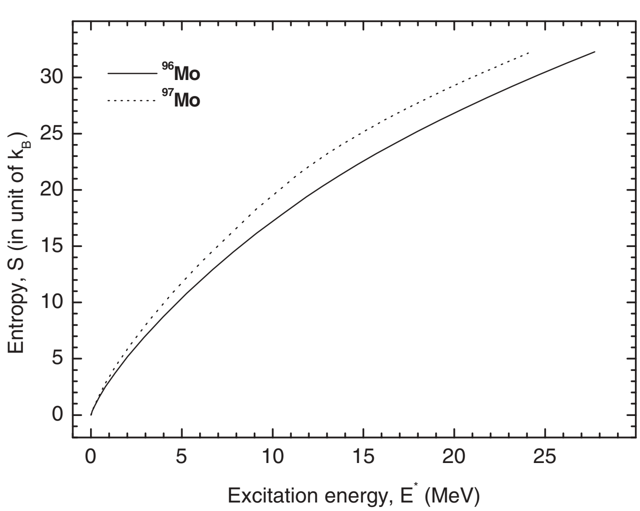


FIG. 4. The entropy as a function of excitation energy for $^{96,97}$Mo nuclei.

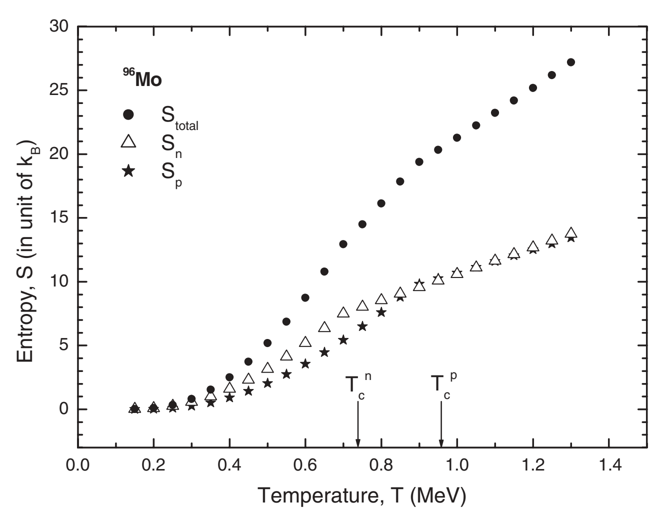


FIG. 6. The individual contributions of the neutrons and protons to the total entropy for the $^{96}$Mo nucleus. The arrows show the critical temperatures for neutrons and protons at 0.69 MeV and 0.89 MeV, respectively.

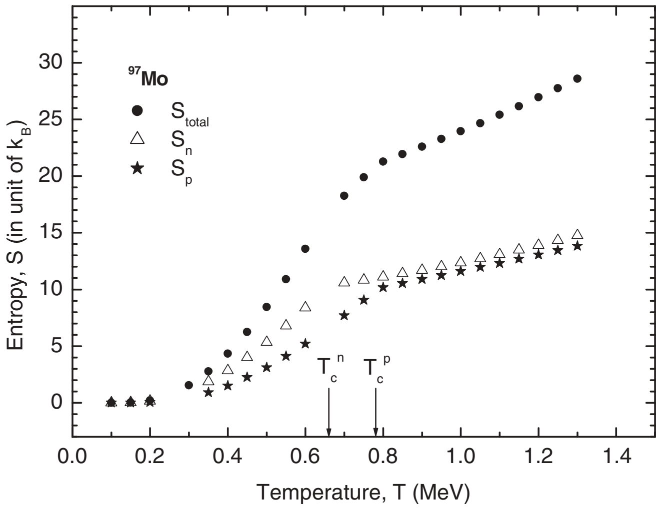


FIG. 7. The individual contributions of the neutrons and protons to the total entropy for the $^{97}$Mo nucleus. The arrows show the critical temperatures for neutrons and protons at 0.66 MeV and 0.78 MeV, respectively.

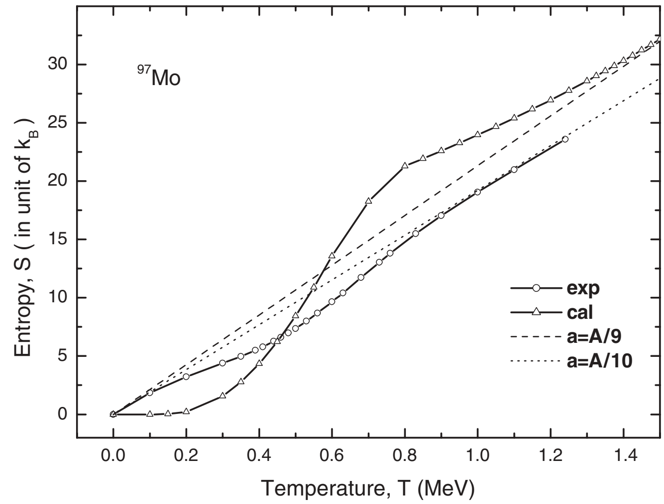


FIG. 9. The entropy as a function of temperature for the $^{97}$Mo nucleus. The open triangles are the calculated entropy, as in Fig. 5, and the open circles are the entropy obtained from the heat capacities extracted from the experimental level density [17]. The dashed and dotted lines are the Fermi-gas values with the level density parameter $a = A/9$ and $a = A/10$, respectively.

system and the proton system to the total entropy are shown. The critical temperatures for neutron part and proton part are $T_c^n = 0.69$ MeV and $T_c^p = 0.89$ MeV for the $^{96}$Mo nucleus and $T_c^n = 0.66$ MeV and $T_c^p = 0.78$ MeV for the $^{97}$Mo nucleus. The arrows on Figs. 6 and 7 indicate the critical temperatures. The calculated critical temperatures are in good agreement with the experimental values $T_c \sim 0.7$–1.0 MeV [6] for Mo isotopes.

The calculated entropies as well as the observed entropies obtained from the relation $C_V = T(\frac{\partial S}{\partial T})_V$ are plotted in Figs. 8 and 9 for $^{96}$Mo and $^{97}$Mo nuclei. The experimental heat capacities are extracted from the measured level densities as described in [6]. Both theoretical and experimental entropies show structure, although the values at a given temperature are different. The dashed and dotted lines on the figures denote the Fermi-gas values.

Using Eqs. (12) and (13), the spin cut-off factor has been calculated at temperature $T$. In Fig. 10 the spin cut-off factor is plotted as a function of temperature for $^{96}$Mo and $^{97}$Mo nuclei. Below the critical temperatures they show structures, while with increasing temperature the vanishing of pairing interaction is seen.

In summary, using the saddle-point approximation the experimental level densities of $^{96}$Mo and $^{97}$Mo nuclei are

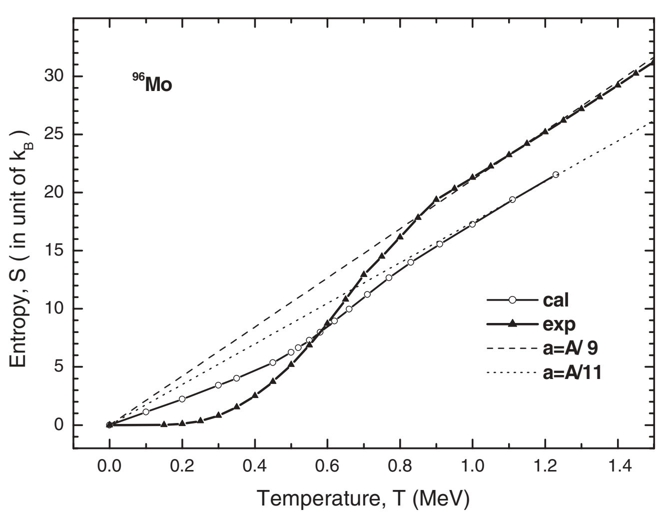


FIG. 8. The entropy as a function of temperature for the $^{96}$Mo nucleus. The filled triangles are the calculated entropy, as in Fig. 5, and the open circles are the entropy obtained from the heat capacities extracted from the experimental level density [17]. The dashed and dotted lines are the Fermi-gas values with the level density parameter $a = A/9$ and $a = A/11$, respectively.

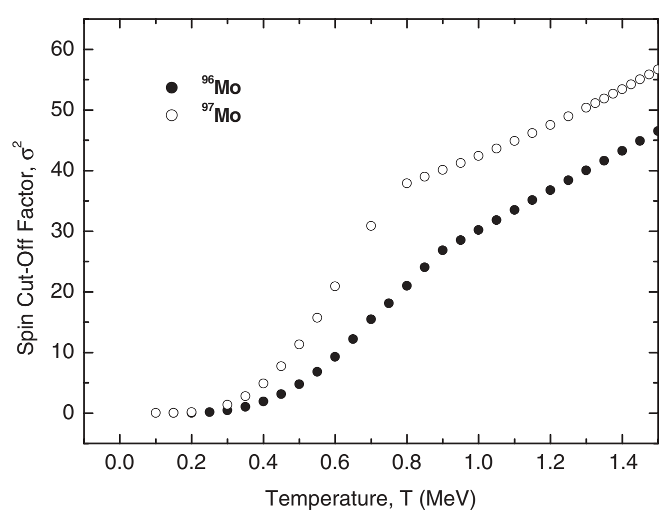


FIG. 10. The spin cut-off factor versus temperature for $^{96,97}$Mo nuclei.

reproduced well. We have shown that the pairing correlations can be well described by the Bardeen-Cooper-Schrieffer theory of superconductivity. Also, by using this theory the thermodynamical properties of nuclear pairing show structure, reflecting the nuclear phase transition. The calculation of the critical temperatures for quenching of the pairing transition yields $T_c \sim 0.7$–$0.9$ MeV for $^{96}$Mo and $^{97}$Mo nuclei. Very good agreement between experimental and theoretical critical temperatures is found.

## ACKNOWLEDGMENTS

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