Nuclear level densities in self-consistent field approximation

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Abstract. The effect of two-body nature of the nuclear shell model potential on the recent numerical calculations of the nuclear level density has been examined. For the two most widely used single particle energy level schemes based on harmonic oscillator and Woods-Saxon potential, this effect is shown to significantly modify the excitation energy dependence of the level densities.

Keywords. Nuclear level densities; self-consistency.

1. Introduction

Nuclear level density plays an important role in any statistical analysis of the nuclear reactions. The most commonly used expression for the nuclear level density is from Bethe (1963, 1937), namely $\rho(E_x) = C \exp(\sqrt{2aE_x})$ where the pre-exponential factor C is a slowly varying function of the excitation energy E_x, and a is the level density parameter which is obtained from fits to the available experimental data on neutron evaporation spectra or neutron resonance spacing data, etc. The level density parameters a, obtained from fits to the measured neutron resonance spacing data, are centred around excitation energies $6 \sim 8$ MeV and show strong shell dependence. However, these parameters are not suitable for use at other excitation energy ranges because of the strong excitation energy dependence of the shell effects on the nuclear level densities (Ramamurthy et al 1970). In recent years, several workers have reported numerical calculations of nuclear level densities starting from a set of shell model single particle energy levels (Huizenga and Moretto 1972, Huizenga et al 1973). In these numerical calculations, the nucleus is considered as a non-interacting fermion gas in a shell model potential. The following standard expressions of statistical mechanics for non-interacting Fermion gas are used in these numerical calculations to obtain the nuclear entropy and, therefore, the nuclear level density.

$$S = - \sum_k [n_k \ln n_k + (1 - n_k) \ln (1 - n_k)]$$

$$E_t = \sum_k n_k \, \epsilon_k$$

$$E_0 = \sum_{k=1}^{N} \epsilon_k$$

P—7

$$E_x = E_t - E_g$$

$$\rho(E_x) = C \exp_a(S) \tag{1}$$

where n_k, the Fermi-Dirac occupation probabilities, are given by the expression

$$n_k = \frac{1}{1 + e^{(\epsilon_k - \mu)/t}}.$$

The chemical potential μ is obtained from the number conservation condition, at any temperature t. The energy levels ϵ_k of the fermions are obtained on the basis of a realistic shell model potential namely Nilsson potential or Woods-Saxon potential. In the present work, we have examined the validity of the above expressions in view of the two-body nature of the nucleon-nucleon interaction which generates the effective average potential of the nucleus.

Attempts have been made in the past to examine the extent of validity of these expressions by carrying out detailed temperature dependent Hartree-Fock calculations (Brack and Quentin 1974, Mosel *et al* 1974). However, conflicting conclusions have been drawn on the validity of these expressions in these two papers in spite of their using similar nucleon-nucleon interaction and similar formalism. Further, it may be pointed out here that Hartree-Fock single particle energies ϵ_k show opposite trends in their temperature dependence in the two papers. In the present work we have studied the effect of the two-body nature of the average nuclear potential on nuclear entropy in a simplified way. The temperature dependence of single particle energy eigen values ϵ_k was examined on the basis of a temperature dependent Thomas-Fermi model without carrying out the detailed temperature dependent Hartree-Fock calculations.

2. Theory

In the Hartree-Fock approximation the nuclear wave function is represented by a Slater determinant of one particle wave functions. The excited state of the nucleus is obtained by creating particle-hole configurations. The extension of the Hartree-Fock approximation to finite temperature is well discussed in literature and we only present the essential features of the formalism for the sake of completeness. The total energy of the system is given by the expression

$$H_t = \sum_k n_k \langle k \mid T \mid k \rangle + \tfrac{1}{2} \sum_{j,k} n_j n_k \langle jk \mid V \mid jk \rangle \tag{2}$$

where n_k denotes the probability of occupation of the single particle state $\mid k \rangle$. The Hartree-Fock Hamiltonian is assumed to be diagonal in the states $\mid k \rangle$ at temperature t. The occupation probabilities n_k are obtained by minimising the free energy F, of the nucleus subject to the following condition:

$$N = \sum_k n_k. \tag{3}$$

The free energy of the system at temperature t is given by,

$$F = H_t - tS \tag{4}$$

where S is the entropy and H_t is the total energy of the system. The minimization of the free energy subject to eq. (3) gives the well-known expression for n_k.

$$n_k = \frac{1}{1 + \exp(\epsilon_k - \mu)/t}$$

where

$$\epsilon_k = \langle k \mid T \mid k \rangle + \sum_j n_j \langle jk \mid V \mid jk \rangle \tag{5}$$

If for a given set of n_k, the total energy of the system is minimized by varying the normalised wave functions, $\mid k \rangle$, one gets the following equations for the states $\mid k \rangle$ and the energy eigenvalue ϵ_k.

$$\langle k \mid T \mid k \rangle + \sum_j n_j \langle jk \mid V \mid jk \rangle = \epsilon_k{}^t. \tag{6}$$

Therefore, the parameter n_k and the energy eigen value $\epsilon_k{}^t$, are to be obtained by simultaneous solution of eqs (5) and (6). The total energy of the system at temperature t making use of eq. (6) can be written as:

$$H_t = \sum_k n_k \epsilon_k{}^t - \tfrac{1}{2} \sum_{j,k} n_j n_k \langle jk \mid V \mid jk \rangle \tag{7}$$

or

$$H_t = \sum_k (\epsilon_k{}^t - \tfrac{1}{2} V_k{}^t) n_k$$

where

$$V_k{}^t = \sum_j \langle jk \mid V \mid jk \rangle n_j.$$

Analogous expression for the total energy of the system in ground state can be written as

$$H_g = E_g = \sum_{k=1}^{N} (\epsilon_k{}^0 - \tfrac{1}{2} V_k{}^0).$$

Under the assumption that the terms $(\epsilon_k - \tfrac{1}{2} V_k)$ do not depend on the temperature, the expression for the excitation energy can be immediately written down:

$$E_a = \sum_{k=1} (\epsilon_k - \tfrac{1}{2} V_k) n_k - \sum_{k=1}^{N} (\epsilon_k - \tfrac{1}{2} V_k)$$

or

$$E_a = \sum_k (T_k + \tfrac{1}{2} V_k) n_k - \sum_{k=1}^{N} (T_k + \tfrac{1}{2} V_k) \tag{8}$$

where

$$T_k = \langle k \mid T \mid k \rangle.$$

The assumption involved here is equivalent to the independent particle model assumption, that the average field does not depend on the temperature. However, the expression for the excitation energy in the independent particle model is taken as,

$$E_a = \sum_k n_k \epsilon_k - \sum_{k=1}^{N} \epsilon_k$$

or

$$E = \sum_{k} (T_k + V_k) n_k - \sum_{k=1} (T_k + V_k). \tag{9}$$

Here ϵ_k are the eigen values of the one particle Hamiltonian in a suitable potential. The basis for eq. (9) is said to be Koopman's theorem. Thouless (1972) has given the following expression for the excitation energy of a nucleus with a single particle-single hole state under the assumption that single particle states are unperturbed in one particle-hole excitation.

$$E = \epsilon_k - \epsilon_i + (V_{ki, ki} - V_{ki, ik}) \tag{10}$$

where the term within brackets is the particle-hole interaction energy. This bracketed term is taken to be of the order of $1/N$ and is usually neglected to obtain eq. (9).

For the one particle-one hole excited nuclear state, eqs (8) and (10) are obtained under the same approximations and are exactly equal—*i.e.*,

$$V_{ki, ki} - V_{ki, ik} = \tfrac{1}{2} [(\sum_{k} V_k)^{ph} - (\sum_{i} V_i)^{0}].$$

The antisymmetrized particle-hole matrix element $V_{ki, ki}$ depends strongly on i and k for medium weight mass nuclei, if one of the states is a deep lying state, *e.g.*, 1s, 1p, 1d (Irvine 1972). When both the states, i and k, are near the Fermi surface, matrix element is of the order V/A, where V is the average shell model potential and A is the mass number of the nucleus. For closed shell nuclei, the particle-hole matrix elements are expected to be smaller as compared to mid-shell nuclei. However, the value of the $V_{ki, ki}$ for the first excited state of ^{40}Ca is 1·1 MeV as compared to 8·0 MeV for the leading term in eq. (10). For the first excited state in ^{16}O, the magnitude of $V_{ki, ki}$ is 2·8 MeV (Schaeffer 1971). Therefore, the assumption that the $V_{ki, ki}$ is negligible as compared to leading term is not justified.

3. Calculations

We have also estimated the contribution of the neglected potential energy term in eq. (8) for various single particle potential wells. For very deep potential wells or for very large extended systems, the potential term V_k does not depend on the state k therefore. the neglected term does not contribute to the excitation energy. For the simple harmonic oscillator-model of the nucleus, the kinetic term T_k is equal to the potential energy term V_k and therefore the neglected term in eq. (8) is one-fourth of the leading term. However, for the Woods-Saxon potential well, the potential energy terms depend on the state $|k\rangle$. We have calculated the kinetic term T_k, and the potential term V_k using the single particle eigen functions in the Woods-Saxon potential. Figure 1 shows the plot of the kinetic energy term and the potential energy term as a function of the eigenvalues ϵ_k. It can be seen from the figure that for the deep lying states, the potential energy term varies slowly and the dominant contribution to the excitation energies is from the kinetic energy term. However, for the particle-hole excitation involving the two states

near the Fermi level, the contribution of the potential energy term is comparable to the contribution from the kinetic energy term to the excitation energy as shown by nearly equal values of the quantities $\partial T_k/\partial \epsilon$ and $\partial V_k/\partial \epsilon$ in figure 1. The second term in (10) is approximately 20% of the leading term for the states near the Fermi surface, and therefore, the neglect of this term $V_{ki, \ i_k}$ in eq. (10) is not justified for the Woods-Saxon potential well.

In obtaining eq. (8) it was assumed that the term $(\epsilon_k - V_k/2)$ does not vary as a function of temperature. The following model calculations carried out on the basis of Thomas-Fermi approach, justify this assumption. In the Thomas-Fermi model of nucleus, the potential well depth is proportional to the nuclear matter density. For low temperature region ($T \lesssim 3$ MeV), the nuclear matter density is found to decrease uniformly as function of temperature in the Thomas-Fermi model (Kupper 1972). Therefore, the increment in radius parameter R_0 and decrement in the potential well depth parameter V_0 are related self consistently. The eigen values ϵ_k were computed for Woods-Saxon potential for two such consistent sets of parameters (V_0,R_0) and (V_1,R_1), where (V_0,R_0) refers to the ground state and (V_1,R_1) to the nucleus at temperature T. The calculated differences $\epsilon^0_k - \epsilon_k^1$ and the term $(\epsilon^0_k - V_k^0/2) - (\epsilon_k^1 - V_k^1/2)$ for various single particle
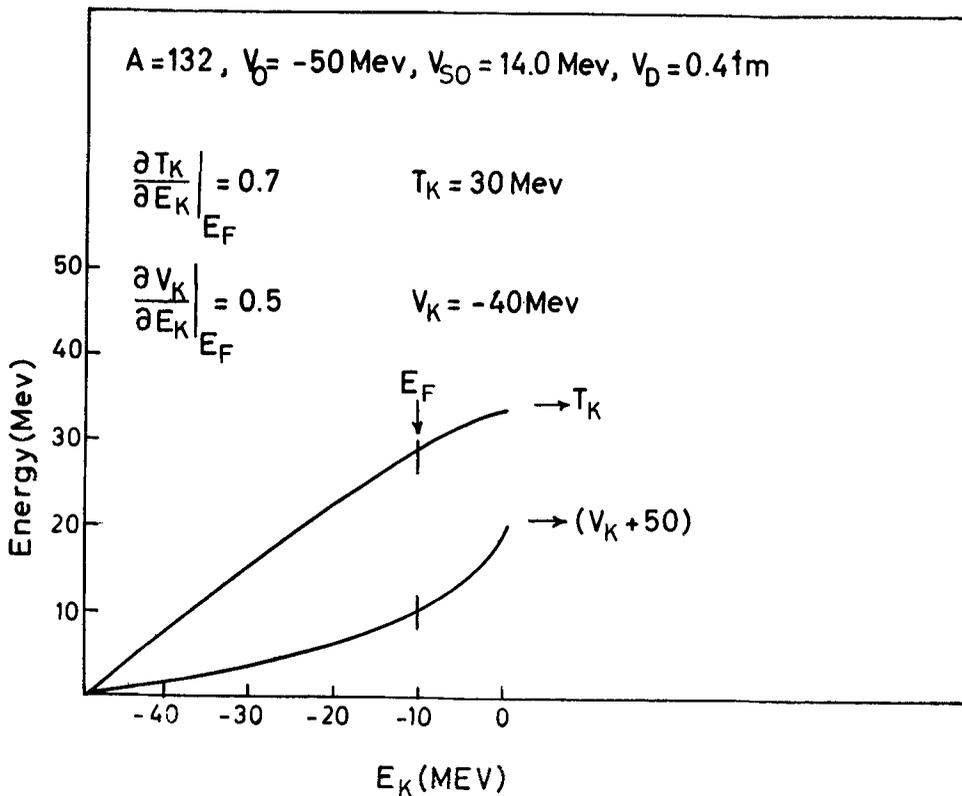

Figure 1. The plot of the kinetic energy term T_k and the potential energy V_k of the energy eigen value ϵ_k in the Woods-Saxon potential as a function of energy eigen value ϵ_k.
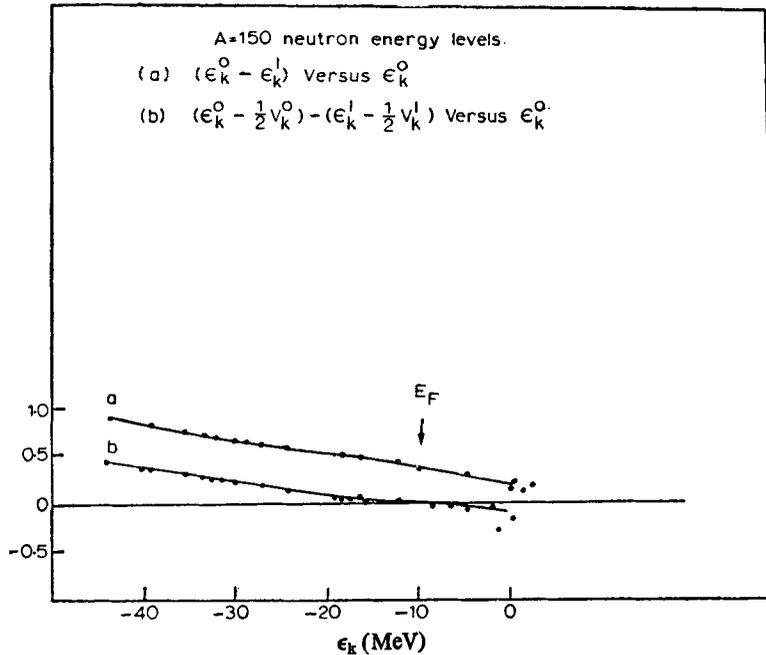
Figure 2. The curve (*a*) represents the differences in the energy eigen value ϵ_k of a given state $| k \rangle$, at two temperatures t_0 and t_1 calculated as described in text. The curve (*b*) shows the differences in the term $(\epsilon_k - \frac{1}{2} V_k)$ at these temperatures.

states are shown in figure 2. It is seen that near the Fermi energy the second term remains almost constant whereas the quantity $(\epsilon_k^0 - \epsilon_k^1)$ decreases uniformly. This supports the assumption that the term $\epsilon_k - V_k/2$ does not depend sensitively on temperature.

4. Results and discussion

Figures 3 *a* and 3 *b* show the calculated nuclear entropies as a function of excitation energy for two nuclei using eqs (8) and (9). The Nilsson model was used to calculate the single particle eigen values ϵ_k and the potential energy terms V_k. It is seen from the figures that for high excitation energies, the nuclear entropy is 20 to 25% higher for a given excitation E_x if eq. (8) is used instead of eq. (9). However, for the low excitation energies no such general conclusion can be drawn, as at low excitation energies the results are sensitive to the shell structure effects.

Experimental verification of the validity of using the eq. (8) instead of eq. (9) can be obtained from the experimental value of the level density parameter *a*. The analysis of the experimental data on nuclear level spacings on the basis of a semi-empirical nuclear level density formula (Gilbert 1968, Ramamurthy *et al* 1975) is consistent with a value of $a^{LDM} \simeq A/7$ for the liquid drop model value of the level density parameter *a* after correction for the nuclear shell effects. However, the theoretical estimate of the parameter a^{LDM} using eq. (9) on the basis of Fermi gas model of the nucleus with $r_0 = 1\cdot2$ f is $A/12$. Also for the realistic single particle energy level scheme based on Nilsson potential or Woods-Saxon potential, the derived values of a^{LDM} on the basis of eq. (9) is $A/10$, However
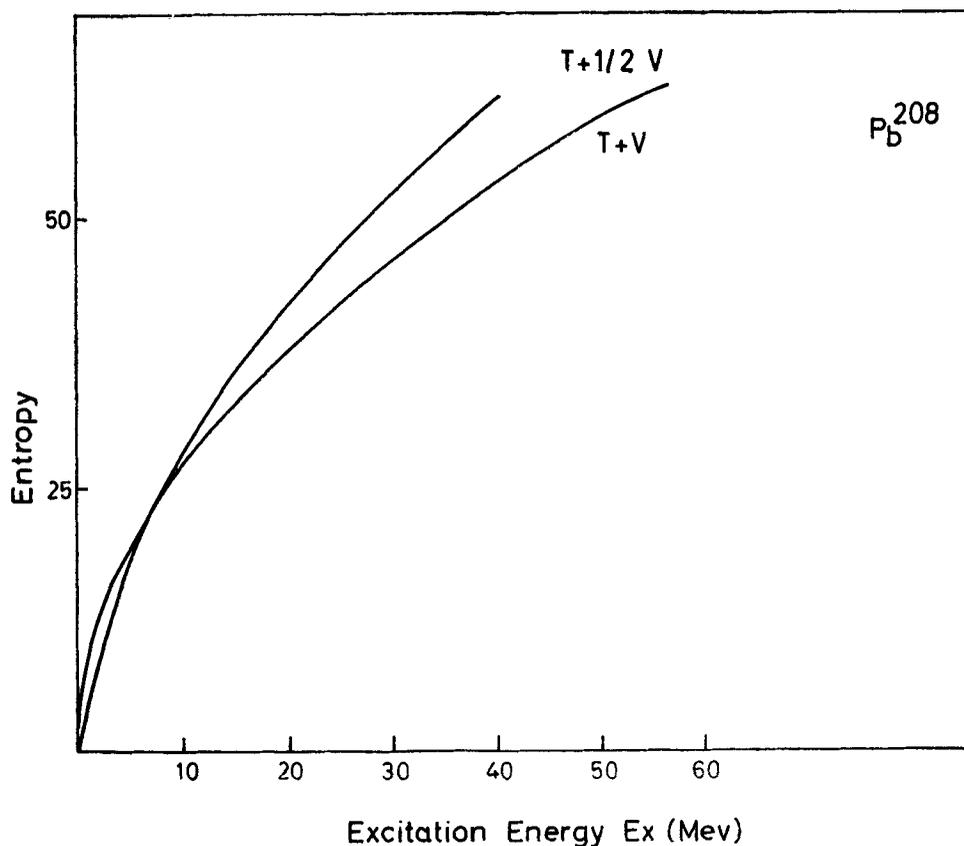
Figure 3 (*a*). The variation of nuclear entropy *S*, as a unction of excitation energy
E_s using eq. (8) (denoted by $T + \frac{1}{2} V$), and using eq. (9) (denoted by $T + V$) for
^{208}Pb with Woods-Saxon potential.

the use of eq. (8) for estimating in both the above-mentioned cases results in the
values of $a^{LDM} \sim A/7$ in agreement with the experimental data. In the above
calculations, we have not included the effect of pairing correlations between the
nucleons. However, it is known that for not too low excitation energies, pairing
effects can be easily taken into account by an energy shift in the level density ex-
pression. Consequently, in these energy ranges, the above analysis remains valid
in spite of neglecting the pairing effects. However, for any quantitative esti-
mate of level densities, it is necessary to include pairing effects.

5. Conclusion

To summarise, we observe that the numerical calculation of level densities in the
independent particle approximation contain significant errors. The use of eq. (8)
in these calculations will give a better estimate of the nuclear entropy *versus*
excitation energy and, therefore, of the level density without recourse to detailed
Hartree-Fock calculations which are yet to attain the required level of confidence
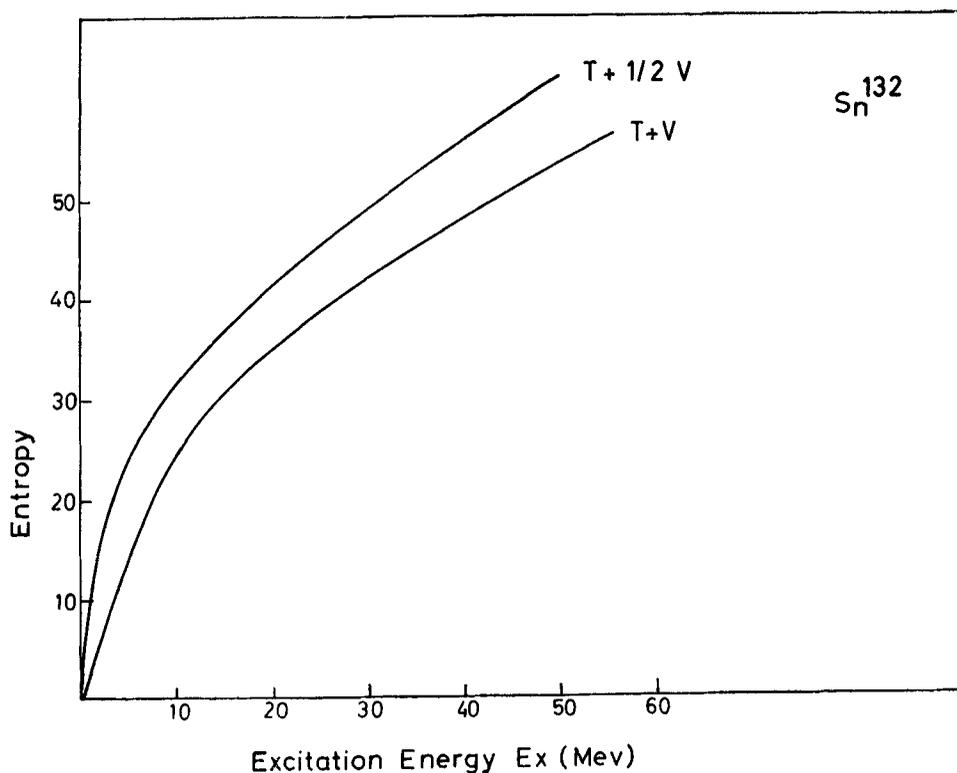for these calculations.

Figure 3 (b).   The variation of nuclear entropy S, as a function of exitation energy E_x using eq. (8) (denoted by $T + \frac{1}{2} V$), and using eq. (9) (denoted by $T + V$) for ^{132}Sn with Woods-Saxon potential.

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