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# Calculating the thermal properties of $^{93,94,95}$Mo using the BCS model with an average value gap parameter

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**Abstract** The gap parameter of the standard BCS model is replaced by the order parameter of the modified Ginzburg–Landau theory. Using this new form of the BCS model, the energy, entropy, and heat capacity of $^{93,94,95}$Mo nuclei are calculated. The results are compared with the experimental data and standard BCS results. Since the order parameter does not drop to zero at a critical temperature, our results for thermal properties are free of singularities. We have shown that the heat capacity as a function of temperature behaves smoothly and it is highly in agreement with the experimental heat capacity, while heat capacity behaves singularly and discontinuously in the standard BCS model. A smooth peak in the heat capacity is observed which is interpreted as a signature of the transition from the superfluid to the normal phase.

**Keywords** BCS · Ginzburg–Landau · Statistical fluctuations

## 1 Introduction

Systems of paired fermions are present in different fields of physics, and their size ranges from astronomical objects, such as neutron stars, to small systems, such as nuclei. Regardless of the origin of the pairing potential between fermions, the BCS [1–8] model and it's number projected versions [9–12] are the most popular tools used in investigations of paired systems. An important step in deriving BCS equations is finding the gap parameter. This parameter is the measure to find whether the system is in the paired phase or not. In the standard BCS model, we choose the most probable values of gap parameter, which are the values of gap parameter that minimize the free energy [2, 13]. This choice seems to be relevant when the number of constituents of the system are from the order of Avogadro's number. But when the number of particles decreases by orders of magnitude and we are dealing with a finite system such as nuclei, this choice is not the best one. In a finite system, the probability which the system remains in the states that are not the free energy minimum can be comparable with the probability of being in the free energy minimum [13]. Based on this fact, some authors used the mean value of gap parameter in place of the most probable value of it [13, 14]. In this method, the grand potential of the BCS model was used as the distribution function that reveals the importance of different values of the gap parameter at each temperature, and finally the mean value of the gap parameter can be calculated by integrating different values of the gap parameter weighted by this distribution function. Since calculating the mean value of the gap parameter is mathematically complicated, we are interested in the replacement method that can do the same job. Static path approximation(SPA) [15, 16] and it's modified versions [17–19] are the methods that systematically take the effect of statistical fluctuations into account and can be used in investigation of the paired finite systems. But

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since these methods are even more complicated than the mean value BCS, we try to use simpler methods.

Recently, an exact version of the Ginzburg–Landau (EGL) [20, 21] theory of second-order phase transitions was used in investigation of the thermal properties of nuclei. The EGL takes the effect of statistical fluctuations in a finite systems into account by averaging all of the possible order parameters. This procedure is in close analogy with the mean value BCS model. The order parameter of EGL plays the same role as the gap parameter of the BCS, and it seems to be a reasonable choice of a gap parameter that takes the effect of statistical fluctuations into account.

In this paper, we use the order parameter of the EGL as the gap parameter of the BCS model. Using this new formula for determining the gap parameter, the thermal properties, such as energy, entropy, and heat capacity of $^{93,94,95}$Mo nuclei, are calculated. In the case of heat capacity, the results are compared with the experimental heat capacities. In the first part of the paper, we express the used theories. In the second part, we discus the numerical method and results, and finally, we summarize the results.

## 2 Model

In the BCS model, all of the thermal properties are extracted from the grand potential, $\Omega$, of the system, which can be written as [2]:

$$\Omega = -\beta \sum (\varepsilon_k - \lambda - E_k) + 2\sum \ln(1+\exp(-\beta E_k)) - \beta\frac{\Delta^2}{G}, \tag{1}$$

where $\varepsilon_k$ is a single-particle energy of particles, $E_k = \sqrt{(\varepsilon_k-\lambda)^2+\Delta^2}$ is quasi-particle energy, $G$ is the pairing strength, $\lambda$ is the chemical potential, and $\beta = \frac{1}{T}$, where $T$ is the temperature. In this equation, $\Delta$ is the gap parameter, which is a measure of the pairing correlation . The standard choice for the gap parameter is the value that minimizes the grand potential:

$$\frac{\partial\Omega}{\partial\Delta} = 0, \tag{2}$$

which leads to the BCS gap equation

$$\sum \frac{1}{E_k}\tanh\left(\frac{1}{2}\beta E_k\right) = \frac{2}{G}. \tag{3}$$

Using this gap equation, the thermodynamic quantities of the system, such as the number of particles, $N$, the energy of the system, $E$, and the entropy, $S$, will be obtained in the following form:

$$N = \frac{\partial\Omega}{\partial\alpha} = \sum\left[1 - \frac{\varepsilon_k-\lambda}{E_k}\tanh\left(\frac{1}{2}\beta E_k\right)\right] (\alpha = \beta\lambda), \tag{4}$$

$$E = -\frac{\partial\Omega}{\partial\beta} = \sum \varepsilon_k\left[1 - \frac{\varepsilon_k-\lambda}{E_k}\tanh\left(\frac{1}{2}\beta E_k\right)\right] - \frac{\Delta^2}{G}, \tag{5}$$

$$S = \Omega - \alpha N + \beta E = 2\sum \ln[1+\exp(-\beta E_k)] + 2\beta\sum\frac{E_k}{1+\exp(\beta E_k)}. \tag{6}$$

Neglecting the small change in $\lambda$ as a function of temperature, the heat capacity, $C$, will be [13]

$$C = \frac{1}{T}\frac{dS}{dT} = \frac{1}{2}\sum \operatorname{sech}^2\left(\frac{1}{2}\beta E_k\right)\left[\beta^2 E_k^2 - \beta\Delta\frac{d\Delta}{dT}\right], \tag{7}$$

where

$$\frac{d\Delta}{dT} = \frac{\frac{1}{2}\sum \operatorname{sech}^2\left(\frac{1}{2}\beta E_k\right)}{\Delta\left(\frac{\beta}{2}\sum\frac{\operatorname{sech}^2\left(\frac{1}{2}\beta E_k\right)}{E_k^2} - \sum\frac{\tanh\left(\frac{1}{2}\beta E_k\right)}{E_k^3}\right)}. \tag{8}$$

Investigation of the thermal properties of finite systems, such as nuclei, with the above formulation predicts unphysical results. For example, when we compare the calculated heat capacity as a function of temperature (Eq. 8) with the experimental data of heat capacity [22–27], an important issue emerges. Calculated heat capacity shows a singularity at the critical temperature, which is observed in the experimental data in the form of a smooth S-shaped peak. This singularity is a consequence of the choice that was made in choosing the gap parameter. In fact, when dealing with the finite systems, the grand potential minimum is the most probable state of the system, but there are other states with considerable probabilities that are not the grand potential minimums and should be taken into account. So it seems necessary to search for such averaged gap parameters and replace them with the standard gap equation (Eq. 3).

The averaged gap parameter that we use in this paper is the order parameter of the EGL model [21]. There are some typos in the relation for the average absolute value of the order parameter (equation 16 of Ref. [21]), and the correct form is:

$$\overline{\Delta(T)} = \frac{T_c\pi^{\frac{3}{2}}\int_0^\infty \lambda^{\frac{1}{2}} e^{-\left(\pi\sqrt{\frac{b}{t\delta}}\lambda + \frac{\pi(t-1)}{2\sqrt{tb\delta}}\right)^2} d\lambda}{\sqrt{\frac{\delta}{2b}}t^{\frac{1}{2}}\left(1 \pm \operatorname{erf}\left(\left|\frac{\overline{\Delta t}}{t^{\frac{1}{2}}}\right|\right)\right)}, \tag{9}$$

where erf is the error function, $\delta$ is the single-particle energy spacing of single-particle energy states, and $T_c$ is the critical temperature of the system. The paired system shows a phase transition at this temperature when the size of the system increases to a macroscopic scale. The upper

sign in denominator applies for $T < T_c$ and the lower sign applies when $T > T_c$. In this formula, $\overline{\Delta t} = \frac{1}{2}\pi(t-1)/\left(b\bar{\delta}\right)^{\frac{1}{2}}$, $t = \frac{T}{T_c}$, $\bar{b} = 7\zeta(3)/16 = 0.526$, and $\bar{\delta} = \delta/k_B T_c$.

Using the averaged value of the gap parameter in place of the gap equation (Eq. 3), we will have the following equations for thermal properties:

$$N = \frac{\partial\Omega}{\partial\alpha} = \sum\left[1 - \frac{\varepsilon_k - \lambda}{E_k}\tanh\left(\frac{1}{2}\beta E_k\right)\right], \tag{10}$$

$$E = -\frac{\partial\Omega}{\partial\beta} = \sum \varepsilon_k\left[1 - \frac{\varepsilon_k - \lambda}{E_k}\tanh\left(\frac{1}{2}\beta E_k\right)\right] - \frac{\bar{\Delta}^2}{G} - \left(\bar{\Delta}^2 + \beta\bar{\Delta}\frac{\partial\bar{\Delta}}{\partial\beta}\right)\left(\sum\frac{\tanh\left(\frac{1}{2}\beta E_k\right)}{E_k} - \frac{2}{G}\right), \tag{11}$$

$$S = 2\sum\ln[1+\exp(-\beta E_k)] + 2\sum\frac{\beta E_k}{1+\exp(\beta E_k)} + \beta^2\bar{\Delta}\frac{\partial\bar{\Delta}}{\partial\beta}\left(\frac{2}{G} - \sum\frac{\tanh\left(\frac{1}{2}\beta E_k\right)}{E_k}\right), \tag{12}$$

where $E_k = \sqrt{(\varepsilon_k - \lambda)^2 + \overline{\Delta}^2}$. It is important to note that since the $\overline{\Delta(T)}$ does not depend on $\alpha$, the above relations for the BCS model with an average gap parameter are the same as the equations expressed in Ref. [14] if we put $\frac{\partial\bar{\Delta}}{\partial\alpha} = 0$. The heat capacity can be numerically calculated, using the relation: $C \approx -\beta\frac{dS}{d\beta}$.

## 3 Results and discussion

In this section, we investigate the thermal properties of $^{93,94,95}$Mo nuclei using both the above formulations of the BCS model and try to clarify the differences between two methods.

In both methods that were mentioned before, two parameters should be calculated at each temperature: gap parameter, $\Delta$, and chemical potential, $\lambda$. The equations that are used in the BCS model for determining these parameters are Eqs. (4) and (3), which should be solved simultaneously at each temperature. When we use the mean value of the gap parameter, Eqs. (9) and (10) should be used.

At the beginning, we should find a set of single-particle energy states. We have used the single-particle energy states of the deformed shell model [28–31] for protons and neutrons. The dipole deformation parameter, $\beta_2$, values were chosen from Ref. [26]. The parameters that were used in our calculations are tabulated in Table 1.

At the first step, we calculate the pairing strength, $G$, by solving Eqs. (3) and (4) simultaneously at zero temperature. The gap parameters at zero temperature were calculated in Ref. [26] using the three-point method. We used these values in the case of neutrons, but in the case of protons, slightly different values of the gap parameters were used which could reproduce the experimental heat capacity better. The three-point and used values of the gap parameter are given in Table 1.

The most probable value of the gap parameter, $\Delta$ (Eq. 3), and the average value of gap parameter, $\overline{\Delta}$, (Eq. 9) of protons and neutrons are plotted as a function of temperature for $^{93,94,95}$Mo in Figs. 1 and 2. The average value gap parameters are normalized to equal the most probable value of gap parameter at zero temperature. We see that $\Delta$ reduces to zero suddenly at a critical temperature, while $\overline{\Delta}$ decreases gradually and smoothly goes to zero. This behavior is in agreement with other theoretical predictions [14, 26] and is correlated with the S-shape of the heat capacity.

In calculating the average value of gap parameter with Eq. (9), two parameters should be used: the single-particle energy spacing of single-particle energy states ($\delta$) and the critical temperature of the system ($T_c$). $\delta$ for each nuclei is calculated from the experimental slow neutron resonances and $(n,\gamma)$ cross sections that were analyzed according to the equidistant spacing model [32]. In the formal BCS model, one can calculate the critical temperature by solving the gap equation and searching for the temperature at which the gap parameter vanishes. These calculations result in approximate relations such as $T_c \approx 0.57\Delta(0)$ [6] or $T_c = 0.6\Delta(0)$ [33] between the critical temperature and the values of $\Delta(0)$. In this work, since we are not using the gap equation, the same relation between $T_c$ and $\Delta(0)$ was not used and we chose a critical temperature that can reproduce the S-shape of the heat capacity well. The calculated and used values of the parameters are given in Table 1.

Using the average value of the order parameter and its derivatives, the energy is calculated from Eq. (11) as a function of temperature. The total energy is $E = E_p + E_n$ and can be calculated by summing the proton energy with the neutron energy. The results are plotted in Fig. 3 for $^{93,94,95}$Mo in comparison with the most probable energy which was calculated using Eq. (5). The results show that both methods are in correspondence at low- and high-temperature regions and the use of average pairing parameter causes the energy graph to behave smoothly near the critical temperature.

Total entropy of a nucleus is calculated by summing the entropy of protons with the neutrons' entropy. The total entropy of the studied nuclei is plotted in Fig. 4 using both the most probable gap parameter formulation, Eq. (6), and the average gap parameter formulation, Eq. (12). The same pattern as in the case of total energy is seen here.

**Table 1** Used parameters in our calculations (For details see the text)

| Nuclei | Used $\Delta_n(0)$(MeV) | $\Delta_n(0)$[26](MeV) | Used $\Delta_p(0)$(MeV) | $\Delta_p(0)$[26](MeV) | $Tc$(MeV) | $\beta_2$[26] | $\delta(\text{MeV})^{-1}$[32] |
|---|---|---|---|---|---|---|---|
| $^{93}$Mo | 0.85 | 0.85 | 1.80 | 1.60 | 1.00 | 0.10 | 0.13 |
| $^{94}$Mo | 1.20 | 1.20 | 1.90 | 1.60 | 0.95 | 0.15 | 0.13 |
| $^{95}$Mo | 1.10 | 1.10 | 1.90 | 1.50 | 0.85 | 0.08 | 0.12 |

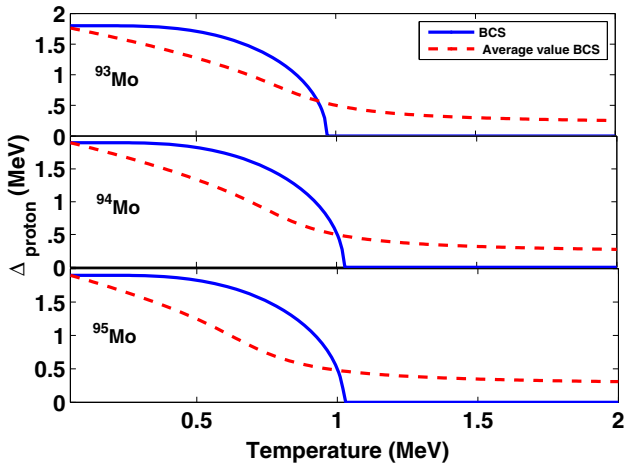


**Fig. 1** (Color online) Pairing gap parameter of protons as a function of temperature. The most probable value and the average value of gap parameter for protons of $^{93,94,95}$Mo are plotted, respectively, by a *solid line* and a *dashed line*

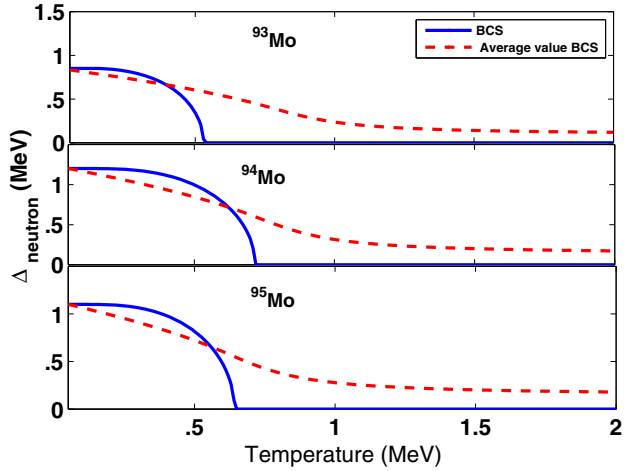


**Fig. 2** (Color online) Pairing gap parameter of neutrons as a function of temperature. The most probable value and the average value of gap parameter for neutrons of $^{93,94,95}$Mo are plotted, respectively, by a *solid line* and a *dashed line*

In Fig. 5, we have plotted the total heat capacities of $^{93,94,95}$Mo. The results of the most probable gap parameter formalism, the average value gap parameter formalism, and the experimental heat capacities [26] are plotted for comparison. It can be observed that using $\bar{\Delta}(T)$ instead of $\Delta(T)$

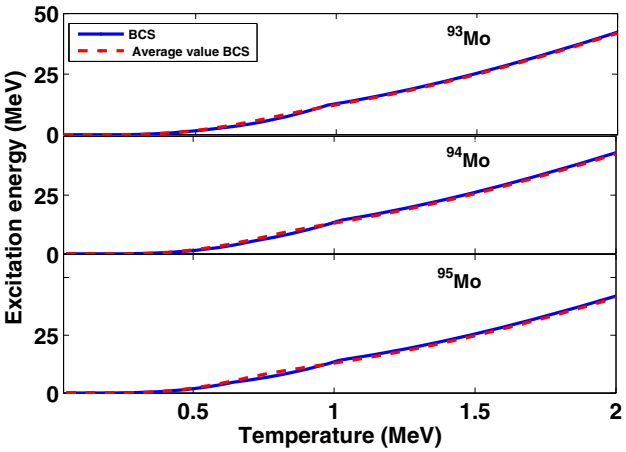


**Fig. 3** (Color online) Total energy versus temperature. Total energy of $^{93,94,95}$Mo has been plotted using the average value and most probable value of the gap parameter

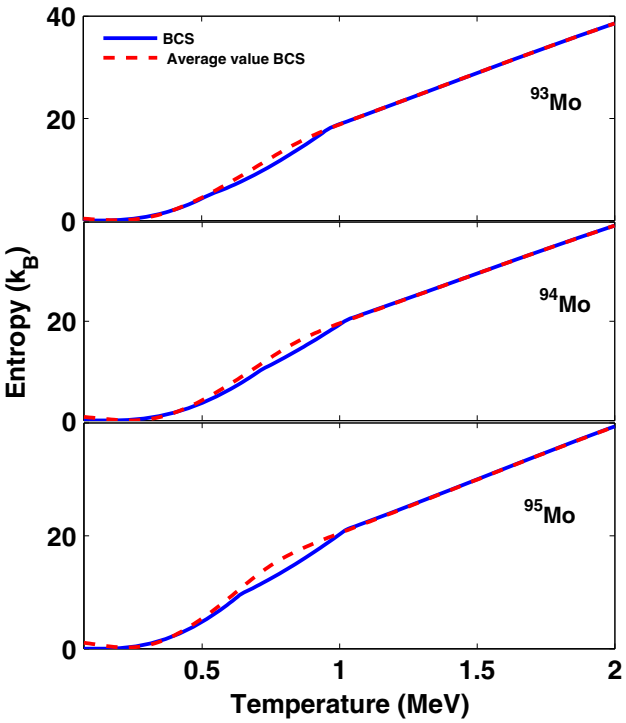


**Fig. 4** (Color online) Total entropy versus temperature. Total entropy of $^{93,94,95}$Mo has been plotted using the average value and most probable value of the gap parameter

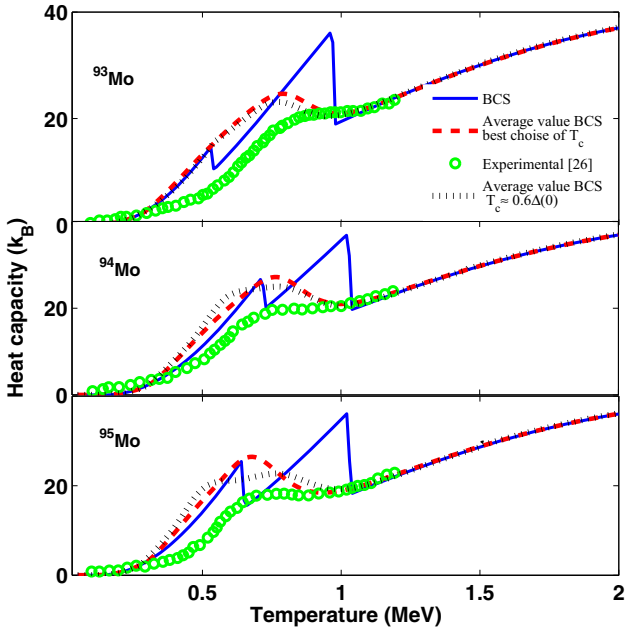


**Fig. 5** (Color online) Total heat capacity as a function of temperature. Total heat capacity of $^{93,94,95}$Mo has been plotted using the average value of the gap parameter with different choices of $Tc$ and a formal BCS model. The experimental heat capacity [26] has been plotted for comparison

and also considering thermal fluctuations cause the singular unreal points in heat capacity to disappear. In order to study the effect of different choices of critical temperature, we have also plotted the heat capacity using the critical temperature of the formal BCS model in this figure. The critical temperature of BCS is approximately equal with $0.6\Delta(0)$. In the case of $^{94,95}$Mo, we can see two smooth peaks in correspondence with the number of peaks of BCS heat capacity, but since they are smooth, they look like a single hump. It should be noted that, as shown in Figure 2 of Ref. [20], if the heat capacity of the paired phase of a small system is calculated using the MGL model, we observe that the smooth peak of the heat capacity of a small system is located at some lower temperature when compared to the critical temperature of the large system. So the smooth peaks of the mean value calculations do not occur at the BCS critical temperatures and are observed at some lower temperatures. In the case of $^{93}$Mo, since the role of neutrons in phase transition is less than the protons (small $\Delta_n(0)$), the neutrons mean value heat capacity is too smooth and does not produce a separate hump, and we just see the hump of the protons heat capacity in the total heat capacity. In fact, the critical temperatures that are listed in Table 1 were chosen to have a single hump in the heat capacity. Calculated heat capacities agree with the experimental data at the high-temperature and low-temperature regions well. Therefore, it can be said that calculated heat capacity using the average value BCS model exhibits an S-shape, which is in harmony with the experimental data.

## 4 Conclusion

In this paper, we have used the BCS model with an average gap parameter to investigate the thermal properties of $^{93,94,95}$Mo. Since the average gap parameter decreases smoothly, the energy and entropy graphs versus temperature behave smoothly near the critical temperature of the BCS model. With the use of the average gap parameter, the singular points in heat capacity, which were predicted by BCS model, disappeared. The heat capacity of the BCS model with average gap parameter shows the S-shape which can be seen in the experimental data of heat capacity.

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