Effects due to the continuum on shell corrections at finite temperatures

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Temperature dependent shell corrections are calculated taking into account the continuum spectrum of a finite depth mean field potential. The effect of the continuum is split up into a discret term which includes Gamow resonances and an integral along a contour in the complex energy plane. The resonances appear in the formalism in the same manner as bound states and at low temperatures they give the main part of the contribution due to the continuum. The method is applied to the particular case of ^{208}Pb. The temperature for which the shell corrections are washed out completly is estimated at $T \approx 2.5$ MeV. [S0556-2813(97)05203-5]

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I. INTRODUCTION

The thermal properties of a nucleus depend on the density of single-particle states around the Fermi level. By thermal excitations these states become equally populated and the single-particle shell structure is washed-out progressively. Above a critical temperature the system displays the behavior of a degenerate Fermi gas, that is the excitation energy increases quadratically with the temperature. For higher excitations the nucleus becomes unstable since nucleons can occupy states of the continuum. In order to describe this process one should consider the excitations of the nucleons in a finite depth potential and to treat properly the continuum part of its energy spectrum.

To deal with the continuum different prescriptions have been used both in self-consistent and phenomenological temperature dependent calculations. One of these prescriptions is to diagonalize the mean field potential in a harmonic oscillator basis and to replace the continuum by the corresponding positive energy solutions [1–3]. The drawback of this approach is that the unbound spectrum depends on the cutoff of the oscillator basis [4].

Another alternative was proposed in Ref. [5] where the continuum was discretized by considering the nucleus in a box at equilibrium with a nucleonic gas. Then the nuclear component of the solution was obtained by extracting the gas solution from the one representing the total system, i.e., nucleus and gas.

In phenomenological temperature dependent calculations, in which the mean field is not changed with the temperature, the continuum contribution is generally introduced through the generalized level density [6,7].

The effects of the continuum on shell corrections was discussed many years ago [8,9] for the case of nuclei in the ground state, but up to now there is not a realistic estimation of these effects for finite temperatures.

In this paper we extend the Strutinsky method as to incorporate in a simple way both the continuum and thermal effects. For evaluating the continuum a general procedure for extracting the main contribution of the resonant states is presented.

II. FORMALISM

Temperature dependent Hartree-Fock (HF) calculations have shown that for values of the temperature (T) less than about 5 MeV the relevant thermodynamical quantities, such as the excitation energy and the entropy, can be described approximatively by using the single-particle spectrum of the "cold" nucleus [1–5]. This justifies a non-self-consistent thermodinamic approach [6,7,10] that will be applied also in the present work. Thus, in what follows we consider that the temperature is externally fixed and that the nucleons move in a temperature independent mean field.

For high excitation energies the particles can be excited into the continuum part of the spectrum. The continuum contributes mainly through the narrow resonances and their effect could be introduced by the generalized level density, $g(\epsilon)$, given by [8,9]

$$g(\epsilon) = \sum_{i \text{bound}} \delta(\epsilon - \epsilon_i) + \Delta g_{\text{cont}}(\epsilon), \tag{1}$$

where

$$\Delta g_{\text{cont}}(\epsilon) = \frac{1}{\pi} \sum_{l,j}^{l_{\max}} (2j+1) \frac{d\delta_{lj}(\epsilon)}{d\epsilon} \tag{2}$$

is the contribution of the continuum to the single-particle level density [11] and δ_{lj} are the phase shifts.

Using the generalized level density one can readily include the contribution of the continuum in the formalism. It is worthwhile to stress that the continuum will contribute not only to the thermal averaging process, but also to the smoothing procedure itself [8,9].

The temperature dependent shell corrections to the free energy are defined by

$$\delta\tilde{F} = F - \tilde{F} = (E - TS) - (\tilde{E} - T\tilde{S}). \tag{3}$$

Here E and S are the HF energy and entropy given by

$$E=\int_{-\infty}^{+\infty}\epsilon g(\epsilon)n(\epsilon)d\epsilon=\sum_{i\text{bound}}\epsilon_i n(\epsilon_i)+\int_0^{+\infty}\epsilon\Delta g(\epsilon)_{\text{cont}}n(\epsilon)d\epsilon \qquad (4)$$

and

$$S=-\int_{-\infty}^{+\infty}g(\epsilon)\{n(\epsilon)\ln[n(\epsilon)]+[1-n(\epsilon)]\ln[1-n(\epsilon)]\}d\epsilon, \qquad (5)$$

where g(ϵ) is the single-particle level density (1) and $n(\epsilon)$ is the Fermi occupation probability

$$n(\epsilon)=\frac{1}{1+e^{(\epsilon-\lambda)/T}}. \qquad (6)$$

The Fermi level for a given temperature, $\lambda(T)$, is fixed by the number of particles

$$N=\int_{-\infty}^{+\infty}g(\epsilon)n(\epsilon)d\epsilon=\sum_{i\text{bound}}n(\epsilon_i)+\int_0^{+\infty}\Delta g(\epsilon)_{\text{cont}}n(\epsilon)d\epsilon. \qquad (7)$$

The smooth energy, $\tilde{E}$, and the smooth entropy, $\tilde{S}$, have similar expressions as the corresponding HF quantities, namely:

$$\tilde{E}=\int_{-\infty}^{+\infty}\epsilon\tilde{g}(\epsilon)\tilde{n}(\epsilon)d\epsilon \qquad (8)$$

and

$$\tilde{S}=-\int_{-\infty}^{+\infty}\tilde{g}(\epsilon)\{\tilde{n}(\epsilon)\ln[\tilde{n}(\epsilon)]+[1-\tilde{n}(\epsilon)]\ln[1-\tilde{n}(\epsilon)]\}d\epsilon. \qquad (9)$$

The quantity $\tilde{n}(\epsilon)$ is the Fermi distribution corresponding to the smooth Fermi level, $\tilde{\lambda}(T)$, which is determined by the condition

$$N=\int_{-\infty}^{+\infty}\tilde{g}(\epsilon)\tilde{n}(\epsilon)d\epsilon. \qquad (10)$$

The level density $\tilde{g}(\epsilon)$ is obtained by folding the corresponding single-particle density with a smoothing function $f(x)$, i.e.,

$$\tilde{g}(\epsilon)=\int_{-\infty}^{+\infty}d\epsilon' g(\epsilon')f\left(\frac{\epsilon-\epsilon'}{\gamma}\right)=\sum_{i\text{bound}}f\left(\frac{\epsilon-w_i}{\gamma}\right)+\int_0^{+\infty}d\epsilon'\Delta g(\epsilon')_{\text{cont}}f\left(\frac{\epsilon-\epsilon'}{\gamma}\right). \qquad (11)$$

In this equation γ is the smoothing parameter, which should be larger than the typical distance between major shells. The function $f(x)$ can be written as a product of a weighting function and the so-called ''curvature correction'' polynomial. Here we use the expression

$$f(x)=\frac{e^{-x^2}}{\gamma\sqrt{\pi}}\sum_0^p c_m H_m(x), \qquad (12)$$

where H_m is the Hermite polynomial of order m and c_m is an expansion coefficient [12].

The shell corrections should not depend strongly on the smoothing parameter γ or on the degree of the curvature polynomial p. These constraints are referred to as the plateau conditions [12].

The quantities defined above contain a discrete sum on bound states and an integral over the phase shifts. To perform these integrals on the real axis may be difficult, particularly if narrow resonances are present. To avoid these difficulties we replace the integral on the real axis by an integration along a contour C in the complex energy plane. Such a contour is shown in Fig. 1. The circles represent the so-called Gamow resonances. They are the outgoing solutions of the time-independent Schrödinger equation corresponding to the finite depth potential.

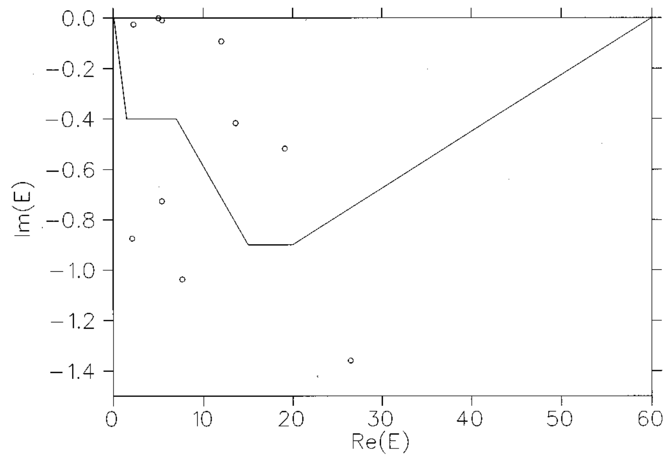

FIG. 1. Contour of the integration path in the complex energy plane used to evaluate the shell correction for neutrons in ^{208}Pb. The open circles are the Gamow-state energies corresponding to a Woods-Saxon potential. Energies are given in MeV.

Changing the path of integration, as displayed in Fig. 1, and applying Cauchy's theorem one obtains from Eq. (11)

$$\tilde{g}(\epsilon)=\sum_i f\left(\frac{\epsilon-w_i}{\gamma}\right)+\int_L d\epsilon'\Delta g(\epsilon')_{\text{cont}}f\left(\frac{\epsilon-\epsilon'}{\gamma}\right). \qquad (13)$$

In this expression the summation runs over all the bound states and resonances enclosed by the contour, while L is the integral path in the complex energy plane of Fig. 1. The contribution of the resonances are evaluated by noticing that near the pole $\mathcal{E}_n=(\epsilon_n,-\gamma_n)$ the derivative of the phase shifts can be written as [15,16]

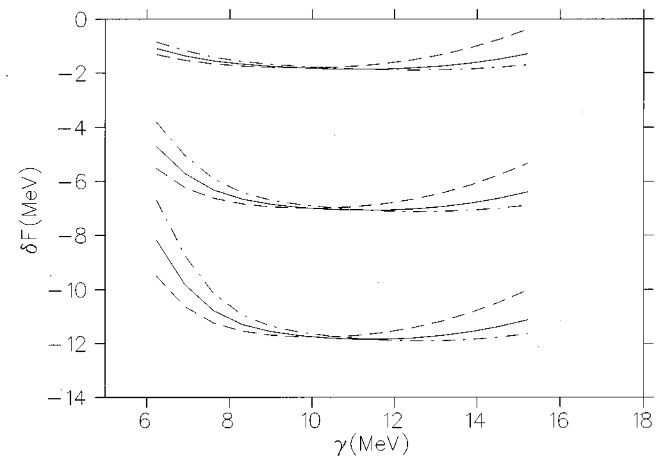

FIG. 2. Shell corrections to the free energy (in MeV), for neutrons in ^{208}Pb, as a function of the smoothing parameter γ and for three different temperatures (from bottom to top) $T=0$, 0.7, and 1.5 MeV, respectively. The dashed, full, and dotted lines correspond to the values of the curvature-order parameter $p=8$, 10, and 12, respectively.

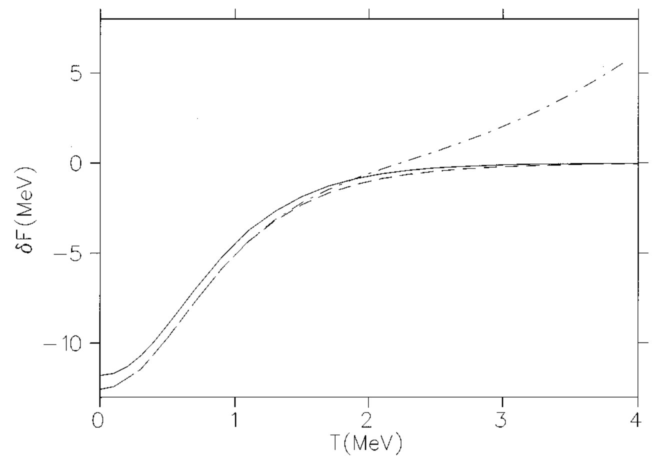

FIG. 3. Shell corrections to the free energy (in MeV) for neutrons in ^{208}Pb as a function of temperature. The full line corresponds to the exact result, the dashed line to the case when only bound and resonant states are included, and the dash-dotted line corresponds to the approximation given in Eq. (15).

$$\frac{d\delta(\mathcal{E})}{d\mathcal{E}}=\frac{\gamma_n}{(\mathcal{E}-\mathcal{E}_n)(\mathcal{E}-\mathcal{E}_n^*)}=\frac{\gamma_n}{(\mathcal{E}-\epsilon_n)^2+\gamma_n^2}. \tag{14}$$

We use the same procedure to evaluate the integrals defining the HF quantities.

The fact that the main contribution due to the continuum can be cast in an analytical form can be used to expand the shell correction formulas in powers of the temperature. This kind of expansion was done in [10] for the case of a harmonic oscillator potential. Neglecting the contribution of the contour integral and keeping only the first term of the expansion in powers of the temperature one gets, for the temperature dependent shell correction to the free energy, the expression

$$\delta\widetilde{F}=\delta\widetilde{E}(T=0)+F^*(T)+\widetilde{a}T^2, \tag{15}$$

where $\delta\widetilde{E}(T=0)$ is the shell correction at zero temperature and $F^*(T)=F(T)-E(T=0)$. Formally the level density parameter $\widetilde{a}$ has the same analitical form as in [10], but now the summation goes over the resonant states as well. One gets

$$\widetilde{a}=\frac{\pi^2}{6\sqrt{\pi}\gamma^2}\sum_j e^{-[(\widetilde{\lambda}-\epsilon_j)/\gamma]^2}\left(0.5\gamma c_p H_{p+2}+\sum_{m=0}^{p} c_m(2\gamma H_m+\epsilon_j H_{m+1})\right). \tag{16}$$

Summarizing this section, we have split up the contribution of the continuum in two parts: a discrete part where resonances are treated in the same footing as bound states, and an integral along a contour in the complex energy plane. This integral can be evaluated without difficulties if one chooses a contour far enough from the poles, where the scattering functions are well behaved. Moreover, if the contour includes only narrow resonances, the contribution of the integral is very small as compared to the discrete term and can be neglected.

In addition to the numerical advantages, this procedure to describe the continuum allows for a transparent interpretation of the results. Thus, one can calculate the occupancy probability of different resonances as a function of temperature as well as their contributions to the thermal averaging and to the smoothing procedure.

III. NUMERICAL RESULTS

We will apply the formalism derived above to the case of ^{208}Pb. For this we utilize as a central field a Saxon-Woods potential with parameters $V_0=44.4$ MeV, $V_{s-o}=16.5$ MeV, $a=a_{s-o}=0.7$ fm, $r_0=r_{s-o}=1.27$ fm. To calculate the complex energies and wave functions of the resonances we use the computer code GAMOW [13], which solves the corresponding Schrödinger equation by imposing outgoing boundary conditions at large distances.

In order to verify the plateau conditions for different temperatures we show in Fig. 2 the results of the shell corrections as a function of the smoothing parameter γ for three values of p. The continuum contribution is important to obtain the plateau, as shown in Ref. [9] for $T=0$. In our calculation the plateau is obtained for resonable cutoff parameters, namely including single-particle states up to $E_{\max}=20$ MeV and for a maximum angular momentum $l_{\max}=11\hbar$. This is to be compared with the values $E_{\max}=100$ MeV and $l_{\max}=20\hbar$ used in Ref. [9]. Our cutoff parameters are the same as those in Ref. [8] where no plateau was found. This could be a manifestation of numerical inaccuracies affecting the integration along the real axis in the region of narrow resonances.

From Fig. 2 one can see that the plateau is stable when the temperature is increased.

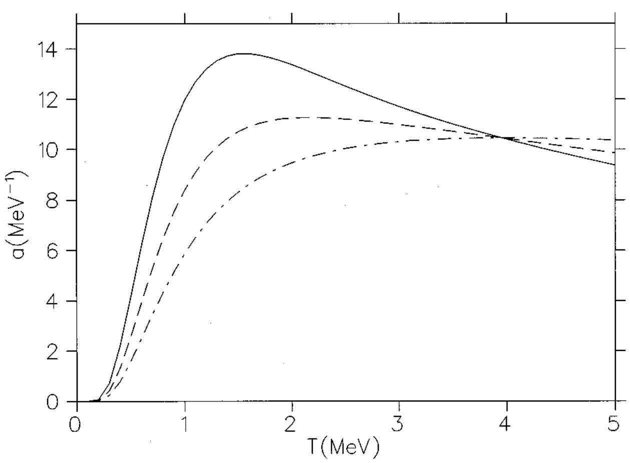

FIG. 4. Variation with the temperature of E^*/T^2 (full line), $S/2T$ (dashed line), and $S^2/4E^*$ (dash-dotted line). All the quantities are in MeV^{-1}.

The results for the temperature dependent shell correction to the free energy are shown in Fig. 3, where $\gamma = 10.6$ MeV and $p = 10$ are used. These values are consistent with the plateau condition, as seen from Fig. 2.

The full curve shown in Fig. 3 gives the exact results, that is when the contribution of the contour is introduced. As one can see, the curve approaches zero exponentially, in agremeent with previous estimations [14]. The temperature for which the shell corrections are completely washed out ($T \approx 2.5$ MeV) is of the same order as the one obtained for the case of the harmonic oscillator potential [10]. The dashed curve shows the results obtained with the discrete part, i.e. by neglecting the contributions of the integrals, both to the HF and to the smoothed quantities. The slope of that curve is almost the same as for the full curve, corresponding to the exact result, and the differences between them are not large. These differences come mainly from the smoothed quantities which include the broader resonances at about 12 MeV. The dash-dotted curve corresponds to the approximation of Eq. (15). One can see that for temperatures below 1.5 MeV this approximation reproduces almost exactly the value given by the discrete term. For higher temperatures the deviation from the exact result increases. This implies that one cannot use the level density parameter $\tilde{a}$ [Eq. (15)] to approximate the value of the shell corrections to the free energy for temperatures much beyond 1.5 MeV. In particular, it would be questionable to implement that approximation for temperatures higher than the 2.5 MeV point of collapse of the shell correction [10].

In Fig. 4 we have plotted the quantities E^*/T^2 (full line), $S/2T$ (dashed line), and $S^2/4E^*$ (dashed-dotted line), where $E^* = E(T) - E(T=0)$ is the excitation energy. In the region where the shell corrections begin to be negligible (i.e., from about 2.5 MeV) those quantities become almost constant. This indicates that the system is in a degenerate Fermi gas regime for high excitation energy, as expected. Therefore, to compare the level density parameter that can be extracted from Fig. 4 to the corresponding Fermi gas value, one has to go to the asymptotic regions of high temperatures. On the other hand, in a Fermi-gas model all the quantities plotted in Fig. 4 would be equal to the level density parameter given by [17]

$$a = \frac{\pi^2}{4} \frac{2m^*}{\hbar^2} \frac{A}{k_F^2}, \tag{17}$$

where m^* is the effective mass and k_F is the Fermi momentum. If one takes for these parameters the values given by a Skyrme interaction [18] then the level density parameter in ^{208}Pb comes at about $a = 11\ \mathrm{MeV}^{-1}$. This agrees well with the asymtotic value extracted from Fig. 4.

An asymtotic behavior for those quantities which is similar to the one seen in Fig. 4 was obtained in Ref. [5] in the framework of a temperature dependent Hartree-Fock calculation (see Fig. 5 of Ref. [5]). However, the asymptotic value of the level density parameter obtained from there is about $15\ \mathrm{MeV}^{-1}$. It is worthwhile to mention that those asymptotic values should not be compared with the level density parameter estimated in Ref. [18], since there one expands the free energy in power of T^2 keeping only the first term, as we did in deriving Eq. (15). But this approximation fails at large temperature, as one can see from Fig. 3. Therefore the value $a = 20\ \mathrm{MeV}^{-1}$ derived in Ref. [18], should rather be compared in our approach to the result given by $\tilde{a}$ in Eq. (15). We thus obtained $\tilde{a} = 17\ \mathrm{MeV}^{-1}$, which is closer to the value of Ref. [18]. The remaining difference may be due to the different interactions used in the calculations, and not to the way the continuum is treated at this low temperature.

For the range of temperatures shown in Fig. 3 only the narrow resonances contribute to the thermal averaging. Indeed, for $T = 2.5$ MeV, the occupancy of the first resonance is about 0.4 while for the next two resonances it is of the order of 0.2. The resonances lying at higher energies are not populated unless unrealistically large values of the temperature are used. For $T = 2.5$ MeV the whole contribution of the continuum to the HF excitation energy is about 2% and to the entropy about 5%. This indicates that in ^{208}Pb the continuum does not play an important role for thermal averaging. But in nuclei that are of interest at present, e.g., nuclei close to the drip line, the low excited states may be above the continuum threshold. In cases like this the treatment of the continuum presented here is a favorable alternative to describe the dynamics of the system.

IV. SUMMARY

In this paper we have presented a method to evaluate the contribution of the continuum part of the spectrum to shell corrections in nuclei at finite temperature. The main part of that contribution is due to outgoing (Gamow) resonances that are not too wide. This is expected, since nucleons moving in wide resonances would not have enough time to feel the interactions induced by the other nucleons in the core.

One appealing feature of the the formalism is that all resonances are treated on the same footing as bound states. That is, formally bound states and Gamow resonances are identical excitations.

The remaining continuum contribution is given by a contour integral which can be easily evaluated. Neglecting this contour integral an analytical expression for the level density parameter, valid for low temperatures, is obtained. The method was applied for the case of ^{208}Pb. The critical temperature for which the shell corrections are completely washed out was estimated at about $T \approx 2.5$ MeV. Beyond this temperature the system behaves as a degenerate Fermi gas. Asymptotically, the value of the level density parameter is close to the value predicted by the Fermi-gas model. In the case of ^{208}Pb the inclusion of the continuum is essential for obtaining the plateau conditions but it does not influence the nuclear thermal properties significantly. One expects that the continuum will be important for thermal excitations in nuclei far from the stability line, where the present method may be an adequate way of treating both shell corrections and thermal properties.

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[1] G. Sauer, H. Chandra, and U. Mosel, Nucl. Phys. **A264**, 221 (1976).
[2] M. Brack and P. Quentin, Phys. Scr. **10**, 163 (1974).
[3] M. Brack and P. Quentin, Nucl. Phys. **A361**, 35 (1981).
[4] M. Bolsterli, E. O. Fiset, J. R. Nix, and J. L. Norton, Phys. Rev. C **5**, 1050 (1972).
[5] P. Bonche, S. Levit, and D. Vautherin, Nucl. Phys. **A427**, 278 (1984).
[6] U. Mosel, Phys. Lett. **46B**, 8 (1973).
[7] D. R. Dean and U. Mosel, Z. Phys. A **322**, 647 (1985).
[8] W. F. Lin, Phys. Rev. C **2**, 871 (1970).
[9] C. K. Ross and R. K. Bhaduri, Nucl. Phys. **A188**, 566 (1972).
[10] O. Civitarese, A. L. De Paoli, and A. Plastino, Z. Phys. A **309**, 177 (1982); **311**, 317 (1983).
[11] E. Beth and G. E. Uhlenbeck, Physica **4**, 915 (1937).
[12] V. M. Strutinsky, Sov. J. Nucl. Phys. **3**, 449 (1996); Nucl. Phys. **A95**, 420 (1967).
[13] T. Vertse, K. F. Pál, and Z. Balogh, Comput. Phys. Commun. **27**, 309 (1982).
[14] A. Bohr and B. Mottelson, *Nuclear Structure* (Benjamin, New York, 1975), Vol. 2.
[15] C. Mahaux and H. A. Weidenmüller, *Shell Model Approach to Nuclear Reactions* (North-Holland, Amsterdam, 1969).
[16] R. Newton, *Scattering Theory of Waves and Particles* (Springer-Verlag, New York, 1982).
[17] H. A. Bethe, Phys. Rev. **50**, 332 (1936).
[18] M. Barranco and J. Treiner, Nucl. Phys. **A351**, 269 (1981).