Specific heat and shape transitions in light sd nuclei

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A systematics of thermal properties, for nuclei with $16 \leq A \leq 30$, is presented. The study has been motivated by previous reports on phase transitions involving nuclei belonging to the 2s-1d shell. We have used the nuclear SU_3 scheme to calculate the specific heat and the temperature dependence of the intrinsic quadrupole moment for each nuclei. We have found that finite size effects and not true phase transitions are affecting the temperature dependence of these quantities, at least within the SU_3 scheme and for the nuclei which we have considered.

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I. INTRODUCTION

In a series of recent papers [1–4] the finding of phase transitions in finite nuclei has been reported. On the other hand, similar calculations, for some of the light nuclei belonging to the 2s1d shell, have shown that the proposed phase transition does not occur [5]. This phase transition was related to a change in the nuclear shape induced by thermal excitations [1]. In the work of Ref. [2] the nuclear specific heat, for the case of ^{24}Mg, was computed using nuclear eigenstates obtained with a number of realistic interactions and also using the available data on the observed energies. The appearance of a prominent peak in the specific heat, for temperatures of the order of $1.7 \leq T \leq 3$ MeV, was interpreted as the signature for a phase transition. Moreover, a change in the nuclear shape was associated with it [2]. However, from the results reported by Dukelsky et al. [5] no change in the sign of the intrinsic quadrupole moment was obtained at these temperatures. In a more recent work [6] the question of the nature of the suggested phase transition is reviewed, this time with reference to finite size effects. In the present work we have computed the specific heat and the intrinsic quadrupole moment, among other temperature dependent quantities, for 11 even-even nuclei in the sd shell and in the context of the nuclear SU_3 model [7, 8]. The results predicted by this model have been tested previously, by Dukelsky et al. [5], against the results obtained by using realistic interactions. Since the nuclear SU_3 model of Elliot allows for a systematics in the above mentioned mass region, we have adopted it in order to include the relatively large number of configurations required for the calculation of mean values at finite temperatures. Because of the relatively good agreement found between descriptions based on the nuclear SU_3 model and realistic interactions for the s-d shell [5], although spin-orbit and pairing effects are not included in the crude SU_3 approach, the present results are expected to show similar overall features as compared with results obtained by using more realistic nuclear Hamiltonians.

II. FORMALISM

A. Classification of states according to SU_3 group

The success of the SU_3 description of collective features in light nuclei has been established long ago [8].

The SU_3 scheme reproduces the overall features of the spectra and transition probabilities involving collective bands. Detailed comparisons between SU_3 descriptions [8] and results obtained using realistic two-body interactions [9] have been reported extensively and we shall not discuss it here again. The clasification of nuclear states according to the SU_3 scheme was proposed by Elliot [7]. The Elliot SU_3 nuclear model has been described in detail in review articles [8]. It has been succesfully applied to nuclei belonging to the 2s1d shell [10]. In terms of the SU_3 quantum numbers (λ, μ) the eigenvalues of the nuclear Hamiltonian are given by the following expression [5, 8]:

$$E(\lambda, \mu, L) = \kappa[A_0 - 4\{\lambda^2 + \mu^2 + \lambda\mu + 3(\lambda + \mu)\} + 3L(L+1)],$$

(1)

where L is the angular momentum. The constants κ (strength of the quadrupole interaction) and A_0 (the energy shift) are adjusted by fitting, for each nucleus, the energy of the first excited $J^\pi = 2^+$ state and by imposing the condition $E(\lambda, \mu, L = 0) = 0$ for the representation (λ, μ) associated to the ground state. Since the model has been extensively described [8], we shall omit further details about it and we shall directly introduce the formalism which we have adopted for the present calculations.

The values of (λ, μ) representations of the SU_3 group for the different nuclei which are included in the calculation, namely, ^{18}O, ^{18}Ne, ^{20}O, ^{20}Ne, ^{22}Ne, ^{22}Mg, ^{24}Ne, ^{24}Mg, ^{26}Mg, ^{26}Si, and ^{28}Si, are taken from the compilation of Perez and Flores [11]. The constants κ and A_0, the number of representations of the SU_3 group, the total number of configurations including the degeneracy in the total angular momentum and in the total isospin, and the experimental energy of the first excited 2^+ state, for each nucleus, are the input of the present calculations. The number of configurations has been calculated, for each case, by applying the rules of Elliot [5, 8] in the following form:

$$K = \min(\lambda, \mu), \min(\lambda, \mu) - 2, ..., 0 \text{ or } 1$$

and

$$L = \begin{cases} K, K+1, ..., K + \max(\lambda, \mu) & \text{if } K \neq 0, \\ \max(\lambda, \mu), \max(\lambda, \mu) - 2, ..., 0 \text{ or } 1 \text{ if } K = 0. \end{cases}$$

For a state belonging to the SU_3 representation, the intrinsic quadrupole moment is given by

$$Q_0(\lambda,\mu) = \begin{cases} (2\lambda + \mu + 3) & \text{if } \lambda \geq \mu, \\ (-\lambda - 2\mu - 3) & \text{if } \lambda < \mu. \end{cases}$$

B. SU_3 model and the partition functions

We shall assume the validity of the SU_3 description and proceed with the calculation of relevant expectation values at finite temperature, such as the intrinsic quadrupole moment, the excitation energy, etc. The canonical partition function is defined by

$$Z(\beta) = \sum_i (2I_i + 1)(2J_i + 1)e^{-\beta E_i}, \qquad (2)$$

where the subscript i labels irreducible representations of the SU_3 group and β is the inverse temperature $\beta = 1/T$ (with T in MeV) [5]. The isospin and the total angular momentum, for each irreducible representation, are denoted by I_i and J_i, respectively. With this partition function one can calculate the mean energy

$$E = -\frac{\partial \ln Z(\beta)}{\partial \beta} \qquad (3)$$

and the specific heat

$$C = \frac{\partial E}{\partial T}. \qquad (4)$$

Other observables are calculated as

$$\langle \Theta \rangle = \frac{\sum_i (2I_i + 1)(2J_i + 1)e^{-\beta E_i}\langle \Theta \rangle_{I_i,J_i}}{Z(\beta)}, \qquad (5)$$

where $\langle \Theta \rangle_{I_i,J_i}$ is the diagonal matrix element of the operator Θ in a given SU_3 representation.

III. RESULTS AND DISCUSSION

We have adopted, for the SU_3 Hamiltonian, a pure quadrupole-quadrupole interaction [8]. The constants entering in the definition of the energy, Eq. (1), have been determined from the data on the excitation energy of the
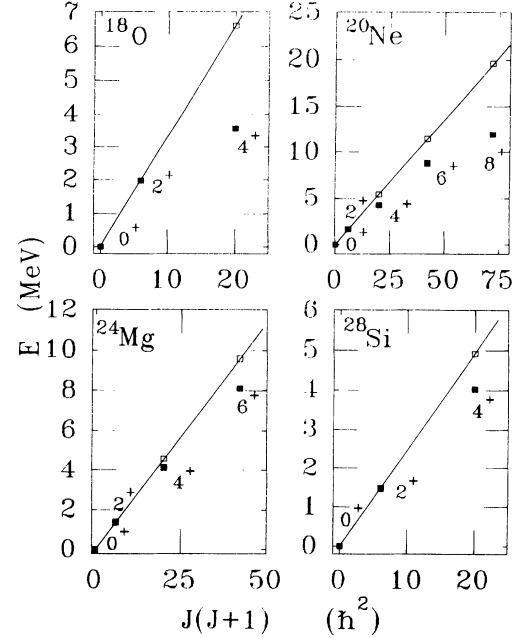

FIG. 1. Yrast line for some of the nuclei considered in the text. Solid lines (with open squares) indicate the energies predicted by the SU_3 model. Experimental values are taken from Refs. [15, 16] and are denoted by solid squares.

first excited quadrupole state. The resulting values for κ and A_0 are listed in Table I together with the number of SU_3 representations and the corresponding number of configurations for each nuclei. These values have been taken from [11]. We have performed our calculations for all the nuclei listed in Table I. To illustrate the results we have selected some cases, which are shown in Figs. 1–7. The predicted yrast line, for some of the nuclei considered in the present analysis, is shown in Fig. 1. The overall agreement between data and the values predicted by the SU_3 scheme is acceptable, as we have verified from the results corresponding to the complete set of nuclei.

The spectral distribution $D(E)$, i.e., the number of eigenstates per unit energy normalized to the total number of eigenstates, corresponding to the set of SU_3 configurations included in the calculations, is shown in Fig.

TABLE I. SU_3 parameters used in the calculations. The constants A_0 and κ have been adjusted to reproduce the energy of the first excited quadrupole state in each nucleus. The number of SU_3 representations and configurations is taken from Perez and Flores [11].

Nucleus	A_0	κ [MeV]	SU_3 representations	SU_3 configurations
^{18}O	112	0.11	3	8
^{18}Ne	112	0.10	3	8
^{20}O	352	0.09	20	78
^{20}Ne	352	0.09	20	84
^{22}Ne	456	0.07	90	493
^{22}Mg	456	0.07	90	500
^{24}Ne	592	0.11	263	170
^{24}Mg	592	0.08	263	625
^{26}Mg	640	0.10	501	417
^{26}Si	640	0.10	501	454
^{28}Si	720	0.08	622	525
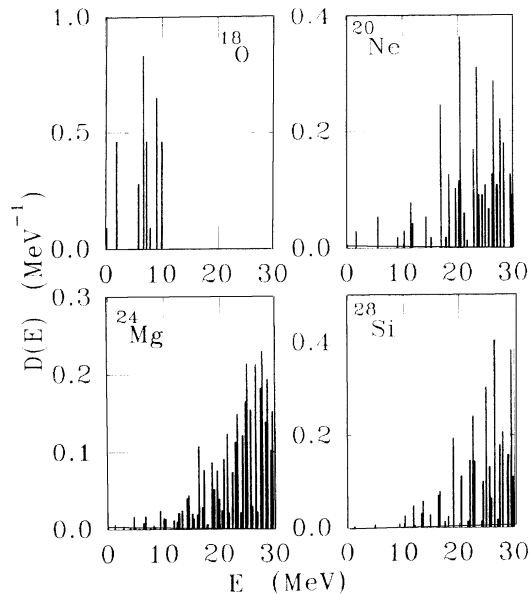
FIG. 2.　Spectral distribution functions $D(E)$ in the SU_3 scheme, as a function of the energy E.

FIG. 3.　Average excitation energy E as a function of the temperature T.

2. It is observed that $D(E)$ is strongly mass dependent but it saturates; i.e., it reaches a maximum value and then decreases at energies of the order of 20–30 MeV. The fragmentation is larger for the heavier isotopes. We have verified that an increase in the number of configurations does not change the structure of $D(E)$ significantly. The same can be said about the maximum excitation energy used in the calculation, which has been fixed at $E_{max} = 30$ MeV, since changing this value to $E_{max} = 50$ MeV does not affect the results. The results for $D(E)$, of Fig. 2, reproduce the observed trend, namely, a dominant rotational ground state band followed by a large number of configurations belonging to other SU_3 representations. The eigenvalue densities, except for collective ground state bands, have a shape which can be described by a distribution similar to the binomial shape reported by Cortes et al. [12]. To summarize the analysis based on the SU_3 model the following features can be mentioned: (a) The rotational ground state band is well reproduced; it goes typically up to energies of the order of 12 MeV for $J^\pi = 8^+$. (b) The spectral distribution $D(E)$ is approximately binomial. (c) The spectral distribution shows, practically in all cases, a number of low-lying collective states followed by a larger number of noncollective excitations. The difference between collective and noncollective excitations is, of course, given by the associated SU_3 clasification.

Statistical expectation values have been calculated with the partition function (2). The structure of $Z(\beta)$ is practically the same for all nuclei, except for ^{18}O and ^{18}Ne where the increase of $Z(\beta)$ with T is less pronounced. The temperature dependence of the mean-value of the energy, Eq. (3), is shown in Fig. 3. All functions displayed in Fig. 3 show an increasing trend with T but this tendency is still far from the linear one which is expected to appear at high temperature and in
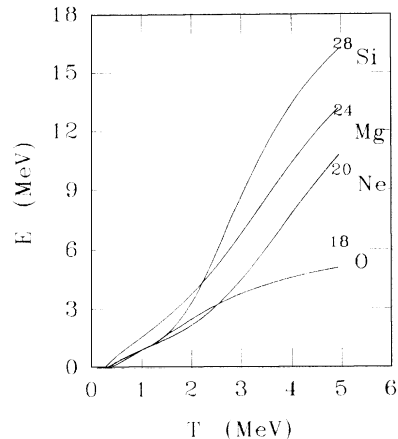
the presence of saturation. For most of the cases a change in the slope is observed at low T.

The specific heat is shown in Fig. 4. The shape of these curves is similar to the one reported in [2, 5]. However, the present systematics shows that the presence of a bump at T of the order of 2–4 MeV is a common feature in all cases. The appearance of a peak at low temperature depends upon the cases; it is more pronounced for ^{20}Ne, ^{22}Ne, and ^{26}Mg and less evident for the other nuclei. The result corresponding to the case of ^{20}Ne reproduces the trend reported by Dukelsky et al. [5]. The interesting question is of course related to the identification of the high temperature bump as a signal for a phase transition [2]. Following the discussion advanced in Ref. [5], and in order to answer the above question, we have calculated the expectation value of the intrinsic quadrupole moment $\langle Q_0 \rangle$. The results are shown in Fig. 5. The important feature shown by these curves is that the intrinsic quadrupole moment, for all the cases considered here, does not change sign. It means that the SU_3 model does not lead to any temperature dependent effect so notorious as the phase transition claimed by the authors of Refs. [1–4]. There is, however, a tendency to decrease the absolute value of the intrinsic quadrupole moment, but the change in shape is well beyond the maximum temperature allowed in the present calculation and well beyond an acceptable value of T for finite nuclei. Concerning the bump at T of the order of 2–4 MeV it can be better explained by the finite size of the configuration space, i.e., the so-called Schottky effect [13]. To clarify this point we have computed the specific heat for a model situation where the spectral density distribution is represented by a rotational band followed by a binomial distribution corresponding to high-lying vibrational states [14]. The results are shown in Fig. 6, together with the results obtained with the SU_3 model. The agreement between both models is good and it gives support to the conclusion of the work of Ref. [5]. Finally, and in order to support this conclusion concerning the structure of the bump shown by the specific heat, we have computed the expectation value of the number of quanta for each degree of freedom described by the SU_3 model. The
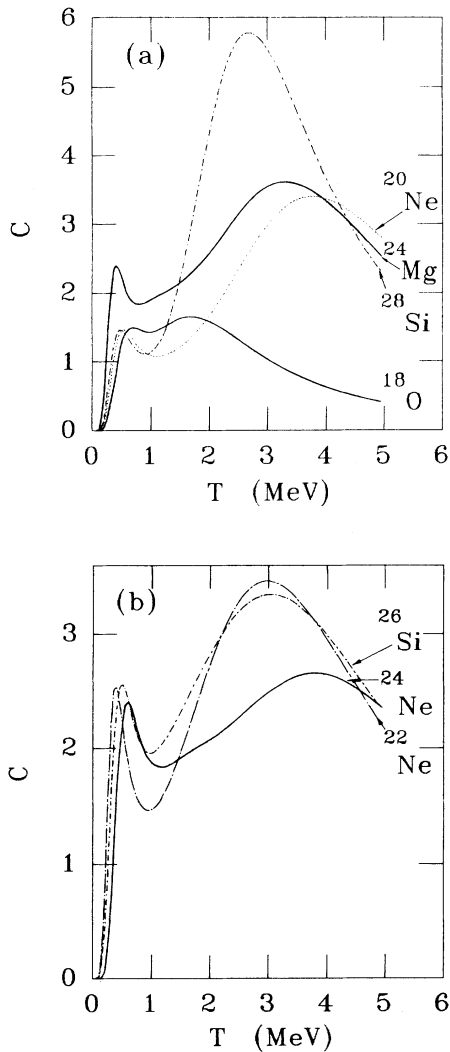
FIG. 4. Temperature dependence of the specific heat C for some of the nuclei listed in Table I.
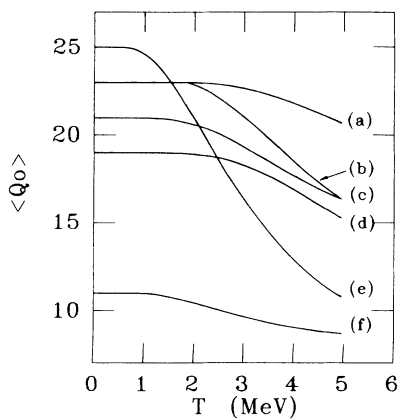
FIG. 5. Temperature dependence of the intrinsic quadrupole moment $\langle Q_0 \rangle$ (in arbitrary units). The cases are denoted by (a) ^{24}Ne, (b) ^{24}Mg, (c) ^{22}Ne, (d) ^{20}Ne, (e) ^{26}Si, and (f) ^{18}O , respectively.
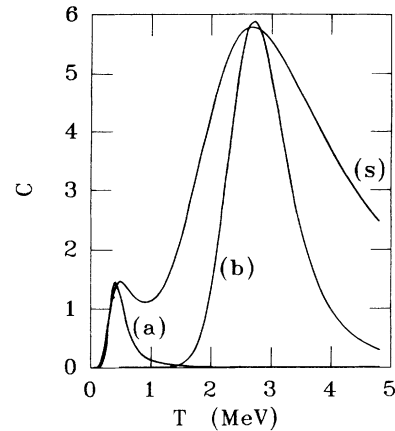
FIG. 6. Specific heat C for the case of ^{28}Si calculated with (a) a simplified model with a low-lying rotational spectrum and (b) a vibrational spectrum; curve s corresponds to the SU_3 model.

results are shown in Fig. 7. Again from these results the occurrence of phase transitions can be safely ruled out.

IV. CONCLUSIONS

In this work we have presented some evidence against the occurrence of phase transitions in light nuclei belonging to the s-d shell. The conclusions are based on calculations performed with the SU_3 model and are, of course, valid within this framework. However, the comparison between results obtained with the SU_3 model and with realistic forces has already shown that the main features of the spectrum of light nuclei calculated with realistic forces are very well reproduced by the SU_3 scheme [3]. In the present case we have also shown that the occurrence of a bump in the specific heat might be due to finite size effect rather to a nuclear structure effect leading to a
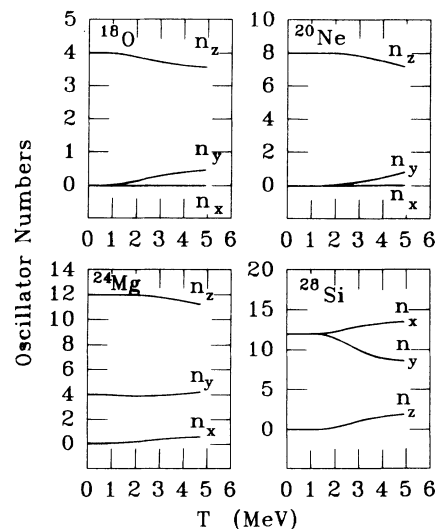
FIG. 7. Temperature dependence of average SU_3 oscillator quantum numbers [9] for some of the cases considered in the calculations.

phase transition. In this respect and taking the value of the intrinsic quadrupole moment as an order parameter its temperature dependence does not show the features expected for phase transitions.

We have shown that the conclusions of Ref. [5] are indeed valid for all the nuclei which we have considered and that they are not restricted to an isolate example, like, i.e, the case of ^{20}Ne.

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