Calculation of microscopic nuclear level densities based on covariant density functional theory Postprint

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Abstract

A microscopic method for calculating nuclear level density (NLD) based on the covariant density functional theory (CDFT) is developed. The particle-hole state density is calculated by combinatorial method using the single-particle levels schemes obtained from the CDFT, and then the level densities are obtained by taking into account collective effects such as vibration and rotation. Our results are compared with those from other NLD models, including phenomenological, microstatistical and non-relativistic HFB combinatorial models. The comparison suggests that the general trends among these models are basically the same, except for some deviations from different NLD models. In addition, the NLDs of the CDFT combinatorial method with normalization are compared with experimental data, including the observed cumulative number of levels at low excitation energy and the measured NLDs. Compared with the existing experimental data, the CDFT combinatorial method can give reasonable results.

Full Text

Preamble

Calculation of Microscopic Nuclear Level Densities Based on Covariant Density Functional Theory

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We develop a microscopic method for calculating nuclear level density (NLD) based on covariant density functional theory (CDFT). The particle-hole state density is computed using a combinatorial method with single-particle level schemes obtained from CDFT, and level densities are then derived by incorporating collective effects such as vibration and rotation. Our results are compared with those from other NLD models, including phenomenological, microstatistical, and non-relativistic HFB combinatorial approaches. The comparison reveals that, aside from minor deviations among different NLD models, the overall trends are essentially consistent. Additionally, NLDs from the CDFT combinatorial method with normalization are compared with experimental data, including the observed cumulative number of levels at low excitation energy and measured NLDs. The CDFT combinatorial method yields reasonable results when compared with existing experimental data.

Keywords: nuclear level density, covariant density functional theory, combinatorial method

Introduction

Nuclear level density (NLD) is fundamental physics input for nuclear reactions and represents a key ingredient for calculating reaction cross sections relevant to nucleosynthesis [**?**, **?**, **?**]. The study of NLDs dates back to the 1930s with Bethe's pioneering work [**?**]. Since then, many theoretical models have been adopted for NLD studies, including the Back-Shifted Fermi Gas Model (BFM) [**?**], the Composite Gilbert-Cameron Model (CTM) [**?**], and the Generalised Superfluid Model (GSM) [**?**]. These phenomenological models are widely used in nuclear reaction calculations. However, they rely more or less on experimental data to adjust their parameters, and such experimental data are limited, particularly for nuclei far from the β-stability line [**?**]. To address these difficulties, microscopic methods have been developed.

Over the last several decades, various microscopic models for NLD have been proposed, ranging from the equidistant spacing model [**?**, **?**, **?**, **?**], the shell-model Monte Carlo method [**?**, **?**, **?**, **?**, **?**], the spectral distribution calculation [**?**, **?**, **?**], to the independent particle model at finite temperature [**?**, **?**, **?**, **?**] and micro-statistical methods [**?**, **?**, **?**, **?**]. Especially in the last two decades, the microscopic method based on the Hartree-Fock-Bogoliubov (HFB) plus combinatorial model [**?**] has been well developed. The combinatorial method can compete with statistical methods in reproducing experimental data and provides energy-, spin-, and parity-dependent NLDs that are beyond the reach of statistical methods [**?**]. Non-relativistic Hartree-Fock-Bogoliubov combinatorial methods based on Skyrme and Gogny effective interactions have successfully reproduced NLDs for various nuclei [**?**, **?**] and been applied to various astrophysical reactions. The accuracy of NLD is related to basic nuclear structure information such as single-particle levels, deformation, and binding energy.

In recent years, covariant (relativistic) density functional theory has attracted

considerable attention in the nuclear physics community due to its successful description of complex nuclear structure and reaction dynamics [?, ?, ?, ?, ?, ?]. For instance, it can reproduce isotopic shifts in Pb isotopes well [?], naturally explain the origin of pseudospin and spin symmetries in the antinucleon spectrum [?], and provide a good description of nuclear magnetic moments [?, ?]. Recently, a micro-statistical method based on CDFT has been developed to describe NLDs [?]. The model has been applied to calculate NLDs of ^{94,96,98}Mo, ^{106,108}Pd, etc., and the NLDs are in very good agreement with experimental data across the entire measured energy range [?]. While the microstatistical method can calculate only energy-dependent NLDs, the combinatorial method can calculate energy-, spin-, and parity-dependent NLDs. Therefore, it is a meaningful endeavor to calculate NLDs using the CDFT plus combinatorial method.

The theoretical framework and methods are introduced in Sec. II. The NLDs calculated based on the CDFT combinatorial method are compared with other NLD predictions and experimental data in Sec. III. Conclusions and prospects are finally drawn in Sec. IV.

II. Theoretical Framework

Covariant density functional theory starts from a Lagrangian, and the corresponding Kohn-Sham equations take the form of a Dirac equation with effective fields S and V derived from this Lagrangian [?, ?, ?, ?, ?]. Specifically, nucleons in the nucleus are described as Dirac particles moving in an average potential field given by meson and photon fields, interacting with each other through the exchange of mesons and photons. By solving the Dirac equation:

$$[\alpha \cdot \mathbf{p} + \beta(m + S) + V]\psi_i = \varepsilon_i \psi_i,$$

where ε_i is the single-particle energy—precisely what we need to calculate the NLDs—and S and V are the relativistic scalar field and the time-like component of the vector field, respectively.

After obtaining the energy ε, spin projection m, and parity p of the single-particle levels through CDFT, this level information is substituted into the generating function defined in the combinatorial method [?] to obtain the particle-hole state density ρ_i. The generating function Z reads:

$$Z(x_1, x_2, x_3, x_4) = \prod_k \prod_i (1 + x_k p_i^k y^{\varepsilon_i^k} t^{m_i^k}).$$

This generating function is a straightforward generalization of that used previously in Ref. [?] to account not only for energy ε_i^k but also for spin projection m_i^k and parity p_i^k. Z can be expanded in powers of x_k as:

$$Z(x_1, x_2, x_3, x_4) = \sum_N F_N(y,t) \prod_k x_k^{N_k},$$

where the symbol N denotes any integer combination (N_1, N_2, N_3, N_4). The function $F(y,t)$ can be expanded into powers of y and t as:

$$F_N(y,t) = \sum_U \sum_M \sum_{P=-1,+1} C_N(U,M,P) y^U t^M,$$

where U, M, and P represent the excitation energy, spin projection, and parity, respectively. The coefficients $C_N(U,M,P)$ are the numbers of solutions. Through these coefficients, the simplest definition for particle-hole state density ρ_i reads:

$$\rho_i(U,M,P) = \frac{C_N(U,M,P)}{\varepsilon_0},$$

but the state density ρ_i turns out to be strongly dependent on any unit energy ε_0. Therefore, another method suggested by Williams [**?**] is employed in this paper to limit the discretization effects as explained below.

Summing all the C_N up to a given excitation energy U, we first obtain the cumulated number of states $N_N(U,M,P)$, which represents the number of particle-hole states with excitation energy E such that $0 \leq E < U$. The particle-hole state density is then defined as:

$$\rho_i(U,M,P) = \frac{dN_N(U,M,P)}{dU}.$$

The particle-hole state density ρ_i calculated is only related to particle-hole excitations. Two special collective effects need to be taken into account to obtain the level density: rotational and vibrational enhancement. If the nucleus under consideration displays spherical symmetry, the intrinsic and laboratory frames coincide, and the level density is trivially obtained through the relation [**?**]:

$$\rho_{\text{sph}}(U,M,P) = \rho_i(U, M=J, P) - \rho_i(U, M=J+1, P).$$

For deformed nuclei, within the axial symmetry hypothesis, the NLD after accounting for rotational effects reads:

$$\rho_{\text{def}}(U,M,P) = \sum_{K=-J}^{K\neq 0} \rho_i(U - E^{\text{rot}}_{J,K}, K, P) + \frac{1}{2}[\delta(J_{\text{even}})\delta(p=+)\rho_i(U - E^{\text{rot}}_{J,K}, 0, P) + \delta(J_{\text{odd}})\delta(p=-)\rho_i(U - E^{\text{rot}}_{J,K}, 0$$

The factor 1/2 accounts for the fact that in mirror axially symmetric nuclei, intrinsic states with spin projections $+K$ or $-K$ give rise to the same rotational levels. Moreover, in the second term of the summation, the symbol $\delta(x)$ (defined by $\delta(x) = 1$ if x holds true, and 0 otherwise) restricts the rotational bands built on intrinsic states with spin projection $K = 0$ and parity P to the level sequences $0, 2, 4, ...$ for $P = +$ and $1, 3, 5, ...$ for $P = -$. Finally, the rotational energy is obtained with the well-known expression [**?**]:

$$E^{\mathrm{rot}}_{J,K} = \frac{J(J+1) - K^2}{2\mathcal{J}_{\perp}},$$

where $\mathcal{J}_{\perp}$ is the moment of inertia of a nucleus rotating around an axis perpendicular to the symmetry axis. In this article, $\mathcal{J}_{\perp}$ is approximated by the rigid-body value $\mathcal{J}_{\mathrm{rigid}}$, which reads:

$$\mathcal{J}_{\mathrm{rigid}} = \frac{2}{5} mR^2 \left(1 + \sqrt{\frac{5}{4\pi}}\beta\right)$$

for an ellipsoidal shape with axial quadrupole deformation parameter β. The vibrational enhancement is approximated by the equation [**?**]:

$$K_{\mathrm{vib}} = \exp[\delta S - (\delta U/T)],$$

where S is the entropy, U is the excitation energy, and T is the nuclear temperature.

Finally, a phenomenological damping function is introduced to avoid sharp transitions between spherical and deformed level densities affecting the NLD predictions. The expression for the NLD after introducing the damping function can be written as [**?**]:

$$\rho(U, M, P) = [1 - f_{\mathrm{dam}}(U)]K_{\mathrm{vib}}\rho_{\mathrm{sph}}(U, M, P) + f_{\mathrm{dam}}(U)K_{\mathrm{vib}}\rho_{\mathrm{def}}(U, M, P).$$

The damping function f_{dam} is expressed as [**?**]:

$$f_{\mathrm{dam}} = 1 - \frac{1}{1 + \exp[(\beta - 0.18)/0.038]},$$

where β is the quadrupole deformation parameter. The parameters 0.18 and 0.038 have been adjusted according to experimental data at the neutron separation energy S_n [**?**]. The expression of f_{dam} has been evolved in Ref. [**?**], which has been simplified to depend only on the nuclear deformation, thus reducing the number of phenomenological parameters. This damping function is used to

suppress discontinuities that occur between spherical and deformed NLDs and ensure a smooth shape transition from deformed to spherical.

III. Results and Discussion

In this section, we present our NLD results from the combinatorial method based on CDFT and compare them with results from other NLD models [**?**] and experiments [**?**, **?**]. The effective meson-exchange interaction parameter PK1 [**?**] is adopted throughout the CDFT calculations. For spherical CDFT calculations, we fix the box size $R_{\rm box} = 20$ fm and step size $\Delta r = 0.1$ fm. In the present deformed CDFT calculations, both the Dirac equation for nucleons and the Klein–Gordon equations for mesons are solved in an isotropic harmonic oscillator basis with 18 major oscillator shells adopted.

[Figure 2: see original paper] (Color online) Comparison of NLDs calculated based on the CDFT combinatorial method with results from HFB combinatorial methods and the microstatistical method (HFB+Sta) [**?**, **?**, **?**]. The experimental data are taken from Refs. [**?**, **?**, **?**, **?**].

[Figure 1: see original paper] (Color online) Comparison of NLDs calculated using different effective interactions under CDFT with experimental data [**?**, **?**]. As the combinatorial results rely on single-particle level properties, to understand the effect of using different effective interactions on the NLDs, the NLDs of ^{112}Cd and ^{162}Dy obtained with different CDFT effective interactions PK1 [**?**], NL3 [**?**], DD-ME2 [**?**], and DD-PC1 [**?**] are presented for comparison in Fig. 1. For nuclei with small deformation, such as ^{112}Cd, the NLDs for the four effective interactions are similar for excitation energies above 4 MeV. However, a significant difference is observed for excitation energies below 4 MeV. This difference arises because the single-particle energies near the Fermi level are very sensitive to the choice of effective interactions, especially when the Fermi level is near proton or neutron shells. Meanwhile, CDFT calculations with the chosen interactions do not reproduce the single-particle levels of the magic nucleus ^{132}Sn [**?**] very well, which explains the deviations of our results from the measurements in Fig. 1. For the well-deformed ^{162}Dy, the NLDs calculated with the four effective interactions deviate from each other across the entire excitation energy region, although the overall trend is consistent. This deviation at low excitation energy is mainly caused by differences in the single-particle energies around the Fermi level. Meanwhile, the entropy S obtained from the four effective interactions is significantly different for nuclei with large deformation, ultimately leading to deviations in NLDs at high excitation energy. Compared with experimental data for ^{112}Cd [**?**] and ^{162}Dy [**?**], the deviation between the NLDs obtained using the PK1 effective interaction and the results from other effective interactions is within a reasonable range.

As non-relativistic HFB combinatorial methods, including Skyrme and Gogny interactions, have been widely used in NLD predictions [**?**, **?**], the NLDs of spherical nuclei (^{55}Co, ^{132}Sn, ^{208}Pb) and deformed nuclei (^{94}Mo, ^{95}Mo, ^{166}Er)

calculated from the present CDFT combinatorial method are given in Fig. 2 and compared with them and the corresponding experimental data.

For ^{55}Co, the CDFT combinatorial method gives a lower NLD compared to experimental data, while the Skyrme combinatorial method gives a higher NLD. Although the result of the Gogny combinatorial method is closer to the experimental data to a certain extent, it shows strong oscillations. For ^{132}Sn and ^{208}Pb, the results of the CDFT combinatorial method are similar to those of the Skyrme combinatorial method, but the results of the Gogny combinatorial method are significantly lower than the other two methods. Compared with experimental data, the CDFT combinatorial method can better describe the NLD of ^{208}Pb. The NLDs of ^{55}Co, ^{132}Sn, and ^{208}Pb from the three combinatorial methods are more or less oscillatory because these three nuclei are spherical with highly degenerate single-particle levels, and there is a strong shell effect.

For ^{94}Mo, both the CDFT and Skyrme combinatorial method results are closer to experimental data than the Gogny combinatorial method. For ^{95}Mo and ^{166}Er, the NLDs obtained by the three combinatorial methods are similar and slightly larger than experimental data. It should be emphasized that the deformed nuclei ^{94}Mo, ^{95}Mo, and ^{166}Er break single-particle level degeneracy, thus obtaining smoother NLDs as shown in Fig. 2. It is worth noting that the CDFT combinatorial method gives higher NLDs for ^{94}Mo and ^{95}Mo. One possible reason is that the CDFT combinatorial method uses the rigid-body value when considering rotational effects, which is not appropriate for soft nuclei [**?**].

In addition, the NLDs of ^{55}Co and ^{94}Mo are well described by the microstatistical model [**?**] relative to the CDFT combinatorial method, while the description of the NLDs of ^{95}Mo and ^{166}Er is similar between these two models. In comparison, the microstatistical model gives relatively smooth results for spherical and deformed nuclei, which do not well reflect shell effects. Therefore, it can be concluded that the CDFT combinatorial method has a similar ability to describe NLDs as the other two combinatorial methods and the microstatistical model.

[Figure 3: see original paper] (Color online) Comparison of NLDs obtained from the CDFT combinatorial method with other NLD predictions [**?**] and experimental data [**?**, **?**, **?**, **?**]. The full asterisk corresponds to the experimental data at the neutron separation energy S_n [**?**].

At the same time, it is also necessary to compare with phenomenological models (BFM, CTM, and GSM) that have been widely applied. In particular, phenomenological models can well describe experimental data at the neutron separation energy by fitting experimental data. The NLDs of even-even nuclei (^{112}Cd, ^{162}Dy), odd-A nuclei (^{51}V, ^{97}Mo, ^{119}Sn), and odd-odd nucleus (^{60}Co) calculated from the present CDFT combinatorial method are given in Fig. 3 and compared with results from phenomenological models and experimental data. It can be seen from Fig. 3 that the CDFT combinatorial method has a similar ability to phenomenological models in reproducing experimental data at neutron separation energy, especially in describing the NLD of ^{51}V well. In addition,

the overall description of experimental data below neutron separation energy by the CDFT combinatorial method is also similar to that of phenomenological methods. In conclusion, while there are some differences in the results for each NLD model, the overall ability to describe experimental data is similar.

The most extensive and reliable source of experimental information on NLD remains the s-wave neutron resonance spacings D_0 [**?**] and the observed low-energy excited levels [**?**]. To measure the dispersion between theoretical and experimental D_0, the $f_{\rm rms}$ factor is defined as:

$$f_{\rm rms} = \exp\left[\frac{1}{N_e}\sum_{i=1}^{N_e}\ln^2\left(\frac{D_i^{\rm th}}{D_i^{\rm exp}}\right)\right]^{1/2},$$

where $D^{\rm th}$ ($D^{\rm exp}$) is the theoretical (experimental) resonance spacing and N_e is the number of nuclei in the compilation. The results for the ratios of $D^{\rm th}$ and $D^{\rm exp}$ are shown in Fig. 4 [Figure 4: see original paper], with $f_{\rm rms} = 3.62$ for a total of 66 nuclei counted. Under the same calculation conditions, the $f_{\rm rms}$ of the Gogny (D1S) interaction based on HFB plus combinatorial method is 7.25 [**?**]. At present, the result of the CDFT combinatorial method is larger than the $f_{\rm rms} = 1.8$ deviation of the phenomenological back-shifted Fermi gas model [**?**] and the $f_{\rm rms} = 2.1$ value obtained with the microstatistical method [**?**]. However, the HFB combinatorial method based on the Skyrme effective interaction improved pairing correlation [**?**] and collective effects, achieving $f_{\rm rms} = 2.3$ [**?**]. In subsequent work, it is expected to improve the CDFT combinatorial method in the same way.

[Figure 5: see original paper] (Color online) The NLDs obtained from the CDFT combinatorial method with (red) and without (black) normalization. The experimental data are taken from Refs. [**?**, **?**, **?**].

When phenomenological NLDs are used in nuclear physics applications, such as nuclear data evaluation or accurate and reliable estimation of reaction cross sections, one often adjusts the few parameters on which phenomenological expressions depend. The results of the combinatorial method can also be normalized to both the experimental level scheme at low excitation energy and the neutron resonance spacings at $U = S_n$ in a way similar to what is usually done with analytical formulas. More precisely, the normalized level density can be obtained by the expression [**?**]:

$$\rho(U, J, P) = e^{\alpha U - \delta} \times \rho(U - \delta, J, P),$$

where the energy shift δ is essentially extracted from the analysis of the cumulative number of levels, and α can be obtained through the expression $\rho^{\rm th}(S_n) \times e^{\alpha S_n} = \rho^{\rm exp}(S_n)$. With such normalization, the experimental low-lying states and the D_0 values can be reproduced reasonably well.

[Figure 6: see original paper] Normalized parameters α (left) and δ (right) values are plotted as a function of the atomic mass number.

As an illustration, the variation of NLDs obtained by the CDFT combinatorial method before and after normalization is shown in Fig. 5. When normalization is applied, the NLDs pass through the experimental data at the neutron separation energy S_n. As shown in Fig. 5(a), if the theoretical calculation value is close to the experimental data at the neutron separation energy S_n, the results before and after normalization do not change much. In Fig. 5(b), the results show better agreement with experimental data [**?**] after normalization, especially above 2 MeV. This is because the coefficient e^{α} is related to the excitation energy U, and when U is small, normalization has little effect. Some nuclear α and δ values are shown in Fig. 6.

Finally, the NLDs calculated based on the CDFT combinatorial method are compared with the observed low-energy excited levels, which are the most extensive and reliable source of experimental information on NLDs [**?**]. The cumulative number of nuclear levels $N(U)$ indicates the sum of the number of all levels below some excitation energy U (including $N(U) = \sum_M \sum_P N(U, M, P)$, where $N(U, M, P)$ is the cumulative number of levels under spin M and parity P up to excitation energy E). The predicted cumulative number of levels $N(U)$ is compared with experimental data [**?**] in Fig. 7 [Figure 7: see original paper], including light as well as heavy, spherical and deformed nuclei. Globally, the results of the CDFT combinatorial method are in reasonably good agreement with experimental data at lower excitation energy, especially for light nuclei. At high excitation energy, the theoretically calculated cumulative number of nuclear levels is higher than the experimental value. NLDs increase rapidly with increasing excitation energy, and $N(U)$ should also gradually increase at high excitation energy, but the experimental cumulative number gradually stabilizes, likely limited by experimental conditions that prevent complete counting of levels.

[Figure 8: see original paper] (Color online) Comparison between the calculated NLDs based on the CDFT combinatorial method (red lines) and the experimental data [**?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**] (black dots). The full asterisk corresponds to the experimental data at the neutron separation energy S_n [**?**].

In Fig. 8 [Figure 8: see original paper], the CDFT combinatorial method predictions after normalization are compared with experimental data extracted by the Oslo group [**?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**] and particle evaporation spectra [**?**, **?**]. The Oslo method is model-dependent. To extract the absolute value of the total level density from measured data, the so-called experimental NLDs need to be normalized by the total level density at the neutron binding energy, which in turn is derived from the neutron resonance spacing. For a meaningful comparison between the CDFT combinatorial predictions and the Oslo group data, it is therefore important to normalize the NLDs of the CDFT combinatorial method to the level density value at $U = S_n$ considered by the Oslo group. As shown in Fig. 8, the results of the CDFT combinatorial method after normalization agree

well with experimental data below S_n, except for the small NLDs of ^{111}Cd and ^{161}Dy at low excitation energy. The smaller result is due to the larger energy spacing of the theoretically calculated single-particle levels near the Fermi level. Overall, the results obtained by the CDFT combinatorial method are reliable.

IV. Summary and Prospects

The combinatorial method has been adopted to describe nuclear level densities for nuclear reaction calculations. The particle-hole state density is obtained with a combinatorial method using single-particle levels provided by the CDFT-based PK1 effective interaction. After accounting for collective effects, including vibration and rotation, the energy-, spin-, and parity-dependent NLDs are obtained. Our results are compared with those from other NLD models, including phenomenological, microstatistical, and non-relativistic HFB combinatorial models. The comparison suggests that, besides some small deviations from different NLD models, the general trends among these models are basically the same. In conclusion, the CDFT combinatorial method is capable of reproducing experimental data at or below the neutron separation energy. It implies that the CDFT combinatorial method is as reliable as other models for describing NLDs. Finally, the NLDs of the CDFT combinatorial method with normalization are compared with experimental data, obtaining excellent agreement with the observed cumulative number of levels at low excitation energy and the measured NLDs below the neutron separation energy.

Our results exhibit the predictive power of the CDFT combinatorial method, even though pairing correlations are not considered while the collective effects are empirical. In our future work, the CDFT combinatorial method can be improved by including energy-dependent pairing correlations and adopting a partition function approach to treat vibrational enhancement. These results will surely aid our study of important neutron capture processes such as the r-process.

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