

# Generalized particle–hole state densities within the equidistant spacing model

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## Abstract

We present an improved mathematical method to compute particle–hole state densities, with high numerical accuracy, for an arbitrary single particle level scheme. For the simplest case, the equidistant spacing model (ESM), we compare our exact particle–hole state density calculations with several existing and new analytical formulae. The latter are derived using the method of Berger and Martinot and lead to a generalization of the Obložinský formula for the two-component particle–hole state density. Our new formulae, which include correction terms up to any order, are discussed for various particle–hole configurations over a broad energy range. © 1998 Elsevier Science B.V.

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## 1. Introduction

The analysis of pre-equilibrium nuclear reactions is generally based on a statistical approach in which the key role is played by the density of excited states of configurations with a certain number of particles and holes. So far, the only way to obtain simple approximate expressions for this so called particle–hole state density  $\omega_{ph}$  is to derive them analytically within the equidistant spacing model (ESM) framework. The mathematical methods used for such a derivation have been presented in many well-known theoretical papers [1–5], where more or less accurate analytical formulae for  $\omega_{ph}$  are provided.

In this paper we will present a new and general analytical formula for  $\omega_{\text{ph}}$  for the ESM, and compare it with the expressions derived by Williams [2], Běták and Doběš [3], Stankiewicz et al. [4] and Obložinský [5]. In order to check the accuracy of these various analytical formulae, we first present in Section 2 a general combinatorial approach – based on the formalism developed by Berger and Martinot [6] – which provides the exact  $\omega_{\text{ph}}$  values for any particle–hole excitation in the general independent particle model (GIPM). Details of our numerical method, which gives accurate results for even the most complex particle–hole configurations, are outlined. Our new analytical formula is then derived in Section 3. Finally, the results obtained with this new formula are discussed in Section 4 and compared with the usually employed expressions and with our exact combinatorial results obtained within the ESM. Although our new expression has not yet been applied in nuclear reaction calculations, we discuss its possible impact on pre-equilibrium models.

## 2. Exact particle–hole state densities in the GIPM

In this section, we present the formalism and method to compute exact particle–hole state densities as functions of the excitation energy within the GIPM. We first define particle and hole states. We then display the basic equations that we want to solve, and briefly discuss the numerical method we use.

### 2.1. Particles and holes in the GIPM

In the GIPM, a nucleus with  $Z$  protons and  $N$  neutrons is represented by two energy level schemes, namely  $(\varepsilon_1^\pi < \varepsilon_2^\pi < \dots < \varepsilon_n^\pi < \dots)$  for protons, and  $(\varepsilon_1^\nu < \varepsilon_2^\nu < \dots < \varepsilon_n^\nu < \dots)$  for neutrons, where the  $Z$  (resp.  $N$ ) first single particle states are occupied while the others are empty. As usual, one splits each scheme into two parts: the particle level scheme and the hole level scheme. The proton (resp. neutron) hole states are defined as the  $Z$  (resp.  $N$ ) single particle states filled in the ground state. If we denote by the index  $F_\pi$  (resp.  $F_\nu$ ) the last occupied level in the proton (resp. neutron) single particle level scheme, the excitation energies for particles and holes are defined as:

$$\begin{aligned} \varepsilon_i^1 &= \varepsilon_{F_\pi+i}^\pi - \varepsilon_{F_\pi}^\pi, & i &= 1, 2, \dots, I_1 & \text{for proton particles,} \\ \varepsilon_i^2 &= \varepsilon_{F_\pi}^\pi - \varepsilon_{F_\pi-i+1}^\pi, & i &= 1, 2, \dots, I_2 & \text{for proton holes,} \\ \varepsilon_i^3 &= \varepsilon_{F_\nu+i}^\nu - \varepsilon_{F_\nu}^\nu, & i &= 1, 2, \dots, I_3 & \text{for neutron particles,} \\ \varepsilon_i^4 &= \varepsilon_{F_\nu}^\nu - \varepsilon_{F_\nu-i+1}^\nu, & i &= 1, 2, \dots, I_4 & \text{for neutron holes.} \end{aligned}$$

In this set of equations,  $I_2$  and  $I_4$  are equal to  $Z$  and  $N$ , respectively, while  $I_1$  and  $I_3$  enable us to deal simultaneously with finite and infinite sets of particle states.<sup>1</sup>

## 2.2. The fundamental equations

We want to calculate the number of states  $N_{\mathcal{N}}(U) = N_{(N_1, N_2, N_3, N_4)}(U)$  at excitation energy  $U$  resulting from the excitation of  $N_1$  proton particles,  $N_2$  proton holes,  $N_3$  neutron particles, and  $N_4$  neutron holes. Thus,  $\mathcal{N}$  denotes the specific configuration of particles and holes. The integer  $N_{\mathcal{N}}(U)$  is the total number of solutions of

$$U = \sum_{k=1}^4 \sum_{i=1}^{I_k} n_i^k \varepsilon_i^k, \quad (1)$$

and of the four equations

$$N_k = \sum_{i=1}^{I_k} n_i^k \quad (k = 1, 2, 3 \text{ and } 4), \quad (2)$$

where  $n_i^k = 0$  or 1, depending upon whether the state  $i$  is empty or occupied, respectively.

To calculate  $N_{\mathcal{N}}(U)$ , we start from the grand partition function for multiple particle-hole excited configurations as given by Berger and Martinot [6]:

$$\mathcal{Z}(x_1, x_2, x_3, x_4, y) = \prod_{k=1}^4 \prod_{i=1}^{I_k} (1 + x_k y^{\varepsilon_i^k}). \quad (3)$$

Following Ref. [6], Eq. (3) can be expanded in powers of  $x_k$  as

$$\mathcal{Z}(x_1, x_2, x_3, x_4, y) = \sum_{\mathcal{N}} \mathcal{F}_{\mathcal{N}}(y) x_1^{N_1} x_2^{N_2} x_3^{N_3} x_4^{N_4}, \quad (4)$$

and the integer coefficients  $N_{\mathcal{N}}(U)$  are obtained using the relation

$$\mathcal{F}_{\mathcal{N}}(y) = \sum_U N_{\mathcal{N}}(U) y^U. \quad (5)$$

The mathematical problem consists of computing of the function  $\mathcal{F}_{\mathcal{N}}$  as a polynomial function of the excitation energy. The method we use is now explained.

## 2.3. Calculation of particle-hole state densities

It has been shown [6] that

$$\mathcal{F}_{\mathcal{N}}(y) = \prod_{k=1}^4 \sum_{\{\alpha(N_k)\}} \prod_{j=1}^{N_k} \frac{1}{\alpha_j^k} [\mathcal{F}_j^k(y)]^{\alpha_j^k}, \quad (6)$$

<sup>1</sup> In the general case, one deals with infinite sets (i.e.  $I_1$  and  $I_3$  reach infinity). Yet, one may also be interested in particle-hole excitations involving only bound particles (for multistep compound nuclear reactions).  $I_1$  and  $I_3$  are then the labels of the last bound single particle state in the proton and neutron level schemes, respectively. In this case, the sets are finite.

with

$$\mathcal{F}_j^k(y) = \sum_{i=1}^{I_k} \frac{(-1)^{j+1}}{j} y^{j\epsilon_i^k}, \quad (7)$$

where the symbol  $\sum_{\{\alpha(N_k)\}}$  means the summation over all the integer partitions  $(\alpha_1^k, \alpha_2^k, \dots, \alpha_{N_k}^k)$  that obey

$$\alpha_1^k + 2\alpha_2^k + \dots + N_k \alpha_{N_k}^k = N_k.$$

To compute the coefficients  $N_{\mathcal{N}}(U)$ , it is convenient to assume that any energy appearing in our scheme is an integer multiple of an elementary energy unit  $\varepsilon_0$ .<sup>2</sup> Writing  $U = n \times \varepsilon_0$  and  $\varepsilon_i^k = \nu_i^k \times \varepsilon_0$ , Eq. (1) then reads

$$n = \sum_{k=1}^4 \sum_{i=1}^{I_k} n_i^k \nu_i^k. \quad (8)$$

The problem is now to calculate the integers  $N_{\mathcal{N}}(n)$ , representing the number of solutions of Eqs. (2) and (8) (i.e. the number of nuclear excited states for the configuration  $\mathcal{N}$  in the energy bin  $E_n = [n\varepsilon_0, (n+1)\varepsilon_0]$ ). In Ref. [6], a fast Fourier transform was used to compute these integers. Such a method can be employed with good accuracy only when the number of excited particles and holes is small. When this number becomes large, this method results in a loss of numerical precision. Therefore, a rather different method has been implemented, as is explained below.

We first replace the single particle states energies  $\varepsilon_i^k$  by integers  $\nu_i^k$  such that

$$\varepsilon_i^k \in [\nu_i^k \varepsilon_0, (\nu_i^k + 1) \varepsilon_0].$$

Then Eq. (7) can be written as

$$\mathcal{F}_j^k(y) = \sum_{i=1}^{I_k} \frac{(-1)^{j+1}}{j} y^{j\nu_i^k},$$

provided  $\varepsilon_0$  is the new energy unit.

The new numerical method consists of associating polynomials of this form with the vectors  $\mathcal{V}_{\mathcal{F}_i^k}$  as explained in Appendix A. Then, using the vector operations as defined in Appendix A, the computation of the vector  $\mathcal{V}_{\mathcal{F}_{\mathcal{N}}}$ , associated with the polynomial function  $\mathcal{F}_{\mathcal{N}}$  given by Eq. (6), is easy to handle. One finally deduces the coefficient  $N_{\mathcal{N}}(n)$  from the trivial relation

$$N_{\mathcal{N}}(n) = V_{\mathcal{F}_{\mathcal{N}}}(n).$$

The particle-hole state density associated with the computed vector  $\mathcal{V}_{\mathcal{F}_{\mathcal{N}}}$ , for  $U$  in the energy bin  $E_n$ , is then

$$\omega_{\mathcal{N}}^{(\text{ex})}(U \in E_n) = \frac{1}{\varepsilon_0} V_{\mathcal{F}_{\mathcal{N}}}(n).$$

<sup>2</sup> The best value for  $\varepsilon_0$  is of course equal to  $10^{-n}$  if the single particle state energies are given with  $n$  digits.

In sum, we have related the function  $\mathcal{F}_N$  of the partition function (4) to the *exact* particle–hole state density  $\omega_N^{(\text{ex})}$ . The  $\omega_N^{(\text{ex})}(U)$  values can be computed numerically with a very high precision. They will be compared with more approximate analytical approaches in Section 4.

### 3. Closed expression for particle–hole state densities in the ESM

In this section, we establish a new closed expression for particle–hole state densities in the ESM. It is based on (i) a polynomial expansion of the partition function [5], (ii) a derivation of correction terms following the method of Anzaldo-Meneses [7], and (iii) a multinomial expansion of the type given in Ref. [8]. The relationship between this new formula and the other well known expressions of Williams [2], Běták and Doběš [3], Stankiewicz et al. [4] and Obložinský [5] is also discussed.

#### 3.1. The new formula

In the ESM, the only parameters are the single particle–single hole state densities  $g_1, g_2$  (resp.  $g_3, g_4$ ), which are defined as the average number of states to be found in a 1 MeV interval in the level scheme of the proton (resp. neutron) particles or holes. With these parameters, the four particle–hole level schemes are

$$\begin{aligned} \varepsilon_i^1 &= \frac{i}{g_1}, & i &= 1, 2, \dots, I_1 & \text{for proton particles,} \\ \varepsilon_i^2 &= \frac{i}{g_2}, & i &= 0, 1, \dots, Z-1 & \text{for proton holes,} \\ \varepsilon_i^3 &= \frac{i}{g_3}, & i &= 1, 2, \dots, I_3 & \text{for neutron particles,} \\ \varepsilon_i^4 &= \frac{i}{g_4}, & i &= 0, 1, \dots, N-1 & \text{for neutron holes.} \end{aligned} \quad (9)$$

Setting  $Z = I_2$  and  $N = I_4$ , the partition function (3) simplifies to

$$\mathcal{Z}(x_1, x_2, x_3, x_4, y) = \prod_{k=1,3} \mathcal{Z}_p(x_k, y, g_k, I_k) \prod_{k=2,4} \mathcal{Z}_h(x_k, y, g_k, I_k),$$

with

$$\mathcal{Z}_p(x, y, g, I) = \prod_{i=1}^I (1 + x y^{i/g}), \quad \mathcal{Z}_h(x, y, g, I) = \prod_{i=0}^{I-1} (1 + x y^{i/g}).$$

It can be shown [5] that

$$\mathcal{Z}_p(x, y, g, I) = \sum_{k=0}^I x^k y^{\frac{k(k+1)}{2g}} \prod_{l=1}^k \frac{1 - y^{\frac{l-k+1}{g}}}{1 - y^{l/g}}, \quad (10)$$

$$\mathcal{Z}_h(x, y, g, I) = \sum_{k=0}^I x^k y^{\frac{k(k-1)}{2g}} \prod_{l=1}^k \frac{1 - y^{\frac{l-k+1}{g}}}{1 - y^{l/g}}. \quad (11)$$

The state densities for  $N$  particles (resp.  $N$  holes) are given by the coefficients  $\omega_p(N, U)$  [resp.  $\omega_h(N, U)$ ] of  $x^N y^U$  if we expand  $\mathcal{Z}_p$  (resp.  $\mathcal{Z}_h$ ) in powers of  $x$  and  $y$ . The residual theorem applied to Eqs. (10) and (11) gives after integration over  $x$

$$\omega_p(N, U) = \frac{1}{2i\pi} \oint y^{\frac{N(N+1)}{2g}} \prod_{l=1}^N \frac{1 - y^{\frac{l-N+l}{g}}}{1 - y^{l/g}} \frac{dy}{y^{U+1}},$$

for the particle state density, and

$$\omega_h(N, U) = \frac{1}{2i\pi} \oint y^{\frac{N(N-1)}{2g}} \prod_{k=1}^N \frac{1 - y^{\frac{l-N+k}{g}}}{1 - y^{k/g}} \frac{dy}{y^{U+1}},$$

for the hole state density.

Setting  $y = e^{-\beta}$ ,  $\omega_p(N, U)$  and  $\omega_h(N, U)$  can be considered as inverse Laplace transforms expressed in terms of the variable  $\beta$ . The particle-hole state density  $\omega_N(U)$  is obtained by folding in the four separate particle and hole state densities  $\omega_p(N_1, U)$ ,  $\omega_h(N_2, U)$ ,  $\omega_p(N_3, U)$  and  $\omega_h(N_4, U)$ . Using the convolution theorem for Laplace transforms, it can be written as

$$\omega_N(U) = \frac{1}{2\pi i} \oint e^{\beta(U-A)} \prod_{k=1}^4 U_k(\beta) D_k(\beta) d\beta, \quad (12)$$

where

$$A = \frac{N_1^2 + N_1}{2g_1} + \frac{N_2^2 - N_2}{2g_2} + \frac{N_3^2 + N_3}{2g_3} + \frac{N_4^2 - N_4}{2g_4}, \quad (13)$$

$$U_k(\beta) = \prod_{i=1}^{N_k} \left[ 1 - e^{-\beta \frac{I_k - N_k + i}{g_k}} \right], \quad (14)$$

$$D_k(\beta) = \left[ \prod_{i=1}^{N_k} \left( 1 - e^{-\beta i/g_k} \right) \right]^{-1}. \quad (15)$$

We now have to express the  $U_k(\beta)$  and  $D_k(\beta)$  terms in a way that enables us to calculate the inverse Laplace transform in Eq. (12).

### 3.1.1. Expansion of $U_k(\beta)$

So far, the formalism presented for the ESM is exact. We now consider two alternative approximations, both applied on the expansion (14), that lead to establishing the new analytical formulae.

In the first approximation, labelled  $\mathcal{H}_1$ , we assume that  $I_k \gg N_k$ . In the second approximation, labelled  $\mathcal{H}_2$ , the subscript  $i$  of Eq. (14) is replaced by its average value  $(N_k + 1)/2$ . This gives the following closed form for the function  $U_k$

$$U_k(\beta) \approx \sum_{i=0}^{N_k} \binom{N_k}{i} (-1)^i e^{-\beta i \frac{I_k}{g_k}}, \quad (16)$$

with

$$J_k = I_k \quad (\text{Approximation } \mathcal{H}_1), \quad (17)$$

or

$$J_k = I_k - \frac{1}{2}(N_k - 1) \quad (\text{Approximation } \mathcal{H}_2). \quad (18)$$

These are the only approximations made throughout the whole derivation of our new analytical formulae.

### 3.1.2. Expansion of $D_k(\beta)$

The derivations of the analytical formulae of Refs. [2,3,5] are all based on approximation  $\mathcal{H}_1$ . In addition, the calculation of  $D_k(\beta)$  is performed by assuming

$$1 - e^{-t} \approx te^{-t/2},$$

which actually is an approximation to the identity [9]

$$1 - e^{-t} = te^{-t/2} \prod_{m=1}^{+\infty} \left[ 1 + \frac{t^2}{4\pi^2 m^2} \right]. \quad (19)$$

In Ref. [7] Anzaldo-Meneses has shown how the whole identity can be used in the Williams formula [2]. However, he only uses Eq. (19) up to  $m = 2$  and gives a new, but restricted analytical expression including corrections to the Williams formula that lead to a better agreement with the exact values of state densities. Here, we use the expansion (19) throughout to obtain a general closed expression for these corrections without any limitation on the  $m$  value. The calculation of  $D_k(\beta)$  is straightforward, as outlined in Appendix B, and the result reads

$$D_k(\beta) = \frac{e^{\beta N(N+1)/4}}{N! \beta^N} \left[ 1 + \sum_{k=1}^{+\infty} C_{2k}(N) \beta^{2k} \right], \quad (20)$$

where the coefficients  $C_{2k}(N)$  are also defined in Appendix B.

### 3.1.3. The general formula

Inserting Eqs. (16) and (20) into Eq. (12) leads to the expression

$$\omega_{\mathcal{N}}(U) = G \sum_{i=0}^{N_1} \sum_{j=0}^{N_2} \sum_{k=0}^{N_3} \sum_{l=0}^{N_4} K_{ijkl} \frac{1}{2\pi i} \oint e^{\beta U_{ijkl}} \sum_{m=0}^{+\infty} E_{2m}^{\mathcal{N}} \beta^{(2m-M)} d\beta, \quad (21)$$

where

$$G = \frac{g_1^{N_1} g_2^{N_2} g_3^{N_3} g_4^{N_4}}{N_1! N_2! N_3! N_4!},$$

$$K_{ijkl} = (-1)^{i+j+k+l} \binom{N_1}{i} \binom{N_2}{j} \binom{N_3}{k} \binom{N_4}{l},$$

$$U_{ijkl} = U - A + B - E_{ijkl}, \quad (22)$$

with  $A$  defined in Eq. (13),

$$B = \frac{N_1^2 + N_1}{4g_1} + \frac{N_2^2 + N_2}{4g_2} + \frac{N_3^2 + N_3}{4g_3} + \frac{N_4^2 + N_4}{4g_4}, \quad (23)$$

and

$$E_{ijkl} = i \frac{J_1}{g_1} + j \frac{J_2}{g_2} + k \frac{J_3}{g_3} + l \frac{J_4}{g_4}. \quad (24)$$

The  $J_n$ 's in Eq. (24) have been defined in Eq. (17) or Eq. (18), and  $E_{2m}^{\mathcal{N}}$  reads

$$E_{2m}^{\mathcal{N}} = 1 \quad \text{for } m = 0,$$

and

$$E_{2m}^{\mathcal{N}} = \sum_{i=0}^m D_{2m-2i}(N_1, N_2) D_{2i}(N_3, N_4) \quad \text{for } m \neq 0,$$

while  $D_{2k}$  is given by

$$D_{2k}(N_i, N_j) = \sum_{l=0}^k \frac{C_{2k-2l}(N_i) C_{2l}(N_j)}{g_i^{2k-2l} g_j^{2l}}.$$

The coefficients  $C_{2k}(N)$  are defined in Appendix B, and  $M$  in Eq. (21) reads

$$M = N_1 + N_2 + N_3 + N_4.$$

The inverse Laplace transforms in Eq. (21) can now be performed term by term in the sum over  $m$ . The result is

$$\begin{aligned} \omega_{\mathcal{N}}(U) = G \sum_{i=0}^{N_1} \sum_{j=0}^{N_2} \sum_{k=0}^{N_3} \sum_{l=0}^{N_4} K_{ijkl} \Theta(U_{ijkl}) \\ \times \left[ \sum_{m=0}^{\left\lfloor E \left[ \frac{M-1}{2} \right] \right\rfloor} E_{2m}^{\mathcal{N}} \frac{U_{ijkl}^{(M-2m-1)}}{(M-2m-1)!} + \sum_{m=E \left[ \frac{M-1}{2} \right] + 1}^{+\infty} \frac{\delta^{(2m-M)}(U_{ijkl})}{(2m-M)!} \right], \quad (25) \end{aligned}$$

where  $\Theta(x)$  is the unit step function (i.e.  $\Theta(x) = 1$  for  $x \geq 0$  and  $\Theta(x) = 0$  for  $x < 0$ ),  $E[(M-1)/2]$  the integer part of  $(M-1)/2$ , and  $\delta^{(n)}$  is the  $n$ th derivative of the Dirac delta function.

The state density  $\omega_{\mathcal{N}}$  critically depends upon the energy shift  $A$  (i.e. the Pauli energy) which represents the energy necessary to create the particle-hole combination  $\mathcal{N}$ . Indeed  $\omega_{\mathcal{N}}(U)$  must vanish for  $U < A$ , and be strictly positive for  $U \geq A$ . This last property is implicitly included in Eq. (25) for  $U \geq A$ . To secure the validity of Eq. (25) for  $U < A$ , we must change  $\Theta(U_{ijkl})$  into  $\Theta(U_{ijkl} - B)$ , where  $B$  is defined in Eq. (23). As a consequence, the  $n$ -th derivatives of the  $\delta$ -function in Eq. (25) vanish and we finally obtain



$$\omega_{\mathcal{N}}(U) = G \sum_{i=0}^{N_1} \sum_{j=0}^{N_2} \sum_{k=0}^{N_3} \sum_{l=0}^{N_4} K_{ijkl} \Theta(U_{ijkl} - B) \left[ \sum_{m=0}^{E \left[ \frac{M-1}{2} \right]} E_{2m}^{\mathcal{N}} \frac{U_{ijkl}^{(M-2m-1)}}{(M-2m-1)!} \right], \quad (26)$$

which is our new and general particle–hole state density formula for the Equidistant Spacing Model.

In this expression, the terms with  $m > 0$  inside the square brackets are called “correction terms”. An example showing how to compute them is given in Appendix C. In the following, the particle–hole state density formula (26) is noted  $\omega_{\mathcal{N}}^{(1)}$  or  $\omega_{\mathcal{N}}^{(2)}$  depending upon whether approximation  $\mathcal{H}_1$  or  $\mathcal{H}_2$  is made in the expansion of  $U_k(\beta)$  [see Eqs. (17) and (18)], respectively, leading to two different values for  $U_{ijkl}$  [see Eqs. (22) and (24)].

### 3.2. Connection with the usual analytical formulae

The densities  $\omega_{\mathcal{N}}^{(1)}$  and  $\omega_{\mathcal{N}}^{(2)}$  reduce to well-known analytical formulae if simplifications are made to Eq. (26). These simplifications are now discussed. We stress that throughout our work, we distinguish between neutrons and protons, whereas Refs. [2–5] deal with one-component configurations. When we mention these more approximate formulae, we actually mean their two-component versions.

First, if we neglect the correction terms in Eq. (26), (i)  $\omega_{\mathcal{N}}^{(1)}$  reduces to the Obložinský formula  $\omega_{\mathcal{N}}^{(o1)}$  [5]

$$\omega_{\mathcal{N}}^{(o1)}(U) = G \sum_{i=0}^{N_1} \sum_{j=0}^{N_2} \sum_{k=0}^{N_3} \sum_{l=0}^{N_4} K_{ijkl} \Theta(U_{ijkl} - B) \frac{U_{ijkl}^{(M-1)}}{(M-1)!},$$

and (ii)  $\omega_{\mathcal{N}}^{(2)}$  reduces to  $\omega_{\mathcal{N}}^{(o2)}$ , another formula also suggested, but not further considered, in Ref. [5]. The expression  $\omega_{\mathcal{N}}^{(o2)}$  has the same functional form as  $\omega_{\mathcal{N}}^{(o1)}$  but the energy shifts  $E_{ijkl}$  [Eq. (24)] entering the definition of  $U_{ijkl}$  [Eq. (22)] are now defined in terms of the  $J_k$ 's of Eq. (18) instead of those of Eq. (17).

Second, in the limit where  $J_1$  and  $J_3$  reach infinity (i.e. the number of particle states becomes infinite while the number of hole states remains finite),  $\omega_{\mathcal{N}}^{(o1)}$  reduces to the expression derived by Běťák and Doběš [3]. This expression is here labelled as  $\omega_{\mathcal{N}}^{(b1)}$ . Analogously, a second state density closely related to that of Běťák and Doběš, labelled  $\omega_{\mathcal{N}}^{(b2)}$ , may also be deduced from  $\omega_{\mathcal{N}}^{(o2)}$ . In contrast, if  $J_2$  and  $J_4$  reach infinity (i.e. the number of hole states is infinite and the number of particle states is finite),  $\omega_{\mathcal{N}}^{(o1)}$  reduces to the expression  $\omega_{\mathcal{N}}^{(s1)}$  derived by Stankiewicz et al. [4], and a similar expression  $\omega_{\mathcal{N}}^{(s2)}$  can also be obtained from  $\omega_{\mathcal{N}}^{(o2)}$ .

Third, if we assume (i) an infinite potential well depth (i.e. an infinite number of hole states) and (ii) an infinite number of particle states, the  $J_k$ 's of Eqs. (17) and (18) all reach infinity. In this case, we obtain the Williams formula [2], here labelled  $\omega_{\mathcal{N}}^{(w)}$

$$\omega_{\mathcal{N}}^{(w)}(U) = G \Theta(U - A) \frac{(U + B - A)^{M-1}}{(M-1)!}.$$

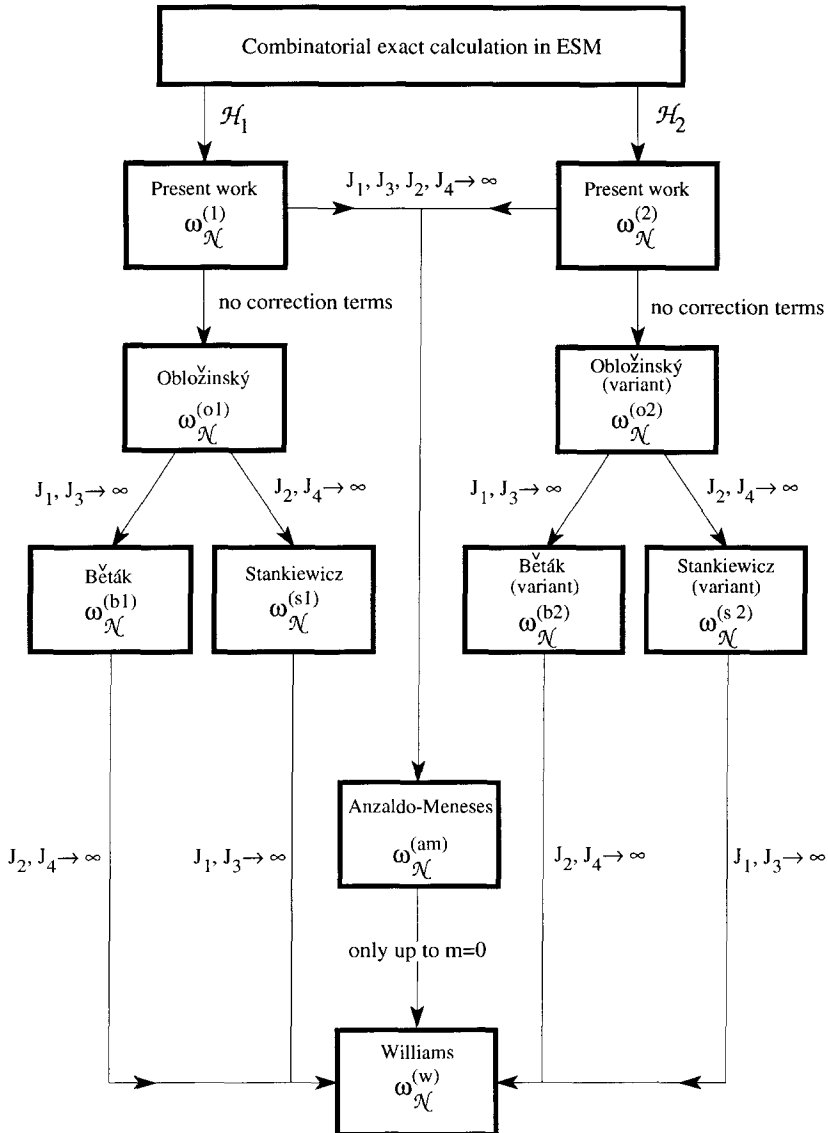


Fig. 1. Family tree of ESM particle-hole state densities, showing from top to bottom the various state density formulae which may be derived through successive approximations from exact ESM calculations. The symbols are defined in Section 3.2.

The correction terms could of course also be included in the Williams formula. This leads to an alternative formula  $\omega_{\mathcal{N}}^{(am)}$ , which is the general form of the Anzaldo-Meneses formula, developed up to  $m = 2$  in Ref. [7].

All successive approximations can be assembled in a family tree of ESM particle-hole state densities, which is shown in Fig. 1.

## 4. Results and discussion

With our exact calculations as the reference basis, we test the reliability of the state densities predicted by our new analytical formulae  $\omega_{\mathcal{N}}^{(1)}$  and  $\omega_{\mathcal{N}}^{(2)}$  for various particle–hole configurations, and compare them with some of the more simple analytical expressions cited in Section 3.2. In all the cases considered, we use an Equidistant Spacing Model with  $g_1 = g_2 = g_\pi$  and  $g_3 = g_4 = g_\nu$ , and furthermore assume  $g_\pi = g_\nu = g_0$  for simplicity. Therefore, all the energies will be expressed in units of  $g_0^{-1}$  MeV. Moreover, as a physical constraint, we always use a number of neutron (resp. proton) holes identical to the number of neutrons (resp. protons) of the nucleus (i.e. we set  $J_2 = Z$  and  $J_4 = N$ ). Hence, the formula of Stankiewicz et al. [4] is not included in our comparison. Finally, since the various state densities may take either very low or very large values, depending on the excitation energy, we always present the ratio between analytical and combinatorial, exact results.

### 4.1. Effect of the corrections terms

First, we consider configurations involving many correction terms in order to study their effects and to see to what extent correction terms are needed or not. In this case we consider an infinite number of accessible particle levels (i.e. we take the limits  $J_1 \rightarrow \infty$  and  $J_3 \rightarrow \infty$ ). We thus compare  $\omega_{\mathcal{N}}^{(1)}$ ,  $\omega_{\mathcal{N}}^{(2)}$ ,  $\omega_{\mathcal{N}}^{(b1)}$ ,  $\omega_{\mathcal{N}}^{(b2)}$ ,  $\omega_{\mathcal{N}}^{(w)}$  and  $\omega_{\mathcal{N}}^{(am)}$  predictions with our exact combinatorial results. This is performed for two nuclei, namely  $^{96}\text{Mo}$  and  $^{208}\text{Pb}$ , so that the mass dependence can be studied as well.

#### 4.1.1. The role of the correction terms

The results for the neutron configuration  $\mathcal{N} = (0, 0, 6, 6)$  in  $^{96}\text{Mo}$  are shown in Fig. 2. In Figs. 2a and 2b the plotted ratios are  $\omega_{\mathcal{N}}^{(b1)}/\omega_{\mathcal{N}}^{(\text{ex})}$ ,  $\omega_{\mathcal{N}}^{(b2)}/\omega_{\mathcal{N}}^{(\text{ex})}$  and  $\omega_{\mathcal{N}}^{(w)}/\omega_{\mathcal{N}}^{(\text{ex})}$ , for excitation energies lower than  $150g_0^{-1}$  MeV and between  $150g_0^{-1}$  and  $500g_0^{-1}$  MeV, respectively. In Fig. 2c the corrections terms have been added, so that the plotted ratios are  $\omega_{\mathcal{N}}^{(1)}/\omega_{\mathcal{N}}^{(\text{ex})}$ ,  $\omega_{\mathcal{N}}^{(2)}/\omega_{\mathcal{N}}^{(\text{ex})}$  and  $\omega_{\mathcal{N}}^{(am)}/\omega_{\mathcal{N}}^{(\text{ex})}$ .

Near the Pauli energy of this configuration (i.e.  $A = 36g_0^{-1}$  MeV), the ratios  $\omega_{\mathcal{N}}^{(i)}/\omega_{\mathcal{N}}^{(\text{ex})}$  ( $i = b1, b2$  or  $w$ ) are identical and overestimate the exact value by a large amount [see Fig. 2a]. With increasing excitation energy  $U$  up to about  $140g_0^{-1}$  these ratios decrease and get close to unity. Beyond  $U \approx 140g_0^{-1}$  [see Fig. 2b], the three ratios display a distinct behaviour. First, as expected,  $\omega_{\mathcal{N}}^{(w)}/\omega_{\mathcal{N}}^{(\text{ex})}$  (dashed-dotted curve) increases sharply, while the two other ratios remain close to unity. This different behaviour illustrates the crucial influence of the finite depth of the single particle potential. Second, we observe that the ratio  $\omega_{\mathcal{N}}^{(b1)}/\omega_{\mathcal{N}}^{(\text{ex})}$  (dashed line) increases slowly with  $U$  while  $\omega_{\mathcal{N}}^{(b2)}/\omega_{\mathcal{N}}^{(\text{ex})}$  (dotted line) decreases and gets practically equal to unity. Similar patterns are observed for the curves in Fig. 2c only for  $U \geq 140g_0^{-1}$ . Below this energy, the ratios are very close to unity, which illustrates the key role played by the corrections terms in Eq. (26). Near the Pauli energy of this configuration, we observe a small departure from unity for all the ratios. This feature results from the fact that the ana-

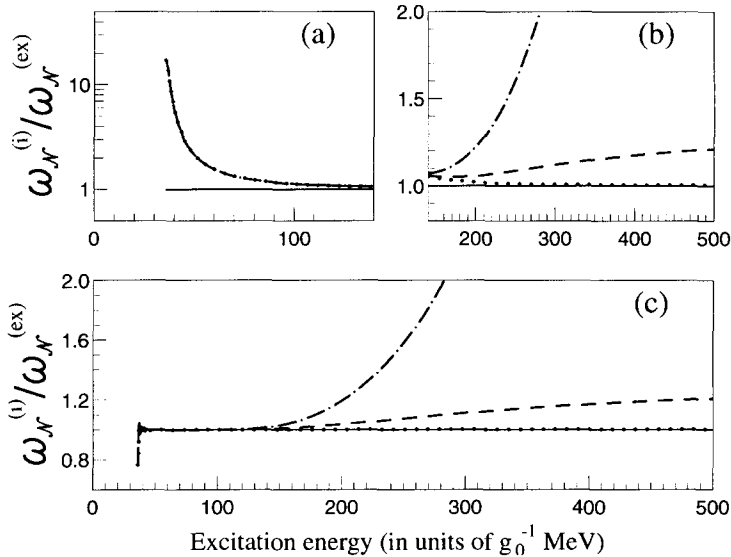


Fig. 2. Comparison between exact calculations and analytical formulae predictions for the neutron configuration  $\mathcal{N} = (0, 0, 6, 6)$  in  $^{96}\text{Mo}$ : (a), (b), (c) The solid curves represent unity, (a), (b) the dot-dashed curve gives the ratios  $\omega_{\mathcal{N}}^{(w)}/\omega_{\mathcal{N}}^{(\text{ex})}$ , the dotted curve gives  $\omega_{\mathcal{N}}^{(b2)}/\omega_{\mathcal{N}}^{(\text{ex})}$  and the dashed curve gives  $\omega_{\mathcal{N}}^{(b1)}/\omega_{\mathcal{N}}^{(\text{ex})}$  (no correction terms), (c) the dot-dashed curve gives  $\omega_{\mathcal{N}}^{(am)}/\omega_{\mathcal{N}}^{(\text{ex})}$ , the dotted curve gives  $\omega_{\mathcal{N}}^{(2)}/\omega_{\mathcal{N}}^{(\text{ex})}$  and the dashed curve gives  $\omega_{\mathcal{N}}^{(1)}/\omega_{\mathcal{N}}^{(\text{ex})}$  (correction terms included).

lytical formulae (continuous functions) only represent the exact state density (discrete function) on average. In sum, the improvement obtained by including the correction terms and by using  $\mathcal{H}_2$  instead of  $\mathcal{H}_1$  is evident.

From this comparison between various ratios with and without correction terms, we observe that  $\omega_{\mathcal{N}}^{(2)}$  is the best approximation of  $\omega_{\mathcal{N}}^{(\text{ex})}$ , and that the Williams formula (corrected or not) is the worst approximation at high excitation energy. The same statement applies to all other possible configurations and all other nuclei. Therefore  $\omega_{\mathcal{N}}^{(w)}$ ,  $\omega_{\mathcal{N}}^{(am)}$ , and all the analytical formulae derived from  $\mathcal{H}_1$  (see Section 3.1.1) are no longer considered in the rest of our discussion.

An example of a state density for the more complex proton–neutron configuration  $\mathcal{N} = (8, 8, 8, 8)$  in  $^{96}\text{Mo}$  is shown in Fig. 3.

Figs. 3a and 3b display the ratio  $\omega_{\mathcal{N}}^{(b2)}/\omega_{\mathcal{N}}^{(\text{ex})}$ , for excitation energies lower than  $300g_0^{-1}$  MeV and between  $300g_0^{-1}$  and  $500g_0^{-1}$  MeV, respectively, and Fig. 3(c) displays  $\omega_{\mathcal{N}}^{(2)}/\omega_{\mathcal{N}}^{(\text{ex})}$ . These ratios have a behaviour similar to those shown in Fig. 2. However,  $\omega_{\mathcal{N}}^{(b2)}/\omega_{\mathcal{N}}^{(\text{ex})}$  deviates more from unity at both the Pauli energy and at high energies than it does in Figs. 2a and 2b. As for the ratio  $\omega_{\mathcal{N}}^{(2)}/\omega_{\mathcal{N}}^{(\text{ex})}$ , we see again that the correction terms to the state density have a large effect near the Pauli energy of this configuration (i.e.  $A = 128g_0^{-1}$  MeV). Furthermore, we observe that these terms now give a significant improvement over the  $\omega_{\mathcal{N}}^{(b2)}$  predictions at high energies, which was not yet evident in Fig. 2c. The same configuration  $\mathcal{N} = (8, 8, 8, 8)$  has also been considered for  $^{208}\text{Pb}$  (see Fig. 4).

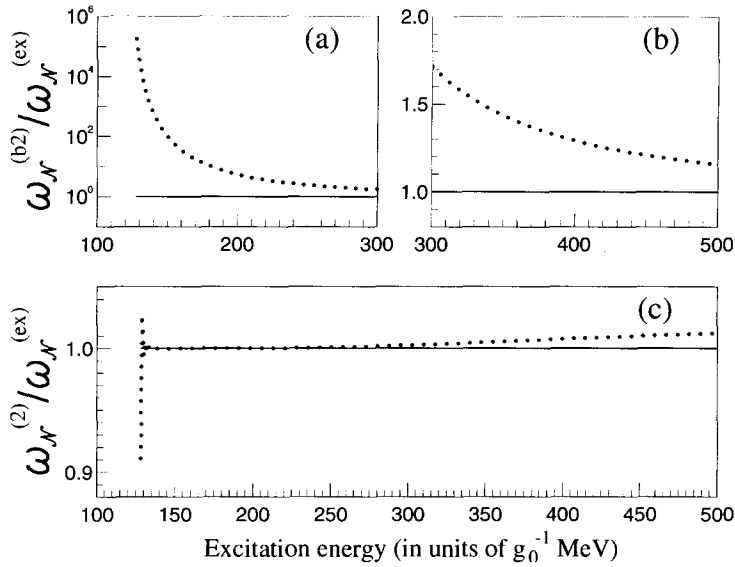


Fig. 3. Comparison between exact calculations and analytical formulae predictions for the proton-neutron configuration  $\mathcal{N} = (8, 8, 8, 8)$  in  $^{96}\text{Mo}$ . (a),(b),(c) The solid curves represent unity, (a),(b) the dotted curves the ratio  $\omega_{\mathcal{N}}^{(b2)}/\omega_{\mathcal{N}}^{(\text{ex})}$  (no correction terms), (c)  $\omega_{\mathcal{N}}^{(2)}/\omega_{\mathcal{N}}^{(\text{ex})}$  (correction terms included).

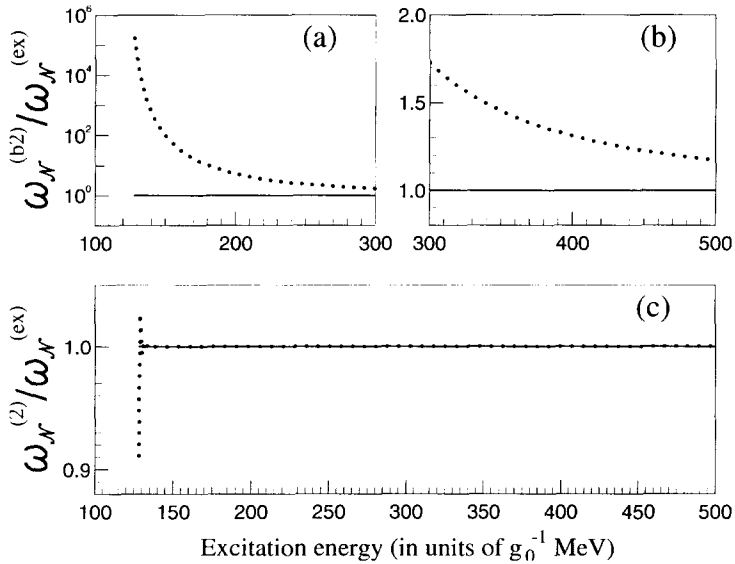


Fig. 4. Comparison between exact calculations and analytical formulae predictions for the proton-neutron configuration  $\mathcal{N} = (8, 8, 8, 8)$  in  $^{208}\text{Pb}$ . The curves have the same meaning as in Fig. 3.

A comparison between Figs. 3a and 3b, and Figs. 4a and 4b shows that the ratios are nearly identical. The only sizeable differences occur for the  $\omega_{\mathcal{N}}^{(2)}/\omega_{\mathcal{N}}^{(\text{ex})}$  ratio [Fig. 4c]. While this ratio deviates by 1% from unity at high energy for  $^{96}\text{Mo}$ , it is nearly equal

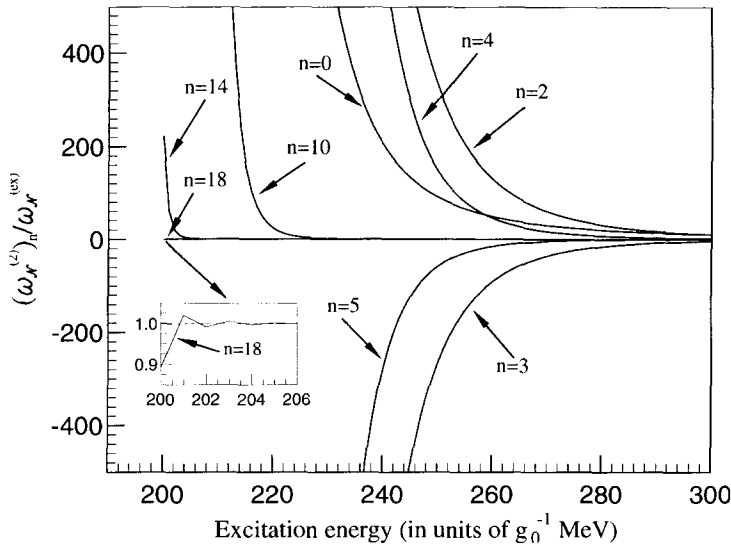


Fig. 5. Comparison between exact calculations and the truncated state density  $(\omega_{\mathcal{N}}^{(2)})_n$  predictions for various values of  $n$  in the case of the proton–neutron configuration  $\mathcal{N} = (10, 10, 10, 10)$  in  $^{208}\text{Pb}$ .

to unity for  $^{208}\text{Pb}$  over the same excitation energy range. The ratio  $\omega_{\mathcal{N}}^{(2)}/\omega_{\mathcal{N}}^{(\text{ex})}$  begins to depart from unity for  $U > 500g_0^{-1}$  [not shown in Fig. 4c]. This difference in deviation is related to the increase of potential well depths with increasing mass.

In practice, the sum  $g_{\pi} + g_{\nu}$  of the single particle–single hole state density is usually taken equal to  $A/13$ . Since we have assumed  $g_0 = g_{\pi} = g_{\nu}$ , our  $g_0$  value is equal to  $A/26$ . Therefore,  $g_0 \approx 3.5$  for  $^{96}\text{Mo}$  and  $g_0 \approx 8.0$  for  $^{208}\text{Pb}$ . Translating our results to practical cases, we conclude that the inclusion of all correction terms may influence nuclear reaction calculations already in the tens of MeV excitation energy range.

#### 4.1.2. Truncated corrections

We now investigate the effect of truncating the sum over the correction terms in Eq. (26), and discuss its impact on the predictions. For convenience, we define the truncated state density  $(\omega_{\mathcal{N}}^{(2)})_n$  by

$$\left(\omega_{\mathcal{N}}^{(2)}\right)_n(U) = G \sum_{i=0}^{N_1} \sum_{j=0}^{N_2} \sum_{k=0}^{N_3} \sum_{l=0}^{N_4} K_{ijkl} \Theta(U_{ijkl} - B) \left[ \sum_{m=0}^n E_{2m}^{\mathcal{N}} \frac{U_{ijkl}^{(M-2m-1)}}{(M-2m-1)!} \right], \quad (27)$$

with  $n < E \left[ \frac{M-1}{2} \right]$ .

In Fig. 5 the ratios  $(\omega_{\mathcal{N}}^{(2)})_n/\omega_{\mathcal{N}}^{(\text{ex})}$  are plotted for various orders of the correction (namely  $n = 0, 2, 3, 4, 5, 10, 14$  and  $18$  for the proton–neutron configuration  $\mathcal{N} = (10, 10, 10, 10)$  in  $^{208}\text{Pb}$ ). We see that all the ratios get close to unity when  $U$  increases. With increasing  $n$  values, we also observe that  $(\omega_{\mathcal{N}}^{(2)})_n/\omega_{\mathcal{N}}^{(\text{ex})}$  reaches unity alternatively from below or from above, depending upon whether  $n$  is odd or even, respectively. Furthermore, we notice that the truncated state density can take negative

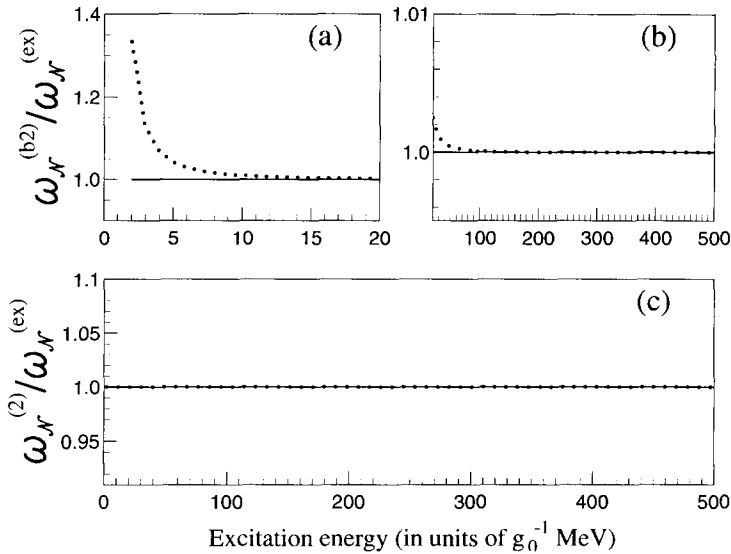


Fig. 6. Comparison between exact calculations and analytical formulae predictions for the proton-neutron configuration  $\mathcal{N} = (1, 1, 1, 1)$  in  $^{208}\text{Pb}$ . The curves have the same meaning as in Fig. 3.

values for  $n = 3$  and  $n = 5$ . To avoid such a pathology, it is therefore mandatory to impose an even  $n$  value when using Eq. (27). Moreover, it is interesting to observe that  $(\omega_{\mathcal{N}}^{(2)})_0$  may be a better approximation at low excitation energy than  $(\omega_{\mathcal{N}}^{(2)})_2$  and  $(\omega_{\mathcal{N}}^{(2)})_4$ . As a result, it is clear that for any  $\mathcal{N}$ -configuration all the correction terms must be kept in the low excitation energy range. This holds true especially near the Pauli energies.

#### 4.2. Configurations relevant to nuclear reaction models

So far, we have investigated the effect of the correction coefficients for configurations with a large number of particles and holes. While these configurations are important for the construction of total state densities as a sum over particle-hole state densities, in practice, pre-equilibrium calculations rely on state densities with few particles and holes. Therefore, we discuss the effect of our approach on even configurations (for multi-step direct reactions [10]) and odd configurations (for multi-step compound reactions [11], the exciton model [12] and the hybrid model [13]).

##### 4.2.1. Even configurations

For multistep direct calculations, where a leading-particle is followed independently of the excited nucleus, one deals with particle-hole configurations of the type  $(1, 1, 0, 0)$ ,  $(2, 2, 0, 0)$  or  $(1, 1, 1, 1)$  (i.e. configurations having the same number of particles and holes) with no limit imposed on the number of particle levels involved. For  $\mathcal{N} = (1, 1, 0, 0)$ , no correction terms are needed [see Eq. (26)], and the agreement between  $\omega_{\mathcal{N}}^{(b2)}$  predictions and our exact combinatorial results is perfect. Hence, correction terms do not apply to the multi-step direct formula of Feshbach, Kerman and Koonin [14],

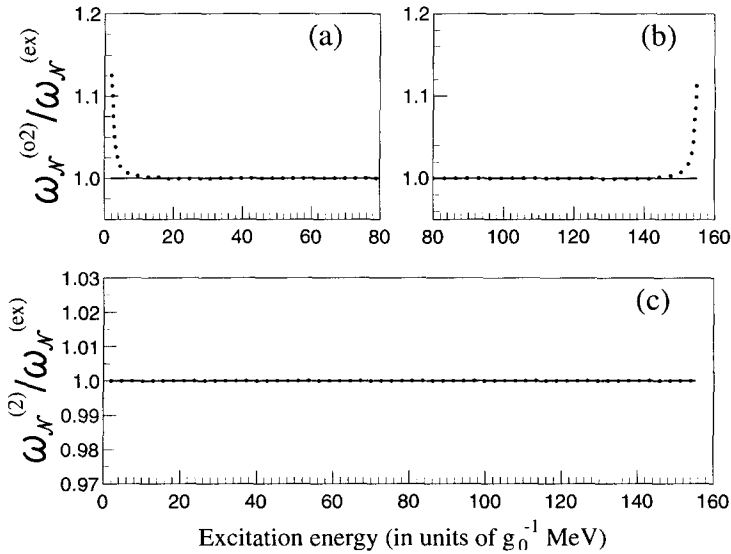


Fig. 7. Comparison between exact calculations and analytical formulae predictions for the proton-neutron configuration  $\mathcal{N} = (1, 0, 1, 1)$  in  $^{208}\text{Pb}$ . (a), (b), (c) The solid curves represent unity, (a), (b) the dotted curves the ratio  $\omega_{\mathcal{N}}^{(o2)}/\omega_{\mathcal{N}}^{(ex)}$  (no correction terms), (c)  $\omega_{\mathcal{N}}^{(2)}/\omega_{\mathcal{N}}^{(ex)}$  (correction terms included).

which contains a convolution of one particle-one hole state densities. When one has more than two particles and holes, which appear in more sophisticated multi-step direct theories, such as that of Nishioka, Weidenmüller and Yoshida [15], the correction terms are needed if one uses an ESM. As an example, we show in Figs. 6a and 6b the ratio  $\omega_{\mathcal{N}}^{(b2)}/\omega_{\mathcal{N}}^{(ex)}$  for the proton-neutron configuration  $\mathcal{N} = (1, 1, 1, 1)$  for  $^{208}\text{Pb}$ . In Fig. 6c the ratio  $\omega_{\mathcal{N}}^{(2)}/\omega_{\mathcal{N}}^{(ex)}$  is also plotted. We see that the correction terms do not have a very large effect but nevertheless improve the predictions at low excitation energy. The same effects are obtained for  $\mathcal{N} = (2, 2, 0, 0)$  (not shown).

#### 4.2.2. Odd configurations

In the other pre-equilibrium models, namely the multi-step compound model (the complement of the multi-step direct model) and semi-classical exciton and hybrid models, the propagation of the projectile + target is treated as a composite system, without distinction of a leading particle. Therefore, the configurations involved usually have a different number of particles and holes (i.e.  $\mathcal{N} = (1, 0, 1, 1)$ ,  $\mathcal{N} = (3, 2, 0, 0)$  ...). Furthermore, in the case of multi-step compound reactions, one has to deal with a restricted number of particle levels since only bound particles are considered. The standard analytical formula corresponding to such a situation is given by Obložinský [5]. In Figs. 7, 8 and 9 we show the ratios  $\omega_{\mathcal{N}}^{(o2)}/\omega_{\mathcal{N}}^{(ex)}$  and  $\omega_{\mathcal{N}}^{(2)}/\omega_{\mathcal{N}}^{(ex)}$  for the proton-neutron configurations  $\mathcal{N} = (1, 0, 1, 1)$ ,  $\mathcal{N} = (3, 2, 0, 0)$  and  $\mathcal{N} = (3, 2, 1, 1)$  for  $^{208}\text{Pb}$ . We observe that the correction terms have a significant effect near the Pauli energy and for energies close to the maximum energy (i.e., above which the state density vanishes). This effect becomes larger when the number of excited particle-holes increases.



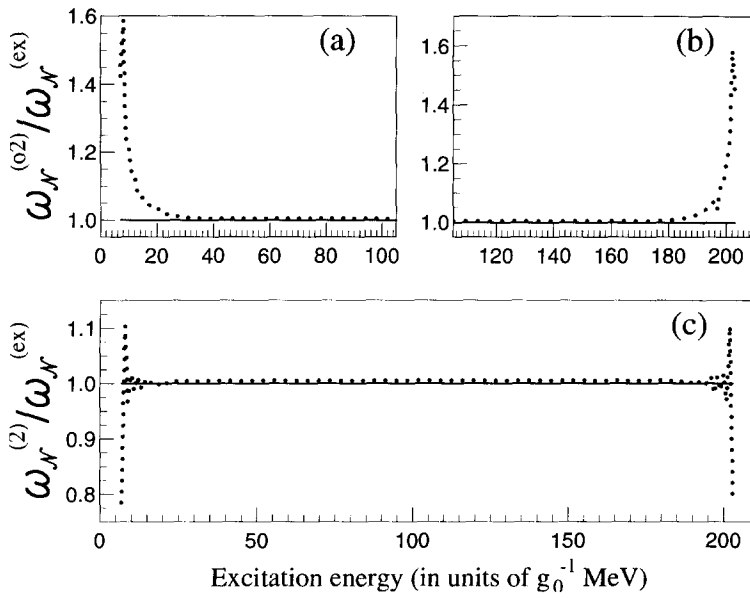


Fig. 8. Comparison between exact calculations and analytical formulae predictions for the proton configuration  $\mathcal{N} = (3, 2, 0, 0)$  in  $^{208}\text{Pb}$ . The curves have the same meaning as in Fig. 7.

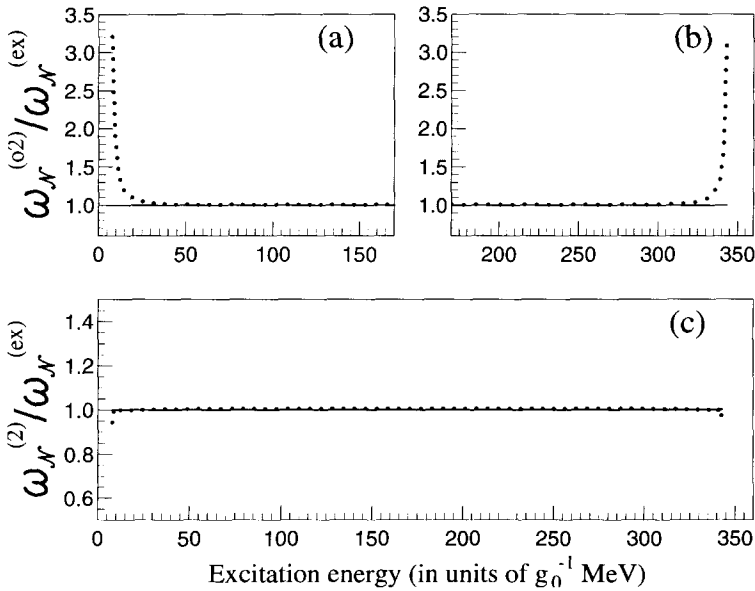


Fig. 9. Comparison between exact calculations and analytical formulae predictions for the proton-neutron configuration  $\mathcal{N} = (3, 2, 1, 1)$  in  $^{208}\text{Pb}$ . The curves have the same meaning as in Fig. 7.

## 5. Conclusions

We have presented a new combinatorial method to compute exact particle–hole state densities within the General Independent Particle Model. This method, which employs an improved, accurate numerical formalism, has been applied to the Equidistant Spacing Model yielding exact state densities for any particle–hole configuration. On the same mathematical basis, we have established a new analytical particle–hole state density formula in the ESM framework, which we present here again, now separated from the mathematical derivation. Our general particle–hole state density for the configuration  $\mathcal{N}$  including  $N_1$  proton particles,  $N_2$  proton holes,  $N_3$  neutron particles and  $N_4$  neutron holes at an excitation energy  $U$  reads

$$\omega_{\mathcal{N}}(U) = \frac{g_1^{N_1} g_2^{N_2} g_3^{N_3} g_4^{N_4}}{N_1! N_2! N_3! N_4!} \sum_{i=0}^{N_1} \sum_{j=0}^{N_2} \sum_{k=0}^{N_3} \sum_{l=0}^{N_4} (-1)^{i+j+k+l} \binom{N_1}{i} \binom{N_2}{j} \binom{N_3}{k} \binom{N_4}{l} \\ \times \Theta(U_{ijkl} - B) \left[ \sum_{m=0}^{E[\frac{M-1}{2}]} E_{2m}^{\mathcal{N}} \frac{U_{ijkl}^{(M-2m-1)}}{(M-2m-1)!} \right], \quad (28)$$

where

$$U_{ijkl} = U - \frac{N_1^2 + N_1}{4g_1} - \frac{N_2^2 - 3N_2}{4g_2} - \frac{N_3^2 + N_3}{4g_3} - \frac{N_4^2 - 3N_4}{4g_4} \\ - i \frac{J_1}{g_1} - j \frac{J_2}{g_2} - k \frac{J_3}{g_3} - l \frac{J_4}{g_4},$$

and

$$B = \frac{N_1^2 + N_1}{4g_1} + \frac{N_2^2 + N_2}{4g_2} + \frac{N_3^2 + N_3}{4g_3} + \frac{N_4^2 + N_4}{4g_4}.$$

The formula that gives the closest approximation to the exact results,  $\omega_{\mathcal{N}}^{(2)}$ , is obtained with

$$J_k = I_k - \frac{1}{2}(N_k - 1) \quad (\text{Approximation } \mathcal{H}_2),$$

whereas the alternative approximation, giving  $\omega_{\mathcal{N}}^{(1)}$ , is obtained with

$$J_k = I_k \quad (\text{Approximation } \mathcal{H}_1).$$

Here,  $I_2 = Z$ ,  $I_4 = N$ , and  $I_1, I_3$  are either infinite (unbound configurations) or the labels of the last bound single-particle states in the level scheme of proton and neutron particles, respectively. Furthermore,  $E[\frac{M-1}{2}]$  is the integer part of  $\frac{M-1}{2}$  (where  $M = N_1 + N_2 + N_3 + N_4$ ),  $\Theta$  the unit step function, and the correction term  $E_{2m}^{\mathcal{N}}$  is given by

$$E_{2m}^{\mathcal{N}} = \sum_{i=0}^m D_{2m-2i}(N_1, N_2) D_{2i}(N_3, N_4) \quad (E_0^{\mathcal{N}} = 1),$$

with

$$D_{2k}(N_i, N_j) = \sum_{l=0}^k \frac{C_{2k-2l}(N_i) C_{2l}(N_j)}{g_i^{2k-2l} g_j^{2l}}.$$

The calculation of the  $C_{2k}(N)$ -coefficients is outlined in Appendices B and C.

From this formula, all older analytical formulae can be derived using various simplifications (see Fig. 1). The only mathematical approximation throughout the whole derivation has been performed in the factor  $U_k(\beta)$  of Eq. (14). Further improvement of our analytical formula, within the ESM, can only be obtained with a less restrictive approximation than Eq. (18), a mathematical task we have not further pursued. Such a further generalization is practically not important anyway, since the agreement between  $\omega_N^{(2)}$  and exact calculations is impressive for any particle–hole configuration and excitation energy.

The ESM is arguably the simplest single-particle model, and the only model that easily leads to analytical formulae. Therefore, it is used extensively in pre-equilibrium reaction models, which justifies our desire to generalize the analytical approach as far as possible. We realize, however, that the physical basis of the ESM is limited. Since our general combinatorial method can be applied to any level scheme, we are presently performing exact partial and total level density calculations using single-particle levels derived with the Hartree–Fock and Hartree–Fock–Bogoliubov method and a reliable effective nucleon–nucleon interaction. Parity and angular momentum conservation are then automatically taken into account.

## Acknowledgements

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## Appendix A. Numerical method

The computation of Eq. (6) involves products and sums of polynomials. To handle such an expression, it is convenient to represent any polynomial function

$$P(y) = \sum_k p_k y^k$$

by a vector

$$\mathcal{V}_P = [V_P(1), V_P(2), \dots, V_P(n)]$$

defined by

$$V_P(i) = p_i.$$

The product of two polynomials  $P$  and  $Q$ , with

$$P(y) = \sum_k p_k y^k$$

and

$$Q(y) = \sum_k q_k y^k$$

is thus represented by the vector  $\mathcal{V}_{PQ} = \mathcal{V}_P \times \mathcal{V}_Q$  that reads

$$V_{PQ}(l) = \sum_{i+j=l} p_i q_j, \quad (\text{A.1})$$

or

$$V_{PQ}(l) = \sum_{i+j=l} V_P(i) V_Q(j).$$

A vector for the sum  $P + Q$  is represented by  $\mathcal{V}_{P+Q} = \mathcal{V}_P + \mathcal{V}_Q$  defined by

$$V_{P+Q}(l) = V_P(l) + V_Q(l).$$

With such conventions the products and sums of polynomials are easy to compute numerically.

## Appendix B. Expansion of $\prod_{i=1}^N \frac{1}{1 - \exp(-i\beta)}$

We need to develop the product

$$\frac{1}{(e^{-\beta})_N} = \prod_{i=1}^N \frac{1}{1 - e^{-i\beta}}. \quad (\text{B.1})$$

With the relation

$$1 - e^{-i\beta} = 2e^{-i\beta/2} \sinh(i\beta/2),$$

and the development of  $\sinh(x)$  [9] as an infinite product,

$$\sinh(x) = x \prod_{i=1}^{+\infty} \left( 1 + \frac{x^2}{\pi^2 i^2} \right),$$

we obtain

$$1 - e^{-i\beta} = i\beta e^{-i\beta/2} \prod_{m=1}^{+\infty} \left[ 1 + \frac{(i\beta)^2}{4\pi^2 m^2} \right]. \quad (\text{B.2})$$

Combining (B.1) and (B.2) yields

$$\frac{1}{(e^{-\beta})_N} = \frac{e^{\beta \frac{N(N+1)}{4}}}{N! \beta^N} \left[ \frac{1}{\prod_{i=1}^N \prod_{m=1}^{+\infty} \left( 1 + \frac{(i\beta)^2}{4\pi^2 m^2} \right)} \right].$$

Setting

$$A(N) = \left[ \prod_{i=1}^N \prod_{m=1}^{+\infty} \left( 1 + \frac{(i\beta)^2}{4\pi^2 m^2} \right) \right]^{-1}, \quad (\text{B.3})$$

and using the Taylor series expansion of  $\ln(1+x)$  yields

$$\ln A(N) = \sum_{i=1}^N \sum_{m=1}^{+\infty} \sum_{k=1}^{+\infty} \frac{(-1)^k}{k} \left( \frac{i\beta}{2\pi m} \right)^{2k}.$$

Then we obtain

$$A(N) = \exp \left[ \sum_{k=1}^{+\infty} \beta^{2k} B_{2k} S_{2k}(N) \right], \quad (\text{B.4})$$

with

$$B_{2k} = \frac{(-1)^k}{k 4^k \pi^{2k}} \sum_{m=1}^{+\infty} \frac{1}{m^{2k}},$$

and

$$S_{2k}(N) = \sum_{i=1}^N i^{2k}.$$

We then use the Taylor series expansion of  $\exp(x)$  to write

$$A(N) = \sum_{n=0}^{+\infty} \frac{\left[ \sum_{k=1}^{+\infty} \beta^{2k} B_{2k} S_{2k}(N) \right]^n}{n!}. \quad (\text{B.5})$$

Since the multinomial expansion of an infinite sum reads [8]

$$\left( \sum_{k=1}^{+\infty} \frac{x_k}{k} t^k \right)^m = m! \sum_{n=m}^{+\infty} t^n \sum_{\{a(n)\}} \prod_{i=1}^n \frac{1}{a_i!} \left( \frac{x_i}{i} \right)^{a_i}, \quad (\text{B.6})$$

where  $\sum_{\{a(n)\}}$  means summing over all the integer combinations  $(a_1, a_2, \dots, a_n)$  that obey

$$a_1 + 2a_2 + \dots + na_n = n,$$

and

$$a_1 + a_2 + \dots + a_n = m,$$

we can finally expand Eq. (B.5) as

$$A(N) = 1 + \sum_{k=1}^{+\infty} C_{2k}(N) \beta^{2k},$$

with

$$C_{2k}(N) = \sum_{\{\alpha(k)\}} \prod_{i=1}^k \frac{[B_{2i} S_{2i}(N)]^{\alpha_i}}{\alpha_i!}.$$

Here, the symbol  $\sum_{\{\alpha(k)\}}$  denotes the summation over all the combinations  $(\alpha_1, \dots, \alpha_k)$  that obey

$$\alpha_1 + 2\alpha_2 + \dots + k\alpha_k = k.$$

All the formulae derived in this appendix are valid for  $k \neq 0$  and  $N \neq 0$ . In the cases that require the coefficients  $C_0(N)$  or  $C_{2k}(0)$ , we must consider particular values to get the correct results. As shown in Appendix C, we must impose

$$C_0(N) = 1 \quad \text{for } N \geq 0,$$

and

$$C_{2k}(0) = 0 \quad \text{for } k > 0.$$

### Appendix C. Calculation of the correction coefficients

The correction coefficients  $E_{2m}^{\mathcal{N}}$  can be calculated easily using both

$$E_{2m}^{\mathcal{N}} = \sum_{i=0}^m D_{2m-2i}(N_1, N_2) D_{2i}(N_3, N_4) \quad (E_0^{\mathcal{N}} = 1), \quad (\text{C.1})$$

and

$$D_{2k}(N_i, N_j) = \sum_{l=0}^k \frac{C_{2k-2l}(N_i) C_{2l}(N_j)}{g_i^{2k-2l} g_j^{2l}}. \quad (\text{C.2})$$

once the coefficients  $C_{2i}(N)$  have been obtained. The calculation of these  $C_{2i}(N)$  is the most complicated part and may need more explanation.

First we must compute the partitions  $(\alpha_1, \dots, \alpha_N)$  of  $N$  defined by

$$\alpha_1 + 2\alpha_2 + \dots + N\alpha_N = N.$$

As an example, in Table C.1 these partitions are shown for  $N = 5$ .

Table C.1

The seven partitions of  $N = 5$ 

Number	$\alpha_1$	$\alpha_2$	$\alpha_3$	$\alpha_4$	$\alpha_5$
1	5	0	0	0	0
2	3	1	0	0	0
3	2	0	1	0	0
4	1	2	0	0	0
5	1	0	0	1	0
6	0	1	1	0	0
7	0	0	0	0	1

Table C.2

Number  $D(N)$  of partitions of  $N$ 

$N$	1	7	13	20	27	34	41	49
$D(N)$	1	15	101	627	3010	12 310	44 583	173 525

Table C.2 shows the number of partitions  $D(N)$  for various  $N$  values. It is clear that this number increases rapidly with  $N$ . Therefore, we only compute these partitions once and store them to keep the time for successive state density calculations limited.

Once these partitions are known, we can compute the coefficients  $C_{2k}(N)$ . They are given by

$$C_{2k}(N) = \sum_{\{\alpha(k)\}} \prod_{i=1}^k \frac{[B_{2i} S_{2i}(N)]^{\alpha_i}}{\alpha_i!}. \quad (\text{C.3})$$

For our example, this yields

$$\begin{aligned} C_{10}(N) = & \frac{[B_2 S_2(N)]^5}{5!} + \frac{[B_2 S_2(N)]^3 [B_4 S_4(N)]^1}{3! 1!} + \frac{[B_2 S_2(N)]^2 [B_6 S_6(N)]^1}{2! 1!} \\ & + \frac{[B_2 S_2(N)]^1 [B_4 S_4(N)]^2}{1! 2!} + \frac{[B_2 S_2(N)]^1 [B_8 S_8(N)]^1}{1! 1!} \\ & + \frac{[B_4 S_4(N)]^1 [B_6 S_6(N)]^1}{1! 1!} + \frac{[B_{10} S_{10}(N)]^1}{1!}, \end{aligned}$$

where the shortened notations

$$S_{2k}(N) = \sum_{i=1}^N i^{2k},$$

and

$$B_{2k} = \frac{(-1)^k}{k 4^k \pi^{2k}} \sum_{m=1}^{+\infty} \frac{1}{m^{2k}},$$

have been adopted. Two particular cases may appear when one has to calculate coefficients such as  $C_0(N)$  or  $C_{2k}(0)$ . Let us consider the configuration  $\mathcal{N} = (2, 2, 0, 0)$  for

instance. In this case, we only have to compute  $E_2^{\mathcal{N}}(2, 2, 0, 0)$  [see Eq. (26)]. Using Eq. (C.1), we can write

$$E_2^{\mathcal{N}} = D_2(2, 2)D_0(0, 0) + D_0(2, 2)D_2(0, 0),$$

where the coefficients  $D_{2k}(N_i, N_j)$  are given, following Eq. (C.2), by

$$\begin{aligned} D_2(2, 2) &= \frac{C_2(2)}{g_1^2} \frac{C_0(2)}{g_2^0} + \frac{C_0(2)}{g_1^0} \frac{C_2(2)}{g_2^2}, \\ D_0(0, 0) &= \frac{C_0(0)}{g_3^0} \frac{C_0(0)}{g_4^0}, \\ D_0(2, 2) &= \frac{C_0(2)}{g_1^0} \frac{C_0(2)}{g_2^0}, \\ D_2(0, 0) &= \frac{C_2(0)}{g_1^2} \frac{C_0(0)}{g_2^0} + \frac{C_0(0)}{g_1^0} \frac{C_2(0)}{g_2^2}. \end{aligned}$$

For such a simple configuration the coefficient  $E_2^{\mathcal{N}}$  has been given by Anzaldo-Meneses [7] and reads

$$E_2^{\mathcal{N}} = -\frac{1}{24} \left[ \frac{S_2(2)}{g_1^2} + \frac{S_2(2)}{g_2^2} \right]. \quad (\text{C.4})$$

From Eq. (C.3) we have

$$C_2(2) = -\frac{1}{24}S_2(2),$$

but the coefficients  $C_0(0)$ ,  $C_0(2)$  and  $C_2(0)$  do not follow the closed form of Eq. (C.3). To get agreement between Eq. (C.4) and our closed formulae we must impose

$$C_0(0) = 1, \quad C_0(2) = 1, \quad C_2(0) = 0.$$

Analogous arguments apply to more complicated configurations, so that we always have, as stated in Appendix B

$$\begin{aligned} C_0(N) &= 1 & \text{for } N \geq 0, \\ C_{2k}(0) &= 0 & \text{for } k > 0. \end{aligned}$$

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