Brief critical analysis of the Darwin-Fowler method

F. B. Guimaraes

Instituto de Estudos Avançados/DCTA,
12228-001 São José dos Campos, São Paulo, Brazil
e-mail: fbraga@ieav.cta.br

Abstract

We present a brief numerical study of the Darwin-Fowler method applied to the analysis of the energy partition of ensembles of bosons and fermions. We analyze the assertion of the existence of a “strong maximum” made in the original paper of Darwin and Fowler and other studies and show that although the presumed saddle point along the real axis of the grand canonical parameters may exist it cannot, in general, be characterized as “strong”, in the sense of having much larger magnitude than the other points along the path of integration.
In addition, we show that in some cases the saddle point is not even present and the various approximations of the method can be interpreted as a tricky reformulation of usual thermodynamic relations.
The close connection of the method with the formalism of the Laplace transform may produce wrong results if the internal energy of the components of the ensemble is not large enough.
Therefore, although useful in many applications the Darwin-Fowler method may not be suitable, in general, for a detailed microscopic analysis of the nuclear structure in connection with the Shell Model approach, as it is usually done in studies of the pre-equilibrium stage of nuclear reactions.

1. Introduction

The seminal paper of Darwin and Fowler[1] proposed a method for the statistical determination of how the energy is partitioned in an ensemble of a large number of microsystems, which should be used to replace the traditional approach based on the direct computation of probabilities. The statistical analysis of these ensembles showed that the “most probable arrangement” would have a much greater probability than the others and their effort intended to avoid the use of the Stirling’s approximation for factorials, which they recognized as “illegitimate” in many cases.
In nuclear physics the method of Ref. [1] is often used as an auxiliary formalism in the description of the pre-equilibrium stage of nuclear reactions (PE) and the nuclear density in connection with the Shell Model and the exciton model (EXM). [2] [3] [4] [5]

In particular, it can be used with the traditional Shell Model approach to define the moments of the Hamiltonian in terms of Laplace transforms and their inverses to obtain the nuclear density [3] and in the microscopic description of PE dynamics to obtain the transition strengths. [6]

In the formalism of Ref. [6] some problems were observed in connection with the Darwin-Fowler method, due to the statistical nature of its approximations, which may not be very precisely defined at the microscopic level and can obscure the analysis of some details of the microscopic interaction in the description of the PE process. [7]

In the Darwin-Fowler formalism the level density can be defined as the pole of the grand canonical generating function \( f(x, y) \) divided by adequate factors \( x^{A+1}y^{E+1} \), where \( x \) is a parameter associated with the total number of single particle levels (sp-levels), \( A \), and \( y \) is a parameter associated with the total energy, \( E \). The sp-levels are supposed to have well defined energies, which can be degenerate or not.

Either for bosons or fermions \( f(x, y) \) can be expanded as a sum of products of terms of the type \( (xy^{\nu}) \), where \( \nu \) is an integer. Then, \( f(x, y) \) can be interpreted, in the continuous approximation limit (CAP), as the inverse Laplace transform of a linear combination of nuclear densities for given \( A \) and \( E \), which is very useful in practical applications. [2] [3] [6]

For this description to be physically meaningful the terms of the expansion must decrease in modulus when \( y \) vary over complex circles around the origin in comparison with its value at the positive real axis, and this point of maximum should also be a minimum along the positive real axis. [1] [2] Therefore one must have a "saddle point" located on the positive real axes of \( y \).

In Ref. [1] the existence of the saddle point is then considered in connection with the method of "steepest descents." The formalism uses a qualitative analysis of the generating function of the ensemble to conclude that, for large \( E \), this point is also a "strong maximum" along the direction of the path of integration, taken to be the circle centered at the origin with radius equal to the abscissa on the positive real axis where the minimum occurs.

Reference [1] then establishes that, if the integrand has a saddle point with these characteristics, this would be sufficient to obtain approximate equations of state in the usual form for a system of bosons, fermions, etc., for given \( A \) and \( E \).

In this paper, we briefly analyze the assertion of the existence of this "strong maximum" for bosons and fermions and show that although the saddle point may exist the maximum cannot be
characterized in general as “strong”, in the sense of having much larger magnitude than the other points along the path of integration.

In Sec.2 we review some basic definitions of the Darwin-Fowler statistics, the Shell Model formalism and the definition of the level density to better explain the details of the arguments presented in this Introduction.

In Sec.3 we present the simplest cases of partition functions that can be considered as physically meaningful, following closely the development of Ref.[1], and show that the “strong maximum” hypothesis does not necessarily holds for these functions. Similar results are obtained in Sec.4 for more realistic functions of ensembles with fixed number of “particles” and non degenerate levels, in the fundamental state or for non null excitation. The influence of the statistical parameter associated with the chemical potential is also analyzed.

At last, we present in Sec.5 a quick review of the use of the Laplace transform in connection with the Darwin-Fowler method, an explanation of why the approximated equations obtained with the method are correct for various applications and the general conclusion.

2. The level density of a system of bosons or fermions

The analysis of Ref.[1] is focused on a set of “Planck vibrators” (PV), obeying the Bose-Einstein statistics, with a given energy distribution, i.e., $a_r$ vibrators with energy $\epsilon r$, for fixed energy unit $\epsilon$ and variable integer $r$, and the statistical ensemble is defined by the constants for the total energy, $E$, and the total number of vibrators, $M$, satisfying

$$\sum_{(r)} a_r = M, \quad \text{and} \quad \sum_{(r)} r a_r = E.$$  \hspace{1cm} (2.1)

Due to the indistinguishability of the PV with the same energy, the number of different sets satisfying the first equation in (2.1) is given by

$$\frac{M!}{a_0!a_1!a_2!...} \hspace{1cm} (2.2)$$

and the second equation constrains the possible sets $\{a_0, a_1, a_2...\}$ so that their total number could be symbolically written as

$$C = \sum_{M,E=\text{fixed}} \frac{M!}{a_0!a_1!a_2!...}, \hspace{1cm} (2.3)$$
which Ref.[1] calls the total number of “complexions” representing the ensemble, for given $M$ and $E$. Now, if one considers the following series

$$(1 + x^{\epsilon} + x^{2\epsilon} + \cdots)^M = (1 - x^{\epsilon})^{-M}$$

(2.4)

in which $M$ is supposed to be a finite number, possibly very large, then the multinomial expansion gives

$$\sum_{(a_0+a_1+a_2+\ldots=M)} \frac{M!}{a_0!a_1!a_2!\ldots} 1^{a_0}(x^{\epsilon})^{a_1}(x^{2\epsilon})^{a_2}\ldots = \sum_{(a_0+a_1+a_2+\ldots=M)} \frac{M!}{a_0!a_1!a_2!\ldots} x^{\sum_{(r)}rea_r}$$

(2.5)

and, therefore, the first equation of (2.1) is always satisfied. Then, Eq. (2.4) corresponds to the statistical description of an ensemble with fixed number of PV and variable energy, given by $\sum_{(r)}rea_r$, and $C$ can also be written as the sum of the coefficients of the expansion (2.5) in which the exponent of $x$ satisfies the energy equation in (2.1).

Notice that $x$ is an arbitrary algebraic parameter with no specific physical meaning so far and one may also eventually let $M$ vary, to obtain the usual grand canonical description with variable number of microsystems and variable energy.

Then, equation (2.3) can be rewritten using Cauchy’s theorem applied over function (2.4) along a path around the origin of the $x$-complex plane with $|x|<1$,

$$C = \frac{1}{2\pi i} \int_{|x|<1} \frac{dx}{x^{E+1}(1 - x^{\epsilon})^M} ,$$

(2.6)

and one may interpret $C$ as the total degeneracy of the PV with energy $E$.

To obtain an approximate solution of (2.6) Ref.[1] makes use of the steepest descents method and consider that for $x$ along the positive axis, the integrand becomes infinite at $x=0$ and $x=1$, therefore it has at least one minimum in the interval, $|x|\in(0,1)$ with $\text{arg}(x)=0$. A direct computation shows that this minimum is in fact unique and situated at a point $\xi \in \mathbb{R}$, $0 < \xi < 1$, and the integration path (contour) can be taken as the circumference centered at the origin with radius $\xi$. Then, Ref.[1] states that “for values of $x$ on the contour, $x=\xi$ corresponds to a strong maximum” for which the “whole value of the integral is contributed by the contour in the neighborhood of this point”.

This important statement is one of the essential aspects of the entire method, but it is presented as self-evident and without further proof.
The bosonic formalism outlined above is analogous to the usual statistical description of the nucleus (many fermions system) inspired by the Shell Model, in which the nuclear grand canonical ensemble, for all energies \((E)\) and mass numbers \((A)\), can be defined by the following relations\(^{[2]}\)

\[
A = \sum_{(i)} n_i ,
\]

(2.7)

where \(n_i \in \{0,1\}\), are all possible occupation numbers of the single particle (sp) states associated with the corresponding set of sp-levels with energies

\[
\epsilon_i = \nu_i \epsilon .
\]

(2.8)

and total nuclear energy given by

\[
E = N \epsilon = \sum_{(i)} n_i \nu_i \epsilon .
\]

(2.9)

Here \(\nu_i\) are integers and \(\epsilon\) is usually considered as an arbitrarily fixed real number, defining the approximate “equidistant spacing” between any two consecutive sp-levels or an “average spacing” of more realistic bases for the sp-states as, e. g., the H.O. basis, etc.

In this context, the nuclear level density at the energy \(E\), \(\rho(E)\), can be defined as the ratio between the nuclear degeneracy and the sp-level spacing \(\epsilon\), using a formal description based on the Darwin-Fowler method.\(^{[2, 1]}\) In this description, the generating function of the grand canonical ensemble is given by the following expression

\[
f(x, y) = \prod_{i} (1 + xy^{\nu_i}) = \prod_{i} (1 + x_i) ,
\]

(2.10)

where \(x\) and \(y\) are independent parameters associated with \(A\) and \(E\), respectively, and the last simpler form takes into account the fact that \(x\) is the same for all sp-states.\(^{[7]}\)

In the grand canonical ensemble, describing a statistical set of many-body systems with variable number of microsystems and variable energy, the parameter \(x\) has a more strictly combinatorial meaning while \(y\) is related with the probability distribution associated with the various component systems of the ensemble.

Then, the nuclear level density can be directly defined as an adequate pole of the generating function divided by \(\epsilon\),\(^{[2]}\)

\[
\rho(A, E) = \frac{1}{(2\pi i)^2 \epsilon} \oint \oint \frac{f(x, y) dx dy}{x^{A+1} y^{N+1}} ,
\]

(2.11)
therefore, a first drawback in the formalism of [1] when applied to nuclear systems, although a not necessarily an important one, is that expressions like (2.11) for the nuclear density can only be considered as an exact definition if $x$ and $y$ are continuous variables, which is equivalent to assume the continuous approximation limit (CAP).[7]

The generating function in (2.10) can be rewritten as

$$f(x, y) = 1 + x \sum_{(j)} y^{\nu_j} + x^2 \sum_{(j_1, j_2)} y^{(\nu_{j_1} + \nu_{j_2})} + \cdots + x^A \sum_{(j_1, \cdots, j_A)} y^{(\nu_{j_1} + \cdots + \nu_{j_A})} + \cdots, \quad (2.12)$$

which, therefore, describes all nuclear systems with all possible “mass numbers” and energies (nuclear temperature). In other words, for a given nuclear system each configuration of sp-states is also a microstate of the canonical ensemble with fixed mass number and temperature,[8] and the term proportional to $x^A$ is the sum over all possible configurations with fixed nuclear mass $A$ and variable energy.

For each nuclear level, $E_k$, corresponds usually many different configurations of sp-states and to each nuclear mass $A$ a term, $\mathcal{Y}_A$, is defined in Eq. (2.12) as follows,

$$\mathcal{Y}_A = \sum_{(j_1, \cdots, j_A)} y^{(\nu_{j_1} + \cdots + \nu_{j_A})}, \quad (2.13)$$

which can be rewritten in terms of the degeneracies for the various nuclear levels, $D_k$, as

$$\mathcal{Y}_A = \sum_{(k)} D_k y^{N_k}, \quad (2.14)$$

where

$$N_k = \sum_{i=1}^A \nu_{ki} = \frac{E_k}{\epsilon}, \quad (2.15)$$

and $D_k = D_k(E_k, A)$ is the degeneracy of the nuclear level $E_k$, for a given nuclear mass number $A$.

Taking Eq. (2.14) into Eq. (2.12) and using the definition (2.11) for the nuclear level density yields

$$\rho(E_k, A) = \frac{1}{\epsilon} D_k(E_k, A), \quad (2.16)$$

which is a natural result in a microscopic description.[7] Therefore, equation (2.12) can be rewritten as

$$f(x, y) = 1 + x \sum_{(k_1)} D_{k_1}(E_{k_1}, 1) y^{N_{k_1}(1)} +

x^2 \sum_{(k_2)} D_{k_2}(E_{k_2}, 2) y^{N_{k_2}(2)} + \cdots + x^A \sum_{(k)} D_k(E_k, A) y^{N_k(A)} + \cdots, \quad (2.17)$$
where different indices have been used for each term to reinforce the fact that the corresponding nuclear levels may not be the same. In these expressions the sum over \( k \) is equivalent to the sum over the nuclear energy \( E_k \) and \( f(x,y) \) can be written as a sum over nuclear energies

\[
f(x, y) = \sum_{(A,U)} D(A, U) x^A y^{U/\epsilon},
\]

and also as a sum over individual configurations, with all degeneracies equal one,

\[
f(x, y) = \sum_{(\text{conf})} x^A y^{U/\epsilon}.
\]

3. The simplest partition functions

The simplest cases of physically meaningful partition functions corresponding to the description of an ensemble of degenerate fermions or bosons can be directly calculated algebraically and show the main problems with the analysis of Refs. [1] and [2].

The essential part of the integrand of the generating function of the ensemble of identical bosons analyzed by [1] can be written as

\[
f(y) = \frac{1}{y^{E+1}(1 - y)^M},
\]

which obviously approaches infinite for real positive values of \( y \to 1 \) and \( y \to 0 \). A more general definition similar to the integrand of (2.11) would be

\[
f(x, y) = \frac{1}{x^{M+1}y^{E+1}} \prod_{i=1}^{M} \frac{1}{(1 - xy^{i})}.
\]

Equations (3.1) or (3.2) represent a set of \( M \) “Planck vibrators” (bosons) with total energy \( E \). In particular, (3.1) is closer to the expression analyzed in [1] with each vibrator possessing the same set of possible energies \( P=\{n\epsilon; n = 0, \cdots, \infty\} \), where \( n \) is an integer \( \epsilon \) is the energy of the basic vibrating mode. In a slightly more general case than (3.1) and still using only one statistical parameter, one could associate a different basic energy for each boson to obtain

\[
f(y_1, \cdots, y_M) = \frac{1}{w^{E+1}} \prod_{i=1}^{M} \frac{1}{(1 - y_i)},
\]
where $y_i = w^\epsilon_i$, $w = e^{-\beta}$ and

$$E = \sum_{l=1}^{M} r_l \epsilon_l ; \quad r_l \in \{0, 1, \cdots, \infty\}. \quad (3.4)$$

Therefore, the simpler description at (3.1) can be obtained by setting $\epsilon_i = \epsilon = \text{fixed}$, $\forall i$, and it contains the essential numerical characteristics of the more general case (3.3), allowing (3.1) to be used to analyze the general analytical behavior of (3.3).

The above simple expressions for $f(y)$ imply that it has at least one minimum in the interval $(0,1)$ which can be determined analytically

$$\frac{d}{dy} \left[ y^{-(E+1)(1-y)^{-M}} \right] = \frac{1}{y^{E+1}(1-y^{M})} \left( \frac{-(E+1)}{y} + \frac{M}{(1-y)} \right) = 0, \quad (3.5)$$

then

$$y_{\text{min}} = \frac{E + 1}{M + E + 1} \quad (3.6)$$

and the minimum is unique. Now, following Ref.[1], we need to analyze what happens when one considers the values of $f(y)$ for $y$ belonging to the circumference centered at the origin of the complex $y$-plane with radius $y_{\text{min}}$. In the qualitative analysis of [1] it is suggested that $f(y_{\text{min}})$ would correspond to a “strong maximum” in comparison with the other points of the circumference, but the following simple analysis shows that this conclusion is not necessarily true.

For example, consider a simple proportionality

$$E = \frac{M}{k}, \quad (3.7)$$

to analyze the behavior of (3.6) for large $M$. Then,

$$y_{\text{min}} = \frac{M + k}{M(k + 1) + k}, \quad (3.8)$$

and the point of minimum along the real axis will also be the maximum ($f_{\text{max}}$) along the circumference of radius $y_{\text{min}}$ centered at the origin, giving

$$(y_{\text{min}}^{E+1}) f_{\text{max}} = (1 - y_{\text{min}})^{-M} = \left[ \frac{Mk}{(M(k+1)+k)} \right]^{-M} = \left[ \frac{M(k+1)+k}{Mk} \right]^{M}, \quad (3.9)$$

and the minimum along the circumference, $f_{\text{min}}$, is located at the point $y$ where $(1-y)$ is maximum, corresponding to arg($y$)=π or $y=-y_{\text{min}}$, is given by

$$(-y_{\text{min}})^{E+1} f_{\text{min}} = (1 + y_{\text{min}})^{-M} = \left[ \frac{M(k+2)+2k}{M(k+1)+k} \right]^{-M} = \left[ \frac{M(k+1)+k}{M(k+2)+2k} \right]^{M}. \quad (3.10)$$
Now, one can estimate how “strong” the maximum along the real axis is by calculating the ratio, 
\[ \rho = \left| \frac{f_{\text{max}}}{f_{\text{min}}} \right|, \]
which gives
\[ \rho = \left( \frac{k + 2}{k} + \frac{2}{M} \right)^M = \left( \frac{k + 2}{k} \right)^M \left( 1 + \frac{2(k + 2)}{M} \right)^M, \tag{3.11} \]
then,
\[ \lim_{M \to \infty} \left( \frac{f_{\text{max}}}{f_{\text{min}}} \right) = \left( \frac{k + 2}{k} \right)^M e^{(2k/k+2)}, \tag{3.12} \]
which for any \( k > 1 \) would produce \( \left( \frac{f_{\text{max}}}{f_{\text{min}}} \right) \to \infty \) for \( M \to \infty \), in agreement with the qualitative reasoning of [1].

On the other hand, one may also take \( E \) fixed and \( k \) varying with \( M \) in (3.6), to analyze the behavior of the subsets consisting of the microcanonical ensembles with \( E \) and \( M \) fixed, or systems with energy non greater than an arbitrarily fixed maximum. In this case the first term of (3.11) becomes
\[ p(M, E) = \left( \frac{k + 2}{k} \right)^M = \left( \frac{(M + 2E)/E}{M/E} \right)^M = \left( 1 + \frac{2E}{M} \right)^M, \tag{3.13} \]
giving
\[ \lim_{M \to \infty} p(M, E) = e^{2E}, \tag{3.14} \]
while the second term gives
\[ q(M, E) = e^{2k/k+2} = e^{2M/M+2E} = e^{[2/1+2(E/M)]} M \to \infty e^{2}, \tag{3.15} \]
then, the total expression in (3.11) yields
\[ \lim_{M \to \infty} p(M, E)q(M, E) = e^{2(E+1)}, \tag{3.16} \]
which can be “very large” or not, depending on \( E \).

One may ask also how these results translate for the analysis of an ensemble of fermions, as in the study of Ref.[2], in which the number of particles is also variable and the energies of the fermions cannot be considered the same in general. In this case we have to deal with various levels with different energies and a generating function given by (2.10), in which we shall neglect for a
while the term “$x$” associated with the chemical potential. Then, the generating function can be rewritten as

$$f(y) = \prod_i (1 + y^\nu_i)$$  \hspace{1cm} (3.17)

where the $\nu_i$ are different integers in general for each $i$, characterizing the different single particle level for each fermion. Each term in the parenthesis can be compared with the expansion of the terms $1/(1-y^\nu_i)$ in (3.3) and the absence of the corresponding terms proportional to $y^{2\nu_i}$, $y^{3\nu_i}$, etc., is an expression of the exclusion principle.

For $y = e^{-\beta \epsilon} < 1$, the various terms in $y^\nu_i$ contribute less to the magnitude of $f(y)$ than if they were replaced by $y$ only. Therefore, to analyze the asymptotic behavior of the magnitude of $f(y)$ for a “large number” of fermions one may consider all the $\nu_i$ as equal to 1, which will imply that the magnitude of the generating function is necessarily smaller than that of the analyzed $f(y)$. In general, this simplification is not physically possible for an actual system of fermions due to the exclusion principle, unless all them belong to the same set of degenerate sp-states.

We then make this approximation and analyze the following simpler expression for the integrand of (2.11)

$$f(y) = \frac{1}{y^{(E+1)}} \prod_i (1 + y) = \frac{(1 + y)^M}{y^{(E+1)}} ,$$  \hspace{1cm} (3.18)

A more general definition similar to (2.10) and (2.11) would be

$$f(x, y) = \frac{1}{x^{M+1}y^{M+1}} \prod_i (1 + xy_i) .$$  \hspace{1cm} (3.19)

where $y_i = w^{\epsilon_i}$, $w = e^{-\beta}$ and

$$E = \sum_{\{l=1\}}^M r_l \epsilon_l ; \quad r_l \in \{0, 1\} .$$  \hspace{1cm} (3.20)

Using the interpretation $y = e^{-\beta \epsilon}$, equation (3.18) would correspond to a set of degenerate fermions with energy $\epsilon$, while (3.19) describes fermions with different energies, for example, $\epsilon_i = \epsilon \nu_i$ with $\nu_i$ integer.

From (3.18) one readily conclude that, for $y$ belonging to the positive real axis and $M > (E+1)$, $f(y)$ is an increasing function of $y$ and it is also divergent for $y \to 0$. Then, it has at least one minimum for $y > 0$, which can be determined analytically,

$$f'(y) = \frac{d}{dy} \left[ \frac{(1 + y)^M}{y^{(E+1)}} \right] = \left( \frac{(1 + y)^{M-1} y^E}{y^{(2E+2)}} \right) (M y - (E + 1)(1 + y)) = 0 ,$$  \hspace{1cm} (3.21)
giving

\[ y_{\text{min}} = \frac{(E + 1)}{M - (E + 1)}. \]  

(3.22)

Then, \( y_{\text{min}} \) is unique and \( f(y_{\text{min}}) \) will also be the maximum along the circumference centered at the origin with radius \( y_{\text{min}} \). Taking as before \( E = M/k \), results

\[ f_{\text{max}} = \frac{1 + (M + k)/(M(k - 1) - k)]^M}{(M + k)/(M(k - 1) - k)} = \frac{1}{[M(k - 1) - k]^{M-1}} \left( \frac{(kM)^M}{M + k} \right), \]  

(3.23)

and the corresponding minimum along this circumference is

\[ f_{\text{min}} = f(-|y_{\text{min}}|) = \frac{(Mk - 2M - 2k)^M}{(M + k)[M(k - 1) - k]^{M-1}}, \]  

(3.24)

then,

\[ \frac{|f_{\text{max}}|}{f_{\text{min}}} = \left( \frac{Mk}{Mk - 2M - 2k} \right)^M = \left( \frac{k}{k - 2} \right)^M \left[ \frac{1}{[1 - 2k/M(k - 2)]^M} \right], \]  

(3.25)

and for \( k \) fixed and greater than 2 results

\[ \lim_{M \to \infty} \frac{f_{\text{max}}}{f_{\text{min}}} = \left( \frac{k}{k - 2} \right)^M e^{(2k/k - 2)}, \]  

(3.26)

which is very similar to (3.9). Now, taking \( E = M/k = \) constant yields

\[ \frac{k}{k - 2} = \frac{M}{M - 2E}, \]  

(3.27)

and (3.25) becomes

\[ \frac{|f_{\text{max}}|}{f_{\text{min}}} = \left( \frac{M}{M - 2E} \right)^M \left[ \frac{1}{[1 - 2/(M - 2E)]^M} \right] = \left( \frac{1}{1 - 2E/M} \right)^M \frac{M(1 - 2E/M)^M}{M(1 - 2E/M + 2/M)^M}, \]  

(3.28)

then,

\[ \lim_{M \to \infty} \frac{f_{\text{max}}}{f_{\text{min}}} = e^{2(E + 1)}, \]  

(3.29)

which coincides with (3.13) and is not necessarily a “very large” ratio. Notice that in the general case one should consider \( \nu_i \) greater than 1, which would produce even smaller ratios in this case.
Figure 1. Simplified generating function for bosons $f(y)$ of Eq.(3.1), for variable $y$ in the case of $M=20$ sp-states.

Figure 2. Projection of the graph of Fig. 1 on the plane containing $|y|$ and the $z$-axis. The various values of $\arg(y)$ are highlighted with different colors.
Figure 3. Simplified generating function for fermions \( f(y) \) of Eq. (3.17), for variable \( y \) in the case of \( M=20 \) sp-states.

Figure 4. Projection of the graph of Fig. 2 on the plane containing \(|y|\) and the \( z \)-axis. The various values of \( \arg(y) \) are highlighted with different colors.
Figures 1 and 3 show the simplified generating function for bosons and fermions, corresponding to Eqs. (3.1) and (3.17) respectively, for variable \( y \) in the case of \( M=20 \) “particles” ("bosons" or "fermions") and \( E=0 \), the fundamental state. The minimum along the real axis as given by Eqs. (3.5) and (3.19), can be seen as a broader white band crossing the graph parallel to the \( \arg(y) \) axis, close to the points with \(|y|=0\). It is clear in both graphs that the minimum along the real axis is a saddle point, but it is not a strong maximum along the band.

Figures 2 and 4 show the corresponding projections of the three dimensional graphs on the plane containing the \(|y|\) axis and the \( z \)-axis. In these graphs it becomes evident that the maximum along the real axis for \( y=y_{\min} \) is no more than 10 times greater than the minimum along the circumference containing \( y_{\min} \), in agreement with (3.16) and (3.29).

Therefore, for the simple approximate partition functions considered in this section, either for bosons or for fermions, the assumption of “strong maximum” along the direction of the contour, in equations like (2.6) or (2.11), cannot be considered as generally valid as it is assumed in the method of Ref.[1].

4. The saddle point problem

A saddle point of a function is one that is stationary but not a local extremum. For functions of two variables, it is a maximum for the variation of one variable and a minimum for the variation of the other. More precisely, it is a point \((x_\star, y_\star) \in \mathcal{R}^{n+m}\) that satisfies\[8\]

\[
L(x_\star, y) \leq L(x_\star, y_\star) \leq L(x, y_\star), \quad \forall x \in \mathcal{R}^n \text{ and } \forall y \in \mathcal{R}^m,
\]

or, equivalently,

\[
\min_x \max_y L(x, y) = L(x_\star, y_\star) = \max_y \min_x L(x, y),
\]

and the definition for complex variables would correspond to the dimensions \(n=m=2\) for two variables, or \(n=m=1\) along perpendicular directions for one variable.

In a first stage of the formal application of the method of Ref.[1] for partition functions, either for fermions in the integrand of Eq.(2.11) or bosons in (3.2), the variables \( x \) and \( y \) can be thought as possessing no direct physical meaning and to have been created only to keep track of the counting of the number of particles and the energy of the nuclear levels. As we saw in Sec.2 this tracking is formally performed using the Cauchy’s Theorem in the definition of the "density" associated with \( y \) for a given \( A \) (number of particles, excitons, Planck vibrators, etc.).
For given $y$ the analysis of the dependence of $f(x,y)$ with $x$ in (2.10) is similar to the “simplest cases” of Sec.3 and essentially reduces to an additional phase on the $y$ term. Therefore, one can limit the analysis to the dependence on $y$ to have an idea of the general behavior of the partition function.

In a general expression like (3.2) or (3.18) one cannot deduce algebraically the point of maximum in a straightforward way as happened in (3.5) and (3.21), but due to the smooth analytical behavior of these functions one can rely on numerical procedures to determine this point.

These functions can be easily calculated numerically by fixing one variable, for example fixed $|x|$ and $\arg(x)$, and varying $|y|$ with values smaller than one (in accordance to its physical interpretation as $y = e^{-\beta \epsilon}$, with $\beta$ and $\epsilon$ real and positive) and variable $\arg(y)$ with a grid of points dense enough and reasonable range, for example between 0 and $2\pi$, with steps of $2\pi/16$.

We used the Newton-Raphson method\[10\] to obtain the maximum along the real axis of $y$ and compared it with the values in other directions with the same $|y|$. The results are presented in the following figures and are analogous to the simpler cases of Sec.3, i.e., although the saddle point along the real axis is well defined the maximum cannot be considered as “very strong” in the sense of Ref.[1].

**Figure 5.** Simplified generating function for bosons $f(y_1,\ldots,y_M)$ of Eq.(3.3) in the case of $M=20$ sp-states, with $E=0$ and $\epsilon_l=l$ in (3.4).
Figure 6. Projection of the graph of Fig. 5 on the plane containing $|y|$ and the $z$-axis. The various values of arg($y$) are highlighted with different colors.

Figure 7. Simplified generating function for fermions $f(x,y)$ of Eq.(3.19), in the case of $M=20$ sp-states and $E=0$ and $\epsilon_l=l$ in (3.20).
As expected, from the reasoning of the previous section, the maximum along the real axis results “weaker” than in the simplified cases because the magnitude of $y$ is less than 1. This is reflected by flatter surfaces obtained now in comparison with the previous section, as we can see in figures 5 and 7. These figures show the simplified partition functions for bosons and fermions, corresponding to Eqs. (3.3) and (3.19), for $M=20$ “particles” in the fundamental state, using $\arg(x)=0$.

The minimum along the real axis can be seen as a broader white band crossing the graph approximately at its middle, parallel to the $\arg(y)$ axis. It is clear in both graphs that the minimum along the real axis is also a saddle point, but it is not a strong maximum along the band as a function of $\arg(y)$.

Figures 6 and 8 show the projections, corresponding to figures 5 and 7 respectively, on the plane containing the $|y|$ axis and the $z$-axis. These graphs clearly show that the maximum along the real axis for $y=y_{\text{min}}$ has an even smaller ratio to other points along the band than the cases considered in the previous section, which is expected due to the higher powers of $y$ involved in the present functions.

Figures 9 and 11 show the partition functions for bosons and fermions, corresponding to Eqs. (3.2) and (3.19), for $M=20$ “particles” in the fundamental state, using now $\arg(x)=7\pi/8$. 

**Figure 8.** Projection of the graph of Fig. 7 on the plane containing $|y|$ and the $z$-axis. The various values of $\arg(y)$ are highlighted with different colors.
Figure 9. Simplified generating function for bosons $f(x,y)$ of Eq. (3.2), for variable $y$ and fixed $x$, with $\arg(x) = 7\pi/8$, in the case of $M=20$ sp-states, in the fundamental state.

Figure 10. Projection of the graph of Fig. 9 on the plane containing $|y|$ and the $z$-axis. The various values of $\arg(y)$ are highlighted with different colors.
**Figure 11.** Simplified generating function for fermions $f(x,y)$ of Eq.(3.19), for variable $y$ and fixed $x$, with $\arg(x)=7\pi/8$, in the case of $M=20$ sp-states, in the fundamental state.

**Figure 12.** Projection of the graph of Fig. 11 on the plane containing $|y|$ and the $z$-axis. The various values of $\arg(y)$ are highlighted with different colors.
The non null argument of $x$ not only introduces an additional phase in the general functional dependence of the partition function, but also changes its behavior along the real axis from a set of points of maximum to a set of minima.

Figures 13 to 16 show results analogous to figures 9 to 12, but now for $M=10$ “particles”, $\arg(x)=7\pi/8$ and non null excitation, $E=4$ in arbitrary units. One important difference with respect to figures 9 to 12 is the steeper increase of the partition function for $|y|$ close to 0.

Figure 13. Simplified generating function for bosons $f(x,y)$ of Eq.(3.2), for variable $y$ and fixed $x$, with $\arg(x)=7\pi/8$, $M=10$ sp-states and $E=4$ in arbitrary units.
Figure 14. Projection of the graph of Fig. 13 on the plane containing $|y|$ and the $z$-axis. The various values of $\text{arg}(y)$ are highlighted with different colors.

Figure 15. Simplified generating function for fermions $f(x,y)$ of Eq.(3.19), for variable $y$ and fixed $x$, with $\text{arg}(x)=7\pi/8$, $M=10$ sp-states and $E=4$ in arbitrary units.
Figure 16. Projection of the graph of Fig. 15 on the plane containing $|y|$ and the $za$-axis. The various values of arg($y$) are highlighted with different colors.

Therefore, for arg($x$) = $7\pi/8$ the reasoning of Darwin-Fowler method becomes *totally flawed*.

Notice that for fermions in a nuclear system the low number of “particles” and low nuclear excitation are *usual* assumptions in the study of pre-equilibrium dynamics,$^{[11]}$ therefore in this regard the above analysis is realistic.

In Ref.$^{[1]}$ the number of PV’s is implicitly assumed to be large in agreement with the usual statistical approach. On the other hand, the above results clearly show that an increase in $M$ or $E$ would only introduce more oscillations for $|y|$ close to 1 and increase the steepness of the variation of the partition function for $|y|$ close to 0, but would not change the main results, which show that although the maxima on the real axis of $x$ and $y$ may exist and be saddle points of the partition function they cannot be considered, in general, as strong maxima unless $E$ is very large. In addition, if $x$ is considered as a complex variable, the saddle points can only be defined in certain directions of its complex plane.

Therefore, one obtains here the same conclusion as in the previous section, i.e., that the hypothesis of the existence of a “strong maximum” along the direction of the contour cannot be considered as generally valid as assumed in the method of Ref.$^{[1]}$. 
5. Final comments and conclusion

The analysis presented in the previous sections indicates that the whole idea of using the Cauchy theorem in the study of the partition functions of the canonical and grand canonical ensemble, for bosons or fermions, and the consequent connection with the Laplace transform (via CAP), as proposed by the Darwin-Fowler method can be misleading.

In general, the Laplace transform formalism results from the usual statistical interpretation of $y$ as $e^{-\beta \epsilon}$, where $\beta = 1/\kappa T$, $\kappa$ is Boltzman constant, $T$ is the nuclear temperature and $\epsilon$ is the average interspacing among single particle levels, complemented by the hypothesis that $\epsilon$ is infinitesimally small in accordance with CAP. Then, one can rewrite for example (2.18) as

$$f(x,y) = \sum_{(A,U)} D(A,U) x^A y^U / \epsilon \approx \sum_{(A)} \int_{E_{\text{min}}}^{E_{\text{max}}} \omega(A,U) x^A e^{-\beta U} dU ,$$

where the nuclear density $\omega(A,U)$ and degeneracy $D(A,U)$ are related by

$$\omega(A,U,M) \approx D(A,U,M) / \delta U ,$$

and

$$\delta U = U - U_{\text{prev}} ,$$

where $U_{\text{prev}}$ is the highest (discrete) nuclear level energy smaller than $U$. Therefore, with the approximate replacement of $(E_{\text{min}},E_{\text{max}})$ by $(0,\infty)$, which is reasonable if $U$ is for example the nuclear excitation, $f(x,y)$ becomes the Laplace transform of $\omega(A,U)$.

The approximations involved here are not drastic having in sight the usually high density of nuclear levels per MeV observed experimentally, which makes the use of CAP, in general, a very reasonable approach. Then, because the connection of approximated expressions involving the Cauchy’s theorem, like (2.6) or (2.11), with the inverse Laplace transform is also immediate under CAP, the various formalisms become intimately related and tend to be used together, which may be a source of errors if one of these approximations is at least partially incorrect.

For example, in Ref. it was shown that the direct use of the Laplace transform may lead to inconsistencies in the description of transitions in which a given sp-state is destroyed and subsequently re-created.

In this case, the Laplace transform is not able to describe the details of the variation of the set of available states from initial to intermediary and final stages, due to the approximations involved in the definition of the nuclear density. In this case, the imprecise definition of the density may give a wrong result for the moments of the transition if not seconded by an independent analysis.
of the involved microscopic processes and their influence on the definition of the available states at each stage.

Although this problem with the Laplace transform is essentially independent of the Darwin-Fowler method it would not have appeared if the method was not employed in the first place, as the Laplace transform is not a necessary tool for the description of pre-equilibrium nuclear systems.

One may ask, if the method of Ref. [1] has this essential inconsistency and it is not so general as it is usually supposed to be then why does it work so well in many applications? A possible answer for this may be found in the details of the method itself and the meaning of the functions that the method is supposed to be applied to.

For a given analytical function $g(y)$ that is non zero at $y$ the following relation is always valid,

$$g'(y) = \frac{d}{dy}[\log(g(y))]g(y).$$  \hspace{1cm} (5.3)

In the case of an ensemble of bosons or fermions $g(y)$ is the partition function of the ensemble, $f(y)$, divided by terms like $y^{N+1}$, where the total energy is $E=N\epsilon$. Therefore, the minimum is given by the following equation

$$\frac{d}{dy}[\log(g(y))] = \frac{d}{dy}[\log(f(y)) - (N+1)\log(y)] = 0,$$ \hspace{1cm} (5.4)

and by making the usual connection between the partition function and the thermodynamic potential, i.e. $\log(f(y)) = -\beta\Omega$, where $\Omega$ is given by [12]

$$\Omega = E - TS - \mu M = N\epsilon - TS - \mu M,$$ \hspace{1cm} (5.5)

results

$$-\beta\Omega = (N+1)\log(y) + e,$$ \hspace{1cm} (5.6)

where $e$ is a constant of integration that is not a function of $E$, therefore one can take $e$ as equal to $\beta(TS+\mu M)$ to obtain

$$-\beta E = (N+1)\log(y) \approx N\log(y) \quad \text{if } N \text{ is very large},$$ \hspace{1cm} (5.7)

which is the usual thermodynamic interpretation of the statistical parameter $y$.

Therefore, the condition of minimum in (5.4) can be interpreted as an approximate expression of the usual relation between the thermodynamic potential and the elementary energy associated with the single particle quantum levels,

$$\frac{\partial\Omega}{\partial\epsilon} = -\beta N,$$ \hspace{1cm} (5.8)
showing that the entire use of the Cauchy theorem in connection with expressions involving the partition functions, for an ensemble of either fermions or bosons, can be seen as a tricky reformulation to obtain the usual thermodynamic expressions from the microscopic description defined by the partition functions.

In other words, the above reasoning shows that the condition of focusing on the minimum of the integrand instead of the entire integral defined by the Cauchy theorem would work well in the case of partition functions even if the integrands do not define a saddle point with the characteristics assumed in Ref.\[1\].

Therefore, the use of the Darwin-Fowler method can be considered as a convenient tool for many applications, but cannot be taken as the foundation of the analysis of ensembles of fermions or bosons, as suggested by Ref.\[2\].

Consequently, the use of direct algebraic approaches, as the one presented in Ref.\[7\] for the analysis of pre-equilibrium dynamics, can be more appropriate for a microscopic description of the Shell Model, even in the CAP limit and either for fermionic or bosonic systems, unless the total energy $E$ is very large.

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