Latest development of the combinatorial model of nuclear level densities

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Abstract. The combinatorial model of nuclear level densities has now reached a level of accuracy comparable to that of the best global analytical expressions without suffering from the limits imposed by the statistical hypothesis on which the latter expressions rely. In particular, it provides, naturally, non-Gaussian spin distribution as well as non-equipartition of parities which are known to have an impact on cross section predictions at low energies [1, 2, 3]. Our previous global models developed in Refs. [1, 2] suffered from deficiencies, in particular in the way the collective effects - both vibrational and rotational - were treated. We have recently improved this treatment using simultaneously the single-particle levels and collective properties predicted by a newly derived Gogny interaction [4], therefore enabling a microscopic description of energy-dependent shell, pairing and deformation effects. In addition for deformed nuclei, the transition to sphericity is coherently taken into account on the basis of a temperature-dependent Hartree-Fock calculation which provides at each temperature the structure properties needed to build the level densities. This new method is described and shown to give promising results with respect to available experimental data.

1. Introduction

Global microscopic models of nuclear level densities (NLD) have been developed for the last decades [2] but are almost never used for practical applications, because of their lack of accuracy in reproducing experimental data or because they do not offer the same flexibility as do highly parameterized analytical expressions. We have therefore developed a combinatorial approach and demonstrated that it can clearly compete with the statistical ones in the global reproduction of experimental data [1, 2]. In addition, we have shown that such tabulated NLD can be normalized, if need be, to perform experimental fits of cross sections [5, 6]. Such an approach provides the energy, spin and parity dependence of NLD and, at low energies, describes the non-statistical limit which, by definition cannot be described by the traditional statistical formulas though it can have a significant impact on cross section predictions (e.g. [3]). However, our combinatorial method still includes phenomenological ingredients that could hamper its microscopic nature, and consequently its predictive power.

Our combinatorial method has been extensively described in Refs. [1, 2, 7] and we just summarize here the main features. It consists in using the single-particle level scheme and pairing properties obtained from axially symmetric Hartree-Fock-Bogoliubov (HFB) method to construct incoherent particle-hole (ph) state densities as functions of the excitation energy,
the spin projection and the parity. These incoherent ph state densities are then folded with vibrational excited states to yield total state densities [2, 7]. Level densities are then obtained by constructing rotational bands if any (i.e. if the nucleus is deformed) or using the classical expression relating state and level densities for a spherical nucleus [2]. Although it is well established that at increasing energies, a deformed nucleus becomes spherical, this effect has not been taken microscopically into account up to now.

2. Improvements to the combinatorial NLD model

If the combinatorial level densities we had obtained (and tabulated) so far provide quite good results when compared to available experimental data [1, 2] or for cross section estimates [6], it still suffers from several approximations, as (i) the determination of the vibrational energy levels and (ii) the evolution of the collective enhancement at increasing excitation energies. Both approximations have been improved in the present study.

For the prediction of vibrational energy levels, the five-dimensional collective Hamiltonian based on the Gogny interaction which has proven its ability to estimate systematically the properties of the quadrupole vibrational levels [8] is now followed to replace the previously used systematics. Theoretical predictions of the octupole mode can be obtained using the Quasiparticle Random Phase Approximation [9], but such a systematic study has not been performed yet. For coherence, the D1M Gogny force [4] (i.e the first Gogny-type interaction capable of reproducing measured masses with a high degree of accuracy) is adopted to extract systematically all nuclear ingredients of relevance in NLD calculations.

Figure 1. Left: Excitation energy $U$ and and quadrupole deformation $\beta_2$ as a function of the nuclear temperature $T$ for $^{238}$U. Right: Total NLD for positive parities of $^{238}$U calculated for several temperatures connected smoothly thanks to the procedure described in the text. The points not affected by the smoothing procedure and the $T = 0$ level density are also shown.

Concerning the expected transition from deformed to spherical shape at increasing excitation energies, the temperature-dependent HFB approach is now used, following the method described in Ref. [10]. The calculations have been performed with the same D1M interaction [4] and are based on the minimization of the free energy $F = E - TS$ (where $E$ is the binding energy, $T$ the temperature and $S$ the entropy). The approach followed here consists in determining, at a selected temperature $T_i$ (corresponding to a given excitation energy $U_i$) the most probable deformation $\beta_i$ through an unconstrained HFBCS calculation minimizing $F$. The corresponding evolution of the excitation energy $U$ and quadrupole deformation $\beta_2$ with increasing temperatures are illustrated in Fig. 2 for $^{238}$U. The well-known approximative relation $U \propto T^2$ as well as the deformed to spherical shape transition can be observed. To estimate the
NLD at an excitation energy $U_i$ and thus at the corresponding deformation $\beta_i$, the combinatorial method described above is used with the corresponding single-particle level scheme and pairing properties at the temperature $T_i$. The NLD are sensitive to the corresponding $T$-dependent nuclear inputs and display discontinuities stemming from the non-continuous disappearance of shell and pairing effects due to the finite set of temperatures considered. Indeed, the NLD determined at a given temperature is only valid at the corresponding excitation energy. However, for practical reasons, we consider the NLD at $T_i$ to be valid over the interval $[U_i, U_{i+1}]$. To suppress the discontinuities, an differential energy shift is applied to the NLD above $U_i$ (up to $U_{i+1}$) in such a way as to recover the NLD calculated at $U_{i+1}$ on the basis of the HFB ingredients obtained at $T_{i+1}$. With this treatment, the discontinuity in the $T$-dependent NLD are smoothed out, as shown in Fig. 2. The $T$-dependent NLD is found to be significantly different from that traditionally obtained at $T = 0$ (Fig. 2). Such a temperature effect may also affect the s-wave spacings at the neutron separation energy. To check that, we have applied the previously described method to all the nuclei for which experimental s-wave spacings are available. In terms of the rms deviation on all the experimental spacings [11], we find $f_{rms} = 3.6$ without accounting for the temperature dependence, and $f_{rms} = 2.7$ otherwise (for the definition of $f_{rms}$, see Ref. [2]). It should also be mentioned that contrary to what has been done in Ref. [2], no contribution from hexadecapole vibrational phonons are now included for nuclei with $Z < 85$.

\[\text{Figure 2. Ratio of HFB plus combinatorial (} D_{th}\text{) to the experimental (} D_{exp}\text{) s-wave neutron resonance spacings compiled in [11] with the temperature dependent treatment (red circles) and using the HFB ingredients obtained for } T = 0 \text{ (blue squares).}\]

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