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ANALYTIC NUMBER THEORY AND THE NUCLEAR LEVEL DENSITY

A. Anzaldo Meneses

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ABSTRACT

We are presenting here an alternative approach to obtain a better description of the nuclear level density, its shell effects and energy dependency. Our method is statistical and considers a system of neutrons and protons in a single particle energy spectrum. We are applying methods from Analytic Number Theory systematically. The obtained results are formally related to other areas of Mathematical and Theoretical Physics, where the estimation of the coefficients of (formal) Fourier series of partitions functions, e.g. dimensions of root spaces, densities of states and the like, play an important role. The acid test of this approach and the primary reason to develop it is a comparison of an explicit theoretical calculation with experimental data.

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Mach ticmatih occeppa mohualhuiliz,
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CHAPTER 1

INTRODUCTION

The existence of closely spaced resonances in the total nuclear cross sections for nuclear reactions with slow neutrons has its roots in the many body problem of strongly interacting nucleons. The introduction of the concept of a compound nucleus by N. Bohr (1936) plays a central role up to the present. In Fig. 1.1, the total cross-section for the reaction ^{238}U + n with slow neutrons shows some near lying sharp resonances, as a function of the incident neutron energy. The mean spacing between adjacent resonances is of only about 20 eV and their widths are of only few eV.

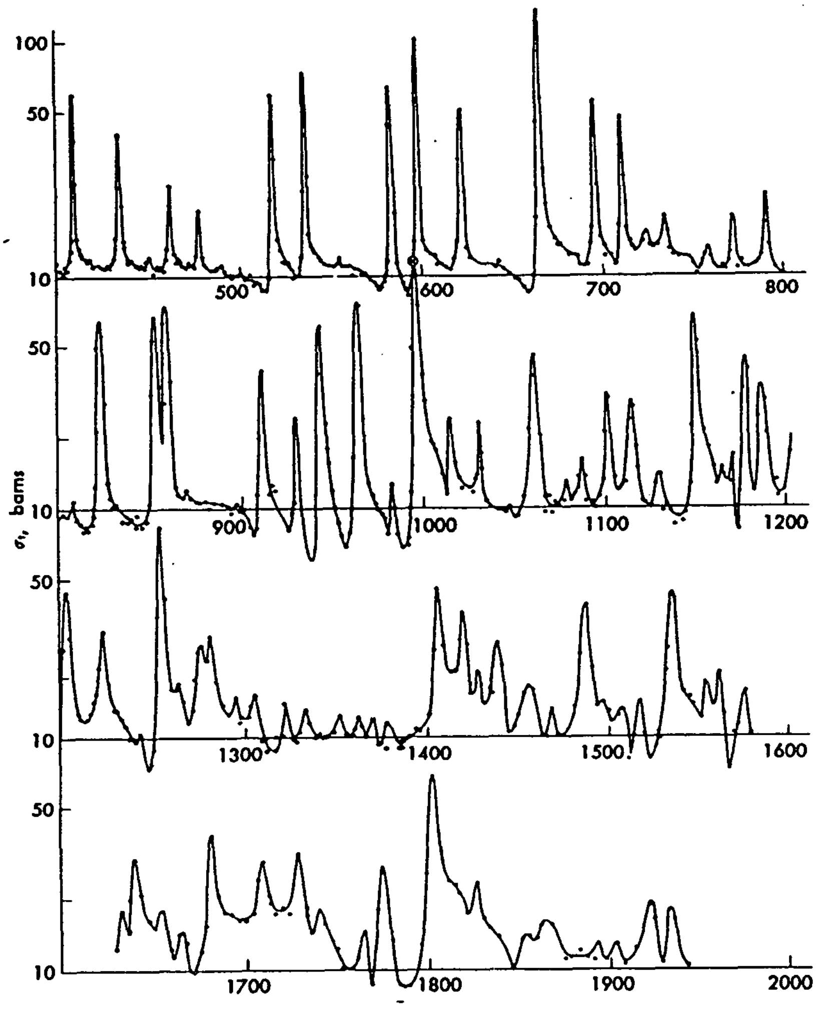


Figure 1.1 Total cross section for ^{238}U+n against the incident neutron energy [taken from F. W. K. Firk et al. (1960)].

These features cannot be explained by simple potential scattering or in terms of energy differences between neighbouring single particle states. For larger incident neutron energies the region of unresolved resonances is reached.

For many applications it is essential to know the average number of resonances in a given interval as well as the statistics of their spacings and widths. Clearly, this problem is very complicated in general because it concerns the description of a finite quantum system of strongly interacting Fermions, whose interactions are not yet well understood. Therefore it is quite important that a relevant part of the calculation of the nuclear level density can be performed using the statistical description. This description treats the neutrons and protons as particles distributed according to the Fermi-Dirac statistics in a fixed set of energy levels. The calculation is reduced in that way to a number theoretical problem. It is still a very difficult task since the knowledge of the physically relevant quantities must be clearly included. The single particle spectra are in general very irregular and their explicit form depends largely on the adopted nuclear model. Rotational and vibrational contributions will appear in general. Pairing effects could also be present. The shell effects must always be considered carefully. Only this last and most important aspect will be studied in detail in this work.

This contribution was motivated by the original work of H.A. Bethe (1936/37), N. Bohr (1936), S. Goudsmit (1937), C. van Lier and G.E. Uhlenbeck (1937) and some other researchers. These authors obtained a formula which showed with very simple analytical relations the most important behaviour of the nuclear level density, parametrized by means of quantities with a clear physical meaning. Let $\rho_o(U)dU$ be the number of levels between the excitation energies U and U+dU. Bethe considers a Fermi gas of A non-interacting neutrons and protons enclosed in a sphere of radius $R= r_oA^{1/3}$, $r_o=1.48 \cdot 10^{-13}$cm, and gives the formula:

$$\rho_o(U)= \frac{\pi^{1/2}}{12\ a^{1/4}U^{5/4}} \exp\ (2\ a^{1/2}U^{1/2})\ ,\ a= \pi^2A/4\varepsilon_F \approx (A/15)\ \mathrm{MeV}^{-1}, \quad (1.1)$$

where $\varepsilon_F=(3^{4/3}\pi^{2/3}/8)\ \hbar^2A^{2/3}/MR^2$ is the average Fermi energy for protons and neutrons. The number of states with a given total angular momentum I is given by:

$$\rho(U,I)= \frac{(2I+1)}{2^{3/2}\sigma^3\pi^{1/2}} \exp[-(I+1/2)^2/2\sigma^2]\ \rho_o(U). \qquad (1.2)$$

Here $\sigma^2 = nj(j+1)/3$, $n = 6 \cdot 2^{1/2} \log(2) (UA)^{1/2}/\pi\varepsilon_F$ is the average number of neutrons and protons having energies larger than ε_F plus the number of unoccupied states of energy smaller than ε_F, j is the average angular momentum of the individual particles $<(j+1/2)^2> = 3^{4/3}\pi^{2/3}A^{2/3}/10$. This angular momentum distribution is based on the very general notion of random coupling of the angular momenta of the individual nucleons.

Van Lier and Uhlenbeck soon noticed that the "a-parameter" introduced by Bethe was given in general simply by $a = \pi^2[g_n(\varepsilon_{Fn}) + g_p(\varepsilon_{Fp})]/6$, in terms of the (smooth) densities of individual levels for neutrons and protons at the Fermi level. Clearly, no parameter was introduced in an ad-hoc way to reproduce experimental results. The connection to number theoretical problems was also known, although at a very elementary level. Nevertheless, their results are only a crude approximation which still today needs to be improved. This occurs mostly because their methods rely completely on the Sommerfeld method for electrons in a metal. Sums over discrete energy levels are substituted by integrals.

Experimental data of the mean resonances spacings have essentially two origins. The first are the level schemes obtained from high resolution (n,γ) and transfer reaction data. These schemes provide the lowest excited levels but are limited from above because it turns easy to miss resonances with increasing energies or because of experimental reasons. In **Fig. 1.2**, the level scheme of ^{237}U obtained by resonant neutron capture in ^{236}U by T. von Egidy et al. (1979) is shown. The second source of experimental values of the nuclear level densities are the neutron resonance data arising from reactions iniciated by low-energy neutrons. These data yield experimental values at energies just above the neutron binding energies. Low energy neutrons are obtained for example from nuclear reactors or from reactions with bursts of particles from accelerators falling on specific targets. It is possible to obtain incident neutron energies in a range of some eV up to some MeV above the binding energies and to deduce from the resulting cross sections (like in Fig. 1.1) the average spacings. This can be done assuming that the resonances are evenly distributed if the energy range is not too large and the resonances are well resolved.

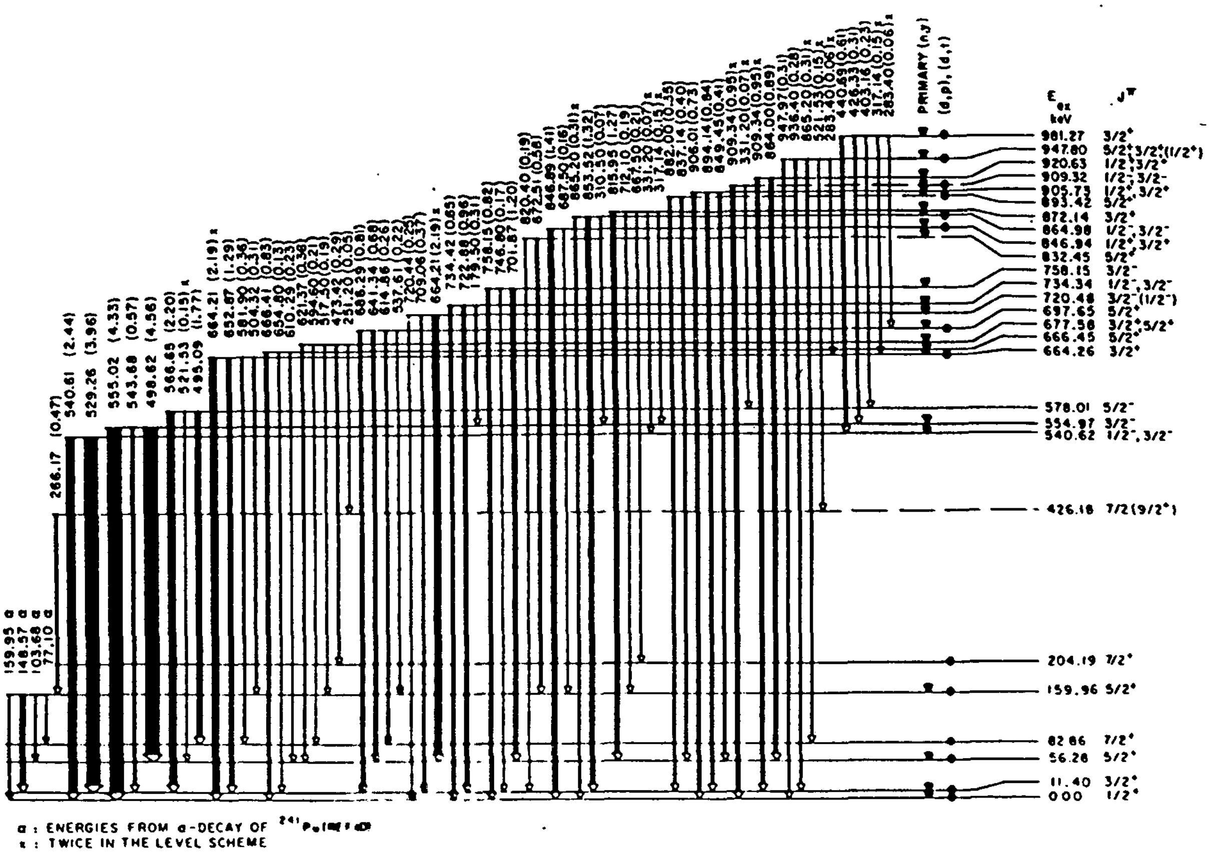


Fig. 1.2. Level scheme of ^{237}U obtained from resonant neutron capture [taken from T. von Egidy et al. (1979)].

In the latter developments it becames clear that adjusting the a-parameter, a good agreement with experimental results could be achieved for fixed excitation energies. Nevertheless, a predictive mathematical method able to reproduce the energy dependency of the shell structure effects for the a-parameter does not exist. It is a common practice to compare distinct approaches by calculating the corresponding a-parameters. In studies where the nuclear level density is the outcome, a Bethe type formula can be fitted to the theoretical data which makes comparisons easier. The staircase functions from the level schemes (like those of Fig. 1.2) are fitted by a Bethe type formula or by a constant temperature formula for low energies. For energies near the neutron binding energy, the mean spacings are determined from the cross-sections and their inverses are fitted similarly. For example, from Fig. 1.1 follows an average resonance spacing of circa 20 eV and thus a total density of about 50 KeV^{-1}.

In Fig. 1.3 some curves for the number of levels N(E) up to energy

E, fitted to experimental level schemes are shown (cf. T. von Egidy et al., 1986). One of the curves was computed using the shifted Bethe formula and the other using a constant temperature relation (see chapter 5 for more details).

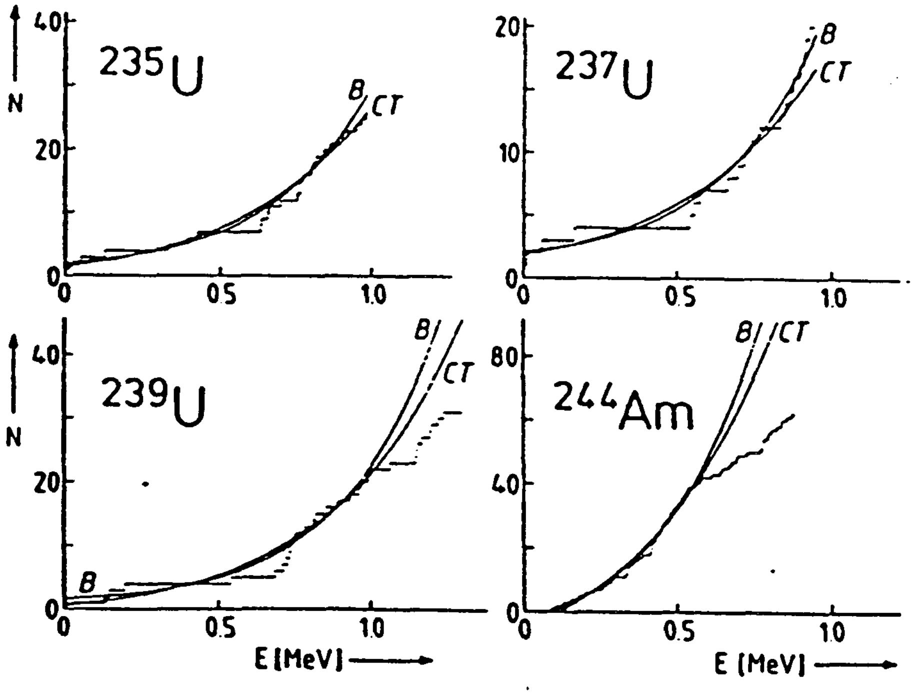


Figure 1.3 Number of levels N(E) up to an energy E for ^{235}U, ^{237}U, ^{239}U and ^{244}Am. The fitted curves are the Bethe and the constant temperature formulae.

By means of a careful consideration of the shell structure present in the (discrete) single particle spectra, we obtain in this work new results expressed with simple formulas. For this purpose, we used as guide methods taken from the modern Analytic Number Theory (see for example T.M. Apostol, "Introduction to Analytic Number Theory", Springer Verlag, 1976). In this way it becomes easier to recognize the relevant mathematical quantities which must be related to the physical parameters. With the generality presented here, the use of analytical number-theoretical methods to this problem has been initiated by the author [cf. A. Anzaldo-Meneses (1982, 1983)].

The study of the resonances spacings and their widths distributions will not be addressed here. The methods necessary for it are very different.

However, also in similar questions there are many well known examples in Analytic Number Theory. Two examples par excellence are the distribution of zeros of a Dirichlet series and the distribution of the prime numbers.

Within the saddle point approximation, we succeeded to obtain here a thorough analytical description for the relevant quantities involved in the nuclear level density. This means that only a minimum of numerical computer calculations is needed to carry out the comparison with experimental results. During the last 30 years, there have been many extensive numerical works under the title "microscopic calculations". But unfortunately they are done without the existence of a consistent fundamental ("microscopic") nuclear theory. It is well known since many years that different spectra lead to the same average results for the level density. There is no unique way to fix the "correct" nuclear Hamiltonian from these considerations. Furthermore, extense numerical computer results are of no aid at problems where the nuclear level density forms only a small (although important) part. The underlying physical understanding becomes nearly as complicated as to obtain the experimental results themselves.

Here we take a different point of view. We consider classes of single particle spectra with common analytic properties. We stress the importance to recognize the most relevant parameters, which must be common to all single particle spectra, whenever they are to reproduce the experimental data. In this way we do not need to limit ourselves to a special kind of Hamiltonian and it is also not necessary to diagonalize it. We attempt rather to introduce nuclear structure properties in the form of well founded mathematical quantities with a corresponding physical interpretation. This approach should conduce to the study of invariants associated to complex nuclei.

In **Chapter 2** we state the problem and the saddle point approximation which we follow. In **Chapter 3** we present our method for a wide class of single particle spectra and obtain explicit expressions for all relevant quantities mentioned in the preceeding chapter. The consideration of the local structure of the single particle spectra is studied in **Chapter 4** for a periodic spectrum in some detail and observations for more general cases are done. In particular, the three dimensional harmonic oscillator with spin-orbit coupling and the three dimensional anisotropic oscillator are briefly touched. With the results of chapter 4, we finally compute explicitly a physically relevant quantity and compare it with experimental data in **Chapter 5**.

At the same time we attempt to introduce as many mathematical devices that we consider reasonable for a serious study of nuclear spectra and to find a common basis for all analytic studies up to now, as well as for future developments. The most important criterium we observed is the achievement of a method for explicit numerical calculations ready to be compared with available experimental data.

We report further some results concerning particle-hole state densities in **Chapter 6** to correct a wrong formula frequently used in practical pre-equilibrium calculations.

It is remarkable that many results are formally related with other branches of mathematical and theoretical Physics as the reader can see. We have included some observations on this theme in **Chapter 7**. The topics of mathematical Physics are the exact evaluation of the Fourier coefficients of modular forms and some related results of the theory of Kac-Moody algebras. Concerning theoretical Physics, we refer to recent investigations on shell structures in clusters and mesoscopic systems. We obtain some new results.

We show in **Chapter 8** an elementary method to obtain colored graphs which contain the most relevant information of a given analytic function and which we have used during this work to improve our understanding of the functions of Analytic Number Theory.

CHAPTER 2

THE STARTING EQUATIONS

In this chapter, the general equations needed for the calculation of the nuclear level density are given. Following the statistical description the calculation is performed by estimating the number of accessible states of a system of fixed numbers of neutrons and of protons distributed in single particle level spectra. Therefore, the nuclear level density is defined combinatorially in a form particularly favorable for the application of analytical number-theoretical methods. The saddle point method leads to an explicit form in terms of functions evaluated at the saddle point. These functions, including the grand partition function, will be analyzed in the forthcoming chapters.

We follow the **Darwin-Fowler method** to obtain an analytic expression for the level density (see R. Fowler, 1936). The **density of excited states** of a system of N neutrons and Z protons with total energy E and total angular momentum projection M is given by $\rho(N,Z,M,E)$ in the expression for the **grand partition function** :

$$Z(\alpha,\beta)=\prod[1 + \exp(\alpha_n+\alpha_3 m_{3\nu_n}- \beta\varepsilon_{\nu_n})]\prod[1 + \exp(\alpha_p+\alpha_3 m_{3\nu_p}- \beta\varepsilon_{\nu_p})] =$$

$$= \sum_{Z,N,M,E} x_p^Z\, x_n^N\, x_3^M\, y^E\, \rho(N,Z,M,E)\ ,\quad \alpha_n,\alpha_p,\alpha_3,\ \beta \in \mathbb{C}\ , \tag{2.1}$$

where:

$$N = \sum n_{\nu_n}\ ,\quad Z = \sum n_{\nu_p}\ ,\quad M = \sum n_{\nu_n} m_{\nu_n} + \sum n_{\nu_p} m_{\nu_p}\ , \tag{2.2}$$

and

$$E = \sum n_{\nu_n}\varepsilon_{\nu_n} + \sum n_{\nu_p}\varepsilon_{\nu_p}\ , \tag{2.3}$$

with $x_k=e^{\alpha_k}$, $y=e^{-\beta}$ and the **single particle spectrum** $\{\varepsilon_{\nu_{n(p)}}\}$ for neutrons, respectively for protons. Further, $n_{\nu_{n(p)}}$ are the occupation numbers associated with the single particle energy level $\varepsilon_{\nu_{n(p)}}$ with magnetic quantum number $m_{\nu_{n(p)}}$. The sums for E run over different values of $\varepsilon_{\nu_{n(p)}}$. Although the numbers ε_ν are in general real numbers, we choose a sufficiently small energy unit and consider them as integer numbers.

The objective is to obtain a simple expression for $\rho(N,Z,M,E)$ valid for all energies E in a certain interval. We assume that the excitation energy $U=E-E_o$, where E_o is the ground state energy, is not large enough to excite the lowest lying nucleons in the spectrum. This means that we study only so-called "**degenerated systems**". The estimation of $\rho(N,Z,M,E)$ can also be interpreted as the evaluation of the coefficients for the Fourier series of $Z(\alpha,\beta)$.

The Darwin-Fowler method consists now in the evaluation of the contour integral:

$$\rho(N,Z,M,E)= \frac{1}{(2\pi i)^4}\int_{-i\infty}^{i\infty} d\alpha_n \int_{-i\infty}^{i\infty} d\alpha_p \int_{-i\infty}^{i\infty} d\alpha_3 \int_{-i\infty}^{i\infty} d\beta \; \exp[\ln Z(\alpha,\beta)+\beta E-\alpha_n N-\alpha_p Z-\alpha_3 M], \tag{2.4}$$

where the "**entropy**" of the system is defined by:

$$S(\alpha,\beta) = \ln Z(\alpha,\beta) + \beta E - \alpha_n N - \alpha_p Z - \alpha_3 M , \tag{2.5}$$

The series in eq.(1) is only formal within a combinatorial interpretation, but if we restrict the complex variables to suitable complex regions we can also understand the series as defining relations of specific analytic functions. In particular we can deform the integration path to evaluate the integrals in eq.(2.4) by means of the **saddle point method.** To this end we need to know the behaviour of $S(\alpha,\beta)$ in $\mathbb{C}^4$ to be able to select properly the integration contour in the best way. For the spectra we consider this is always possible as follows from the rapid oscillatory behaviour of $S(\alpha,\beta)$. The entropy is developed locally around the stationary point (α_o,β_o) given by the solution of the **saddle point equations** :

$$\partial_{\alpha_n} S(\alpha_o,\beta)= 0 \; , \; \partial_{\alpha_p} S(\alpha,\beta)= 0 \; , \; \partial_{\alpha_3} S(\alpha,\beta)= 0 \; , \; \partial_{\beta} \, S(\alpha,\beta)= 0 \; , \tag{2.6}$$

disregarding higher order contributions :

$$S(\alpha,\beta) \approx S(\alpha_o,\beta_o) + \sum_{i,j} (\alpha_i-\alpha_{io})(\alpha_j-\alpha_{jo}) \, \partial_{\alpha_i\alpha_j} S(\alpha_o,\beta_o)/2 \; , \tag{2.7}$$

we set here $\alpha_1=\alpha_n$, $\alpha_2=\alpha_p$ and $\alpha_4=\beta$.

The resulting quadratic form can be easily diagonalized by a linear orthogonal transformation and the resulting integrals are of Gaussian form leading to the expression:

$$\rho(N,Z,M,E) = \frac{\exp S}{(2\pi)^2\sqrt{D}} \;, \tag{2.8}$$

where D is the determinant of the 4×4 matrix formed with the second order partial derivatives of $\ln Z(\alpha,\beta)$ evaluated at the saddle point :

$$D = \det \left[\, \partial_{\alpha_i}\partial_{\alpha_j} \ln Z(\alpha,\beta) \, \right] , \qquad i,j = n,\, p,\, 3{,}4 \;,\; \alpha_4 = \beta \;, \tag{2.9}$$

The equations we like to solve are thus the following :

$$N = \sum 1/[1+\exp(-\alpha_n-\alpha_3 m_{\nu_n}+\beta\varepsilon_{\nu_n})] \;,\; Z = \sum 1/[1+\exp(-\alpha_p-\alpha_3 m_{\nu_p}+\beta\varepsilon_{\nu_p})] \;, \tag{2.10}$$

$$E = \sum \varepsilon_{\nu_n}/(1+\exp(-\alpha_n-\alpha_3 m_{\nu_n}+\beta\varepsilon_{\nu_n})) + \sum \varepsilon_{\nu_p}/(1+\exp(-\alpha_p-\alpha_3 m_{\nu_p}+\beta\varepsilon_{\nu_p})) \;,$$

$$M = \sum m_{\nu_n}/(1+\exp(-\alpha_n-\alpha_3 m_{\nu_n}+\beta\varepsilon_{\nu_n})) + \sum m_{\nu_p}/(1+\exp(-\alpha_p-\alpha_3 m_{\nu_p}+\beta\varepsilon_{\nu_p})) \;,$$

for the determination of the saddle-point. All sums run over all single particle energies available and include also equal ε_ν according to their degeneracy.

The entropy is given by:

$$S(\alpha_o,\beta_o) = \ln Z(\alpha_o,\beta_o) + \sum (\beta\varepsilon_{\nu_n}-\alpha_n-\alpha_3 m_{\nu_n})/(1+\exp(-\alpha_n-\alpha_3 m_{\nu_n}+\beta\varepsilon_{\nu_n})) \;+$$
$$+ \text{ similar terms for protons} \;, \tag{2.11}$$

and for the determinant we need further :

$$\partial^2_{\beta\beta} \ln Z = \sum \varepsilon^2_{\nu_n}/4\cosh^2((\beta\varepsilon_{\nu_n}-\alpha_n-\alpha_3 m_{\nu_n})/2) \quad + \text{ similar for protons} \;,$$

$$\partial^2_{\alpha_3\beta} \ln Z = -\sum \varepsilon_{\nu_n} m_{\nu_n}/4\cosh^2((\beta\varepsilon_{\nu_n}-\alpha_n-\alpha_3 m_{\nu_n})/2) \; - \text{ similar for protons} \;,$$

$$\partial^2_{\alpha_3\alpha_3} \ln Z = \sum m^2_{\nu_n}/4\cosh^2((\beta\varepsilon_{\nu_n}-\alpha_n-\alpha_3 m_{\nu_n})/2) \quad + \text{ similar for protons} \;,$$

$$\partial^2_{\alpha_n\alpha_n} \ln Z = \sum \; 1/4\cosh^2((\beta\varepsilon_{\nu_n}-\alpha_n-\alpha_3 m_{\nu_n})/2) \;,$$

$$\partial^2_{\alpha_p\alpha_p} \ln Z = \sum \; 1/4\cosh^2((\beta\varepsilon_{\nu_p}-\alpha_p-\alpha_3 m_{\nu_p})/2) \;, \tag{2.12}$$

$$\partial^2_{\alpha_n\beta} \ln Z = -\sum \varepsilon_{\nu_n}/4\cosh^2((\beta\varepsilon_{\nu_n}-\alpha_n-\alpha_3 m_{\nu_n})/2) \;,$$

$$\partial^2_{\alpha_p \beta} \ln Z = -\sum \varepsilon_{\nu_p} / 4\cosh^2((\beta\varepsilon_{\nu_p} - \alpha_p - \alpha_3 m_{\nu_p})/2) ,$$

$$\partial_{\alpha_n \alpha_3} \ln Z = \sum m_{\nu_n} / 4\cosh^2((\beta\varepsilon_{\nu_n} - \alpha_n - \alpha_3 m_{\nu_n})/2) ,$$

$$\partial_{\alpha_p \alpha_3} \ln Z = \sum m_{\nu_p} / 4\cosh^2((\beta\varepsilon_{\nu_p} - \alpha_p - \alpha_3 m_{\nu_p})/2) ,$$

$$\partial_{\alpha_n \alpha_p} \ln Z = 0 ,$$

If we introduce additional constants of motion coming from e.g. further kinds of fermions, the resulting equations retain the form given above with additional terms of the same type for the added chemical potentials.

We shall follow Bethe's original work (1936) for the consideration of the angular momentum dependency and compute the level density $\rho_0(N,Z,E)$ without the introduction of M and its Lagrange multiplier in the above equations. We will follow in this way the common practice and compute the nuclear level density with total angular momentum I dependency by:

$$\rho(N,Z,I,E) \approx \frac{2I+1}{2\sqrt{2\pi}\,\sigma^3}\, \rho_0(N,Z,E) \exp\left[-\frac{(I+1)^2}{2\sigma^2}\right] , \tag{2.13}$$

where σ^2 is the **spin cut-off parameter** and gives the width of the Gaussian angular momentum projection M distribution. Although the determination of σ^2 is still not a well settled problem, it is the only analytical way able to approximate the angular momentum dependency. The values commonly used are those proposed by A. Gilbert and A.G.W. Cameron (1965), which have a reasonable experimental support (see chapter 5 for more details).

From this point on our calculation departs from the usual one. Normally, see for example T. Ericson (1958), the partition function is expressed as an integral over a smooth single particle level density. Different simple Ansätze for the latter function lead to the well known results [see for example the review by V.S. Ramamurthy (1989)] . Instead of doing so, we will retain the discrete structure of the single particle spectra in form of properties associated with number theoretical functions. Working in this way we will be able not only to understand much better all the preceding works, but also to improve them and achieve a better description of experimental results.

A major improvement of the saddle point approximation would be to include further terms in the expansion of the entropy around the saddle point or/and to select a better integration path as that used to obtain the Gaussian integrals. Nevertheless, this can only be done once we know better the analytic properties of the entropy as a function of its variables. In this work we study more in detail the entropy and other related quantities and show that, without going beyond the saddle-point approximation, we can obtain a better agreement with experimental data as we have already mentioned. In chapter 6, we shall make some observations connected with this problem.

CHAPTER 3

USE OF METHODS FROM ANALYTIC NUMBER THEORY

We prefer to continue the use of functions from the Analytic Number Theory. The formal series and products as those of equation (2.1) have a precise analytic meaning if the complex variables are restricted to a particular region of the complex plane. We will not consider the angular momentum dependence in this chapter.

Let us now sketch the contents here. First, we introduce a mathematical assumption to allow the introduction of mathematical methods which help us to consider a large number of single particle spectra physically reasonable. This assumption affords to substitute the single particle spectrum energies by a small number of constants with a clear analytic meaning. Only global aspects of the behaviour of general single particle spectra can be considered in this way. The inclusion of general irregularities in the spectra ("shell effects") will be treated in the next chapter.

Next, in Sec. 3.1 we introduce the powerful concept of a Dirichlet series through the partition function. The analytic properties of the obtained function are analyzed in Sec. 3.2. The logarithm of the grand partition function (Sec. 3.3) is also expressed in terms of Dirichlet series by means of an integral transform. After some algebraic and analytic transformations the logarithm of the partition function will be expressed in terms of ("q") series with good convergence properties for large "temperatures". The saddle point equations are considered in Sec. 3.4. The transformation properties of infinite products of the type we are considering under certain modular transformations are treated in Sec 3.5. Another exact relation for the logarithm of the grand partition function is deduced in Sec. 3.5b, but now with good convergence properties for small "temperatures". Finally, in Sec 3.5c, both obtained relations for the grand partition function are proved to be equivalent. This means that there are two equivalent exact expressions with good convergence properties in distinct regions. This is of course of large advantage, wherever we are interested in the whole energy range.

As mentioned, although the single particle energies ε_ν are real numbers, we substitute them by integer numbers using a sufficiently small energy unit. The involved error can be made as small as we like. The rather intrincate subtleties associated with general real ε_ν will not be regarded. Furthermore, we take $\varepsilon_n = 1,2, \ldots$, and describe a general single particle spectrum by an adequated selection of **degeneracy numbers** a_n . Clearly, we can in this way approximate locally any prescribed finite sequence of levels. Hence, the a_n give the degeneracy of the corresponding ε_n. We are still allowed to impose additional conditions on the degeneracy numbers a_n to consider particular spectra.

To introduce a physically motivated mathematical **assumption**, which also allows explicit calculations, we proceed as follows. Consider the number of particles which can be allocated in the given spectrum up to the level n starting from the lowest level. For this number of particles we assume:

$$\sum_{j=1}^{n} a_j \approx \sum_{m} \frac{A_m}{d_m} n^{d_m} \qquad , \ d_m > d_n \text{ for } m>n \ , \ d_m>0, \tag{3.1}$$

where we have introduced a finite set of **parameters** $\{A_m, d_m\}$, which, for physical reasons, must be real.

The assumption given by eq.(3.1) can be interpreted as a description of the increase of the single particle level density. It expresses the maximal number of particles which can be allocated up to level n. Of course, in particular cases we start from single particle spectra which satisfy eq.(3.1) identically and for which we can write instead of the sign "$\approx$" an equality sign "=". The physical motivation for eq.(3.1) is simply to include the constant single particle spectrum (all $d_m = 1$) as well as spectra of the harmonic oscillator type ($d_m = 1,2,3$) and other similar spectra in a simple way to allow the necessary computations for applications and comparison with experimental data. The assumption (3.1) can be generalized to include spectra with more general shell structure. Some observations and calculations are given in the next chapter.

Of course, we could introduce first a similar assumption for the a_n themselves and deduce a relation like eq.(3.1) with adequate coefficients, but we prefered to work directly with the partial sums since in doing so we simplify our treatment of infinite series later. Further, the numbers a_n are in general very irregular arithmetical functions, whereas their partial sums are easier to handle. We shall later see also the importance to have simple expressions for the ground state energy and the number of particles.

In our present method we find thus :

$$a(n) \approx \sum_{j=1}^{n} a_j - \sum_{k=1}^{n-1} a_k \approx \sum_{m} \frac{A_m}{d_m} (n^{d_m} - (n-1)^{d_m}) = \sum_{m} \frac{A_m}{d_m} \sum_{k=1} \binom{d_m}{k} (-1)^{k+1} n^{\,d_m - k}; \tag{3.2}$$

We write a_n for the discrete function and a(n) for the continuous function with a variable n not necessarely integer. The sum over k will have a finite number of terms if all d_m are integers.

3.1. Introduction of Dirichlet Series

In our statistical investigation the **partition function** plays of course a very important role. We write:

$$Z(x) = \sum \exp(-x\varepsilon_n) = \mathrm{Tr}\, e^{-xH} \quad , \quad \varepsilon_n > 0 \, , \tag{3.1.1}$$

In Analytic Number Theory series of the form

$$\sum a_n \, e^{-s\lambda(n)} , \quad s \in \mathbb{C} \, , \ \lambda(n) > 0 \, , \ a_n \geq 0 \, ,$$

are called **general Dirichlet series** if $\{\lambda(n)\}$ is a strictly increasing sequence of real numbers such that $\lambda(n) \to \infty$ as $n \to \infty$. (see T.M. Apostol, "Modular Functions and Dirichlet Series in Number Theory", Springer Verlag, 1976) . The function associated with the series, in its domain of uniform convergency, can further be seen as the generating function of the numbers a_n.

The series is called **ordinary Dirichlet series** if $\lambda(n) = \ln(n)$. We assume that all Dirichlet series we consider are absolutely convergent for the half-plane $s > \delta > 0$. Further, we assume that they possess an analytic continuation in the region $s > -c$, $0 < c < 1$, and that in such a region they are analytic except for a finite number of real simple poles. We write, using the single particle spectrum description introduced in the last section:

$$Z(s) = \sum_{n>0} a_n \, e^{-sn} \quad , \quad a_n \geq 0, \ \ \mathrm{Re}\, s > \delta > 0, \tag{3.1.2}$$

Thus, we can see Z(s) as the generating function of the degeneracies a_n with respect to the functions exp(-sn).

We are thus naturally lead to study the function $Z(x)$ in the complex plane. In particular, $Z(it)$ is a periodic function of unit period for $t \in \mathbb{R}$. Further, we will analyse the corresponding ordinary Dirichlet series:

$$D(z) = \sum \left(\frac{1}{\varepsilon_m}\right)^z = \sum_{n>0} \frac{a_n}{n^z} = \frac{1}{\Gamma(z)} \int_0^{\infty} dx\, x^{z-1}\, Z(x)\ ,\ \varepsilon_m \neq 0,\ \mathrm{Re}\ z>0\ , \tag{3.1.3}$$

which will play a central role.

Formula (3.1.3) follows from the integral representation of the Γ-function :

$$\Gamma(z) = \int_0^{\infty} dx\, e^{-x} x^{z-1},\ \mathrm{Re}\ z > 0, \text{ and } e^{-x} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dz\, \Gamma(z)\, x^{-z},\ c>0,\ \mathrm{Re}\ x>0, \tag{3.1.4}$$

(see for example Erdelyi A. et al (1953)).

The function $D(z)$ will contain all the relevant information of this problem. The most famous and simple case results from $\varepsilon_\nu \in \mathbb{Z}^+$ leading to the Riemann ζ-function:

$$\zeta(z) = \sum_{n>0} n^{-z} = \frac{1}{\Gamma(z)} \int_0^{\infty} dx\ \ x^{z-1}/(\exp(x) - 1)\ \ ,\ \ \mathrm{Re}\ z > 1, \tag{3.1.5}$$

this function has a simple pole at $z=1$ with residue 1; and in this case $Z_0(x) = 1/(\exp(x)-1)$.

The integral in eq.(3.1.3) is called the **Mellin transform** of $Z(x)$ (see I.N. Sneddon, "The Use of Integral Transforms", McGraw-Hill Book Company, New York, 1972). Thus $\Gamma(z)$ is the Mellin transform of $\exp(-x)$.

3.2. Poles and Residues of the Dirichlet Series.

The function $Z(x)$ can be obtained, once we know $D(x)$, using the inverse Mellin transform:

$$Z(x) = \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} dz\, x^{-z}\, \Gamma(z)\, D(z)\ ,\ \mathrm{Re}\ x > \delta > 0,\ \ \sigma>0, \tag{3.2.1}$$

where we assumed that $D(z)$ has only poles, localized to the left of the contour. For simplicity, we will further assume that these poles are simple (higher order poles can be also included). In **Figure 3.1** we show the integration contour.

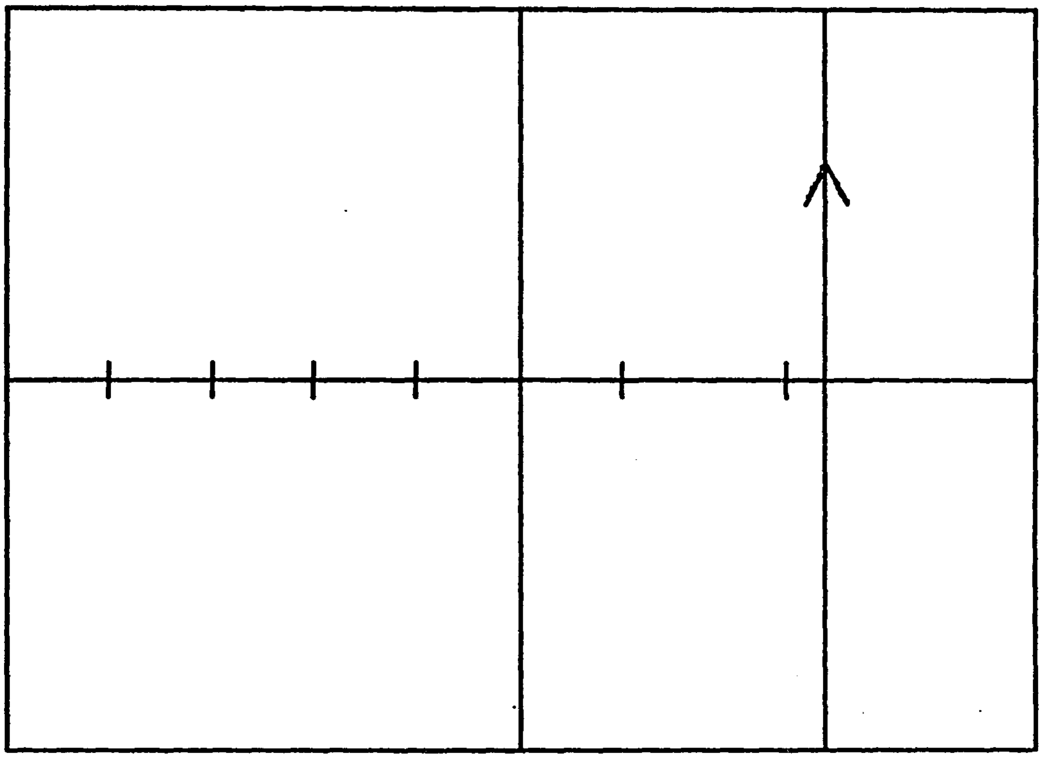


Figure 3.1 Contour integration for eq.(3.2.1)

We will study now the analytic consequences of the form of the spectrum introduced by eq.(3.1) on the series Z(x) and D(s).

From relation (3.2.1) we see that the quantities to which we have to give a physical interpretation are the residues and the position of the poles of D(x), which determine the analytic structure of the infinite sum.

From (3.1), using partial summation, we can approximate D(s) as follows:

$$D(s) = \sum_{n=1}^{\infty} n^{-s}\left[\sum_{j=1}^{n} a_j - \sum_{j=1}^{n-1} a_j\right] \approx \sum_{n=1}^{\infty} n^{-s} \sum_{m} \frac{A_m}{d_m}\left(n^{d_m} - (n-1)^{d_m}\right), \qquad (3.2.2)$$

and then :

$$D(s) \approx \sum_{m} \frac{A_m}{d_m} \sum_{k=1} \binom{d_m}{k} (-1)^{k+1} \zeta(s - d_m + k), \qquad (3.2.3)$$

and this means that D(s) has simple poles at $s = d_i - k + 1$. The leading poles are localized at d_i with residues A_i . For d_m integer the sum over k is finite. Nevertheless, for simplicity, we shall consider only finite sums, disregarding the remaining terms which arise if d_m is non integer.

From Riemann's functional equation for $\zeta(s)$:

$$\zeta(s)=2\Gamma(1-s)(2\pi)^{s-1}\sin(\pi s/2)\zeta(1-s), \text{ or: } \zeta(1-s)=2(2\pi)^{-s}\Gamma(s)\cos(\pi s/2)\zeta(s), \quad (3.2.4)$$

(see Abramowitz M. et al. (1964)).

We find further:

$$D(s)\approx\sum_m \frac{A_m}{d_m}\sum_{k=1}\binom{d_m}{k}(-1)^{k+1}2\Gamma(1-s+d_m-k)(2\pi)^{s-d_m+k-1}\sin(\pi(s-d_m+k)/2)\zeta(1-s+d_m-k), \quad (3.2.5)$$

This equation gives us the **analytic continuation** of D(s) to the left of its poles. Additionally, we can use eq.(3.2.5) to obtain D(-k) entirely in terms of the set $\{d_i,A_j\}$. We need only to remember the values: $\zeta(0) = -1/2$, $\zeta(-2m) = 0$ and $\zeta(1-2m) = -B_{2m}/2m$ for $m=1,2,\ldots$, where the B_n are the Bernoulli numbers ($B_0=1$, $B_1=-1/2$, $B_2=1/6$, $B_3=0$, $B_4=-1/30$, etc.). Note also that if we naively write $z=0,-1,-2,\ldots$ in eq.(3.1.3) we obtain an infinite number, the analytic continuation eq.(3.2.5) gives the correct answer.

The last observation leads to the ζ-function regularization in quantum gravity (see for example D. Ray and I. Singer (1971) or S.W. Hawking (1977)) , where the determinant of the operator H with eigenvalues ε_n is given by the product of all its eigenvalues and is formally :

$$\det H = \prod_{n>o} \varepsilon_n \mathrel{\hat{=}} \exp\{-\partial_s D(s)|_{s=o}\}$$

where the Dirichlet series D(s) is called the Minakshisundaran-Pleijel zeta function and its corresponding series Z(x) is related to the heat kernel by:

$$Z(x) = \int d\alpha(t) \sum_n \psi_n(t)\, \psi_n^{*}(t)\, e^{-\varepsilon_n x} = \int d\alpha(t)\, G(t,t;x)$$

where the eigenfunctions $\{\psi_n\}$ are assumed to be orthonormal with respect to the measure $d\alpha$. Some further technical assumptions are needed.

If we now compute the inverse Mellin transform to D(s) we find from eqs.(3.2.1) and (3.2.3) :

$$Z(x)\approx\sum_{m}A_m(d_m-1)!\sum_{k=1}^{d_m}\frac{1}{k!}(-1)^{k+1}x^{-d_m+k-1}+\sum_{k=0}^{\infty}(-1)^k x^k D(-k)/k!\ ,\ \mathrm{Re}\ x>\delta>0, \tag{3.2.6}$$

We can recognize in the first sum over k the first terms in the expansion of the exponential function and thus we can write:

$$Z(x)\approx\sum_{m}A_m(d_m-1)!\ \mathrm{S.P.}\{x^{-d_m-1}(1-e^{x})\}\ +\sum_{k\geq 0}(-1)^k x^k D(-k)/k!, \tag{3.2.7}$$

where the symbol S.P.{f(x)} means the singular part of f(x) for x→0. Another way to express this result can be found using the incomplete gamma function:

$$\sum_{k=0}^{d_m}\frac{(-x)^k}{k!}=e^{-x}\,\Gamma(d_m+1,-x)\ =\ \int_{-x}^{\infty}dt\ t^{d_m}e^{-x-t}, \tag{3.2.7a}$$

The infinite series on the right hand side of eq.(3.2.6) converges only for a restricted set of values of x. For example, for the simple case of a constant spectrum as mentioned before, we obtain $D(s)=\zeta(s)$ and using :

$$xZ_0(x)\ =\ \frac{x}{\exp(x)-1}\ =\sum_{n=0}^{\infty}\frac{B_n}{n!}x^n\ \ ,\ |x|\ <\ 2\pi, \tag{3.2.8}$$

from the definition of the Bernoulli numbers B_n , we find the condition $0<|x|<2\pi$. In this simple example we note the transformation formula:

$$Z_0(x)\ =\ -e^{-x}\,Z_0(-x)\ ,\quad \text{or well :}\qquad Z_0(t)\ =\ -(1/t)Z_0(1/t)\ ,\ \text{if}\quad t=e^x\ , \tag{3.2.9}$$

this result motivates us to study the general case nearer.

Similarly as we have done for D(s) using partial sums, we can obtain for Z(x) the relation:

$$Z(x)\approx\sum_{n=1}^{\infty}e^{-xn}\sum_{m}\frac{A_m}{d_m}\left(n^{d_m}-(n-1)^{d_m}\right)=\sum_{m}\frac{A_m}{d_m}\sum_{k=1}\binom{d_m}{k}(-1)^{k+1}\sum_{n=1}^{\infty}n^{d_m-k}e^{-xn}\ , \tag{3.2.10}$$

for x outside the negative real axis. If we transform x↦-x, the infinite series must be substituted by its analytic continuation. To perform this transformation we define:

$$Z_\alpha(x) = \sum_{n>o} n^\alpha\, e^{-xn} = (-1)^\alpha \partial^\alpha\, Z_o(x)\,, \tag{3.2.11}$$

this functions have the simple transformation properties:

$$Z_\alpha(x) = (-1)^{\alpha+1} Z_\alpha(-x)\,,\ \alpha=1,2,\ \dots\,, \tag{3.2.12}$$

For non integral α there exists also a transformation rule with an additional term, but for our purposes it is not necessary. Using these functions we rewrite Z(x) as:

$$Z(x) \approx \sum_m \frac{A_m}{d_m} (-1)^{d_m+1} \sum_{k=1} \binom{d_m}{k} \partial^{d_m-k} Z_o(x) = \sum \frac{A_m}{d_m}\Big((-\partial)^{d_m} - (-\partial-1)^{d_m}\Big) Z_o(x), \tag{3.2.13}$$

and recalling the form of the function a(x) given by eq.(3.2):

$$Z(x) = a(-\partial)\, Z_o(x)\,,\ \text{ and: } Z(-x) = -a(\partial)\, e^x Z_o(x) = -a(\partial)\, (Z_o(x)+1)\,, \tag{3.2.14}$$

we remark here that, in general, the function a(x) has not well defined parity, i.e. $a(x) \neq \pm a(-x)$.

Let us now resume some important facts. We started with the estimation of a sum over the set $\{\varepsilon_\nu\}$, say :

$$S(x) = \sum_\nu f(x\varepsilon_\nu) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} ds\, f_M(s)\, D(s)\, x^{-s}\quad,\ c>0,\ \mathrm{Re}\ x>0, \tag{3.2.15}$$

where the function f(t) has a Mellin transform given by (Mellin's inversion formulae) :

$$f_M(s) = \int_o^\infty dt\, f(t)\, t^{s-1}\ ,\qquad f(t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} ds\, f_M(s)\, t^{-s}\quad,\ c>0,\ \mathrm{Re}\ t>0. \tag{3.2.16}$$

Here, $f_M(s)$ with $s=\sigma+i\tau$ is assumed to be regular in the strip: $\{z|a<\sigma<b\}$ and $c\in(a,b)$. We have introduced the Dirichlet series D(s) defined by eq.(3.1.3). The residue theorem leads us now to a result if we know the analytic structure of the functions $f_M(s)$ and D(s). In our case we set f(t) = exp(-t) and we express the function D(s) using relation (3.2) and finally we obtain eq.(3.2.6) for Z(x).

Let us express now our final result for Z(x) in a different form. Mellin transforms satisfy the following relation:

$$x^{-s} f_M(s) = \int_0^\infty dy\, f(xy)\, y^{s-1}, \tag{3.2.17}$$

using this formula for $f_M(s)=\Gamma(s)$, $s=d_m-k+1$, we rewrite eq.(3.2.6) as:

$$Z(x) \approx \int_{0-}^{\infty} dt\, e^{-xt} \left[\sum_m \frac{A_m}{d_m} \sum_{k=1} \binom{d_m}{k} (-1)^{k+1} t^{d_m-k} + \sum_{k=0}^{\infty} D(-k)\delta^{(k)}(t)/k! \right] ,$$

or (cf. eq.(3.1.1)) :

$$Z(x) = \sum \exp(-x\varepsilon_n) \approx \int_{0-}^{\infty} dt\, e^{-xt}\, g(t) \ , \tag{3.2.18}$$

where we have introduced what we will call the **single particle level density**, which is thus naturally defined by:

$$g(t) = \sum_m \frac{A_m}{d_m} \sum_{k=1} \binom{d_m}{k} (-1)^{k+1} t^{d_m-k} + \sum_{k=0}^{\infty} D(-k)\delta^{(k)}(t)/k! \ , \tag{3.2.19}$$

or :

$$g(t) = \sum_m \frac{A_m}{d_m} \left[t^{d_m} - (t-1)^{d_m} \right] + \sum_{k \geq 0} D(-k)\, \delta^{(k)}(t)/k! \ , \tag{3.2.19a}$$

we recognize, of course, in the first term, the expression for $a(n)$ given by eq.(3.2). Hence, for any $t>0$ both functions $g(t)$ and $a(t)$ are equal. From this relation we can evaluate approximately for example the accumulated number of levels up to a given energy by simple integration. Such a procedure is of practical interest if we know from independent considerations (say geometrical, like Weyl's area rule) the coefficients of the corresponding asymptotic expansion.

We stress here again the fact that for a_n , for which for all n, expression (3.1) is an equality, we can also in all other formulae of this section write the equality sign "=" instead of the sign "≈". This will occur for example in the case when the numbers a_n are given by a polynomial in the integer n. In this case, the function $a(n)$ is given trivially by the same polynomial, but of a complex variable and the partial sums of eq.(3.1) can be readily computed using:

$$\sum_{k=1}^{n} k^m = \frac{B_{m+1}(n+1) - B_{m+1}}{m+1} \ , \quad m,n = 1,2, \ldots , \tag{3.2.20}$$

where the Bernuolli polynomials $B_m(t)$ are generated by:

$$\frac{xe^{xt}}{e^{x}-1}=\sum_{n\geq 0}\frac{x^{n}}{n!}B_n(t)\ ,\quad |x|<2\pi\ ,\ \text{and}\quad B_n(t)=\sum_{k=o}^{n}\binom{n}{k}B_k\, t^{n-k}\ , \qquad (3.2.21)$$

with $B_n=B_n(0)$. The first polynomials are: $B_o(t)=1$, $B_1(t)=t-1/2$, $B_2(t)=t^2-t+1/6$, $B_3(t)=t^3-3t^2/2+t/2$.

Remarks. It is important to note that in our approach, we start from the single particle spectra in the form given by assumption (3.1). Thus we do not consider directly the problem related with the calculation of the single particle spectra for a given spectral operator H and associated boundary conditions. The analytic form we assume, also avoids the problem connected with the calculation of a "smooth single particle level density" obtained from a given sequence of eigenvalues $\{\varepsilon_n\}$. For both mentioned problems exist large amounts of efforts and important results, but for our purposes, we find much more adequate to start directly from a simple explicit and general expression for the eigenvalues themselves.

We remark the different interpretation of $g(\varepsilon)$. In the literature $g(\varepsilon)$ is the result of a smoothing procedure starting from a given discrete spectrum. Here $g(\varepsilon)$ is defined for any discrete spectrum by eq.(3.2.19). For $\varepsilon\to 0$, the derivatives of $\delta(\varepsilon)$ lead to additional contributions not present in the formula coming from any smoothing procedure of a discrete spectrum. These contributions are physically important for the description of the shell effects and mathematically indispensable for reasons which will appear clearer in the course of this work.

3.2a. An Alternative Procedure.

In the method we have presented, the partial sums, eq.(3.1), contain all the necessary information about the single particle spectrum we consider. Alternatively, we could proceed in the following different way. Suppose we start with the knowledge of the position of the poles (here assumed to be simple) and their residues of the Dirichlet series.

In such a case we can again obtain directly Z(x) and $g(\varepsilon)$ in the same way as we have done before. If for example D(s) has poles at $z=b_j>0$, with residues B_j, then from eq.(3.2.1) we find :

$$Z(x)=\sum_{m} x^{-b_m}\ \Gamma(b_m)B_m\ +\sum_{k\geq 0}(-1)^{k} x^{k} D(-k)/k!\ , \tag{3.2.22}$$

and:

$$g(\varepsilon)=\sum_{m} \varepsilon^{b_m-1} B_m\ +\sum_{k\geq 0} D(-k)\ \delta^{(k)}(\varepsilon)/k!\ , \tag{3.2.23}$$

Similarly, many of the results we will obtain later can be found also directly.

Nevertheless, to obtain the partial sums given by eq.(3.1) or to write the numbers a_n in terms of the position of the poles and the corresponding residues of D(s) is a non trivial problem. By a formula due to Perron (c.f. T.M. Apostol, 1976), we know that:

$$\sum_{n\leq\mu_0}\frac{a_n}{n^s} = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} dz\ D(z+s)\ \frac{\mu_0^z}{z}\ , \qquad c>0,\ \mu_0>0,\ \mathrm{Re}\ s > \sigma_a - c\ , \tag{3.2.24}$$

where the last term in the sum must be multiplied by 1/2 if μ_0 is an integer. Here, σ_a is the abscisa of absolute convergency of D(z) and the integral is understood as a principal value. From this formula for $s=0$ and if D(z) has only simple poles at d_j with residues A_j, we shoud obtain eq.(3.1). Actually, Perron's formula is not quite useful for our purposes as it stands, since if we write the complete expression for D(s) given by eq.(3.2.3) we do not obtain easily eq.(3.1). The result of a contour integration around the (simple) poles of D(s) gives for $s=0$, instead of the partial sum over a_n, the integral of the continuous function a(y) up to μ_0. We can see this as follows. From eq.(3.2) we obtain after integration:

$$\int d\mu\ a(\mu)= \sum_{m}\frac{A_m}{d_m}\sum_{k=1}\binom{d_m}{k}(-1)^{k+1}\mu^{d_m-k+1}/(d_m-k+1)\ +\ \text{constant}\ , \tag{3.2.25}$$

and this is the expression we obtain after the mentioned contour integration in Perron's formula using the explicit form for D(s) and setting the constant equal to D(0). Of course, this is possible only when we can assume that the a(y) are integrable functions. Nevertheless, it is clear that, once we know the position of the poles of D(s), we can find readily the leading term of the partial sums over a_n without a previous explicit knowledge of them. The reason of the discrepancy is that the integral in Perron's formula is a principal value integral and we have interpreted it as a contour integral around the poles of the integrand.

The assumption (3.2) can be understood as follows. In general, the series D(s) will be defined in terms of discrete functions a_n of the integer n, which can not be easily described by a continuous function a(n) (for n not necessarely integer). But with expression (3.2) being at least approximately valid, we have such a continuous function a(n) and for D(s) we find eq.(3.2.3) described in terms of the Riemann ζ-function, but only as far as there are only a finite number of poles. It is not difficult to construct examples of Dirichlet series with an infinite number of poles, but we shall assume that all the Dirichlet series D(s) that we study have only a finite number of poles.

Since the straightforward application of Perron's formula is difficult in general, a simple method equivalent to assumption (3.2) for the partial sums could be quite useful.

The following formula solves our particular problem:

$$\frac{1}{2\pi i}\int_{\Gamma} dz\ D(z+s)\sum_{n=1}^{m} n^{z-1} \approx \sum_{n=1}^{m} \frac{a_n}{n^s} \qquad , m=1,2, \ldots , \qquad (3.2.26)$$

where the contour Γ encloses all poles (here assumed to be simple) of D(z) and supposed to be different from zero. If we set $s=0$ and insert eq.(3.2.3) for D(z) we obtain eq.(3.1) for the partial sums. Only if all d_m are integer numbers we can write signs "=" instead of "$\approx$" signs. For $s=-k$, $k=1,2, \ldots$, we obtain also closed expressions for the partial sums if all d_m are integer numbers. The similitude of eq.(3.2.26) with Perron's formula can be made clearer if we note that:

$$\sum_{n=1}^{m} n^{z-1} = \frac{m^z}{z} + \frac{m^{z-1}}{2} + \frac{zm^{z-2}}{12} + \ldots , \qquad \mathrm{Re}\ z \geq 1, \qquad (3.2.27)$$

obtainable from the Euler-Maclaurin summation formula. The first terms result from the integration of n^{z-1}. Thus, if we replace in relation (3.2.26) the sum by m^z/z (viz. we replace the finite sum in the contour integral by the integral over n^{z-1}) we find the smooth result.

From relation (3.2.26) for $s=0$, we find:

$$a_j = \frac{1}{2\pi i}\int_{\Gamma} dz\ D(z)\ j^{z-1} \quad , \qquad (3.2.28)$$

this relation yields eq.(3.2) if we use eq.(3.2.3) for D(s). It is interesting to note the similitude of (3.2.28) with the expression for the coefficients of the

Laurent series of a function f(z) holomorphic in the outer region bound by a contour C surrounding the origin:

$$f(z)=\sum_{n\geq o} \alpha_n z^{-n}\ , \quad \text{and} \quad \alpha_n=\frac{1}{2\pi i}\int_C dz\ f(z)\ z^{n-1}\ , \tag{3.2.29}$$

This similitude results from the fact that the Dirichlet series Z(x) (see eq.(3.1.2)) can be written as a Laurent series if we do the change of variables $z=\exp(x)$.

3.3. Expression of the Grand Partition Function by the Poles and Residues.

In this section we introduce one further element. We consider the additional complex variable α which accounts for the chemical potential introduced to fix the number of particles.

In the next section we will analyse the saddle point equations, the solution of which will then be parametrized by the set of constants $\{d_j, A_i\}$. But first we need to estimate $Z(\alpha,\beta)$ which we rewrite as:

$$\ln Z(\alpha,\beta)=\sum_{k>0} (-1)^{k+1}\ \frac{1}{k}\ e^{k\alpha}\ Z(k\beta)= \frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} dz\ \frac{\pi e^{\alpha z}\ Z(\beta z)}{z\ \sin(\pi z)}\ ,\ 0<\sigma<1, \tag{3.3.1}$$

The last integral on the far right hand side can be shown to be equivalent to the infinite series of this equation using the Laurent series:

$$\frac{\pi}{\sin \pi z} = \frac{1}{z} + 2z\sum_{k=1}^{\infty} \frac{(-1)^k}{z^2 - k^2}\ , \tag{3.3.1a}$$

and evaluating the residues at $z=1,2,\ldots$.

With eq.(3.2.9) we have, for a restricted kind of spectrum, a Laurent series for Z(x) which allows a very simple integration of eq.(3.3.1), under the condition that the sums are well defined, at least asymptotically.

The integration in eq.(3.3.1) has now **three different contributions:**

a) The pole at $z=0$ with terms of different multiplicities, resulting from the poles of D(x).

b) The simple poles of $1/\sin(\pi z)$ for $z<0$ integer.

c) The singularities from the function given by the infinite series in eq.(3.2.6) with coefficients D(-k).

Let us write these contributions separately as:

$$\ln Z(\alpha,\beta) = I_a + I_b + I_c \,, \qquad (3.3.2)$$

In **Figure 3.2**, we show the integration contours. For the contribution (a), we have a small circle around the origin. For (b), the contour encloses all negative integers. And for (c), the contour encloses all the positive and all the negative imaginary integer numbers. The straigth line parallel to the imaginary axis is the integration path used in eq.(3.3.1) .

We evaluate them now further. First we have from eqs.(3.3.1) and (3.2.6), expanding 1/sin x around x=0 :

$$\frac{1}{\sin x} = \frac{1}{x} + \sum_{k=1}^{\infty} \frac{(-1)^{k-1} 2(2^{2k-1}-1) B_{2k}\, x^{2k-1}}{(2k)!} \quad , \ |x| < \pi \,, \qquad (3.3.3)$$

the expression:

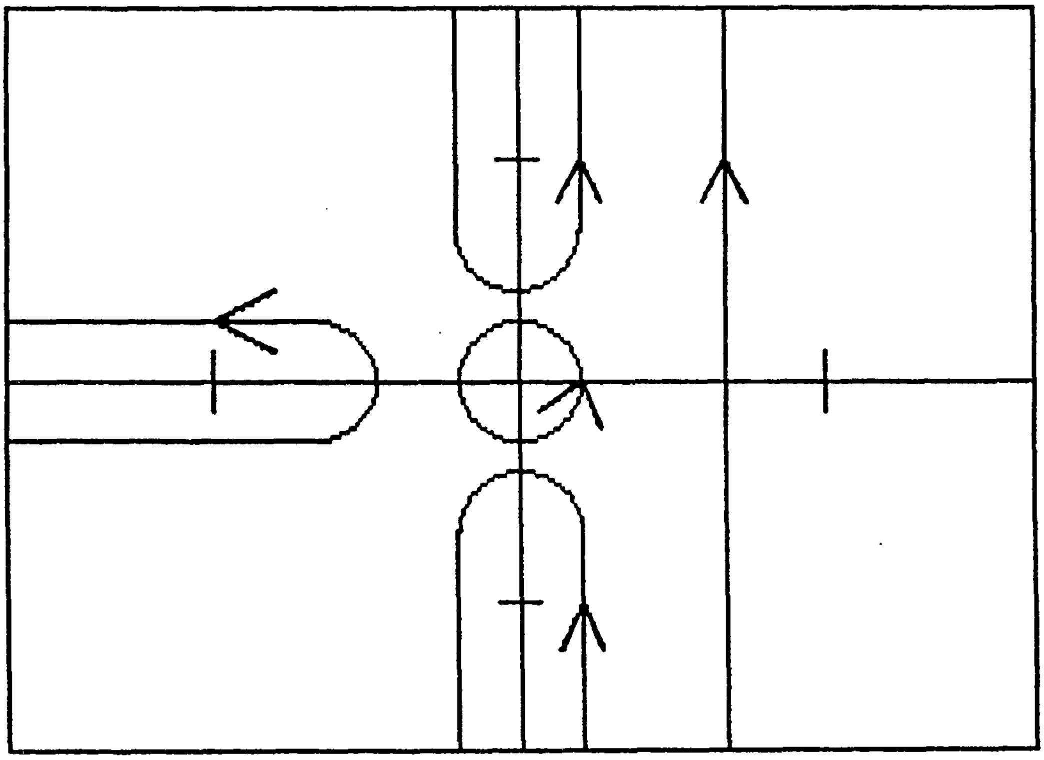


Figure 3.2 Integration contours for eq.(3.3.2) .

$$I_a = \frac{\pi^2}{2\pi i} \int_{C_o} dz\, e^{\alpha z} \Big(\sum_m \frac{A_m}{d_m} \sum_{k=1} \binom{d_m}{k} (-1)^{k+1} \Gamma(d_m-k+1)\, z^{-d_m+k-1} \beta^{-d_m+k-1} + \sum_{k=o}^{\infty} (-1)^{-k} (z\beta)^k D(-k)/k! \Big) \cdot \qquad (3.3.4)$$

$$\cdot \left[\frac{1}{\pi^2 z^2} + \frac{1}{6} + \frac{7}{360} (\pi z)^2 + \cdots + \frac{(-1)^{k-1}\, 2(2^{2j-1}-1)}{(2j)!} (\pi z)^{2j-2} B_{2j} + \cdots \right],$$

where C_o is a small contour enclosing the origin.
We find after contour integration:

$$I_a = \pi^2 \sum_m \frac{A_m}{d_m} \sum_{k=1} \binom{d_m}{k} (-1)^{k+1} (d_m-k)!\, \beta^{-d_m+k-1} \Big[\frac{\alpha^{d_m-k+2}}{(d_m-k+2)!\,\pi^2} + \frac{\alpha^{d_m-k}}{(d_m-k)!\,6} + \frac{7\pi^2 \alpha^{d_m-k-2}}{(d_m-k-2)!\,360} +$$

$$+ \frac{(-1)^{j-1}\, 2(2^{2j-1}-1)\pi^{2j-2}}{(2j)!\,(d_m-2j-k+2)!} \alpha^{d_m-2j-k+2} B_{2j} + \cdots \Big] + \alpha\, D(0) - \beta\, D(-1), \qquad (3.3.5a)$$

where the sum in the bracket has a finite number of terms. If we take into account all terms, the only approximation involved would be the assumption (3.1) for the partial sums of the a_n, which for particular spectra are anyway satisfied exactly. Using now the definition for $g(\mu)$, eq.(3.2.19), we arrive at :

$$I_a = \int_{o-}^{\mu} d\varepsilon\, g(\varepsilon)(\alpha - \beta\varepsilon) + \sum_{j>0} \frac{(-1)^{j-1}\, 2(2^{2j-1}-1)\pi^{2j}}{(2j)!\,\beta^{2j-1}} B_{2j} g^{(2j-2)}(\mu), \qquad (3.3.5b)$$

or:

$$I_a = \int_{o-}^{\mu} d\varepsilon\, g(\varepsilon)(\alpha - \beta\varepsilon) + \frac{\pi^2}{6\beta} g(\mu) + \frac{7\pi^4}{360\beta^3} g''(\mu) + O(g^{(iv)}(\mu)),$$

which is formally equal to the known results obtained using a "smooth" single particle level density (see Bohr A. & Mottelson B. (1968)). Nevertheless, this is only one part of our results and we have additionally a deeper understanding of the analytic behaviour of the involved functions as well as a better method for practical explicit computation, as we shall see in chapter five.

For the second integral around the negative integers we obtain formally from eq.(3.3.1), shifting the contour to the left:

$$I_b = \ln Z(-\alpha, -\beta) = \sum_{k>o} (-1)^{k+1} k^{-1} e^{-k\alpha} Z(-k\beta), \tag{3.3.6}$$

We shall disregard this term later in the calculation with the saddle point method (see section 3.4), since we shall consider degenerated systems for which $\alpha \gg 1$. Nevertheless, let us mention that this term is very relevant for another reason. It reflects important properties associated with modular forms (see for example H. Rademacher, "Topics in Analytic Number Theory", Springer-Verlag, N.Y., 1973). Actually, this occurs for the simple case where the single particle spectrum consists only of equally spaced levels with equal degeneracy. But as our calculation shows, it is possible to extend some important properties to the more interesting case we are considering. In a later section and in the next chapter we will analyse these aspects more in detail.

Finally, for the last integral we need a similar estimation as for the first case. Since we evaluate the integral in eq.(3.3.1) over the imaginary axis (without the origin), we need to know the behaviour of $Z(s+it)$ for $s \to +0$ and fixed $|t| > 0$.
The last infinite sum in eq.(3.2.10) can be rewritten using (see for example K. Chandrasekharan (1985)) :

$$\sum_{n=1}^{\infty} n^{\rho-1} \exp(-nz) = \Gamma(\rho) \sum_{n=-\infty}^{\infty} (z+2\pi i n)^{-\rho} , \quad \rho > 1, \ \mathrm{Re}\, z > 0, \tag{3.3.7}$$

yielding for $d_m > k$:

$$Z(x) \approx \sum_m \frac{A_m}{d_m} \sum_{k=1}^{d_m-1} \binom{d_m}{k} (-1)^{k+1} \Gamma(d_m-k+1) \sum_{n=-\infty}^{\infty} \frac{1}{(x+2\pi i n)^{d_m-k+1}}, \tag{3.3.8}$$

we see clearly that this function will have for $|\mathrm{Im}\, x| > 0$ poles of order d_m-k+1 at $x = \pm 2\pi n i$, $n \neq 0$. With eq.(3.3.8) we have an analytic continuation for $Z(x)$, which gives us also the residues of the poles located at the imaginary axis. The terms with $d_m = k$ give additional contributions which are regular for the integration contour considered for I_c and thus, they disappear after integration. Explicitly :

$$\sum_{n>0} e^{-nz} = \frac{\cosh(z/2)}{2\sinh(z/2)} - 1/2 = z^{-1} - 1/2 + \sum_{\substack{-\infty \\ n\neq 0}}^{+\infty} \left[\frac{1}{z+2\pi i n} - \frac{1}{2\pi i n} \right], \qquad (3.3.9)$$

where we see clearly that the first two terms do not contribute to I_c .

The series given in eq.(3.3.8) are also expressible in terms of the logarithmic derivative of the Γ-function and its derivatives :

$$\psi(z) = \Gamma'(z)/\Gamma(z) \text{ , and } \psi^{(n)}(z) = (-1)^{n+1} n! \sum_{k\geq o} \frac{1}{(z+k)^{n+1}} \qquad (3.3.10)$$

Finally, the terms with $k>d_m$ have no poles at the imaginary axis and so they also do not contribute to I_c .

We obtain from eqs.(3.3.1) and (3.3.7), for d_m all integers:

$$I_c = \sum_m \frac{A_m \pi}{d_m} \sum_{k=1}^{d_m} \binom{d_m}{k} \frac{(-1)^{k+1}}{\beta^{d_m-k+1}} \sum_{\substack{-\infty \\ n\neq 0}}^{\infty} \partial_z^{d_m-k} \left[\frac{e^{\alpha z}}{z \sin(\pi z)} \right]_{z=2\pi i n/\beta}, \qquad (3.3.11)$$

where the $(d_m$-k)-th derivative respect to z is to be evaluated at $2\pi i n/\beta$. With the change of variable $z=2\pi i n t$, $t=1/\beta$ and $\sin(ix) = i\sinh(x)$ we find:

$$I_c = \sum_m \frac{A_m \pi}{d_m} \sum_{k=1}^{d_m} \binom{d_m}{k} \frac{i(-1)^k}{(2\pi i \beta)^{d_m-k+1}} \partial_t^{d_m-k} \frac{2}{t} \sum_{n>o} \frac{\sigma_{d_m-k}\cos(2\pi\alpha n t) + i\sigma_{d_m-k+1}\sin(2\pi\alpha n t)}{n^{d_m-k+1}\sinh(2\pi^2 n t)} \qquad (3.3.12a)$$

with $\sigma_{2m}=1$ and $\sigma_{2m+1}=0$. for $m=0,1,2, \dots$, or :

$$I_c = \sum_m \frac{A_m \pi}{d_m} \sum_{k=1}^{d_m} \binom{d_m}{k} \frac{i(-1)^k}{(2\pi i\beta)^{d_m-k+1}} \partial_t^{d_m-k} \frac{2}{t} \Big[\sigma_{d_m-k} C_{d_m-k+1}(\alpha/\beta, \pi/\beta) + i\sigma_{d_m-k+1} S_{d_m-k+1}(\alpha/\beta, \pi/\beta) \Big], \qquad (3.3.13)$$

where we have introduced the following q-series (set $q=\exp(2\pi t)$) :

$$C_{2m+1}(z,t) = \sum_{n>o} \frac{\cos(2\pi n z)}{n^{2m+1}\sinh(2\pi n t)}, \quad S_{2m}(z,t) = \sum_{n>o} \frac{\sin(2\pi n z)}{n^{2m}\sinh(2\pi n t)}, \qquad (3.3.14)$$

for $|\mathrm{Im}(z)| < \pi \mathrm{Re}(t)$. We recognize further that, for each $t= i\tau$ and τ beeing a rational number, these series have a singular point. In other words, the unit circle $|q|=1$ is a natural boundary.

But, for z in the strip of uniform convergency, we can differentiate and integrate the series term by term and in this way we relate both q- series to each other:

$$\begin{aligned} \partial_z C_{2m+1} &= -2\pi\, S_{2m}\,, & 2\pi\int dz\, C_{2m+1} &= S_{2m+2}\,, \\ \partial_z S_{2m} &= 2\pi\, C_{2m-1}\,, & 2\pi\int dz\, S_{2m} &= -\,C_{2m+1}\,, \end{aligned} \qquad (3.3.15)$$

for $m=0,\pm1,\pm2,\ldots$. Thus, we can select any of them as "fundamental". For us $C_1(z,\pi t)$ is the most important because, save a constant, it is precisely the well known q-series for the logarithm of Jacobi's ϑ_0-function (see later). Furthermore, C_1 is the coefficient of the largest power of the chemical potential for I_c as we shall see and it is always present for the kind of spectra we study.

The expression (3.3.13) for I_c is exact if the spectrum satisfies eq.(3.1) also exactly. For practical calculations, however, we can simplify the expression much more, if we consider the problem of a system at large temperature (small $|\beta|$). In this case, we need only to consider the largest powers in the chemical potential α/β . We compute now explicitly the derivatives appearing in eq.(3.3.12). We begin with:

$$\partial_t^{\kappa}\sum_{n\geq1}\frac{\exp(2\pi in\alpha t)}{tn^{\kappa+1}\sinh(2\pi^2nt)} = (2\pi i)^{\kappa}\sum_{n\geq1}\Bigg[\frac{2\alpha^{\kappa}\cos(2\pi n\alpha t)}{tn\,\sinh(2\pi^2nt)} - \frac{\kappa\alpha^{\kappa-1}\sin(2\pi n\alpha t)}{\pi t^2n^2\sinh(2\pi^2nt)} - \qquad (3.3.16)$$
$$- \frac{\kappa\alpha^{\kappa-1}2\pi\sin(2\pi n\alpha t)\cosh(2\pi^2nt)}{tn\,\sinh^2(2\pi^2nt)}\Bigg] + O(\alpha^{\kappa-2}e^{-2\pi^2t}),$$

we set now $\kappa=d_m-k$, $t=1/\beta$, $\mu=\alpha/\beta$:

$$I_c=\sum_m\frac{A_m}{d_m}\sum_{k=1}^{d_m}\binom{d_m}{k}\frac{(-1)^k}{2\beta^{d_m-k+1}}\Bigg[\sum_{n\geq1}\Bigg[\frac{2\beta\alpha^{d_m-k}\cos(2\pi n\mu)}{n\,\sinh(2\pi^2n/\beta)} - \frac{(d_m-k)\beta^2\alpha^{d_m-k-1}\sin(2\pi n\mu)}{\pi n^2\sinh(2\pi^2n/\beta)} - \qquad (3.3.17)$$
$$- \frac{(d_m-k)\beta\alpha^{d_m-k-1}2\pi\sin(2\pi n\mu)\cosh(2\pi^2n/\beta)}{n\,\sinh^2(2\pi^2n/\beta)}\Bigg] + O(\alpha^{d_m-k-2}e^{-2\pi^2t})\Bigg]\,,$$

we evaluate now the summations over k and m using eq.(3.2.19) for $g(\mu)$ and find:

$$I_c = \sum_{n\geq 1}\left[-\frac{g(\mu)\cos(2\pi n\mu)}{n\sinh(2\pi^2 n/\beta)} + \frac{g'(\mu)\sin(2\pi n\mu)}{2\pi n^2 \sinh(2\pi^2 n/\beta)} + \right.$$

$$\left. + \frac{g'(\mu)\,\pi\sin(2\pi n\mu)\cosh(2\pi^2 n/\beta)}{\beta n \sinh^2(2\pi^2 n/\beta)} \right] + O(g''(\mu)e^{-2\pi^2 t}),$$

and finally, using the q-series defined by eq.(3.3.14) :

$$I_c = -g(\mu)C_1(\mu,\pi t) + \frac{1}{2\pi}g'(\mu)S_2(\mu,\pi t) - \frac{1}{2\pi\beta}g'(\mu)\partial_t S_2(\mu,\pi t) + O(g''(\mu)e^{-2\pi^2 t}), \tag{3.3.18}$$

The contributions given explicitly in eq.(3.3.18) are the only terms necessary for practical calculations for spectra of the class we consider (those which fulfil eq.(3.1)). Of course, only if the "temperature" $|1/\beta|$ is large enough.

We have thus obtained relations useful for applications for a large class of spectra. Nevertheless, here too, it becomes possible to write the full series in terms of the derivatives of $g(\mu)$. We find from eq.(3.3.11):

$$I_c = \sum_m \frac{A_m}{d_m}\pi \sum_{k=1} \binom{d_m}{k} \frac{(-1)^{k+1}}{\beta^{d_m-k+1}} \sum_{n\neq 0} \sum_{j=0}^{d_m-k} \binom{d_m-k}{j} \alpha^{d_m-k-j} e^{\alpha z} \partial_z^j \frac{1}{z\sin\pi z}\bigg|_{2\pi i n/\beta},$$

we interchange now the sums over j and k and find :

$$I_c = -\sum_{j>0} \frac{g^{(j-1)}(\mu)}{\beta^j (j-1)!(2\pi i)^{j-1}} \partial_t^{j-1} t^{-1} D_j(\mu,\pi t), \tag{3.3.12b}$$

where we defined (cf. eq.(3.3.14) :

$$D_j(\mu,\pi t) = \sigma_{j-1}C_j(\mu,\pi t) + i\sigma_j S_j(\mu,\pi t), \tag{3.3.19}$$

(remember that : $\sigma_{2m}=1$, $\sigma_{2m+1}=0$).

Now, we can add all contributions to obtain the **final formula** for the grand partition function:

$$\ln Z(\alpha,\beta) = \ln Z(-\alpha,-\beta) + \int_{0-}^{\mu} d\varepsilon\, g(\varepsilon)(\alpha-\beta\varepsilon) + \sum_{j>0} \frac{(-1)^{j-1} 2(2^{2j-1}-1)\pi^{2j}}{(2j)!\beta^{2j-1}} B_{2j} g^{(2j-2)}(\mu) - \tag{3.3.20}$$

$$- \sum_{j>0} \frac{g^{(j-1)}(\mu)}{\beta^j (j-1)!(2\pi i)^{j-1}} \partial_t^{j-1} t^{-1} D_j(\mu,\pi t),$$

where the single particle level density $g(\varepsilon)$ is given by eq.(3.2.19). With this expression in terms of the derivatives of the single particle level density we can conclude that also for the general case where the numbers d_m are non integers, we obtained a relation for the partition function with $g(\varepsilon)$ given by eq.(3.2.19a). With this expression we arrive thus essentially to a Fourier series for the logarithm of the partition function $Z(\alpha,\beta)$.

In a later section we will find expressions which are completely equivalent to the equations we have obtained in this section, but are given only in terms of β itself. Such expressions will be important if the temperature is low.

From eqs.(3.3.12) we recognize an oscillatory behaviour as function of the "chemical potential" $\mu=\alpha/\beta$ and damped by the "temperature" $1/\beta$. This contribution leads to the energy dependent shell effects which will allow a better description as that given in the current formulae for nuclear level densities. This term is in some respect the most interesting, also from a mathematical point of view. As we already mentioned, it can be related to the logarithm of a Jacobi theta function for a constant single particle spectrum. This is important since these functions have a very far developed theory.

3.4. Explicit Expressions for the Saddle Point Equations.

The saddle point equations can now be readily written using the two contributions for ln $Z(\alpha_j,\beta)$ given by equations (3.3.5) and (3.3.11). The parameter set $\{d_j,A_k\}$ could be selected for protons in a different way as for neutrons.

The partial derivation with respect to β of eq.(3.3.5a) leads to an "asymptotic" series in positive powers of the chemical potential $\mu=\alpha/\beta$ and the temperature $1/\beta$ plus a constant term :

$$\partial_\beta I_a = -\sum_m \frac{A_m}{d_m} \sum_{k=1} \binom{d_m}{k} (-1)^{k+1} \left[\mu^{d_m-k+2} \frac{1}{(d_m-k+2)} + \mu^{d_m-k} \frac{(d_m-k+1)\pi^2}{6\beta^2} + \ldots \right] - D(-1), \tag{3.4.1a}$$

where the sum in square braquets is finite. This contribution constitutes what is usually called the "smooth part" of the excitation energy. The constant term is a shift of the ground state energy. This is the proper origin of what leads to the so called "back-shifted" formulas of the literature of nuclear level densities. On the other hand, this constant is intimately related to the "dimensions" of the modular forms mentioned after eq.(3.3.6).

We can express all the coefficients of powers of $1/\beta$ by $g(\alpha/\beta)$ and its derivatives using eq.(3.2.19), for example:

$$\sum_{m} \frac{A_m}{d_m} \sum_{k=1} \binom{d_m}{k} (-1)^{k+1}(d_m-k+1)\mu^{d_m-k} = g(\mu) + g'(\mu)\mu \quad , \quad \mu>0 \qquad (3.4.2)$$

is the coefficient of $1/\beta^2$ in eq.(3.4.1). The first term in eq.(3.4.1) plus the constant term can be easily recognized as the **"smooth" ground state energy** defined by:

$$\widetilde{E}_o = \int_{o-}^{\tilde{\mu}_o} d\varepsilon \, g(\varepsilon) \, \varepsilon = \sum_{m} \frac{A_m}{d_m} \sum_{k=1} \binom{d_m}{k} (-1)^{k+1} \frac{\tilde{\mu}_o^{d_m-k+2}}{d_m-k+2} + D(-1), \qquad (3.4.3a)$$

if $\tilde{\mu}_o$ is the "smooth" Fermi level. This quantity can be obtained in terms of the particle number solving eq.(3.4.5a). We call it "smooth" since an integral replaces the sum appearing in the **ground state energy** E_o, given by:

$$E_o = \sum_{\varepsilon_n \leq \mu_o} \varepsilon_n + \delta = \sum_{n \leq \mu_o} n \, a_n + \delta \approx \sum_{m} \frac{A_m}{d_m} \sum_{k=1} \binom{d_m}{k} (-)^{k+1} \sum_{n \leq \mu_o} n^{d_m-k+1} + \delta \, , \quad (3.4.3b)$$

where μ_o is the Fermi level, situated anywhere between the last (partially) filled level and the following empty level. Here, δ is the contribution from the last (partially) filled level. We can express μ_o in terms of the particle number solving eq.(3.4.5b). Note that if we replace in the last sum of eq.(3.4.3b) the sum by an integral from 0 up to $\tilde{\mu}_o$, we obtain eq.(3.4.3a) up to a constant. The sum is rather given, for d_m integer, in closed form in terms of the Bernoulli polynomials (see eq.(3.2.21).)

Remark. The "ground state energies" E_o and $\widetilde{E}_o$ have no physical meaning. Only their difference will play a relevant role. The "smooth" energy will be replaced by the liquid drop ground state energy to make comparisons with experimental data.

We have the following alternative expression to eq.(3.4.1a), using the definition of $g(\mu)$ given by eq.(3.2.19):

$$\partial_\beta I_a = -\int_{o-}^{\mu} d\varepsilon g(\varepsilon)\varepsilon - \sum_{j>0} \frac{(-1)^{j-1} 2(2^{2j-1}-1)\pi^{2j}}{(2j)!\ \beta^{2j}} \ B_{2j}\left[(2j-1)g^{(2j-2)}(\mu) + \ \mu g^{(2j-1)}(\mu)\right] ,$$

or :

$$\partial_\beta I_a = -\int_{o-}^{\mu} d\varepsilon \ g(\varepsilon)\varepsilon - \frac{\pi^2}{6\beta^2}\left[\mu g'(\mu) + g(\mu)\right] - \frac{7\pi^4}{120\beta^4} \ g'' - \frac{7\pi^4\mu}{360\beta^4} g''' + O\left(g^{iv}(\mu)\right), \quad (3.4.1b)$$

which, of course, follows also directly from eq.(3.3.8b).

The partial derivation of I_a with respect to α is:

$$\partial_\alpha I_a = \sum_m \frac{A_m}{d_m} \sum_{k=1} \binom{d_m}{k} (-1)^{k+1} \left[\mu^{d_m-k+1} \frac{1}{(d_m-k+1)} + \ \mu^{d_m-k-1} \frac{(d_m-k)\pi^2}{6\beta^2} + \ \dots \right] + D(0) , \quad (3.4.4a)$$

where again we can express all coefficients in terms of $g(\alpha/\beta)$ and its derivatives. In particular, if again $\mu \approx \tilde{\mu}_o$ (the smooth Fermi level), then we recognize in the first term the particle number :

$$N = \int_{o-}^{\tilde{\mu}_o} d\varepsilon \ g(\varepsilon) = \sum_m \frac{A_m}{d_m} \sum_{k=1} \binom{d_m}{k} \ (-1)^{k+1} \frac{\tilde{\mu}_o^{\,d_m-k+1}}{d_m-k+1} \ + \ D(0) , \quad (3.4.5a)$$

in contrast with the formula (cf. eq.(3.1), exact for d_m all integer):

$$N = \sum_{n \le \mu_o} a_n + \gamma \approx \sum_m \frac{A_m}{d_m} \ [\mu_o]^{\ d_m} \ + \ \gamma , \quad (3.4.5b)$$

where γ is the number of particles in the last (half) filled level. Here [x] means the integer part of x.

Using $g(\mu)$ we write (3.4.4a) as follows:

$$\partial_\alpha I_a = \int_{o-}^{\mu} d\varepsilon g(\varepsilon) \ + \ \sum_{j>0} \frac{(-1)^{j-1} 2(2^{2j-1}-1)\pi^{2j}}{(2j)!\ \beta^{2j}} \ B_{2j} g^{(2j-1)}(\mu) ,$$

or also :

$$\partial_\alpha I_a = \int_{o-}^{\mu} d\varepsilon \ g(\varepsilon) \ + \frac{\pi^2}{6\beta^2} \ g'(\mu) \ + \ O(g''(\mu)) , \quad (3.4.4b)$$

and this expression results also from eq.(3.3.8b) directly.

The second order derivatives are:

$\partial^2_{\alpha\alpha} I_a = g(\mu)/\beta + \sum_{j>o} c_j g^{(2j)}(\mu)$, with: $c_j = (-)^{j-1} 2(2^{2j-1}-1)\pi^{2j} B_{2j}/(2j)!\beta^{2j+1}$,

$$\partial^2_{\beta\beta}I_a = \mu^2\partial^2_{\alpha\alpha}I_a + \sum_{j>o} 2jc_j\left[(2j-1)g^{(2j-2)}(\mu) + 2\mu g^{(2j-1)}(\mu)\right] ,$$

$$\partial^2_{\alpha\beta}I_a = -\mu\partial^2_{\alpha\alpha}I_a - \sum_{j>o} 2jc_j g^{(2j-1)}(\mu).$$

If we consider only the contributions given explicitely in eq.(3.4.1) to the saddle point eqs.(2.6), we obtain a result valid for large excitation energies but without energy dependent shell corrections. That is, if we disregard the second saddle point equation $\partial_\alpha S=0$ and write $\mu=\tilde{\mu}_o$. Nevertheless, also in such a situation, we have a good explanation for the constant shiftings in the excitation energy dependency. We find easily neglecting terms expressed in higher order derivatives of $g(\tilde{\mu}_o)$ in eq.(3.4.1) as well as the contribution coming from I_c :

$$U + (E_o - \widetilde{E}_o) \approx \frac{\pi^2}{6\beta^2} \sum_m \frac{A_m}{d_m} \sum_{k=1} \binom{d_m}{k} (-1)^{k+1} (d_m-k+1)\, \tilde{\mu}_o^{d_m-k} , \qquad (3.4.6)$$

where U is the excitation energy , E_o is the ground state energy and $\widetilde{E}_o$ is its estimate given by eq.(3.4.3a), where the chemical potential $\tilde{\mu}_o$ is obtained solving eq.(3.4.5a) in terms of N . We will call the difference $E_o-\widetilde{E}_o$ the **ground state shell energy correction $E_{shell}(0)$**. In this crude approximation we would have disregarded all temperature dependent irregularities of the spectra. Thus, for example the chemical potential μ would be approximated by the smooth Fermi level $\tilde{\mu}_o$. The following calculations will remove these restrictions.

From eq.(3.3.15b) we find:

$$\partial_\beta I_c = \sum_{j>0}\left[\frac{g^{(j)}(\mu)\partial_t^{j-1} t^{-1} D_j + 2\pi i g^{(j-1)}(\mu)\partial_t^{j-1} t^{-1} D_{j-1}}{(j-1)!\beta^{j+1}(2\pi i)^{j-1}}\mu + \frac{g^{(j-1)}(\mu)(j+t\partial_t)\partial_t^{j-1} t^{-1} D_j}{\beta^{j+1}\,(j-1)!(2\pi i)^{j-1}} \right]$$

where we have suppressed the arguments for simplicity. The first terms are:

$$\partial_\beta I_c = -\frac{2\pi\mu}{\beta} gS_o - \frac{\mu g''}{2\pi\beta}S_2 + \frac{(g+\mu g')}{\beta^2}\partial_t C_1 + \frac{\mu g''}{2\pi^2\beta^2}\partial_t S_2 + \frac{g'}{2\pi\beta^3}\partial_t^2 S_2 + O(g\, \bar{e}^{2\pi^2 t}) , \qquad (3.4.7)$$

and evaluating the derivative respect to α, we obtain for the last contribution finally:

$$\partial_\alpha I_c = -\sum_{j>0} \frac{g^{(j)}(\mu)\partial_t^{\,j-1} t^{-1} D_j + 2\pi i\, g^{(j-1)}(\mu)\partial_t^{\,j-1} t^{-1} D_{j-1}}{(j-1)!\beta^{j+1}(2\pi i)^{j-1}} \,, \tag{3.4.8}$$

Thus, the complete expressions for the **saddle point** equations are :

$$E = -\partial_\beta \ln Z(\alpha,\beta) = \int_{0-}^{\mu} d\varepsilon g(\varepsilon)\varepsilon + \sum_{j>0} \frac{(-1)^{j-1} 2(2^{2j-1}-1)\pi^{2j}}{(2j)!\beta^{2j}} B_{2j}[(2j-1)g^{(2j-2)} + \mu g^{(2j-1)}] - \tag{3.4.9}$$
$$-\sum_{j>0}\left[\frac{g^{(j)}(\mu)\partial_t^{\,j-1} t^{-1} D_j + 2\pi i g^{(j-1)}(\mu)\partial_t^{\,j-1} t^{-1} D_{j-1}}{(j-1)!\beta^{j+2}(2\pi i)^{j-1}}\mu + \frac{g^{(j-1)}(\mu)(j+t\partial_t)\partial_t^{\,j-1} t^{-1} D_j}{\beta^{j+1}\,(j-1)!(2\pi i)^{j-1}} \right]$$

and:

$$N = \partial_\alpha \ln Z(\alpha,\beta) = \int_{0-}^{\mu} d\varepsilon g(\varepsilon) + \sum_{j>0} \frac{(-1)^{j-1} 2(2^{2j-1}-1)\pi^{2j}}{(2j)!\beta^{2j}} B_{2j} g^{(2j-1)}(\mu) - \tag{3.4.10}$$
$$- \sum_{j>0} \frac{g^{(j)}(\mu)\partial_t^{\,j-1} t^{-1} D_j + 2\pi i\, g^{(j-1)}(\mu)\partial_t^{\,j-1} t^{-1} D_{j-1}}{(j-1)!\beta^{j+1}(2\pi i)^{j-1}} \,,$$

We recognize in these formulae that the infinite sums for N in the last equation are also present in the expression for E (save a common factor μ). This fact leads to further simplifications. For the **entropy** evaluated at the saddle point we arrive at:

$$S(\alpha,\beta) = \ln Z(\alpha,\beta) + \beta E - \alpha N = \sum_{j>0} \frac{(-1)^{j-1} 2(2^{2j-1}-1)\pi^{2j}}{(2j-1)!\beta^{2j-1}} B_{2j} g^{(2j-2)}(\mu) -$$
$$- \sum_{j>0} \frac{g^{(j-1)} \partial_t t^{j+1} \partial_j^{\,j-1} t^{-1} D_j(\mu,\pi t)}{(j-1)!\,(2\pi i)^{j-1}} \,, \tag{3.4.11}$$

The determinant appearing in the formula for the nuclear level density follows after the similar evaluation of the remaining second order derivatives of the contributions I_c [cf. eq.(3.3.12b)] without additional problems.

With these formulae we have explicitly calculated all contributions that we need for an explicit computation. It remains only to give the set of parameters which define the Dirichlet series associated with the spectrum. The series used have precise domains of convergency which of course must be taken into consideration. (Remember the strip of uniform convergency mentioned after eq.(3.3.14).) In the next chapter we shall see some concrete examples. The simplest application is the Bethe formula, which follows disregarding all contributions except the most important for $|\beta|\to 0$. In this case: $U+(E_o-\tilde{E}_o) \approx \pi^2 g(\varepsilon_F)/6\beta_o^2$ and $S(\alpha_o,\beta_o)\approx\pi\left(a(U+E_o-\tilde{E}_o)\right)^{1/2}$ with $a=2g(\varepsilon_F)/3$. Here $g(\varepsilon_F)$ is the smooth single particle level density of eq.(3.2.19) evaluated at the Fermi level.

It is worth mentioning that in the literature, neither the relation with the ϑ-functions for the constant single particle spectrum has been recognized, nor the more general analytic properties we are studying have been considered.

To be able to compute the needed sums also for the cases where the temperature is not large enough or near a discontinuity we need to transform the sums in terms of $1/\beta$ into sums in terms of β. This transformation will be studied in the next section.

3.5. Transformation Properties.

As mentioned in the preceding sections, the obtained relations are all in terms of the temperature $1/\beta$. This is an adequate starting point, if we like to consider problems where $|\beta|$ is small. But if we want to be able to make good estimations for the general problem where $|\beta|$ is not necessarily small or for systems with half filled shells, we need to do additional work.

We can transform all the formulae we have obtained in the last section into relations containing β instead of $1/\beta$. Certain important aspects of the theory of modular forms will appear in the sequel. We will first review some important facts from the theory of Jacobi theta functions and then we will proceed to develope some analogue formulas for our more general problem.

3.5a. Motivation, Theta Functions and Related Results.

In our investigation, the q-series $C_{2m+1}(z,t)$ and $S_{2m}(z,t)$ (see eq.(3.3.14)) are the most important functions for the transformation of β into $1/\beta$, i.e. small into large temperature expansions. For the constant single particle spectrum these functions are directly related to logarithms of the Jacobi theta functions, which in terms of infinite products are given by (see for example H. Rademacher (1973)) :

$$\vartheta_0(z|\tau)=C(\tau)\prod_{n=1}^{\infty}(1-q^{2n-1}e^{2\pi iz})(1-q^{2n-1}e^{-2\pi iz})=\sum_{-\infty}^{\infty}(-1)^n q^{n^2}\exp(2\pi inz)\ , \qquad (3.5.1a)$$

$$\vartheta_1(z|\tau)=2q^{1/4}\sin(\pi z)C(\tau)\prod_{n=1}^{\infty}(1-q^{2n}e^{2\pi iz})(1-q^{2n}e^{-2\pi iz})=i\sum_{-\infty}^{\infty}(-)^n q^{(n-1/2)^2}e^{(2n-1)\pi iz}\ , \qquad (3.5.1b)$$

$$\vartheta_2(z|\tau)=2q^{1/4}\cos(\pi z)C(\tau)\prod_{n=1}^{\infty}(1+q^{2n}e^{2\pi iz})(1+q^{2n}e^{-2\pi iz})=\sum_{-\infty}^{\infty}q^{(n-1/2)^2}e^{(2n-1)\pi iz}\ , \qquad (3.5.1c)$$

$$\vartheta_3(z|\tau)=C(\tau)\prod_{n=1}^{\infty}(1+q^{2n-1}e^{2\pi iz})(1+q^{2n-1}e^{-2\pi iz})=\sum_{-\infty}^{\infty}q^{n^2}\exp(2\pi inz)\ , \qquad (3.5.1d)$$

with $q=\exp(\pi i\tau)$, $\mathrm{Im}\,\tau>0$, and the product:

$$C(\tau)=\prod_{n=1}^{\infty}(1-q^{2n})\ =\ e^{-\pi i\tau/12}\ \eta(\tau)\ =\ \sum_{-\infty}^{\infty}(-)^n q^{3n^2+n}\ , \qquad (3.5.2)$$

where $\eta(\tau)$ is the Dedekind η-function. The equality between the infinite products and the Fourier series in eqs.(3.5.1a-d) are essentially the so-called Jacobi triple product identity. They imply directly similar expansions for $\eta(\tau)$ like: $\eta^3(\tau)=\vartheta_1'(0|\tau)/(2\pi q^{1/4})$, where the prime denotes the derivative with respect to z. The infinite series for $C(\tau)$ was found, first empirically and after some effort proved, by Euler, but can be derived from eq.(3.5.1c) .

From the infinite products, we recognize that, if we write $\beta=-2\pi i\tau$ and $\alpha=2\pi iz$, we obtain from ϑ_2 and ϑ_3 partition functions for fermions and antifermions in constant single particle spectra, with energies $\varepsilon_n=1,2,\ \dots$, and $\varepsilon_n=1/2,\ 3/2$, etc., respectively. And, if Re $\beta>0$ the τ will be in the upper half plane as required. Thus, their appearance in our work is not surprising. The kind of spectra we are considering is much more general, since the single particle levels have in general a degeneracy growing as a(n) (see eq.(3.2)). But nevertheless we will find many similitudes.

The logarithms can be obtained from the infinite products as:

$$\ln\,\vartheta_0(z|\tau)=\ln\,C(\tau)\ -\ 2\sum_{n>0}\frac{q^n\cos(2\pi nz)}{n(1-q^{2n})}\ =\ \ln C(\tau)\ +\ \sum_{n>o}\frac{\cos(2\pi nz)}{in\ \sin(\pi in\tau)}\ , \qquad (3.5.3a)$$

$$\ln\,\vartheta_1(z|\tau)\ =\ \ln\,C(\tau)\ +\frac{\pi i\tau}{4}\ +\ \ln(2\sin(\pi z))\ -\ 2\sum_{n>0}\frac{q^{2n}\cos(2\pi nz)}{n(1-q^{2n})}\ , \qquad (3.5.3b)$$

$$\ln \vartheta_2(z|\tau) = \ln C(\tau) + \frac{\pi i \tau}{4} + \ln(2\cos(\pi z)) - 2\sum_{n>0} \frac{(-1)^n q^{2n}\cos(2\pi n z)}{n(1-q^{2n})}, \tag{3.5.3c}$$

$$\ln \vartheta_3(z|\tau) = \ln C(\tau) - 2\sum_{n>0} \frac{(-1)^n q^{n}\cos(2\pi n z)}{n(1-q^{2n})}, \tag{3.5.3d}$$

and :

$$\ln C(\tau) = -\sum_{n>o} \frac{q^{2n}}{n(1-q^{2n})}, \tag{3.5.3e}$$

where $|\mathrm{Im}\ z| < \mathrm{Im}\ \tau$ for ϑ_1 and ϑ_2 and $2|\mathrm{Im}\ z| < \mathrm{Im}\ \tau$ for ϑ_o and ϑ_3 .

The sums shown for the logarithms of the ϑ's are precisely of the kind we found for the $C_{2m+1}(z,t)$ and $S_{2m}(z,t)$ in eq.(3.3.16), but in general, instead of n in the denominators, we have higher powers of n.

Finally, the most important fact in the theory of the theta functions we have shown, is their transformation properties with respect to the elements of the modular group. The **full modular group** $SL_2(\mathbb{Z})$ is the group of fractional substitutions:

$$\tau' = \frac{a\tau + b}{c\tau + d}, \quad \text{for } a,b,c,d \in \mathbb{Z} \text{ and: } \quad ad - bc = 1, \tag{3.5.4}$$

it is a discontinuous group of infinite order, i.e. for each τ in the definition domain U, the set of images by all elements of the group does not accumulate at any point of U. All its substitutions map the upper half plane $\mathrm{Im}(\tau)>0$ onto itself. The group is generated by the transformations $\tau \mapsto \tau+1$ and $\tau \mapsto -1/\tau$. We will consider in this work only substitutions of this kind and thus show only the most simple transformation properties. These are the following:

$$\vartheta_1(z/\tau|-1/\tau) = -i\sqrt{\tau/i}\; e^{i\pi z^2/\tau}\vartheta_1(z|\tau), \quad \vartheta_1(z|\tau+1) = e^{i\pi/4}\vartheta_1(z|\tau), \tag{3.5.4a}$$

$$\vartheta_2(z/\tau|-1/\tau) = \sqrt{\tau/i}\; e^{i\pi z^2/\tau}\vartheta_0(z|\tau), \quad \vartheta_2(z|\tau+1) = e^{i\pi/4}\vartheta_2(z|\tau), \tag{3.5.4b}$$

$$\vartheta_3(z/\tau|-1/\tau) = \sqrt{\tau/i}\; e^{i\pi z^2/\tau}\vartheta_3(z|\tau), \quad \vartheta_3(z|\tau+1) = \vartheta_0(z|\tau), \tag{3.5.4c}$$

$$\vartheta_0(z/\tau|-1/\tau) = \sqrt{\tau/i}\; e^{i\pi z^2/\tau}\vartheta_2(z|\tau), \quad \vartheta_0(z|\tau+1) = \vartheta_3(z|\tau), \tag{3.5.4d}$$

and for the Dedekind η-function:

$$\eta(-1/\tau) = \sqrt{\tau/i}\;\eta(\tau) , \qquad \eta(\tau+b) = e^{i\pi b/12}\,\eta(\tau) , \qquad (3.5.4e)$$

These relations are relevant for us since, as we mentioned before, β is given by - $2\pi i\tau$ for the constant spectrum and thus to transform β into $4\pi^2/\beta$ corresponds to transform τ into $-1/\tau$. More general spectra satisfy similar relations as we show in the next section. However let us remark that, to some extent, general modular transformations can also be studied for general partitions functions in a similar way as it occurs for the Jacobi ϑ-functions .

We would like to mention further that the transformation properties we have displayed are directly related, by a Mellin transformation, to the functional relation of the Riemann ζ-function, eq.(3.2.4). The key formula is:

$$\zeta(s) = 2^{-1}\pi^{s/2}\Gamma(s/2)^{-1}\int_0^\infty dt\;\{\vartheta_3(0|it) - 1\}\; t^{-1+s/2} , \quad \mathrm{Re}\; s > 1/2 , \qquad (3.5.5)$$

this formula results from the application of the Mellin transform eq.(3.1.4) written as:

$$n^{-s} = \pi^{s/2}\Gamma(s/2)^{-1}\int_0^\infty dt\; t^{s/2-1}\, e^{-n^2 t\pi} , \quad e^{-n^2 t\pi} = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} ds\; n^{-2s}(\pi t)^{-s}\Gamma(s) , \qquad (3.5.6)$$

If we introduce the transformation law for $\vartheta_3(0|\tau)$ from eq.(3.5.4c), we find the functional relation eq.(3.2.4). However, we are not especially interested in such relations, but in series expansions for Z(x). It is noteworthy that the two expressions we have obtained for Z(x), for the particular case of a constant single particle spectrum, transform through adequate Laplace transforms in both functional relations for $\zeta(s)$ and for $\vartheta_3(0|\tau)$. For a constant spectrum we showed with eq.(3.1.5) the well known fact :

$$\zeta(s) = \Gamma(s)^{-1}\int_0^\infty dx\; x^{s-1}\, Z_0(x) , \quad Z_0(x) = \frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty} dz\; x^{-z}\,\Gamma(z)\zeta(z) , \quad \sigma > 0 , \qquad (3.5.7)$$

for $Z_0(x) = 1/(\exp(x)-1)$. By contour deformation and using a Laurent series for $Z_0(x)$ [cf. eq.(3.3.13)], the functional relation eq.(3.2.4) can be obtained [see for example H. Rademacher (1968)].

Similarly, using Laplace transformations it is possible to derive the Laurent series for $Z_0(x)$, for the constant single particle spectrum, from the functional relation for $\vartheta_3(0|\tau)$. We know that [cf. Erdelyi et al. (1953)] :

$$\exp(-nx) = \pi^{-1/2}x \int_0^\infty dt\ t^{-1/2} \exp(-x^2t-n^2/4t) \quad , \ \mathrm{Re}\ x^2 > 0 \ , \tag{3.5.8}$$

and from this we obtain:

$$Z_0(x)=\pi^{-1/2}2^{-1}x \int_0^\infty dt\ t^{-1/2}\exp(-x^2t)\ \{\vartheta_3(0|-1/4\pi it) - 1\} \ , \tag{3.5.9}$$

If we insert now both expressions for $\vartheta_3(0|-1/4\pi it)$, we obtain the transformation relations for $Z_0(x)$. Analogously, from the relations for $Z_0(x)$ we can obtain the transformation formula for $\vartheta_0(0|\tau)$. We see in this way the equivalence of the functional relation for $\zeta(s)$, the transformation for $\vartheta_3(0|\tau)$ under $\tau \mapsto -1/\tau$ and the Laurent expansion for $Z_0(x)$. To these relations we can add the Euler-Maclaurin summation formula, the Poisson summation formula and certain Fourier series expansions, as H. Hamburger (1922) has shown in a different context. In this work we did not use the mentioned summation formulas but some of our results can also be obtained in such a way.

The purpose of the last remarks is just to make plausible why the use of Laurent series help us to transform formulas depending on $1/\beta$ into relations containing β for general spectra in the next sections.

In an analogous way, we can define more general ϑ-functions (or ζ-functions) by similar Fourier series with coefficients n^{-s} with s complex:

$$\vartheta_{3,s}(z|\tau) = \sum_{n>0} (n+\alpha)^{-s} q^{n^2} \cos 2\pi nz \ , \qquad \alpha \neq -1, -2, \ldots ,$$

which for s equal to a negative integer k and $\alpha=0$ is equal to the derivatives of order k of the usual $\vartheta_3(z|\tau)$ as given by the series in eq.(3.5.1d). And in such case they are related to the series C_{2m+1} and S_{2m} defined in eq.(3.3.16) with m negative. In particular for $m \leq -1$ they are elliptic functions. But for k positive they are integrals and we do not know their explicit infinite product representations. However, some properties are easily found like for example that the function $\vartheta_{3,s}$ satisfies the heat equation:

$$\partial_z^2 \vartheta_{3,s}(z|\tau) = 4\pi i\ \partial_t \vartheta_{3,s}(z|\tau) \ ,$$

In the limit $q \to 1$ and $z \to 0$ we obtain essentially Hurwitz ζ-function (if additionally $\alpha=0$ then Riemann's ζ-function.)

On the other hand, the infinite products we have studied are of the following kind (remember $q=\exp(\pi i\tau)$) :

$$T_k(z|\tau) = \prod_{n=1}^{\infty} (1+q^{2n-1} e^{2\pi iz})^{n^k} \quad , \quad k= 0,1, \ldots ,$$

these products are periodic in z and their logarithms are related to the series C_{2m+1} and S_{2m} for m positive. But in this case, we do not know in general simple Fourier series as those for the Jacobi ϑ-functions, i.e. the generalization of Jacobi's triple product identity (obtainable for $k=0$). As we mentioned in section 3.3, eq.(3.3.20) provides us a Fourier series only for the logarithm of the partition function. We obtained several interesting relations for the mentioned products, like for example:

$$T_k(z+\tau|\tau) = (1+q\, e^{2\pi iz})^{-\delta_{k,o}} \prod_{j=o}^{k} \left(T_j(z|\tau)\right)^{\binom{k}{j}(-)^{k-j}}$$

relating $T_k(z+\tau|\tau)$ with $T_j(z|\tau)$ and $j= 0,1, \ldots , k$. In the next section we will show some results for the modular transformation $(z,\tau) \mapsto (z/\tau,-1/\tau)$.

It is needless to say that it is naive to try to generalize the whole theory of theta functions in this way. Fortunately, for our applications in the next chapter, precisely the aspects we need can be generalized with similar methods.

3.5b. The Partition Function as a Function of β.

To obtain a relation, where the partition function is a function of β explicitly, there are two possible ways. The first way consists in starting again from ln $Z(\alpha,\beta)$ and proceed somehow, with a different method, to find such an expression. This is the way we follow in this section. The second possibility is to transform the obtained expressions, in terms of $1/\beta$, into expressions in terms of β itself. This is the procedure we follow in the next section and it constitutes a consistency proof.

We start with:

$$\ln Z(\alpha,\beta)=\sum_{n>o} a_n \ln(1+e^{\alpha-\beta n}) =\sum_m \frac{A_m}{d_m} \sum_{n>o}(n^{d_m} - (n-1)^{d_m-1}) \ln(1+e^{\alpha-\beta n}) , \tag{3.5.10}$$

that is, we apply our method from the beginning. Then, for Re $\beta>0$ and $0<\mathrm{Re}(\alpha/\beta)<1$:

$$\begin{aligned}\ln Z(\alpha,\beta)&=\sum_m \frac{A_m}{d_m}\sum_{k=1}\binom{d_m}{k}(-1)^{k+1}\sum_{n>o} n^{d_m-k}\ln(1+e^{\alpha-\beta n}) = \\ &=\sum_m \frac{A_m}{d_m}\sum_{k=1}\binom{d_m}{k}(-1)^{k+1}\sum_{\nu>o}\frac{(-1)^{\nu+1}}{\nu} e^{\nu\alpha}\sum_{n>o} n^{d_m-k} e^{-\beta\nu n}\end{aligned} \tag{3.5.11}$$

now, for Re $\beta>0$:

$$\sum_{n>o} n^{d_m-k} e^{-\beta\nu n} = (-1)^{d_m-k} \nu^{k-d_m} \partial_\beta^{d_m-k}\left(\frac{e^{-\beta\nu}}{1-e^{-\beta\nu}}\right) , \tag{3.5.12}$$

lead us to:

$$\ln Z(\alpha,\beta)=\sum_m \frac{A_m}{d_m}\sum_{k=1}\binom{d_m}{k}(-1)^{d_m}\partial_\beta^{d_m-k}\sum_{\nu>o}\frac{(-1)^\nu \; e^{\nu(\alpha-\beta)}}{\nu^{d_m-k+1}(1-e^{-\beta\nu})} , \tag{3.5.13}$$

in an analogous way:

$$\ln Z(-\alpha,-\beta)=\sum_m \frac{A_m}{d_m}\sum\binom{d_m}{k}(-1)^k \; \partial_\beta^{d_m-k}\sum_{\nu>o}\frac{(-1)^\nu \; e^{-\nu(\alpha-\beta)}}{\nu^{d_m-k+1}(1-e^{\beta\nu})} , \tag{3.5.14}$$

and now we substract both relations to find:

$$\begin{aligned}\ln Z(\alpha,\beta)=\ln Z(-\alpha,-\beta)+\sum_m\frac{A_m}{d_m}\sum_{k=1}\binom{d_m}{k}\partial_\beta^{d_m-k}\Bigg[\sum_{\nu>o}\frac{(-1)^\nu e^{-\beta\nu/2}}{\nu^{d_m-k+1}} \cdot \\ \cdot\left(\frac{(-1)^{d_m} e^{\nu\alpha}+(-1)^k e^{-\nu\alpha}}{e^{\beta\nu/2}-e^{-\beta\nu/2}}\right) +(-1)^k\sum_{\nu>o}\frac{(-1)^\nu e^{-\nu\alpha}}{\nu^{d_m-k+1}}\Bigg] ,\end{aligned} \tag{3.5.15}$$

the last sum survives, after partial derivation, only for $d_m=k$ as:

$$\sum_{\nu>o}\frac{(-1)^\nu e^{-\nu\alpha}}{\nu} = - \ln(1+e^{-\alpha}) = \frac{\alpha}{2} - \ln(2\cosh(\tfrac{\alpha}{2})) , \tag{3.5.16}$$

and introducing again: $\sigma_{2m}=1$, $\sigma_{2m+1}=0$, we obtain:

$$\ln Z(\alpha,\beta) = \ln Z(-\alpha,-\beta) + \sum_{m} \frac{A_m}{d_m}\Bigg[-(-1)^{d_m} \ln(1+e^{-\alpha}) + \qquad (3.5.17)$$
$$+ \sum_{k=1} \binom{d_m}{k} \partial_{\beta}^{d_m-k} \sum_{\nu>o} \frac{(-1)^{d_m+\nu}\; e^{-\beta\nu/2}}{\nu^{d_m-k+1}} \; \frac{(\sigma_{d_m-k} \cosh(\nu\alpha) + \sigma_{d_m-k+1} \sinh(\nu\alpha))}{\sinh(\beta\nu/2)} \Bigg]$$

We introduce now, in an analogous way as in section 3.3, the Fourier series [q-series or Lambert series cf. eq.(3.3.14)] :

$$\hat{C}_{2m+1}(z,t) = \sum_{n>o} \frac{(-1)^n\, e^{-2\pi nt} \cos(2\pi nz)}{n^{2m+1}\, \sinh(2\pi nt)} \; , \quad \hat{S}_{2m}(z,t) = \sum_{n>o} \frac{(-1)^n\, e^{-2\pi nt} \sin(2\pi nz)}{n^{2m}\, \sinh(2\pi nt)} \quad , \qquad (3.5.18)$$

these series have also the unit circle $|\exp(2\pi t)| = 1$ as a natural boundary. And thus, we write finally:

$$\ln Z(\alpha,\beta) = \ln Z(-\alpha,-\beta) + \sum_{m} \frac{A_m}{d_m}\Bigg[-(-1)^{d_m} \ln(1+e^{-\alpha}) + \qquad (3.5.19)$$
$$+ \sum_{k=1} \binom{d_m}{k} (-1)^{d_m} \partial_{\beta}^{d_m-k}\, \hat{D}_{d_m-k+1}(i\alpha/2\pi, \beta/4\pi) \Bigg] \; ,$$

with :

$$\hat{D}_m(z,t) = \sigma_{m-1}\, \hat{C}_m(z,t) - i\sigma_m\, \hat{S}_m(z,t) \quad , \qquad (3.5.20)$$

[remember $\sin(iz) = i \sinh(z)$]. These are the analogous formulae to those of section 3.3. [see eq.(3.3.19) and eq.(3.3.20)]. In the next section we show their equivalency for Re $\beta > 0$ and $0 < \mathrm{Re}(\alpha/\beta) < 1$.

3.5c. Equivalency of the Two Relations for the Partition Function

With eq.(3.3.20) and eq.(3.5.19) we obtained, by two alternative ways, two expressions for ln $Z(\alpha,\beta)$. We like to show now that these two expressions are indeed equivalent. We will prove this for Re $\beta > 0$ and $0 < \mathrm{Re}(\alpha/\beta) < 1$:

$$\frac{(d_m-k)!\,\beta^{-d_m+k-1}\alpha^{d_m-k+2}}{(d_m-k+2)!} + (d_m-k)!\,\beta^{-d_m+k-1}\sum_{j=1} \frac{(-)^{j-1}2(2^{2j-1}-1)\pi^{2j}\alpha^{d_m-2j-k+2}}{(2j)!(d_m-2j-k+2)!}B_{2j}$$

$$-\frac{2\pi i}{(2\pi i\beta)^{d_m-k+1}}\partial_t^{d_m-k}\, t^{-1}D_{d_m-k+1}\left(\frac{\alpha}{\beta},\frac{\pi}{\beta}\right) + \alpha\zeta(-d_m+k) - \beta\zeta(-1-d_m+k) =$$

$$= \partial_\beta^{d_m-k}\left[\ \ln(1+\bar{e}^{\alpha}) + (-1)^{d_m-k-1}\hat{D}_{d_m-k+1}\left(\frac{i\alpha}{2\pi},\frac{\beta}{4\pi}\right)\right]. \qquad (3.5.21)$$

This relation gives clearly the transformation properties of the Fourier series $D_j(\alpha/\beta,\pi/\beta)$ into the Fourier series $\hat{D}_j(i\alpha/2\pi,\beta/4\pi)$. Because of the parity involved in the definitions eq.(3.3.19) and eq.(3.5.20), we have two sets of equations: one for the cosine series C_j and one for the sine series S_j, which can be treated similarly. We shall show the proof only for the cosine series to save space.

For the hyperbolic functions we shall use Laurent series. Other possible ways are to apply Poisson's summation formula or to use Mellin transforms. We consider first the case $d_m=k$ since it is slightly different, althougth easier, to show the method and afterwards consider the general cosine identity.

We consider thus:

$$\frac{-\alpha^2}{2\beta} - \frac{\pi^2}{6\beta} + \frac{\alpha}{2} - \frac{\beta}{12} + C_1\left(\frac{\alpha}{\beta},\frac{\pi}{\beta}\right) = \frac{\alpha}{2} - \ln(2\cosh\alpha/2) + \hat{C}_1\left(\frac{i\alpha}{2\pi},\frac{\beta}{4\pi}\right), \qquad (3.5.22)$$

now we use the following formulae to transform C_1 (cf. Erdelyi et al.,1953) :

$$\frac{1}{\sinh z} = \frac{1}{z} + \sum_{k>o}\frac{2z(-1)^k}{z^2+\pi^2k^2}\ ;\ \sum_{n>o}\frac{\cos 2\pi nz}{n^2} = \frac{\pi^2}{6} - \pi z + z^2\ ,\ 0<\mathrm{Re}\ z\le 1, \qquad (3.5.23)$$

and :

$$\sum_{n>o}\frac{\cos 2\pi nz}{n^2+a^2} = \frac{\pi\cosh a\pi(1-2z)}{2a\sinh a\pi} - \frac{1}{2a^2}\ ,\ 0<\mathrm{Re}\ z\le 1\ ,\ \text{and}\ \sum_{k>o}(-)^k k^{-2} = -\pi^2/12\ , \qquad (3.5.24)$$

set $a=k/2t$ and get:

$$C_1(z,t) = \frac{\pi}{12t} - \frac{z\pi}{2t} + \frac{\pi z^2}{2\pi t} + \frac{\pi t}{6} + \sum_{k>o}\frac{(-)^k\cosh(k\pi(1-2z)/2t)}{k\sinh(k\pi/2t)}\ , \qquad (3.5.25)$$

here we set $t=\pi/\beta$ and $z=\alpha/\beta$ and recognize the left hand side of eq.(3.5.22) if we put the polynomial terms of eq.(3.5.25) in its right hand side:

$$C_1\left(\frac{\alpha}{\beta},\frac{\pi}{\beta}\right) - \frac{\beta}{12} + \frac{\alpha}{2} - \frac{\alpha^2}{2\beta} - \frac{\pi^2}{6\beta} = \sum_{k>o} \frac{(-)^k \cosh(k\alpha)\cosh(k\beta/2)}{k\,\sinh(k\beta/2)} + \frac{\alpha}{2}\,, \qquad (3.5.26)$$

where we have used the identity : cosh(a-b) = cosh(a)cosh(b)-sinh(a)sinh(b), and also : $\Sigma(-1)^k\sin(kx)/k = -x/2$, $-\pi<\mathrm{Re}\ x<\pi$ (cf. Erdelyi et al., 1953). Finally the r.h.s. of eq.(3.5.26) can be written as:

$$\text{r.h.s.} = \sum_{k>o} \frac{(-)^k e^{-k\beta/2}\cosh(k\alpha)}{k\,\sinh(k\beta/2)} - \ln(2\cosh(\alpha/2)) + \frac{\alpha}{2}\,, \qquad (3.5.27)$$

because: $\Sigma(-)^k\cos(kx)/k = -\ln(2\cos(x/2))$, $-\pi<\mathrm{Re}\ x<\pi$ (cf. Erdelyi et al., 1953). Since this is the right hand side of eq.(3.5.22) this concludes the proof for $d_m = k$. This proof is equivalent to the proof of eq.(3.5.4b) or eq.(3.5.4d), as we can see taking the logarithms of those equations.

To perform now the calculation for $d_m > k$, we can apply the same method, except that we need some additional infinite sums. We need first (cf. Erdelyi et al., 1953) :

$$\sum_{n>o} \frac{\cos(2\pi nz)}{n^{2k}} = \frac{(-)^{k-1}(2\pi)^{2k}}{2(2k)!} B_{2k}(z)\,, \qquad 0<z\leq 1\,, \qquad (3.5.28)$$

and we need the partial fractions expansion for $a \neq 0$:

$$f_\kappa = \frac{1}{n^\kappa(n^2+a^2)} = \frac{1}{a^2 n^\kappa} - \frac{1}{a^2} f_{\kappa-2} = \sum_{j=o}^{\kappa/2-1} \frac{(-)^j}{n^{\kappa-2j} a^{2j+2}} + \frac{(-)^{\kappa/2}}{a^\kappa} f_o\,, \qquad (3.5.29)$$

for κ even. This relation implies, with eq.(3.5.24) and eq.(3.5.28), an elementary identity for $0<\mathrm{Re}\ z<1$ and $\kappa = 0,2,\ldots$:

$$\sum_{n>o} \frac{\cos(2\pi nz)}{n^\kappa(n^2+a^2)} = \frac{(-)^{\kappa/2}\pi\cosh(a\pi(1-2z))}{2a^{\kappa+1}\sinh a\pi} - \frac{(-)^{\kappa/2}}{2a^{\kappa+2}} \sum_{j=o}^{\kappa/2} \frac{(2\pi a)^{\kappa-2j} B_{\kappa-2j}(z)}{(\kappa-2j)!}\,, \qquad (3.5.30)$$

it is interesting to write this relation in the simple form:

$$\sum_{n>o} \frac{\cos(2\pi nz)}{n^\kappa(n^2+a^2)} = \{1 - \text{S.P.}\} \frac{(-)^{\kappa/2}\pi\cosh(\pi a(1-2z)}{2\,a^{\kappa+1}\sinh(\pi a)}\,, \qquad (3.5.30a)$$

where S.P. means the singular part. The sum eq.(3.5.30) enables us to write down [cf. eq.(3.3.14)] with a = k/2t :

$$C_{\kappa+1}(z,t) = \sum_{k>0} \frac{(-)^k}{\pi t} \left[\sum_{j=0}^{\kappa/2} \frac{(-)^{1+\kappa/2} (2\pi)^{\kappa-2j}}{2a^{2j+2}(\kappa-2j)!} B_{\kappa-2j}(z) + \frac{(-)^{\kappa/2} \pi\cosh(a\pi(1-2z))}{2a^{\kappa+1}\sinh a\pi} \right] + $$
$$+ \frac{(-)^{\kappa/2}(2\pi)^{\kappa+2}}{4\pi t(\kappa+2)!} B_{\kappa+2}(z) \,, \quad 0<\mathrm{Re}\, z<1, \tag{3.5.31}$$

this **reciprocity relation** can also be written in the form:

$$\sum_{n>0} \frac{\cos(2\pi nz)}{n^{\kappa+1}\sinh(2\pi nt)} = \sum_{k>0} \frac{(-)^{k+\kappa/2} (2t)^{\kappa} \cosh(k\pi(1-2z)/2t)}{k^{\kappa+1}\sinh(k\pi/2t)} +$$
$$+ (-)^{\kappa/2} (2\pi)^{\kappa+1} \sum_{j=0}^{1+\kappa/2} \frac{(2^{2j-1}-1)\, t^{2j-1} B_{\kappa-2j+2}(z)}{(\kappa-2j+2)!\,(2j)!} (-)^{j-1} B_{2j} \,, \tag{3.5.31a}$$

Corresponding series can also be obtained for negative even κ. This relationship is a generalization of the logarithm of the transformation formulas for the Jacobi ϑ-functions [cf. eqs.(3.5.4a-d)]. Actually, eq.(3.5.31a) corresponds to a generalization of eq.(3.5.4d), but it is also possible (but here omitted because of lack of space) to obtain generalizations for the other identities. With relation eq.(3.5.31) we transform the left hand side of the cosine transformation rule into:

$$\partial_t^{\kappa} t^{-1} C_{\kappa+1}\left(\frac{\alpha}{\beta}, \frac{\pi}{\beta}\right) = \partial_t^{\kappa} \left(\sum_{k>0} \frac{(-)^k}{\pi^2 t^2} \left[\frac{(-)^{\kappa/2} \pi\cosh(k\pi(1-\alpha t)/2\pi t)}{2k^{\kappa+1}\sinh(k/2t)} (2\pi t)^{\kappa+1} + \right.\right.$$
$$\tag{3.5.32}$$
$$\left.\left. + \sum_{j=0}^{\kappa/2} \frac{(-)^{\kappa/2} (2\pi)^{\kappa-2j} (2\pi t)^{2j+2}}{2k^{2j+2}(\kappa-2j)!} \sum_{n=0}^{\kappa-2j} \binom{\kappa-2j}{n} (\alpha t)^{\kappa-2j-n} B_n \right] + \frac{(-)^{\kappa/2} (2\pi)^{\kappa}}{t^2(\kappa+2)!} \sum_{n=0}^{\kappa+2} \binom{\kappa+2}{n} (\alpha t)^{\kappa+2-n} B_n \right),$$

where we used the expression eq.(3.2.21) for the Bernoulli polynomials $B_n(z)$ in terms of the Bernoulli numbers B_n. After some simplifications and using the values $\zeta(1-2m) = -B_{2m}/2m$, $B_0=1$, $B_1=-1/2$, $B_2=1/6$, $B_{2m+1}=0$ for $m>0$, we obtain:

$$t^{\kappa+1}(2\pi)^{-\kappa}(-)^{\kappa/2}\partial_t^{\kappa}\, t^{-1}C_{\kappa+1}(\frac{\alpha}{\beta},\frac{\pi}{\beta})= \frac{\alpha^{\kappa+2}\kappa!}{\beta^{\kappa+1}(\kappa+2)!} - \zeta(-1-\kappa)\beta + \tag{3.5.33}$$
$$+\sum_{j=1}^{\kappa/2+1}\frac{(-)^{j}2\pi^{2j}(1-2^{2j-1})\alpha^{\kappa-2j+2}\kappa!}{(\kappa-2j+2)!(2j)!\beta^{\kappa+1}}B_{2j} + t^{\kappa+1}\partial_t^{\kappa}\, t^{\kappa-1}\sum_{k>o}\frac{(-)^{k}\cosh(k(\alpha-1/2t))}{k^{\kappa+1}\sinh(k/2t)}$$

and thus the equality we like to show reduces to:

$$t^{\kappa+1}\partial_t^{\kappa}\, t^{\kappa-1}\sum_{k>o}\frac{(-)^{k}\cosh(k(\alpha-1/2t))}{k^{\kappa+1}\sinh(k/2t)} = (-)^{\kappa}\partial_\beta^{\kappa}\sum_{k>o}\frac{(-)^{k}e^{-k\beta/2}\cosh(k\alpha)}{k^{\kappa+1}\sinh(k\beta/2)}\ , \tag{3.5.34}$$

but: cosh(a-b)=cosh(a)cosh(b)-sinh(a)sinh(b) leads us to:

$$t^{\kappa+1}\partial_t^{\kappa}\, t^{\kappa-1}\sum_{k>o}\frac{(-)^{k}e^{-k/2t}\cosh(k\alpha)}{k^{\kappa+1}\sinh(k/2t)} =(-)^{\kappa}\partial_\beta^{\kappa}\sum_{k>o}\frac{(-)^{k}e^{-k\beta/2}\cosh(k\alpha)}{k^{\kappa+1}\sinh(k\beta/2)}\ , \tag{3.5.35}$$

Thus both operators acting on the same function must be equal:

$$t^{\kappa+1}\partial_t^{\kappa}\, t^{\kappa-1} = (-)^{\kappa}\partial_\beta^{\kappa}\ , \tag{3.5.36}$$

to prove this equality we introduce the following notation: $s=\partial_t$, $\alpha=\partial_\beta$. These operators satisfy : $[s,t]=1$ and $[\alpha,\beta]=1$ and are related by $[\beta,t]=0$ and the following quadratic relations $[\alpha,t]=-t^2$, $[s,\beta]=-\ \beta^2$, $[\alpha,s]=1-[\alpha,\beta]_+$ and $[\alpha,\beta]_+ + [s,t]_+=2$. The equality we like to prove reads now :

$$t^{\kappa+1}s^{\kappa}\, t^{\kappa-1} = (t^2s)^{\kappa}\ , \tag{3.5.37}$$

the same equality will hold for α and β. "Classically", i.e. if s and t commute, we have indeed an equality. The "quantum" result can be proved by induction using :

$$s^mt^n = \sum_{j=o}^{\min(m,n)} j!\binom{m}{j}\binom{n}{j}\, t^{n-j}s^{m-j}\ , \tag{3.5.38}$$

which leads to:

$$t^{\kappa+1}s^{\kappa}\, t^{\kappa-1}= \sum_{j=o}^{\kappa-1} j!\binom{\kappa}{j}\binom{\kappa-1}{j}\, t^{2\kappa-j}\, s^{\kappa-j}= (t^2s)^{\kappa}\ , \tag{3.5.39}$$

This concludes the proof for all κ even, i.e. the cosine series.

Since the same method can be applied for the sine series without any additional difficulty we suppress the proof here. The only needed **identities** are, for $\kappa=-1, 1, 3, \ldots$:

$$\sum_{n>0}\frac{\sin(2\pi nz)}{n^{\kappa}(n^2+a^2)} = \sum_{j=0}^{[\kappa/2]}\frac{(-)^{\kappa/2+1/2}(2\pi)^{\kappa-2j}}{2a^{2j+2}(\kappa-2j)!}B_{\kappa-2j}(z) + \frac{(-)^{[\kappa/2]+1}\pi\sinh(a\pi(1-2z))}{2a^{\kappa+1}\sinh a\pi}, \tag{3.5.40}$$

and the **reciprocity relation**:

$$\begin{aligned}\sum_{n>0}\frac{\sin(2\pi nz)}{n^{\kappa+1}\sinh(2\pi nt)} &= \sum_{k>0}\frac{(-)^{k+(\kappa+1)/2}(2t)^{\kappa}\sinh(k\pi(1-2z)/2t)}{k^{\kappa+1}\sinh(k\pi/2t)} + \\ &+ (-)^{(\kappa+1)/2}(2\pi)^{\kappa+1}\sum_{j=0}^{(\kappa+3)/2}\frac{t^{2j-1}(2^{2j-1}-1)(-)^{j}B_{2j}}{(\kappa-2j+2)!\,(2j)!}B_{\kappa-2j+2}(z),\end{aligned} \tag{3.5.41}$$

Corresponding series for negative even $\kappa+1$ can also be easily found. We conclude thus that the two obtained expressions for the partition function $Z(\alpha,\beta)$ are equivalent for Re $\beta>0$ and $0<\mathrm{Re}(\alpha/\beta)<1$.

From the obtained transformation properties it is now possible to do the corresponding calculations for the nuclear level density. The infinite sums appearing in the entropy, the saddle point equations and the determinant can be transformed straightforwardly. In the next chapter we show such explicit calculations for periodic spectra introducing at the same time additional elements which are important for physical reasons.

CHAPTER 4

SINGLE PARTICLE SPECTRA WITH SHELL STRUCTURE

Analyzing general spectra, we will notice, besides the growth of the degeneracy of the single particle levels given by a_n, also a local distribution of levels in the form of "shells". By a "shell" we loosely mean a set of levels separated by gaps from the rest of the spectrum. We could think of these shells as a result of a spreading of levels originally degenerated, by a residual interaction. In the preceding chapter, we have addressed only the problem concerned with the general growth of the number of available states in a spectrum up to a given energy. In this chapter, we look at the effects produced on the nuclear level density by a local regularity in the spectra in the form of shells. This is a problem extensively analysed at zero temperature, for the calculation of the shell corrections to the semi-empirical mass formula, using mostly numerical methods. Our method uses the Analytic Theory of Numbers as a basis and is a refinement of the results in the preceding chapter for excited Fermion systems.

In the first section, we consider the simplest spectrum, consisting in equally spaced levels with constant degeneracy. We do this, to show that already at this elementary level the (partial) filling of the levels ("shells") leads to characteristic properties. The second section extends the calculations to a periodic general spectrum. This spectrum is also very simple, but it will be precisely the type of spectrum that will allow us to compare our results with experimental data in the next chapter. It was not necessary for the purposes of this work to attempt the full calculations of shell structures for the more general single particle spectra studied in the preceding chapter. Therefore, we close this chapter with some simple calculations and observations for more general single particle level schemes. The harmonic oscillator with spin-orbit coupling and the anisotropic oscillator are considered as examples.

4.1. Constant Single Particle Spectrum.

We shall show now the simplest possible case. The spectrum consists of equally spaced shells of zero width with constant degeneracy equal to $a_j=\hbar\omega g_0$, where $\hbar\omega$ is the constant distance between adjacent shells, $\hbar\omega g_0$ is the constant number of single particle levels in each shell and g_0 is the constant single particle level density. The single particle levels are thus given by: $\varepsilon_n/\hbar\omega = 1,2, \ldots$. This is the only problem analysed in the consulted literature (using different methods) in a similar way as we have done in the last chapter, but for large excitation energies only. Some results are clarified only using the present method, like for example the temperature dependency of the shell effects or the low energy behaviour.

For the assumption eq.(3.1) we obtain simply:

$$\sum_{j=1}^{n} a_j = \hbar\omega g_o \, n \quad , \tag{4.1.1}$$

Thus, we have only one d_m (equal to one) and the corresponding residue is $A_m = \hbar\omega g_o$. The Dirichlet series is :

$$D(s) = \hbar\omega g_o \zeta(s) = \hbar\omega g_o \sum_{n>o} \frac{1}{n^s} \quad , \tag{4.1.2}$$

this leads to the values $D(0) = -\hbar\omega g_o/2$ and $D(-1) = -\hbar\omega g_o/12$. Furthermore:

$$Z(x) = \frac{\hbar\omega g_o}{\exp(x) - 1} = \hbar\omega g_o \sum_{n>o} \exp(-xn) = \hbar\omega g_o \sum_{n\geq o} \frac{B_n \, x^{n-1}}{n!} \quad , \tag{4.1.3a}$$

and from eq.(3.2.19) :

$$g(\varepsilon) = g_o + g_o \sum_{k\geq o} (\hbar\omega)^{k+1} \zeta(-k) \, \delta^{(k)}(\varepsilon)/k! \; , \tag{4.1.3b}$$

The grand canonical partition function is given by eq.(3.3.20) as:

$$\ln Z(\alpha,\beta) = \ln Z(-\alpha,-\beta) + \frac{\alpha^2}{2\beta}\hbar\omega g_o - \frac{\alpha}{2}\hbar\omega g_o + \frac{\beta}{12}\hbar\omega g_o + \frac{\pi^2}{6\beta}\hbar\omega g_o - \hbar\omega g_o D_1(\mu,\pi t), \tag{4.1.4}$$

with:

$$D_1(\mu,\pi t) = \sum_{n>0} \frac{\cos(2\pi n\mu)}{n \sinh(2\pi^2 nt)} \quad , \tag{4.1.5}$$

For simplicity, we measure μ and $1/\beta$ in units of $\hbar\omega$.

The saddle point equations are now:(see eqs.(3.4.9) and (3.4.10))

$$E/(\hbar\omega)^2 g_o = \frac{\pi^2}{6\beta^2} + \frac{1}{2}\mu^2 - \frac{1}{12} - 2\pi i\mu t \, D_o - t^2(1+t\partial_t)t^{-1}D_1 \; , \tag{4.1.6}$$

with

$$D_o(\mu,\pi t) = i\sum_{n>0} \frac{\sin(2\pi n\mu)}{\sinh(2\pi^2 nt)} , \tag{4.1.7}$$

and

$$(1+t\partial_t)t^{-1}D_1(\mu,\pi t) = -2\pi^2\sum_{n>0} \frac{\cos(2\pi n\mu)\ \cosh(2\pi^2 nt)}{\sinh(2\pi^2 nt)^2} , \tag{4.1.8}$$

The particle number determines the chemical potential μ through:

$$N/\hbar\omega g_o = \mu - \frac{1}{2} - 2\pi i t\ D_o(\mu,\pi t) , \tag{4.1.9}$$

The entropy is given by eq.(3.4.11) :

$$S(\alpha,\beta)/\hbar\omega g_o = \frac{\pi^2}{3\beta} - \partial_t t\ D_1(\mu,\pi t) , \tag{4.1.10}$$

The **smooth ground state energy**, eq.(3.4.3a) :

$$\tilde{E}_o/(\hbar\omega)^2 g_o = \frac{1}{2}\tilde{\mu}_o^2 - \frac{1}{12} \quad \text{, with : } N/\hbar\omega g_o = \tilde{\mu}_o - \frac{1}{2} , \tag{4.1.11a}$$

or :

$$\tilde{E}_o = \frac{N^2}{2g_o} + \frac{N}{2}\hbar\omega + \frac{1}{24}(\hbar\omega)^2 g_o . \tag{4.1.11b}$$

The exact quantities are:

$$E_o/((\hbar\omega)^2 g_o) = \frac{1}{2}[\mu_o]([\mu_o]+1) + x([\mu_o]+1) , \ N/(\hbar\omega g_o) = [\mu_o] + x , \tag{4.1.12a}$$

where [a] denotes the integral part of the real number a. In terms of N :

$$E_o = \frac{N^2}{2g_o} + \frac{N}{2}\hbar\omega + \frac{1}{2}(\hbar\omega)^2 g_o\ x(1 - x) , \tag{4.1.12b}$$

The difference between the smooth and the exact ground state energies is given by:

$$E_{shell}(0)/((\hbar\omega)^2 g_o) = (E_o - \tilde{E}_o)/((\hbar\omega)^2 g_o) = -\frac{1}{24} + \frac{1}{2}x(1 - x) , \tag{4.1.13}$$

and we call it the **ground state shell energy correction.** We want to stress the fact that this "ground state" quantities are obtainable completely from our definition of g(ε) by eq.(3.2.20) after integration. The saddle point approximation will enable us to extend this result to finite excitation energies.

Now we analyse closer the saddle point equations. From eq.(4.1.9) we find μ in terms of N and D_o. We substitute this value into eq.(4.1.6) and find:

$$E/(\hbar\omega)^2 g_o = (U+E_o)/(\hbar\omega)^2 g_o = \frac{\pi^2}{6\beta^2} + \widetilde{E}_o/(\hbar\omega)^2 g_o + 2\pi^2 t^2 D_o^2 - t^2(1+t\partial_t)t^{-1}D_1, \tag{4.1.14}$$

and thus we obtain for the excitation energy U :

$$U = \frac{\pi^2}{6\beta^2}(\hbar\omega)^2 g_o + E_{shell}(t) - E_{shell}(0) , \tag{4.1.15}$$

where we defined the **temperature dependent shell energy correction** by:

$$E_{shell}(t)/(\hbar\omega)^2 g_o = 2\pi^2 t^2 D_o^2(\mu,\pi t) - t^2(1+t\partial_t)\, t^{-1} D_1(\mu,\pi t) . \tag{4.1.16}$$

This definition is unique in the sense that it constitutes that part of the excitation energy which is given in terms of the q-series $D_j(\mu,\pi t)$. These series are periodic functions of the chemical potential μ damped by the temperature. Furthermore, in the limit $t \to 0$ it gives exactly $E_{shell}(0)$ as computed before (cf. eq.(4.1.13)) as we shall show now.

First, we shall transform the given expressions in terms of $1/\beta$ into relations in terms of β itself. As explained in section 3.5, we need only to use the well known results for ϑ-functions under the modular transformation $\tau \mapsto -1/\tau$. Actually, we have solved this problem in section 3.5b explicitely for a much more general case without reference to the theory of modular forms, but we find it important to relate our work to this very developed mathematical field, at least for the simple cases.

We identify now the function D_1 as the logarithm of a theta function (cf. eq.(3.5.3a) and eq.(4.1.5)) :

$$D_1(\mu,\pi t) = \ln C(2\pi i t) - \ln \vartheta_o(\mu|2\pi i t) . \tag{4.1.17}$$

We notice further from the transformation formula of the ϑ-functions, eq.(3.5.4d) :

$$\ln \vartheta_o(\alpha/\beta|2\pi i/\beta) = \ln (\beta/2\pi)^{1/2} - \beta\{\mu\}/2 + \ln \vartheta_2(\alpha/2\pi i|-\beta/2\pi i) , \tag{4.1.18}$$

where $\{\mu\}$ denotes the fractional part of μ . And from the explicit form for the logarithm of the ϑ_2-function, eq.(3.5.3c), we arrive at:

$$D_1(\mu,\pi/\beta) = \frac{\beta}{12} + \frac{\pi^2}{6\beta} + \frac{\beta\{\mu\}^2}{2} - \frac{\beta\{\mu\}}{2} + \sum_{n>o} \frac{(-)^n \cosh(n\beta(\{\mu\}-1/2))}{n \sinh(n\beta/2)}, \qquad (4.1.19)$$

and this is the desired formula, which gives a good approximation for D_1 for small temperatures (i.e. large β) with only few terms of the infinite series.

In terms of theta functions we find further:

$$\vartheta_2^{\hbar\omega g_o}\left(\frac{\alpha}{2\pi i}\Big|\frac{-\beta}{2\pi i}\right) = (2\cosh(\alpha/2))^{\hbar\omega g_o} \exp(-\hbar\omega g_o\beta/2)\, C^{\hbar\omega g_o}(-\beta/2\pi i)\, Z(\alpha,\beta)\, Z(-\alpha,\beta)\ , \qquad (4.1.20)$$

In the analytic theory of numbers, the k-th powers of the zero values of the ϑ-functions are well known, since the coefficients of their Fourier series give the number of ways $r_k(n)$ into which a positive integer number n can be written as the sum of k squares of positive and negative integers n_j , taking care of the order of the summands:

$$\vartheta_3^k(0|\tau) = \sum_{n_1\in\mathbb{Z}} \cdots \sum_{n_k\in\mathbb{Z}} q^{n_k^2} = \sum_{n\geq o} r_k(n)\, q^n\ .$$

We can now analyse the saddle point equations. First we calculate from eq.(4.1.19) the sum appearing in the particle number, i.e. $2\pi i D_o(\mu,\pi t)$ in eq.(4.1.9) :

$$-2\pi\sum_{n>o} \frac{\sin(2\pi n\mu)}{\sinh(2\pi^2 n/\beta)} = \beta\{\mu\} - \frac{1}{2}\beta + \beta\sum_{n>o} \frac{(-)^n \sinh(n\beta(\{\mu\}-1/2))}{\sinh(n\beta/2)}\ , \qquad (4.1.21)$$

Hence, from eq.(4.1.9), we find for the particle number:

$$N/\hbar\omega g_o = [\mu] - \sum_{n>o} \frac{(-)^n \sinh(n\beta(\{\mu\}-1/2))}{\sinh(n\beta/2)} = [\mu_o] + x\ . \qquad (4.1.22)$$

For the sums appearing in the shell energy correction, eq.(4.1.16) :

$$-t^2(1+t\,\partial_t)\, t^{-1} D_1(\mu,\pi t) = -t^2(1+t\partial_t)t^{-1}\sum_{n>o} \frac{(-)^n \cosh(n\beta(\{\mu\}-1/2))}{n \sinh(n\beta/2)} +$$

$$+ \frac{1}{12} - \frac{\pi^2}{6\beta^2} + \frac{\{\mu\}(\{\mu\}-1)}{2}\ , \qquad (4.1.23)$$

and :

$$2\pi^2t^2D_o^2 = -\frac{1}{8} + \frac{x}{2}\,(1-x) - x - \frac{1}{2}(\mu-[\mu_o])^2 + (\mu-[\mu_o])(x+1/2)\ .$$

The complete expression for the shell energy follows from this relations as:

$$E_{shell}(t)/(\hbar\omega)^2g_o = E_{shell}(0)/(\hbar\omega)^2g_o - t^2(1+t\partial_t)\,t^{-1}\sum_{n>o}\frac{(-)^n\cosh(n\beta(\{\mu\}-1/2))}{n\,\sinh(n\beta/2)} +$$

$$- \frac{\pi^2}{6\beta^2} -([\mu]-[\mu_o])(([\mu]-[\mu_o])/2+\{\mu\}-1-x) + x(\{\mu\}-1)\ , \qquad (4.1.24)$$

thus, for the excitation energy, eq.(4.1.15) :

$$U/(\hbar\omega)^2g_o = - t^2(1+t\partial_t)\,t^{-1}\sum_{n>o}\frac{(-)^n\cosh(n\beta(\{\mu\}-1/2))}{n\,\sinh(n\beta/2)} -$$

$$-([\mu]-[\mu_o])(([\mu]-[\mu_o])/2+\{\mu\}-1-x) + x(\{\mu\}-1)\ , \qquad (4.1.25)$$

where all terms containing $[\mu]-[\mu_o]$ or $\{\mu\}-1$ will vanish at zero temperature (see later).

Finally, for the entropy we arrive at the following result inserting eq.(4.1.19) into eq.(4.1.10) :

$$S/\hbar\omega g_o = \beta^2\partial_\beta\,\beta^{-1}\sum_{n>o}\frac{(-)^n\cosh(n\beta(\{\mu\}-1/2))}{n\,\sinh(n\beta/2)}\ , \qquad (4.1.26)$$

The above formulae are particularly useful in the limit for small temperatures, i.e. as $\beta\rightarrow\infty$. For the particle number we find from eq.(4.1.9) and eq.(4.1.21) :

$$N/\hbar\omega g_o \approx [\mu] -\sum_{n>o}(-)^n\exp(n\beta(\{\mu\}-1)) = [\mu] + \frac{1}{1+\exp(-\beta(\{\mu\}-1))}\ ,(4.1.27)$$

we notice now that: $N/\hbar\omega g_o=[\mu_o]+x$ and find:

$$x \approx 1/(1+\exp(-\beta(\{\mu\}-1))\,)\ , \quad \text{or :} \quad \{\mu\} \approx 1 - \frac{1}{\beta}\ln(1/x - 1)\ , \qquad (4.1.28)$$

since $[\mu]=[\mu_o]$ for $\beta\rightarrow\infty$. In Figure 4.1, we show the energy dependent shell filling parameter $y=\{\mu\}-1/2$ computed numerically. It can also be obtained using the lowest order terms appearing in eqs.(4.1.9) and (4.1.22). We show the parameter y for different values of x in steps of 0.1 and for temperatures between zero and $0.3\hbar\omega$. For low temperatures y is described very well by the linear relation eq.(4.1.28) and for larger temperatures by the shell filling x plus an exponentially decreasing correction. This picture shows rather clearly the "washing out" of the shell effects, which also is present in other quantities.

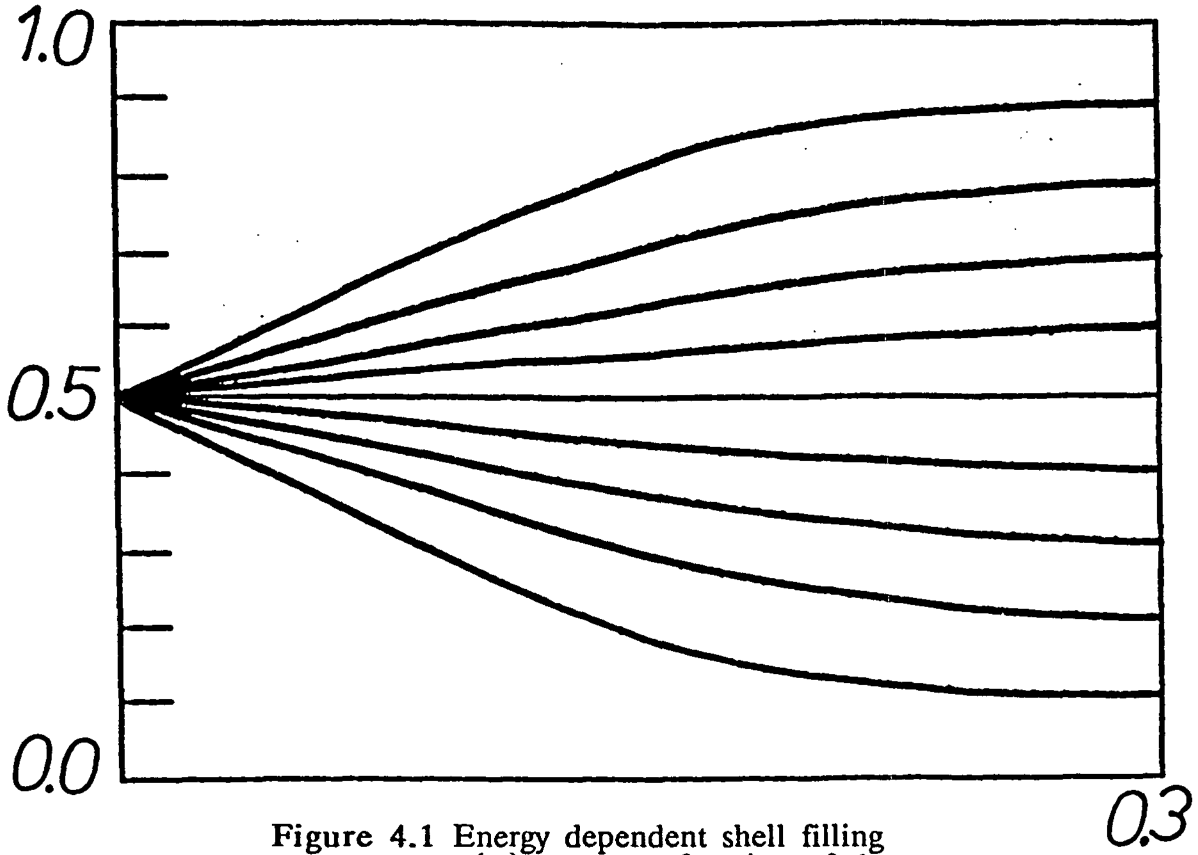


Figure 4.1 Energy dependent shell filling parameter $y=\{\mu\}-1/2$ as a function of the temperature for x=0.0, 0.1, . . . , 0.9, 1.0 and x=0.0 corresponds to the absisas axis, the lowest curve to x=0.1, etc.

For the energy shell correction we evaluate for large β :

$$(1+t\partial_t)t^{-1}D_1(\mu,\pi t) \approx \frac{-1}{12t^2}+\frac{\pi^2}{6}-\frac{\{\mu\}(\{\mu\}-1)}{2t^2}+\frac{\{\mu\} - 1}{t^2(1+\exp(-\beta(\{\mu\}-1)))}, \quad (4.1.29)$$

and thus, in the limit $\beta\rightarrow\infty$ we recover the energy shell correction $E_{shell}(0)$ given by eq.(4.1.13) from eq.(4.1.16) for $E_{shell}(t)$.

Similarly, we find for the entropy in the limit $\beta\rightarrow\infty$ the following result :

$$S/\hbar\omega g_o = - x \ln x - (1 - x) \ln (1 - x) , \quad (4.1.30)$$

the entropy is different from zero at zero excitation energy, since the ground state for this system is degenerated. Note the invariance under the change $x \mapsto (1-x)$ as expected.

4.2. Periodic Single Particle Spectrum

In this section we consider a periodic spectrum studied first by P. Kahn and N. Rosenzweig (1969) (after preliminary work by N. Rosenzweig (1957a), (1957b), (1966)) and given by :

$$\varepsilon_{k,j} = (k + \nu_j)\, \hbar\omega\ , \quad k \in \mathbb{N}\ ;\ j=1,2,\ldots,e \quad ;\ e = \hbar\omega g_o\ , \tag{4.2.1a}$$

where the positive numbers $\nu_j \geq \nu_n$ if $j \geq n$, give the position of level j in each shell, the number e gives the degeneracy of each shell and $\hbar\omega$ is the spacing between any two equivalent levels in adjacent shells. The levels can in general coincide. The absolute width of the shell is given simply by $W = (\nu_e - \nu_1)\hbar\omega$ and we will assume that $W < \hbar\omega$, i.e. that the shells do not overlap. In the limit $W \rightarrow 0$ we obtain clearly the spectrum of the last section with $e = \hbar\omega g_o$.

To analyse the spectrum given by eq.(4.2.1) on the same lines as we have done up to now, we also need to give the numbers ν_j in terms of integer multiples of a certain unit. However, some results are also valid for ν_j all real. As mentioned in chapter 3, this is not difficult, if we choose a sufficiently small energy unit ν_o. We write $\hbar\omega = p\nu_o$ and $\nu_j = n_j/p$ for p a fixed positive integer and n_j an integer $\leq p$. The degeneracies a_n form a periodic sequence of integer numbers with $a_n = a_{n+p}$ and $a_n > 0$ for $n \equiv j \bmod \hbar\omega/\nu_o$ and zero otherwise, where $j\nu_o$ is the position of a level in the first shell. Thus:

$$\varepsilon_n = n\hbar\omega/p\ ,\ \text{for } a_n \neq 0 \quad \text{and} \quad e = \sum_{m=1}^{p} a_m\ ,\ \hbar\omega = p\nu_o\ . \tag{4.2.1b}$$

For the relations in terms of $1/\beta$, however, it is simpler to work explicitly with the ν_j . In **Figure 4.2** we show an example for a periodic spectrum with period $14\nu_o$ and an absolute shell width equal to $10\nu_o$. In general, the distribution of the levels within a period will be arbitrary rational numbers, allowing for example distributions with a smaller or a larger degree of level repulsion.

Assumption eq.(3.1) (with $d_m = 1$) has been extended from the constant spectra to:

$$\sum_{\substack{k>o \\ k\equiv i \bmod(p)}}^{(n-1)p+i} a_k = nA^{(i)} \quad , \quad a_{k\equiv i \bmod(p)} = A^{(i)} \ ; \ \sum_{i=1}^{p} A^{(i)} = e \ . \tag{4.2.1c}$$

with $i=1,2, \ldots ,p$ and $n = 1,2, \ldots$. For $p=1$ this relation reduces to the formula for a constant spectrum.

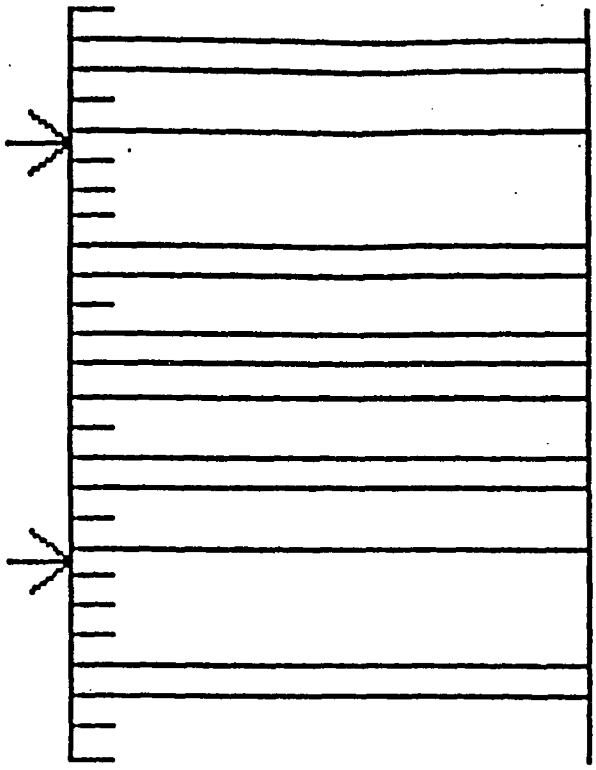


Figure 4.2 A periodic spectrum. The pattern between any two equivalent points (see arrows) repeats upwards and downwards. Here, the period is equal to 14 units (ν_o), $p=14$, the absolute shell width $W=10\nu_o$ and we have 8 different levels ν_j in each shell. If the levels are assumed to be non-degenerated, then $e=8$ and all $a_n=0$ or 1 .

The Dirichlet series is given by :

$$D(s) = \sum_{j=1}^{e} \sum_{n\geq o} \frac{1}{(n+\nu_j)^s} = \sum_{j=1}^{e} \zeta(s,\nu_j) = \sum_{j=1}^{p} a_j \sum_{n\geq o} \frac{1}{(n+j/p)^s} = \sum_{j=1}^{p} a_j\, \zeta(s,j/p) \ , \tag{4.2.2}$$

where $\zeta(s,a)$ is the Hurwitz ζ-function given by:

$$\zeta(s,a) = \sum_{n\geq o}(n+a)^{-s} = \Gamma(s)^{-1}\int_o^\infty dt\; t^{s-1} e^{-at}\,(1-e^{-t})^{-1}, \qquad (4.2.3a)$$

for Re s>1 and Re a>0 , or well :

$$\zeta(s,a) = \frac{1}{2}a^{-s} - \frac{a^{1-s}}{1-s} + \Gamma(s)^{-1}\int_o^\infty dt\; t^{s-1} e^{-at}\left[\frac{1}{e^t-1} - \frac{1}{t} + \frac{1}{2}\right], \qquad (4.2.3b)$$

for Re s>-1 and Re a>0 . From this last relation we recognize that $\zeta(s,a)$ has a single simple pole at s=1 and residue 1 on the rigth half plane. Thus, D(s) has a simple pole at s=1 (i.e. d=1) with residue equal e. Using the well known values $\zeta(0,a)=1/2 - a$ and $\zeta(-m,a)= -B_{m+1}(a)/(m+1)$ for m=0,1, ... , we find : $D(0)= e/2 - \Sigma\nu_j$ and $D(-1)= -e/12 - \Sigma\nu^2{}_j/2 + \Sigma\nu_j/2$.

The analytic continuation for D(s) can be found using the functional relation of Rademacher (1932) for the Hurwitz ζ-function:

$$\zeta(t,j/p)= 2\Gamma(1-t)(2\pi p)^{t-1}\left[\sin\frac{\pi t}{2}\sum_{n=1}^{p}\cos\left(\frac{2\pi jn}{p}\right)\zeta(1-t,\, n/p) + \cos\frac{\pi t}{2}\sum_{n=1}^{p}\sin\left(\frac{2\pi jn}{p}\right)\zeta(1-t,\, n/p)\right], \qquad (4.2.4)$$

and from this equation we found easily :

$$D(s) = 2\Gamma(1-s)(2\pi p)^{s-1}\left[\sin\frac{\pi s}{2}D_c(1-s) + \cos\frac{\pi s}{2}D_s(1-s)\right], \qquad (4.2.5)$$

where the Dirichlet series D_c and D_s are obtained from D(s) after substitution of the numbers a_n respectively by the following finite Fourier cosine and sine transforms :

$$c_n = \sum_{j=1}^{p} a_j \cos\frac{2\pi jn}{p} \quad , \quad s_n = \sum_{j=1}^{p} a_j \sin\frac{2\pi jn}{p} \; . \qquad (4.2.5a)$$

For the partition function holds :

$$Z(x)=\sum_{j=1}^{e}\sum_{n\geq o}\exp(-\,x(n+\nu_j)) = \frac{1}{e^x-1}\sum_{j=1}^{e}\exp(-\,x(1-\nu_j)) \; . \qquad (4.2.6)$$

Its power series around the origin follows immediately from the definition of the Bernoulli polynomials, eq.(3.2.21) :

$$Z(x) = \sum_{j=1}^{e} \sum_{n\geq o} \frac{1}{n!}\, x^{n-1}\, B_n(1-\nu_j) = \frac{e}{x} + \sum_{j=1}^{p} a_j \sum_{n\geq o} \frac{(-x)^n}{n!}\, \zeta(-n, {}^{j}/_{n}) \,, \tag{4.2.7}$$

which can be transformed into a Laurent series using Rademacher's relation eq.(4.2.4) :

$$Z(x) = \frac{e}{x} + \frac{e}{2} - \sum_{j=1}^{e} \nu_j + 2\sum_{j=1}^{p} \sum_{n\geq o} \frac{x c_j + 2\pi(Nn+j)s_j}{4\pi^2(Nn+j)^2+x^2} . \tag{4.2.7a}$$

This relation shows explicitely the position of the poles at the imaginary axis. It is additionally possible to obtain the functional relation for D(s) (cf. eq.(4.2.5)) by a Mellin transformation.

For the single particle level density we find from eq.(3.2.19) :

$$g(\varepsilon)\hbar\omega = e + \sum_{j=1}^{e} \sum_{k\geq o} (\hbar\omega)^{k+1}\, \zeta(-k,\nu_j)\, \delta^{(k)}(\varepsilon)/k! \,. \tag{4.2.8}$$

The grand canonical partition function results from eq.(3.3.20) as the following function :

$$\begin{aligned} \ln Z(\alpha,\beta) = {} & \ln Z(-\alpha,-\beta) + \frac{\pi^2 e}{6\beta} + \frac{\alpha^2 e}{2\beta} + \frac{\alpha e}{2} + \frac{\beta e}{12} + \frac{\beta}{2} \sum_{j=1}^{e} \nu_j(\nu_j-1) - \\ & - \alpha\sum_{j=1}^{e} \nu_j - \sum_{j=1}^{e} D_1(\mu-\nu_j,\pi t) \,, \end{aligned} \tag{4.2.9}$$

where the series $D_1(z,\pi t)$ is given by eq.(4.1.5).

We measure as before μ and $1/\beta$ in units of $\hbar\omega$ for simplicity.

For the particle number relation we find from eq.(3.4.10) :

$$N = \mu e + \frac{e}{2} - \sum_{j=1}^{e} \nu_j - 2\pi i t \sum_{j=1}^{e} D_o(\mu-\nu_j,\pi t) \,, \tag{4.2.10}$$

and for the energy, eq.(3.4.11) leads us to :

$$E/\hbar\omega = \frac{\pi^2 e}{6\beta^2} + \frac{\mu^2 e}{2} - \frac{1}{2}\sum_{j=1}^{e}\nu_j(\nu_j-1) - \frac{e}{12} - 2\pi i\mu t\sum_{j=1}^{e} D_0(\mu-\nu_j,\pi t) - $$

$$- t^2(1+t\partial_t)\, t^{-1}\sum_{j=1}^{e} D_1(\mu-\nu_j,\pi t) \quad . \qquad (4.2.11)$$

For the entropy we easily find (cf. eq.(3.4.3a) :

$$S(\alpha,\beta) = \frac{\pi^2 e}{3\beta} - \partial_t\, t\sum_{j=1}^{e} D_1(\mu-\nu_j,\pi t) \quad , \qquad (4.2.12)$$

here $\mu=\alpha/\beta$ and $t= 1/\beta$.

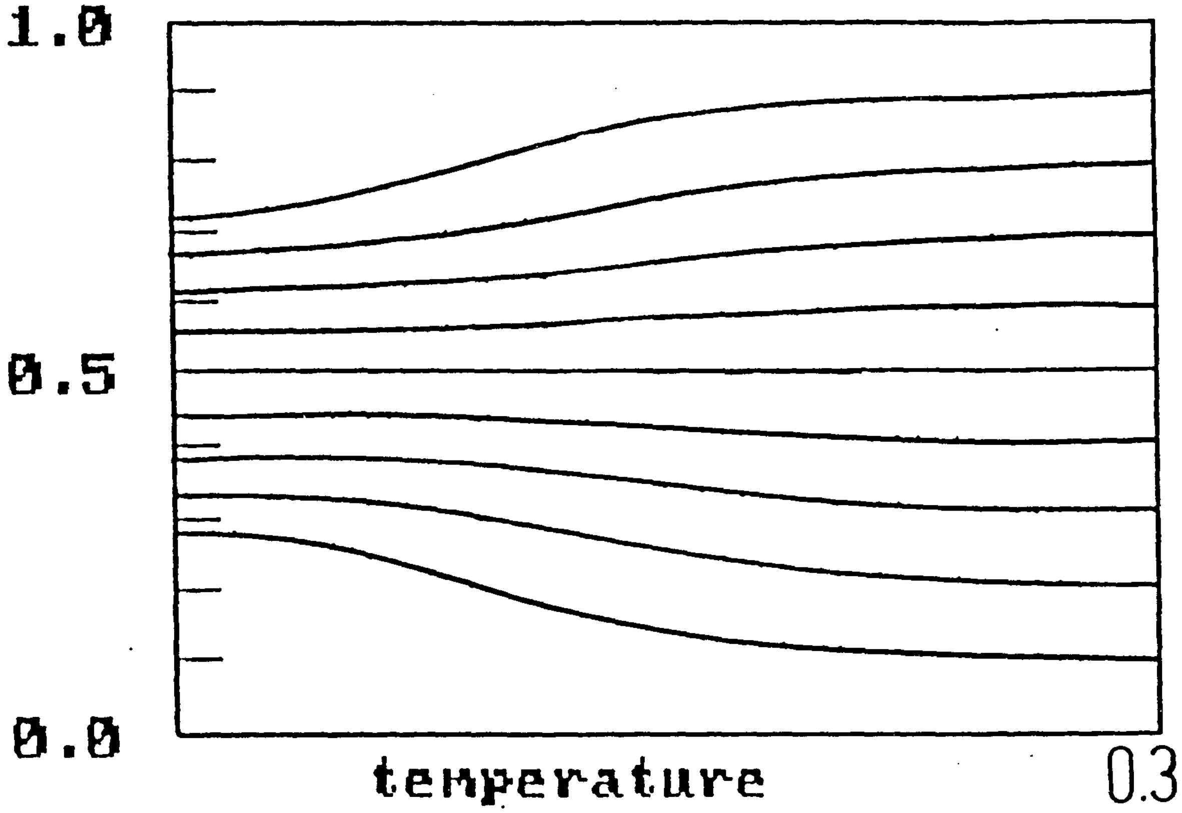


Figure 4.3 Temperature dependent shell filling parameter $y= \{\mu\}-1/2$. Shell width equal to $0.5\hbar\omega$ for a shell of 10 equally spaced levels.

In Figure 4.3, we show the temperature dependent shell filling parameter $y = \{\mu\} - 1/2$ computed numerically. The curves correspond to values of x in steps of 0.1 for a total shell width of $0.5\hbar\omega$ and for a shell consisting of 10 equally spaced levels. The absisas axis corresponds to x=0.0, the lowest curve to x=0.1, etc. . Again, the washing out of the ground state shell structure is clearly observed as the temperature increases.

Now we analyse the smooth ground state formulae. For the ground state we find after integration of $g(\varepsilon)$ directly :

$$\tilde{E}_0/\hbar\omega = \frac{e\tilde{\mu}_0^2}{2} - \frac{e}{12} - \frac{e}{2}(\langle\nu^2\rangle - \langle\nu\rangle) \text{ , and: } N = e\tilde{\mu}_0 + \frac{1}{2}e - \langle\nu\rangle e \text{ .} \quad (4.2.13)$$

In terms of the second and first moments: $\langle\nu^2\rangle = \sum_i \nu_i^2/e$, and $\langle\nu\rangle = \sum_i \nu_i/e$. These relations yield the expression :

$$\tilde{E}_0/\hbar\omega = \frac{N^2}{2e} - \frac{N}{2} + \frac{e}{24} + N\langle\nu\rangle - \frac{e}{2}(\langle\nu^2\rangle - \langle\nu\rangle^2) \text{ .} \quad (4.2.14)$$

Note that the quantity in the last brackets is the variance: $v^2 = \langle\nu^2\rangle - \langle\nu\rangle^2$.

Whereas for the exact quantities we obtain :

$$E_0/\hbar\omega = \frac{e}{2}[\mu_0]([\mu_0]+1) + xe([\mu_0]+1) + ([\mu_0]+1)\langle\nu\rangle + \sum_{j=1}^{xe}\nu_j \text{ ,} \quad (4.2.15)$$

and $N = ([\mu_0]+1)e + xe$. Solving for $[\mu_0]$:

$$E_0/\hbar\omega = \frac{N^2}{2e} - \frac{N}{2} + \frac{e}{2}\,x(1-x) + \sum_{j=1}^{xe}\nu_j + (N - xe)\langle\nu\rangle \text{ .} \quad (4.2.16)$$

Subtracting now the obtained expressions for the exact and the smooth energies we are lead to :

$$E_{\text{shell}}(0)/\hbar\omega = \frac{e}{2}x(1-x) - \frac{e}{24} + \sum_{j=1}^{xe}(\nu_j - \langle\nu\rangle) + \frac{e}{2}(\langle\nu^2\rangle - \langle\nu\rangle^2) \text{ .} \quad (4.2.17)$$

Note that for closed shells (x=0,1) the first and third terms are zero. As expected, this ground state shell correction does not depend on the position of the lowest eigenvalue .

Using now this relation and solving for μ eq.(4.2.10) and substituing it in eq.(4.2.11) for the energy, we obtain for the excitation energy the result:

$$U \approx \frac{\pi^2 e}{6\beta^2}\hbar\omega \;+\; E_{shell}(t) \;-\; E_{shell}(0) \;, \qquad (4.2.18)$$

where the temperature dependent shell energy correction is given by :

$$E_{shell}(t)/\hbar\omega \;=\; \frac{2\pi^2 t^2}{e}\Big(\sum_{j=1}^{e} D_o(\mu-\nu_j,\pi t)\Big)^2 \;-\; t^2(1+t\partial_t)\,t^{-1}\sum_{j=1}^{e} D_1 \;, \qquad (4.2.19)$$

here $\mu=\alpha/\beta$ and $t=1/\beta$.

All the above relations reduce, letting $\nu_j \rightarrow 0$, to the corresponding expressions obtained in the preceding section for vanishing shell width.

The expressions we have obtained can also be transformed into relations containing β instead of $1/\beta$, as shown in the preceding section. From eq.(4.1.19) we obtain the necessary transformation rule. The resulting expressions for the particle number, the excitation energy and the entropy are similar to those of last section, respectively eq.(4.1.22), eq.(4.1.25) and eq.(4.1.26) . The difference is only a sum over the numbers a_n [cf. eq.(4.2.1b)] and, of course, with $E_{shell}(0)$ given by eq.(4.2.17) in this section.

Let us finally mention that now the grand partition function can be expressed in terms of products of **ϑ-functions with characteristics:**

$$\vartheta_{ab}(z|\tau)=C(\tau)\; e^{\pi i a^2\tau + 2\pi i a(z+b)} \prod_{n\geq 0}(1+q^{2n+1}e^{-2\pi i(z+a\tau+b)})(1+q^{2n+1}e^{2\pi i(z+a\tau+b)})$$

$$= \sum_{-\infty}^{\infty} \exp\{\; i\pi(n+a)^2\tau \;+\; 2\pi i(n+a)(z+b)\;\} \;, \qquad (4.2.20)$$

this function satisfies the following transformation formula found by Gauß (1808) :

$$\vartheta_{a,b}(z|\tau) \;=\sqrt{\frac{1}{\tau}}\; e^{-i\pi z^2/\tau \;+\; 2\pi i ab}\;\; \vartheta_{-b,a}(z/\tau|-1/\tau) \;, \qquad (4.2.21)$$

which contains as particular cases the relations eqs.(3.5.4a-d).

Products of these kind of theta functions are called **higher order ϑ-functions** (with characteristics). The order is related for our problem with the shell degeneracy e . The full development of our treatment would involve many properties of these functions, but for now the results we have displayed are sufficient. See section 7.3 for more results.

4.3. General Single Particle Spectra.

The extension we have made in the preceding sections can also be carried out for the general case of chapter three, although the treatment becomes more difficult. We have not yet worked out the general case because the results obtained in the preceding section allowed us to improve the theoretical understanding of certain experimental results we had in mind and which will be explained in the next chapter. Nevertheless, it is still necessary to analyze more in detail the experimental results concerning nuclear level densities to be sure that the periodic single particle spectra considered in the preceding section are sufficiently powerful to cover the most relevant characteristics. At present there is no way to be sure of this fact and it would not be surprising if more general spectra were necessary.

In the preceding chapter we studied spectra with a general single particle level density growing. In the context of this chapter these considerations should be extended to include a clear characterization of the local distribution of the single particle levels, in particular near the Fermi level. Let us remember that in the preceding chapter, the shells were considered as if they would have zero width. But if the single particle level density is an increasing function, a finite shell width will lead to an overlapping of shells. The lowest order approximation to the general problem is already at hand, if the excitation energies are not too high. We need simply to substitute the constant shell degeneracy by the value of the general single particle level density evaluated at the Fermi level.

One part of the forthcoming result can also be visualized now. From the results of the preceding section, the information about the local structure of the spectra is present through the first two moments of the distribution around the Fermi level. Also in the general case we expect to be able to express in a similar way the most relevant quantities associated with the single particle spectrum.

To conclude this chapter some general observations concerning the generalization of the spectra of chapter 3 will be presented. Applications to a three dimensional harmonic oscillator with spin-orbit coupling and to an anisotropic three dimensional oscillator will be initiated.

A first simple generalization can be induced from eq.(4.2.1c). As it can be seen, the simple summation over all integers present in the general assumption eq.(3.1) has been simply divided into sums modulo an integer p. Thus, in general it is reasonable to propose instead of eq.(3.1) the new assumption:

$$\sum_{\substack{k>o\\ k\equiv i\ \mathrm{mod}(p)}}^{(n-1)p+i} a_k = \sum_{m} \frac{A_m^{(i)}}{d_m^{(i)}}\, n^{d_m^{(i)}} , \quad i=1,2, \dots , p; \quad d_m^{(i)} \geq 0. \tag{4.3.1}$$

This means simply that a set of p spectra with single particle level densities of polynomial growth has been introduced. With this assumption a shell structure has been introduced in the spectra. The partition function [cf. eq.(3.1.2)] will be now:

$$Z(x) = \sum_{i=1} \sum_{\substack{k>o\\ k\equiv i\ \mathrm{mod}(p)}} a_k\, e^{-xk/p} , \quad \mathrm{Re}\ x>\delta>0. \tag{4.3.2}$$

Since no essentially new complications have been introduced, the method of chapter 3 can also be applied here. Instead of sums over a single type of spectrum, there will be now sums over the p types introduced. In many cases, to attach a new upper index $i=1, \dots , p$ to the residues A_m and the pole orders d_m and to sum over i will be enough. However, it is necessary to be careful to rewrite the sums over all the integers as sums over the integers modulo p. We do not want to follow this approach further here.

A second simple generalization of the results of chapter 3 to include spectra with shell structure is the following. It occurs offen that instead of a single Dirichlet series a sum of products of series is present, i.e. a sum of terms like:

$$Z(x) = \prod_{i} Z_i(x) , \quad \text{with} \quad Z_i(x) = \sum_{n>o} a_{ni}\, e^{-nx\kappa_i} , \quad \kappa_i>0, \tag{4.3.3}$$

Sometimes the products can be expressed without large efforts as a single series, but the new coefficients will be in general more involved. Alternatively, the methods of chapters 3 and 4 can be applied first to each factor $Z_i(x)$ and in some cases be extended to the grand partition function. We will consider now two examples where this is possible.

A very simple shell model in Nuclear Physics is the harmonic oscillator with spin-orbit coupling and Hamiltonian:

$$H = \frac{-\hbar^2}{2M}\Delta + \frac{1}{2} M\omega^2 r^2 - 2\hbar\omega\,\kappa\,\ell\cdot\sigma \quad , \tag{4.3.4}$$

Here $\hbar\omega \approx 41A^{-1/3}$ and the spectrum is:

$$\begin{aligned} \varepsilon_{j=\ell+1/2} &= (2n_r+\ell+3/2)\hbar\omega - \kappa\hbar\omega\ell \ ; \\ \varepsilon_{j=\ell-1/2} &= (2n_r+\ell+3/2)\hbar\omega + \kappa\hbar\omega(\ell+1) \ , \end{aligned} \qquad n_r,\ell = 0,1,\ldots \ ; \tag{4.3.5}$$

with degeneracies $2(\ell+1)$ and 2ℓ respectively. The parameter $\kappa \approx A^{-1/3}/4$ lies between 0.03 and 0.1 . In Fig. 4.4a, the first levels for the harmonic oscillator with spin-orbit coupling parameter $\kappa \in (0.0,\ 0.1)$ are shown. And in Fig. 4.4b with an additional correction term $(\lambda-1)\ell\hbar\omega$ $(\lambda=0.85)$ to yield a better agreement with the nuclear magic numbers.

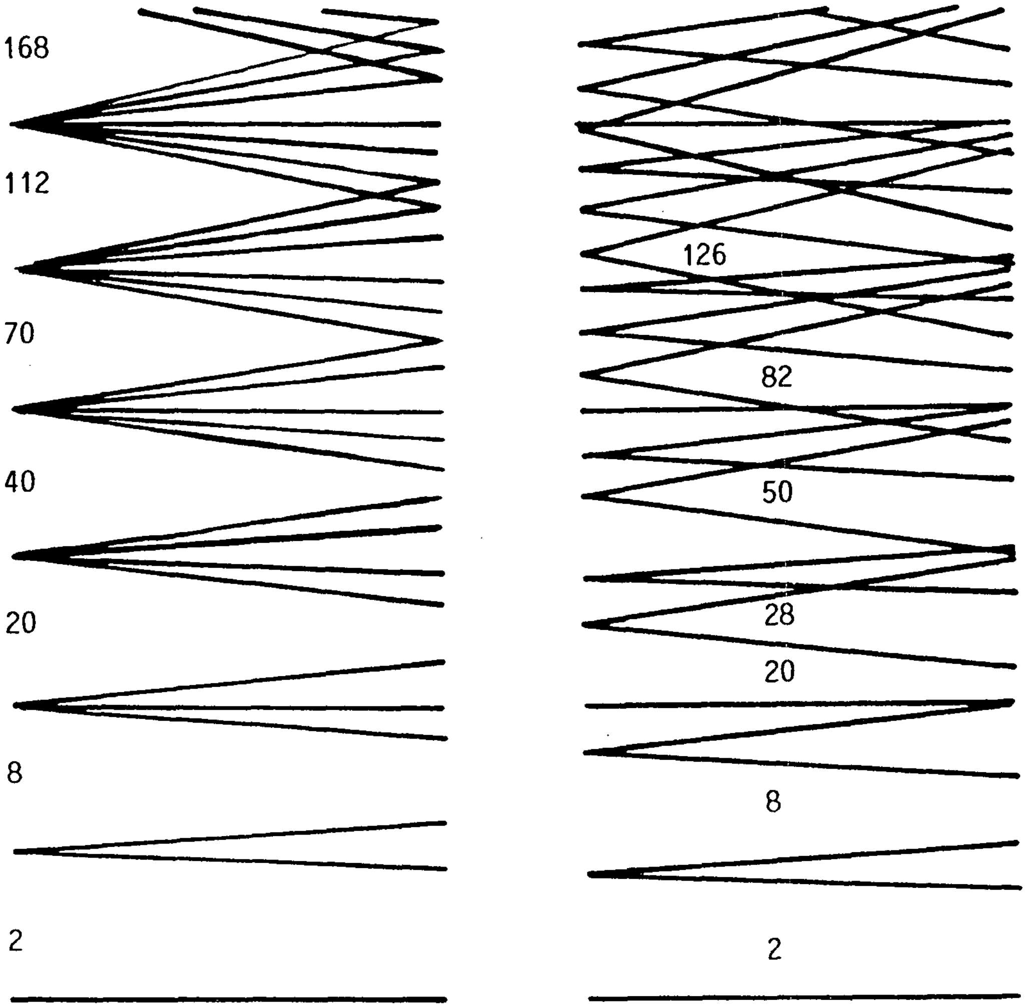


Figure 4.4 Harmonic oscillator spectra. In (a) with spin-orbit and $\kappa \in (0.0,\ 0.1)$. In (b) with an additional term $(\lambda-1)\hbar\omega\ell$ to yield magic numbers as shell closures.

Set now for simplicity $\hbar\omega = 1$. Thus:

$$Z(x) = 2\sum_{n\geq 0} e^{-x(2n+3/2)} \sum_{\ell\geq 0} \left[(\ell+1)e^{-x\ell(\lambda-\kappa)} + \ell e^{-x\ell(\lambda+\kappa)-x\kappa}\right] =$$

$$= \frac{2e^{-3x/2}}{1-e^{-2x}} \left[\frac{e^{-x(\lambda-\kappa)}}{(1-e^{-x(\lambda-\kappa)})^2} + \frac{1}{1-e^{-x(\lambda-\kappa)}} + \frac{e^{-x(\lambda+2\kappa)}}{(1-e^{-x(\lambda+\kappa)})^2} \right]. \qquad (4.3.6)$$

To each sum there is a Dirichlet series associated, for example $\zeta(s,3/2)$ for the first and $\zeta(s-1)+\zeta(s)$ for the second. It is also possible to apply the methods to work out the logarithm of the grand partition function as in chapter 3.

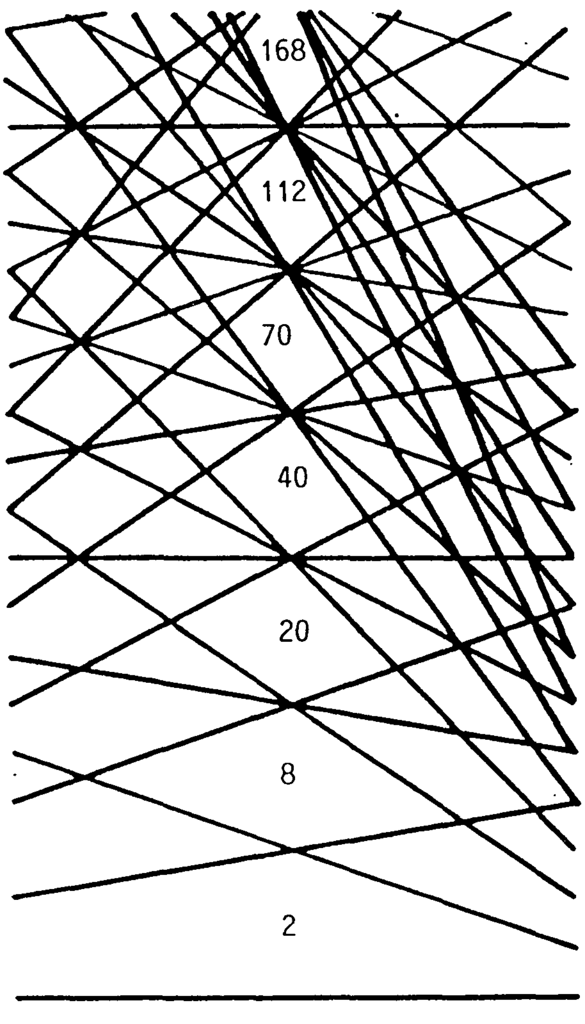


Figure 4.5 Spectrum of the anisotropic oscillator as a function of the deformation parameter $\delta_{osc} \in (-1.0, 1.0)$.

The anisotropic oscillator (see for example A. Bohr and B. Mottelson, 1975) can be considered similarly. The Hamiltonian is now:

$$H= \frac{-\hbar^2}{2M}(\omega_1{}^2\partial_x{}^2 + \omega_2{}^2\partial_y{}^2 + \omega_3{}^2\partial_z{}^2) \,, \tag{4.3.7}$$

with eigenvalues: $\varepsilon(n_1,n_2,n_3)/\hbar = \omega_1 n_1+\omega_2 n_2+\omega_3 n_3+(\omega_1+\omega_2+\omega_3)/2$. In Fig. 4.5, the spectrum for an axially symmetric oscillator is displayed. The eigenvalues are: $\varepsilon(n_3,n)/\hbar\omega_o = N+3/2-\delta_{osc}(2n_3-n)/3$, with $N= n_3+n$, $n= n_1+n_2$, $3\omega_o= \omega_1+\omega_2+\omega_3= 2\omega+\omega_3$ and deformation parameter $\delta_{osc}= 3(\omega-\omega_3)/(2\omega+\omega_3)$. The partition function is now:

$$Z(x)= 2\prod_i \sum_{n\geq 0} e^{-x\hbar\omega_i(n+1/2)} = 2\prod_i e^{-x\hbar\omega_i/2} /(1-e^{-x\hbar\omega_i}). \tag{4.3.8}$$

The associated Dirichlet series for each factor are $(\hbar\omega_i)^{-s}\zeta(s,1/2)$. For the harmonic oscillator $\omega_1=\omega_2=\omega_3$, the Dirichlet series associated to $Z(x)= \sum(n+1)(n+2)\exp[-x\hbar\omega_1(n+3/2)]$ is $\zeta(s-2,3/2)-\zeta(s,3/2)/4$. The further steps of the calculation of the grand partition function will not be presented here. It is clear that our method is also applicable in this case.

CHAPTER 5

COMPARISON WITH EXPERIMENT

In this chapter, some of the theoretical results will be compared with experimental data of nuclear level densities. This is the most important part of this work. We will consider only the simple periodic spectrum as studied in section 4.2 of the preceding chapter and will show that such a simple spectrum, when considered carefully, helps us to understand some aspects of the shell structure observed experimentally. Further, we shall achieve in this way a better theoretical description of the nuclear level density as that currently known. Since the calculation we have in mind is the most simple application of our work in chapter three, we can expect further improvements from the consideration of more general spectra. Such extensions as well as the full computation of all possible quantities usually studied in relation with the nuclear level density are left for the future.

We resume first the formulae that will be needed from last chapter. Next the a-parameter is calculated at the neutron binding energies for the same elements considered in the compilation of T. von Egidy et al. (1986, 1988). After the selection of only few values for the shell width the experimental data are reproduced to a great extent. As a last point, we observe that, although the calculation has been done to compute the a-parameter at the neutron binding energy, there is a by-product. This last corresponds to the shell corrections to the semi-empirical mass-formula [cf. eq.(5.13)]. The experimental values for the correction are taken from the compilation of A.H. Wapstra and G. Audi (1985) and are compared with our results obtained during the a-parameter calculation. A relative good agreement shows the consistency of the procedure.

We will consider only the so-called "a-parameter" which we define by the following relation:

$$a = S^2(\alpha,\beta)/4(U-\delta) \ . \qquad (5.1)$$

This quantity appears as a constant for the constant single particle spectrum or as the lowest order approximation for a general spectrum for large excitation energies. At lowest approximation order it is given by $\pi^2 g(\varepsilon_F)/6$, where $g(\varepsilon_F)$ is the (smooth) single particle level density at the Fermi level. In general it is well known that this parameter is energy dependent and that it shows a shell structure consisting in strong deviations for magic nuclei. The energy shift δ is given naturally as:

$$\delta = E_{shell}(1/\beta) - E_{shell}(0) \ , \tag{5.2}$$

which is clearly energy dependent. Nevertheless, this is not the parametrization used in the relevant literature. As we will explain, the constant δ commonly used is the pairing energy Δ and given according to:

$$\begin{aligned} \Delta &= \Delta_p + \Delta_n \ , && \text{for even-even nuclei,} \\ \Delta &= \Delta_p \ , && \text{for even-odd nuclei,} \\ \Delta &= \Delta_n \ , && \text{for odd-even nuclei,} \\ \Delta &= 0 \ , && \text{for odd-odd nuclei.} \end{aligned} \tag{5.3}$$

From experiments it is well known that approximately $\Delta_{n,p} \approx 11.5\ \mathrm{MeV}/\sqrt{A}$. There is a slight tendency for Δ_p to exceed Δ_n and the sum $\Delta_n + \Delta_p$ is somewhat smaller than $2\Delta_{n,p}$; a possible result of the attractive interaction of the unpaired neutron with the unpaired proton in odd-odd nuclei.

There are several compilations of the a-parameter obtained in a variety of ways. We have selected the work by T. von Egidy and co-workers (1986 and 1988) because it is the most complete recently published contribution with a very clear explanation of the fitting procedure used to tabulate the a-parameter. This aspect is very important since there are very many effects involved, some of them very poorly understood. Von Egidy et al. use a (shifted) Bethe formula for the observable nuclear level density for the Fermi gas model given by:

$$\rho(U) = \sum_I \rho(U,I) \approx \frac{\exp(2\sqrt{a(U-E_1)})}{12\sqrt{2}\ \sigma\ a^{1/4}(U-E_1)^{5/4}} = \frac{1}{(2\pi)^{1/2}\sigma}\ \rho_0(U) \tag{5.4}$$

Here $\rho(U,I)$ is the density of levels of given angular momentum I at an excitation energy U and is given by:

$$\rho(U,I) = \frac{1}{(2\pi)^{1/2}\sigma}\ f(I)\ \rho_0(U) \ , \tag{5.5}$$

with Bethe's Gaussian angular momentum distribution:

$$f(I) = \exp(-I^2/2\sigma^2) - \exp(-(I+1)^2/2\sigma^2) \approx \frac{(2I+1)}{2\,\sigma^2}\exp[-(I+1/2)^2/2\sigma^2], \quad (5.6)$$

The density $\rho_0(U)$ defibed in eq.(5.4) is the total level density:

$$\rho_0(U) = \sum_I (2I+1)\ \rho(U,I)\ ,$$

and includes the degeneracies of the magnetic quantum number.

The level density a-parameter as well as the energy shift E_1 were obtained by a fit to the experimental results. Energy spacings from experimental nuclear level schemes [see for example Fig.(1.2)] for the first excited levels as well as the average neutron resonance spacings were included in a least squares fit. The spin cut off parameter σ is given by the relation of U. Facchini et al. (1968) :

$$\sigma^2 = 0.24\ A^{2/3}\, g(\varepsilon_F)\ t\ , \quad (5.7)$$

where $g(\varepsilon_F)$ is the single particle level density at the Fermi level and t the temperature.

As noticed by H. Hurwitz and H.A. Bethe (1951), the ground state energy should be renormalized by a shift involving shell effects as well as odd-even effects to obtain a better agreement with experiments. Nevertheless, as mentioned by A. Gilbert and A.G.W. Cameron (1965), following the works of T.D. Newton (1956) and of A.G.W. Cameron (1958), both effects cannot be unambiguously separated. These authors considered only a constant shift which takes account of the odd-even differences, whereas the shell structure effects were involved only in the parametrization of the a-parameter. This leads to a clear dependency of the a-parameter on the mass number A=N+Z, with an analogous behaviour as that of the shell correction to the nuclear binding energy. Such dependency does not constitute directly a renormalization of the ground state energy as our results suggest. The efforts of the last decades were directed towards a description of the energy dependency of the obtained a-parameter as defined above. Other possible ways to define the a-parameter have been proposed, but since the way followed by Gilbert and Cameron is by far the best established, we have also adhered to their definition for our present comparison.

We shall take account of the angular momentum of the studied nuclei as usual only by the Gaussian distribution f(J), which multiplies the whole level density as explained in chapter two. This separability of the angular momentum dependency means that for given numbers of neutrons and of protons, we fix the ground state configuration for a given single particle spectrum by filling the corresponding single particle levels without exception starting from the lowest allowed level upwards. Doing so, we forget any possible prescription of the angular momenta associated with each single particle level as required by the shell model. Although this point of view seems to have a rasonable experimental support since its introduction by Bethe, a quantitative analysis of the involved approximation is still lacking and is beyond our goals presently. Effects of collective rotational motion in the nuclear level density have been considered by T. Ericson (1958) and by S. Bjørnholm et al. (1974), but we will not take into account this corrections. However, for strongly deformed nuclei such considerations are important. To include effects like angular momentum selection rules or similar phenomena, it is necessary to select particular configurations from all possible configurations. In our language, this means to consider restricted partitions of integer numbers into smaller numbers under fixed conditions. We have considered in this work only unrestricted partitions (except for chapter seven). Thus the consequent work to include selection rules would be the study of restricted partitions.

As referred before, von Egidy et al. adjusted two parameters. One of them is a normalization of the ground state and the other gives the slope of the exponential growing of the level density. From their reported results, we can recognize, that the behaviour of E_1 is indeed like a pairing correction Δ plus a constant, which does not depend on the parity of the nuclei. Some shell structure is still present but it is much more damped than the shell dependency present in the $a_{\mathrm{experiment}}$-parameter. This difference results from the much larger sensibility of the level density to changes in the a-parameter.

The formulas we obtained in section 4.2 correspond to a general distribution of the single particle levels in a shell. Nevertheless, the relations show us that the important quantities are, besides the filling factor x associated with the ground state, the first two moments $<\nu>$ and $<\nu^2>$. The second moment is present only in the variance $v^2=<\nu^2>-<\nu>^2$ which is a measure of the width of the shell. Thus, a parametrization of the experimental data after our results for the periodic spectra is equivalent with a parametrization according to the spread of the shells, as well as of course taking care of how far the magic numbers are and of the local distribution of levels in a shell.

We quote now the needed equations from chapter four. From eq.(4.2.18), eq.(4.2.19) and eq.(4.2.17) the excitation energy is given by :

$$U = \frac{\pi^2}{6\beta^2} e + E_{shell}(1/\beta) - E_{shell}(0) , \qquad e = e_n + e_p , \tag{5.8}$$

with temperature dependent shell energy contribution :

$$\begin{aligned} E_{shell}(1/\beta)/\hbar\omega = & \frac{-2\pi^2}{e_n^2\beta^2} \left(\sum_{j=1}^{e_n} \sum_{k>o} \frac{\sin(2\pi k(\mu_n - \nu_{j,n}))}{\sinh(2\pi^2 k/\beta)} \right)^2 + \\ & + \frac{2\pi^2}{\beta^2} \sum_{j=1}^{e_n} \sum_{k>o} \frac{\cos(2\pi k(\mu_n - \nu_{j,n}))\cosh(2\pi^2 k/\beta)}{\sinh^2(2\pi^2 k/\beta)} + \text{similar for protons} , \end{aligned} \tag{5.9}$$

with ground state value:

$$\begin{aligned} E_{shell}(0)/\hbar\omega = & \frac{e_n}{2} x_n(1-x_n) - \frac{e_n}{24} + \sum_{j=1}^{x_n e_n} \left(\nu_{j,n}/e_n - \sum_{j=1}^{e_n} \nu_{j,n}/e_n \right) + \\ & + \frac{e_n}{2} \left[\sum_{j=1}^{e_n} \nu_{j,n}^2/e_n - \left(\sum_{j=1}^{e_n} \nu_{j,n}/e_n \right)^2 \right] + \text{similar for protons} . \end{aligned} \tag{5.10}$$

The chemical potential $\mu_{n,p}$ can be determined from eq.(4.2.10) :

$$N_n = \mu_n e_n + \frac{e_n}{2} - \sum_{j=1}^{e_n} \nu_{j,n} + \frac{2\pi}{\beta} \sum_{j=1}^{e_n} \sum_{k>o} \frac{\sin(2\pi k(\mu_n - \nu_{j,n}))}{k \sinh(2\pi^2 k/\beta)} . \tag{5.11}$$

An analogous equation holds for protons. For the entropy we have from eq.(4.2.12) :

$$S(\alpha,\beta) = \frac{\pi^2 e}{3\beta} - \partial_t\, t \sum_{\substack{j=1 \\ i=n,p}}^{e_i} \sum_{k>o} \frac{\cos(2\pi k(\mu_i - \nu_{j,i}))}{k \sinh(2\pi^2 k/\beta)} , \tag{5.12}$$

here $e_{n,(p)}$ give the constant shell degeneracy for neutrons (protons). The numbers $\nu_{j,i}$ (i=n,p) are the positions of the sublevels in a shell.

To find out which distribution of sublevels in a shell is the most adequate we have two different ways. The first consists in the selection of the most simple distribution with a minimum of physical assumptions. The second way follows the opposite path and considers the largest amount of information from other sources. An example for the first possibility could be a selection of the numbers ν_j statistically distributed, e.g. as the eigenvalues of a random matrix subject to general symmetry principles. To take the values ν_j as the single particle levels of the last shell(s) of a shell model calculation with a Nilsson- type or a Woods-Saxon potential could be an example for the second. We have selected an intermediate way and have used the magic numbers as fixed by the harmonic oscillator potential levels with spin-orbit coupling. As an orientation the corresponding shell variances are also used.

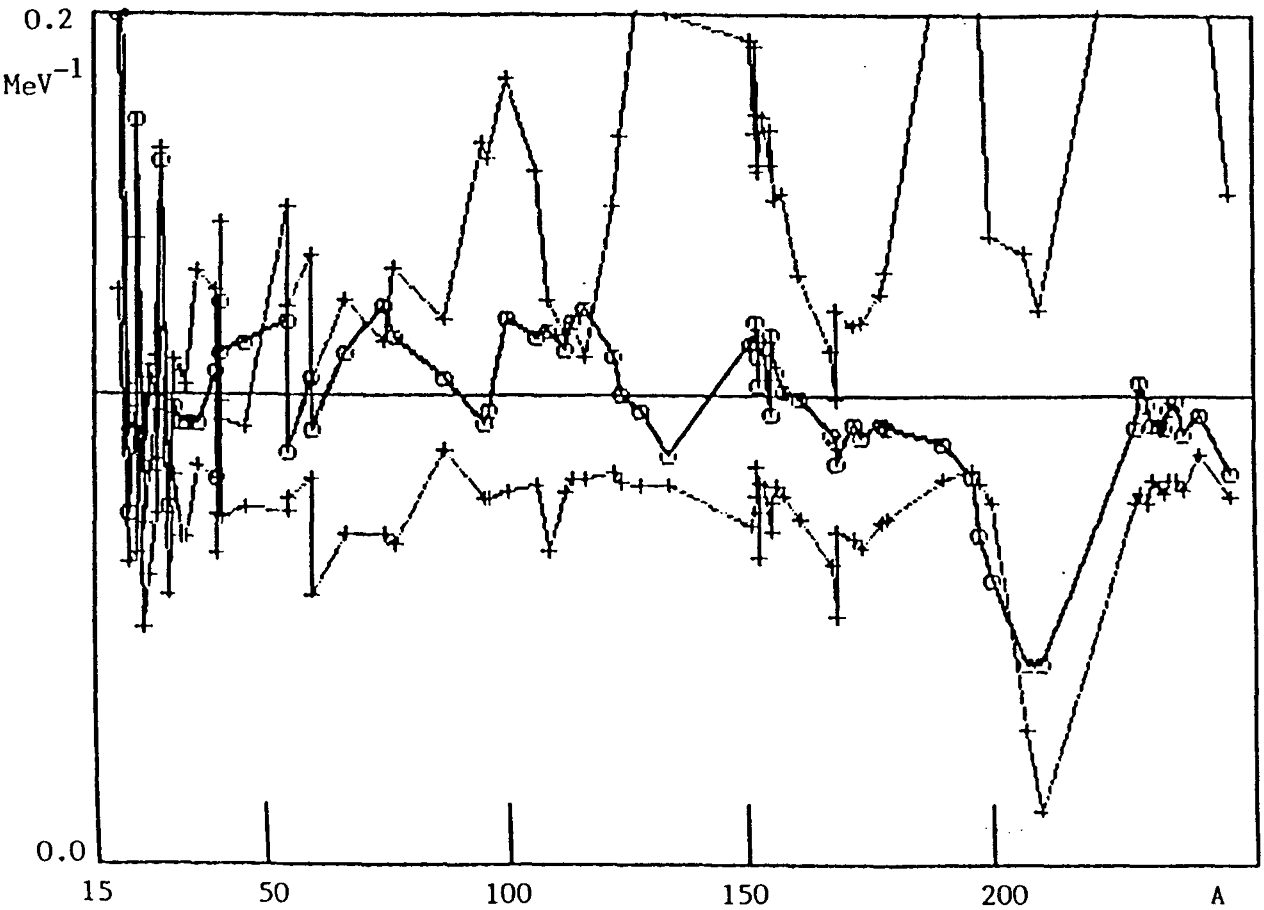


Figure 5.1 We show a/A in MeV^{-1} for the shell widths between $(0.5)\hbar\omega$ and $(0.95)\hbar\omega$ bounded by the upper and lower curves. The central curve displays the experimental data of von Egidy et al. The straight line gives their mean value at about $\hbar\omega/9$ MeV.

The sublevels in a shell have been selected as uniformly distributed in each shell and we associated mostly the same shell width for all nuclei belonging to the same shell at the ground state. We expect that different distributions with the same variances will not lead to strongly different values for the a-parameter.

We show in **Figure 5.1** the a-parameter at the neutron binding energy for the shell widths between $(0.5)\hbar\omega$ and $(0.95)\hbar\omega$, bounded by the upper and lower curves. All neutron binding energies were taken from the tables of A.H. Wapstra and G. Audi (1985b). The central curve represents the experimental results of von Egidy et al. . Since the experimental results are completely embedded into the curves of figure 5.1 (we could use also smaller shell widths). We can reproduce exactly the experimental values if we wish, selecting the adequate shell width for each nucleus. Nevertheless, we prefer a less arbitrary shell widths selection.

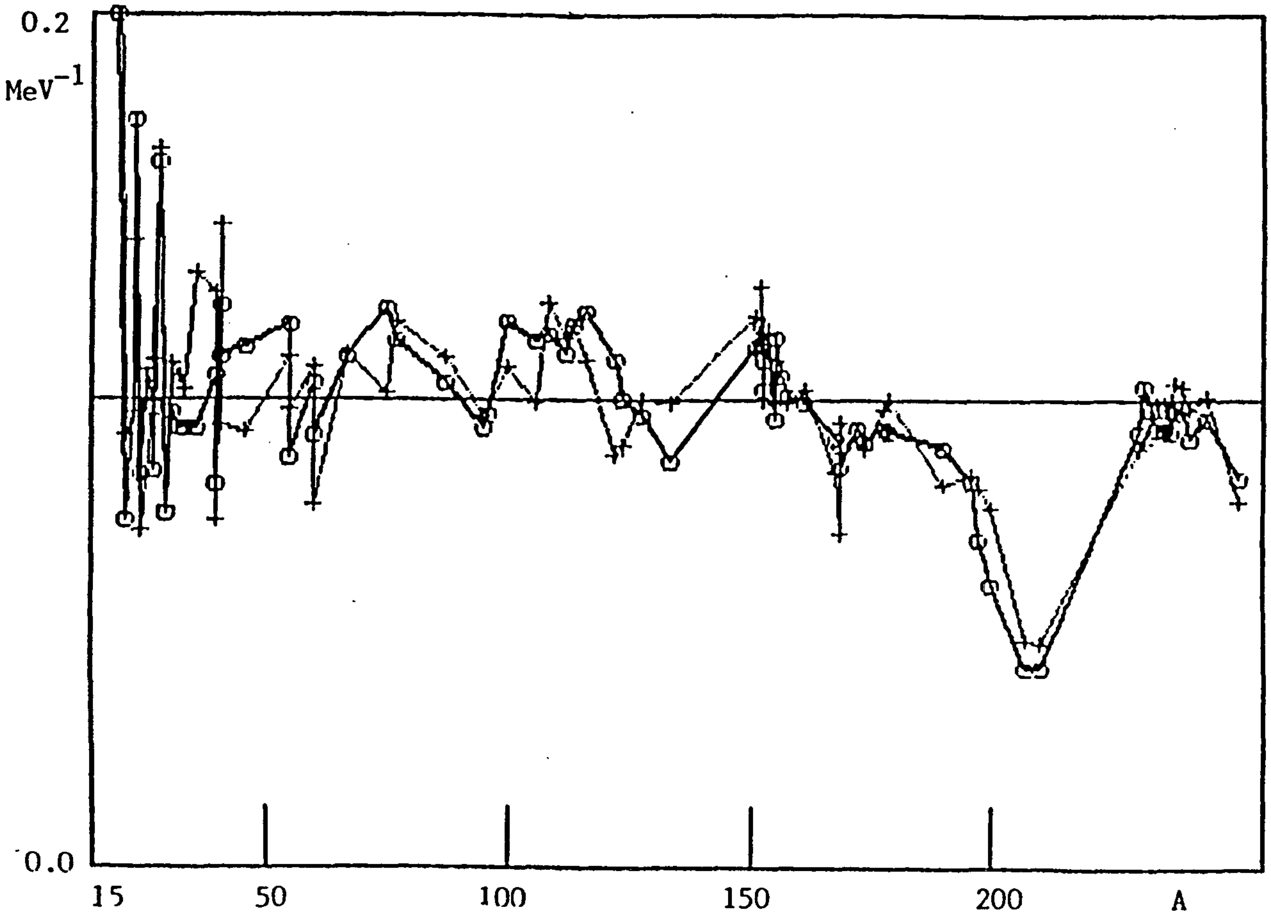


Figure 5.2 Comparison of a particular set of shell widths with the experimental results.

In **Figure** 5.2, the obtained theoretical results can be seen in comparison with the experimental compilation, selecting **the same shell width** for nuclei with neutrons and protons numbers belonging to the **same shells**. The selected shell widths vary between $(0.5)\hbar\omega$ (for ligth nuclei) and $(0.95)\hbar\omega$ (for deformed nuclei). As we can see, we were able, also subjected to the just mentioned restriction, to reproduce the experimental data rather well with our prescription.

As mentioned before, the evaluation of the $a_{exp.}$-parameter at the neutron binding energy corresponds to a selection of the energy dependent $a_{th.}$-parameter at different excitation energies. These energies oscillate in the considered nuclei between 11.417 MeV (for ^{34}S) and 4.604 MeV (for ^{210}Bi).

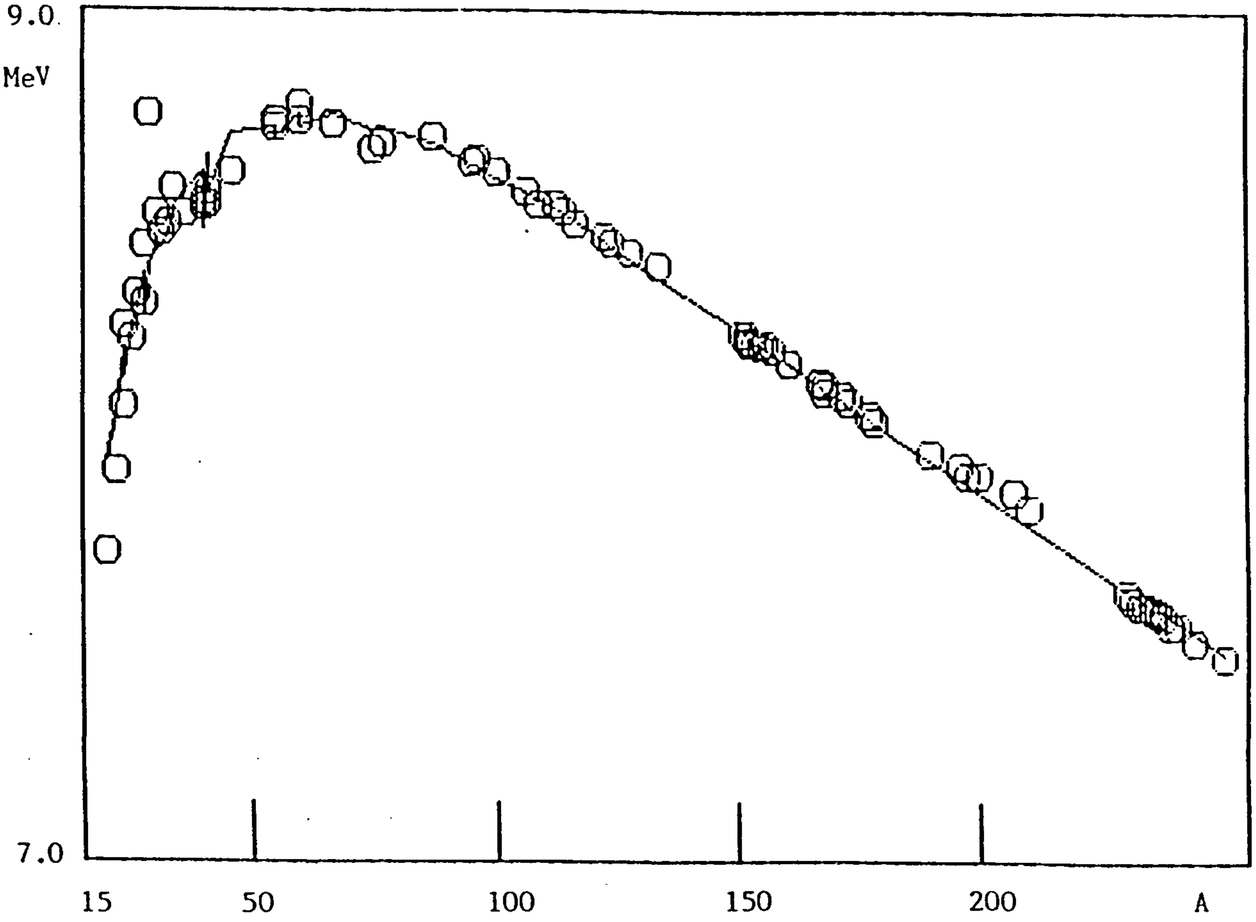


Figure 5.3 Experimental values for the nuclear binding energies in MeV. The curve gives the liquid drop model fit.

This work was oriented only towards the study of the nuclear level density and to a better understanding of the observed shell effects.

Nevertheless, at an early stage the relationship with the ground state properties of nuclei became clear. After we had evaluated the simple formulae for the periodic spectrum as

we have shown in this chapter, we were also interested to see what occurs with the shell effects contributions to the nuclear binding energy. We repeat that the study of this problem is not our primary interest, but a consequence of the treatment of excited nuclei.

In **Figure 5.3**, we show the experimental values for the nuclear binding energy for the same nuclei we have considered before. The values were taken from the compilation of A.H. Wapstra and G. Audi (1985a). The curve is calculated using the well known Bethe-Weizsäcker semiempirical mass formula (von Weizsäcker C.F.(1935), Bethe H.A. and Bacher R.F. (1936)) :

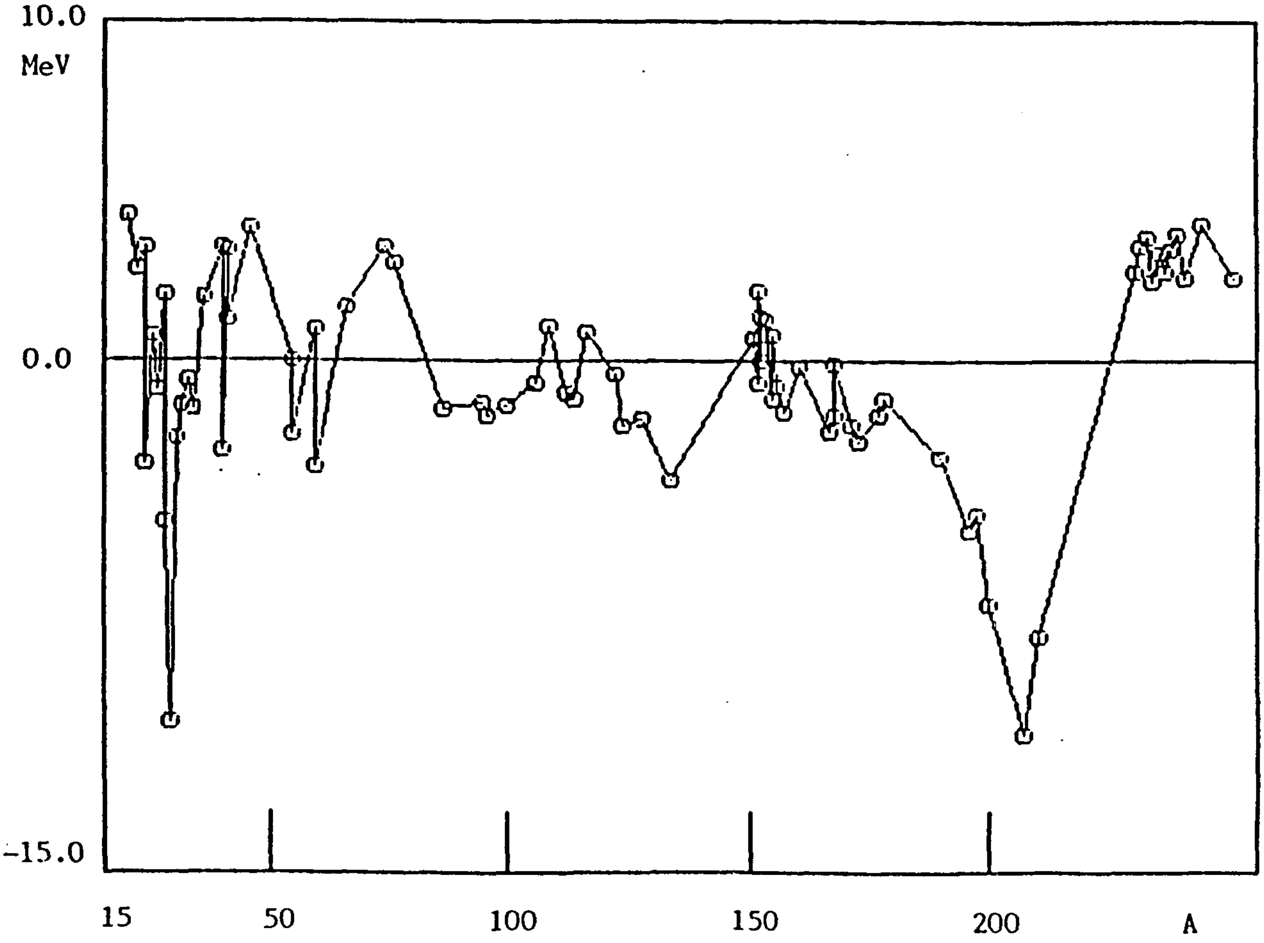


Figure 5.4 The difference between the experimental results and the semi-empirical mass formula.

$$B(N,Z) = b_{vol}A - b_{surf}A^{1/3} - \frac{1}{2}b_{sym}\frac{(N-Z)^2}{A} - b_{Coul}\frac{Z^2}{A^{1/3}} , \qquad (5.13)$$

where we used the parameters of A.E. Green and N.A. Engler (1953): $b_{vol}=15.56$ MeV, $b_{surf}=17.23$ MeV, $b_{sym}=46.57$ MeV, $b_{Coul}=0.697$ MeV. We recognize in the figure a systematic deviation, the shell effects, which can be better appreciated in **Figure 5.4** .

Thus it is natural to compare these "experimental" shell corrections with our simple result for the uniform periodic spectrum for the shell effects (cf. eq.(5.10)), includding of course the pairing energies (cf. eq.(5.3)) taking into account the even-odd effects.

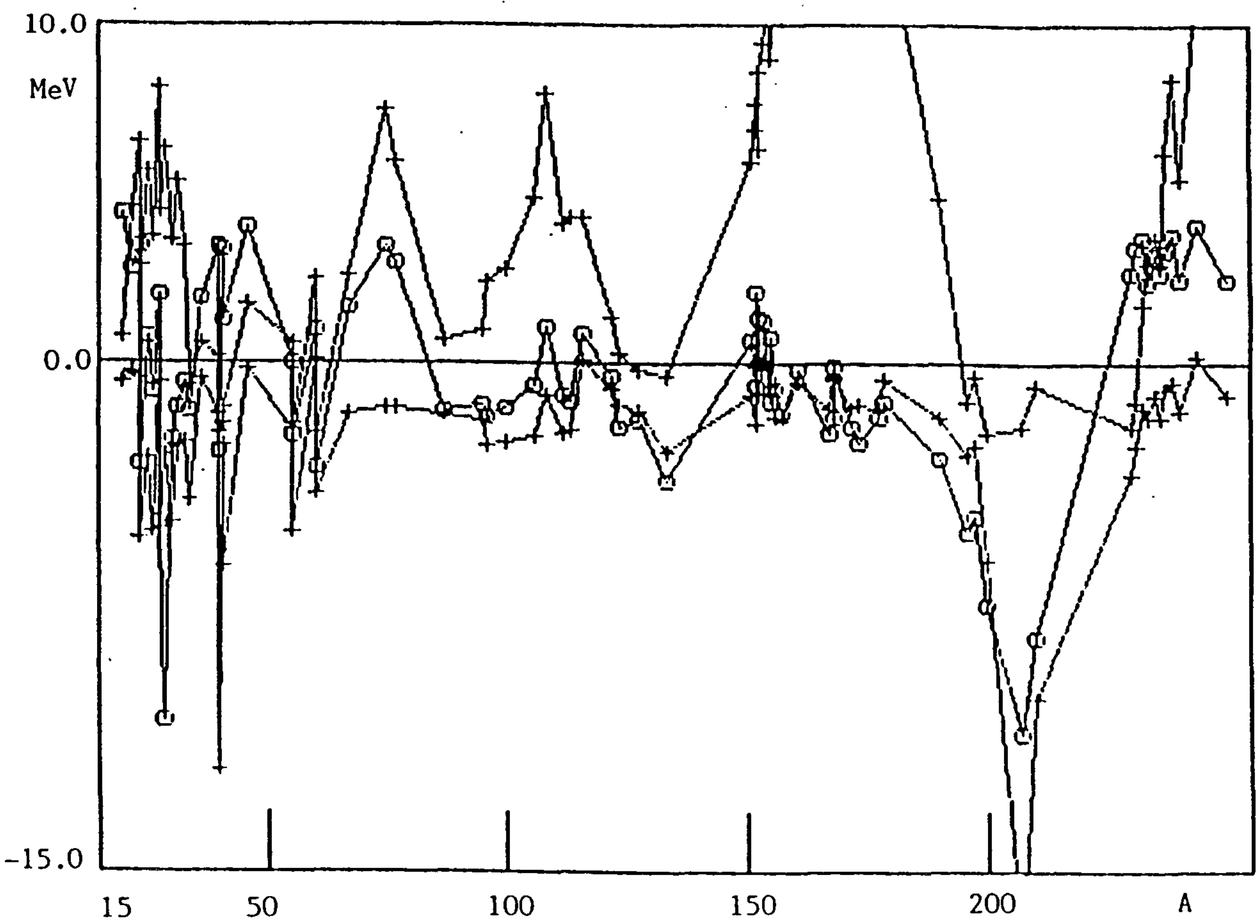


Figure 5.5 The theoretical results for a uniform periodic spectrum, for widths between $(0.5)\hbar\omega$ and $(0.95)\hbar\omega$ are bound by the curves with markers "+". The experimental values are also shown.

In **Figure** 5.5, we show the region of values that we obtain after variation of the shell widths between $(0.5)\hbar\omega$ and $(0.95)\hbar\omega$. The experimental curve cannot be covered as well as we did for the a- parameter (see figure 5.1), but the result is still acceptable, especially if we fit a shell width for each nucleus. Much better is to select precisely the same shell widths as we have done for the a- parameter, i.e. to select the **same shell widths** for those nuclei with protons and neutrons numbers belonging to the **same shell**, respectively .

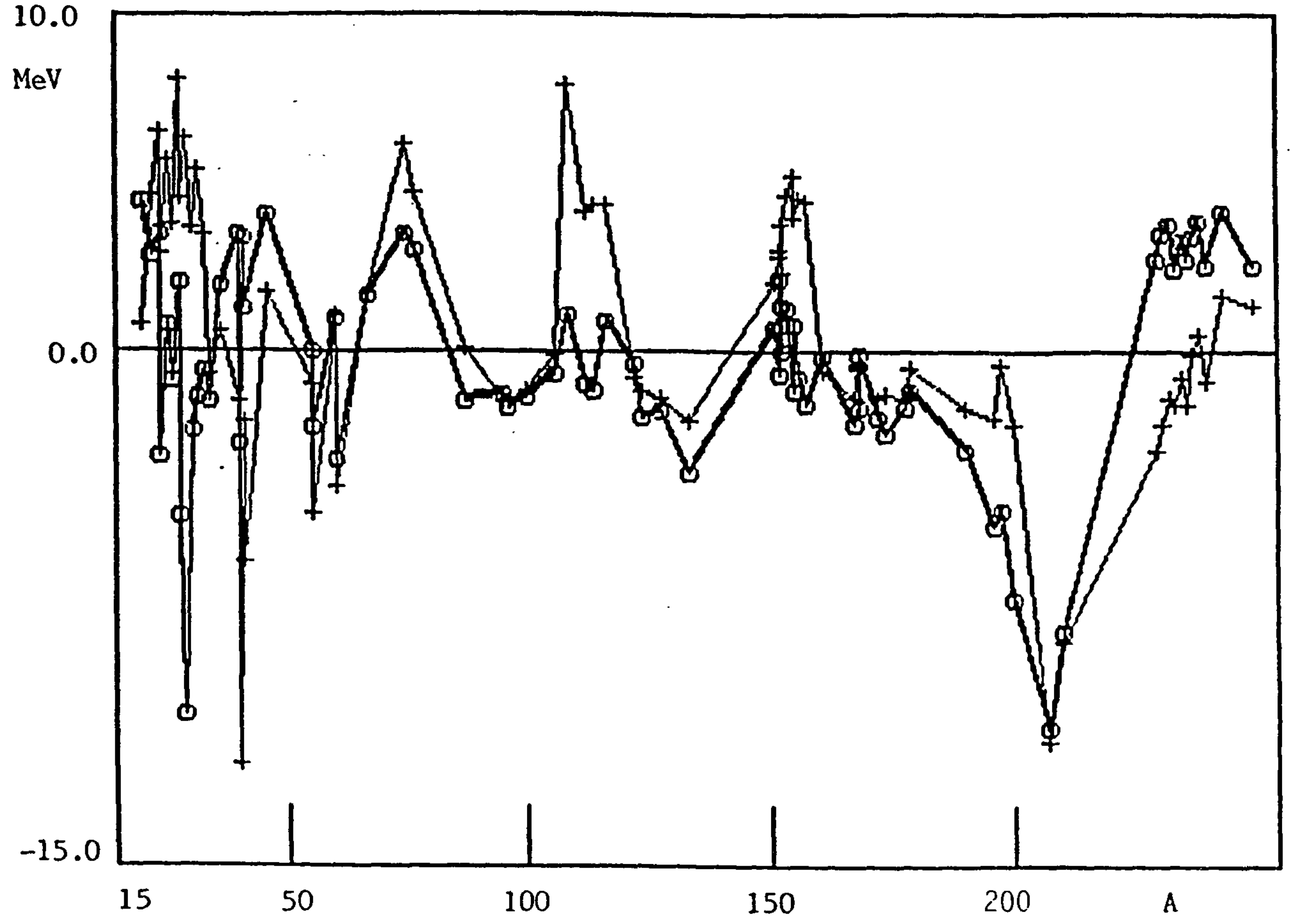


Figure 5.6 Comparison between experiment and the uniform periodic spectrum results for the shell effects. The shell widths are the same as those selected for figure 5.2 .

In **Figure** 5.6 we can see the result of this prescription with relatively good agreement with the "experimental" shell corrections. Let us remember that the present calculation corresponds to the most simple possible application of our analytical results. Furthermore, we are obtaining acceptable results at very different energies.

Let us remark that we have not included error bars in the figures because these calculations are only preliminar. A careful error analysis, also for the theoretical calculations, is necessary, if we want to take more seriously the method presented in this work. However, we do not present such analysis here because it differs largely from our main topic.

The theoretical calculation provides us with an expression valid in an energy range (depending on the mass number) around the neutron binding energies which could be subjected to a comparison with the experimental data in the future. The present computations are still not quite complete since we still need to calculate the whole nuclear level density and not only the a-parameter as we have done. Notwithstanding, we are sure that the adopted method is a very valuable procedure for the study of the level density (at not very large excitation energies) for a large number of nuclei as a function of the excitation energy. We also expect to be able to study other interesting effects related with the nuclear level density, like for example nuclear deformation and some aspects of nuclear reaction theories.

CHAPTER SIX

PARTICLE-HOLE STATE DENSITIES

In this chapter we like to show some results which we obtained some years ago. They are related to the results of the preceding chapters, but are of a somewhat different nature. We consider only non-interacting Fermions in a constant single particle spectrum. We compute the particle-hole state density and give a simple proof for a result we stated long ago [cf. A. Anzaldo-Meneses (1983)]. This result contains a correction to the so-called Williams formula, still in use in almost all pre-equilibrium calculations despite its clear failure for a different number of particles and holes. We give in the following the first correction terms and show that our methods provide also the exact relations after some additional calculations. We show that the particle-hole state densities consist in general of a smooth part and a fluctuating contribution. Both parts increase in absolute value with the excitation energies. At the end of the chapter we show results for the inclusion of pairing correlations when they are taken into account by means of a gap in the single particle spectrum.

The estimation of the cross section for pre-equilibrium reactions involves as a very important quantity the particle-hole state density (cf. H. Jahn, 1984). Because of the complexity of this problem it was up to now only possible to analyse the equidistant spectrum. We begin with only one kind of Fermions. The first relation published was the so called Ericson-formula [c.f. T. Ericson (1960), but see also V. Strutinsky (1958), who includes an additive pairing correction for $p=h$] :

$$\omega(p,h,U) = \frac{U^{p+h-1}}{p!\ h!\ (p+h-1)!} , \tag{6.1}$$

for p particles, h holes and excitation energy U expressed in units of the constant single particle energy separation. This was obtained assuming Boltzmann statistics. Later, F.C. Williams (1971) attempted to do the same calculation for Fermi particles and found:

$$\omega(p,h,U) = \frac{(U-A_w(p,h))^{p+h-1}}{p!\ h!\ (p+h-1)!} \quad , \tag{6.2}$$

where the constant $A_w(p,h)$ accounts for the Pauli principle and reads:

$$A_w(p,h) = \frac{1}{4}(p^2 + h^2) + \frac{1}{4}(p - h) - \frac{1}{2}h \quad , \tag{6.3}$$

which has the drawback of being unsymmetric in p and h. Other attempts after that of Williams' lead to the same failure or to arbitrary ad-hoc symmetrizations (see for example C. Kalbach, 1983). Williams formula remains generally in use.

6.1 The Correct Formula

We prove now that A_w as given by eq.(6.3) is incorrect if $p \neq h$ and give the correct result as well as the first correction terms and a procedure to compute recursively $\omega(p,h,U)$. This discrepancy is of course dependent on the definition. To compare particle-hole state densities from the current literature is not very easy since the definitions do not always coincide. We apply the methods of number theory as presented by G.E. Andrews, "The Theory of Partitions", (1976) for the representation of an integer number by sums of smaller ones. Let us also mention that M. Böhning (1970) observed correctly the combinatorial character of the calculations, but did not arrive at closed expressions.

The most natural way to solve this problem consists first in the construction of the **generating function** for $\omega(p,h,U)$. For a given degenerated system we define particle (hole) states in the following way. The considered spectrum is given by single particle levels at all the integers with occupation numbers zero or one. We define the ground state as formed by filling the spectrum starting from the lowest level upwards leaving no gaps. We define a **reference energy** ε_0 arbitrarily as a positive non-integral number and call a "**particle state**" an occupied level at an energy greater than ε_0 and a "**hole state**" an empty level at an energy smaller than ε_0. Obviously, it is not possible to define unambiguously particles or holes if ε_0 is integer. The reference energy ε_0 differs in general from the **Fermi energy** ε_F defined as an energy between the last filled level and the next empty level in the ground state.

If we consider now the excited system, the number of "**excitons**" $n=p+h$

will increase successively by two units. But |p-h| will remain constant and characterize a class of excitations associated with ε_0. There is no difference between the number of excited states for a (p,h) configuration from a (h,p) configuration as long as the system remains degenerated and thus the result must be necessarily symmetric.

The generating function can now be easily deduced and it consists of three parts. The simplest one is given by the factor q^{ph} since ph is the necessary energy for the first excited state with p particles and h holes. This can be seen starting from the configuration k0 (for $p \geq h$, analogous for $p<h$) at the ground state and observing that to form an excited state with k+1 particle states and one hole state, we need at least k+1 energy units and so succesively to form higher excited states. In general, to form a state with k+h particle states and h hole states, we need at least (k+1)+(k+3)+. . .+(k+2h-1) energy units , that is hk+h(h+1) - h = (k+h)h = ph as stated. The two other factors for the generating functions follow from the well known fact that the number of representations $\omega_N(m)$ of an integer number m by sums of N positive integers has the generating function (cf. Andrews, 1976):

$$\frac{1}{(q)_N} = \frac{1}{(1-q)(1-q^2)\cdots(1-q^N)} = \sum_{m\geq 0} \omega_N(m)\, q^m \quad , \tag{6.4}$$

and thus the complete generating function reads:

$$\frac{q^{ph}}{(q)_p\,(q)_h} = \sum_{m\geq 0} \omega(p,h,m)\, q^m \quad , \tag{6.5}$$

which is symmetric in p and h as required. We were not able to give a closed expression for $\omega(p,h,m)$ and arbitrary p and h, but it is possible to obtain several useful results, which generalize Williams formula for $p \neq h$ and give additional information usually only conjectured. In particular, for $h=0$ and $p>0$, we obtain the generating function for the partitions of an integer number into at most p parts.

First, we prove that the sum of all densities $\omega(p,h,m)$ gives the total exact density $\omega(m)$:

$$\prod_{n>0}\frac{1}{(1-q^n)} = \sum_{m\geq 0} \omega(m)\, q^m = \sum_{p}\frac{q^{ph}}{(q)_p\,(q)_h} = \sum_{p}\sum_{m\geq 0} \omega(p,h,m)\, q^m \ , \tag{6.6}$$

where the sums over p run over all particle states keeping p-h constant. We need now only the following relation due to Cauchy (1893) (cf. Andrews, 1976) :

$$1+\sum_{n>0}\frac{q^{n^2-n}\,z^n}{(1-q)\cdots(1-q^n)(1-z)\cdots(1-zq^{n-1})}=\prod_{k\geq 0}\frac{1}{(1-zq^k)}\ , \tag{6.7}$$

from which we find :

$$\sum_{n>0}\frac{q^{n^2-n(k+1)}}{(1-q)\cdots(1-q^n)(1-q)\cdots(1-q^{n-1-k})}=\prod_{n>0}\frac{1}{(1-q^n)}\ , \tag{6.8}$$

setting here $k=n-1-h$ and $n=p$, we obtain eq.(6.6) concluding the proof of:

$$\omega(n)=\sum_p \omega(p,h,m)\ , \tag{6.9}$$

To obtain a simple way to compute numerically $\omega(p,h,m)$ we deduce a recursion formula directly from eq.(6.5) :

$$\omega(p,h,m+p+h-1)-\omega(p,h,m+h-1)-\omega(p,h,m+p-1)+\omega(p,h,m-1)=\omega(p-1,h-1,m)\ . \tag{6.10}$$

Finally, we obtain the first terms of an expansion for $\omega(p,h,m)$ in powers of $(m-A)$ with A being a constant to be determined. From eq.(6.5) we obtain:

$$\omega(p,h,m)=\frac{1}{2\pi i}\int_{\sigma-i\infty}^{\sigma+i\infty}d\zeta\,\frac{e^{\zeta(m-ph)}}{(e^{-\zeta})_p(e^{-\zeta})_h}\ ,\qquad \sigma>0\ . \tag{6.11}$$

This integral can be evaluated using the following expansion:

$$\frac{1}{(e^{-\zeta})_p}=e^{\zeta p(p+1)/4}\left[\frac{1}{p!\zeta^p}-\frac{s_{2p}}{24p!\zeta^{p-2}}+O(\zeta^{4-p})\right],\quad s_{np}=\sum_{k=1}^{p}k^n\ , \tag{6.12}$$

and similar for holes. The numbers s_{np} can be given in terms of Bernoulli polynomials [cf. eq. (3.2.20)]. We find thus :

$$\omega(p,h,m)=\frac{(m-A)^{p+h-1}}{p!\ h!\ (p+h-1)!}-\frac{(m-A)^{p+h-3}(s_{2p}+s_{2h})}{p!\ h!\ 24(p+h-3)!}\ +$$

$$+\ \frac{(m-A)^{p+h-5}\{(s_{2p}+s_{2h})^2/2\ +\ (s_{4p}+s_{4h})/5\}}{p!\ h!\ 576\ (p+h-5)!}\ +O((m-A)^{\ p+h-7})\ . \qquad (6.13)$$

Higher order terms can be easily found in the same way. The constant energy shift A is given by:

$$A(p,h)\ =\ ph\ -\frac{1}{4}(p(p+1)+h(h+1))\ . \qquad (6.14)$$

This expression is of course symmetric in p and h. Hence, expressions eq.(6.13) and eq.(6.14) are to be preferred over the expressions of Ericson and Williams in general. M.Avrigeanu et al. (1989) use our correct result for A(p,h) in a fast neutron reaction data calculation.

We can rewrite the expansion as follows :

$$\omega(p,h,m)=\ \frac{1}{p!h!(p+h)!}\ \sum_{k>o}\alpha_k(p,h)\ \partial_m^k(m-A)^{p+h}\ , \qquad (6.13a)$$

where the coefficients α_k do not depend on m and thus, if $p>h$ (or $h>p$) , the coefficients of higher order become more important as when $p=h$. We have $\alpha_1=1$, $\alpha_2=0$, $\alpha_3=-(s_{2p}+s_{2h})/24$, etc. .

Let us now return to the total states density obtained after summation of the partial quantities. As shown above [cf. eq.(6.9)], the generating function eq.(6.5) leads to the exact correct result. However, we are also interested to know whether the first term in the expansion eq.(6.13a) leads us to a good approximation. We consider only the case where $p\approx h$, the other cases are more involved and need the consideration of further terms of the expansion. For simplicity we take $p=h+1/2$ and write $\omega_h(m)\approx\ \omega(h+1/2,h,m)$. Then [remember $\Gamma(m+1)=\ m!$]:

$$\omega_h(m)\ =\ \partial_m\frac{m^{2h+1/2}}{\Gamma(h+1/2)\Gamma(h+1)\Gamma(2h+1/2)}\ =\ \frac{2^{3/2}}{\pi}\partial_m\frac{(8m)^{2h+1/2}}{(4h+2)!}\ ,$$

where for the second equality we applied twice the duplication formula $\Gamma(z)\Gamma(z+1/2)\ =\ \pi^{1/2}2^{1-2z}\Gamma(2z)$. The total density reads now :

$$\omega(m) \approx \sum \omega_h(m) \approx \frac{\exp(\sqrt{8m})}{2\sqrt{2}\,\pi\, m} \quad .$$

This formula is in good agreement with the asymptotic result in which instead of 8 in the exponential appears $2\pi^2/3 \approx 6.6$ and in the denominator instead of $2\sqrt{2}\pi \approx 8.9$ appears $\sqrt{48} \approx 6.9$.

As an example for the obtained expansion, we show in **Table 6.1** the particle-hole states densities for p-h=1 and at an "excitation energy" of 80 units. We give the results for the first three terms of our expression eq.(6.13) and the exact values. The exact quantities were computed using the recurrence formula eq.(6.10). As we see, the larger the particle-hole numbers, the more important becomes the relative contribution of the correction terms.

TABLE 6.1

(p,h)	First	Second	Third	Sum	Exact
(1,0)	1	0	0	1	1
(2,1)	1 600	0	0	1 600	1 600
(3,2)	131 852	-203	0	131 649	131 651
(4,3)	1 858 603	-17 698	37	1 840 942	1 840 952
(5,4)	6 573 415	-248 034	2 692	6 328 073	6 328 096
(6,5)	6 742 366	-798 323	31 203	5 975 246	5 974 821
(7,6)	2 043 903	-664 775	77 551	1 456 679	1 452 834
(8,7)	168 373	-140 060	44 171	72 484	66 336
(9,8)	3 062	-6 365	5 219	1 916	185
Sum	17 523 175	-1 875 458	160 873	15 808 590	15 796 476

In **Figure 6.1**, we show the logarithm of the particle-hole states density for excitation energies below 80 units. The upmost curve is the total density and the lower curves correspond from left to right (see n-axis intersection points at ph=n) to ω(2,1,n), ω(3,2,n), ω(4,3,n), ω(5,4,n), ω(6,5,n), ω(7,6,n) and ω(8,7,n) respectively.

In principle, we can calculate explicitely the **exact** expressions for any number of particles and holes using the same procedure as above. As example of this fact we give now the exact expressions for some distributions:

$$\omega(1,0,m) = 1 \,, \tag{6.15a}$$

$$\omega(2,1,m) = m^2/4 + ((-1)^m-1)/8 \,, \quad m = 2, \ldots , \quad A_{2,1}=0 \,, \tag{6.15b}$$

$$\omega(3,2,m) = (m-3/2)^4/288 - (m-3/2)^2\, 57/1728 + (m-3/2)(1,-1) \text{ circ } 2_m + $$
$$+ \left(\frac{53}{512}, \frac{-35}{4608}, \frac{-35}{4608}\right) \text{circ } 3_m \,, \quad m = 6,7,\ldots, \quad A_{3,2}=3/2 \,, \tag{6.15c}$$

where $(a_o,a_1, \ldots ,a_{r-1})$circ r_m is Cayley's circulator which takes the value a_s when $m= s+rk$, $k=0,1,2, \ldots$.

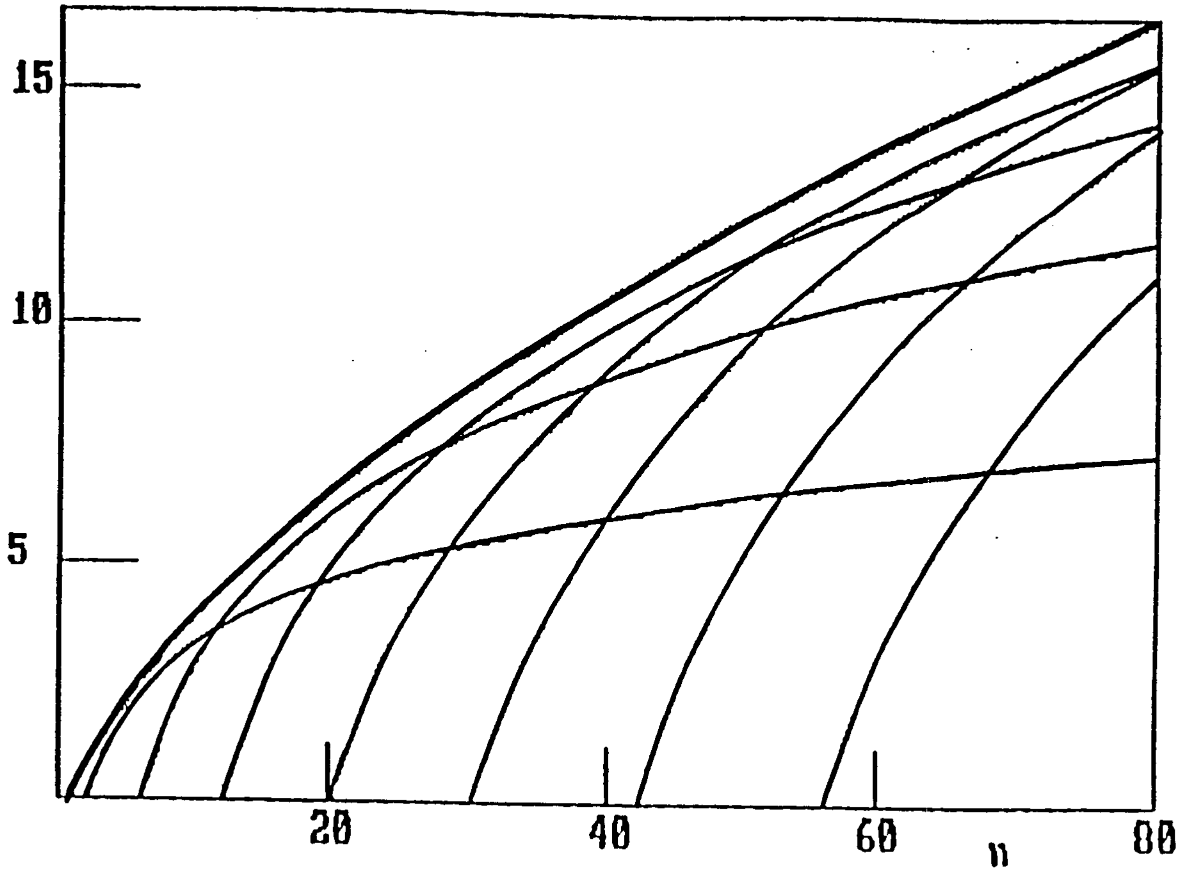


Figure 6.1 Logarithms of the exact particle-hole states densities $\omega(p,h,n)$ for $p-h=1$ and up to $n=80$. The upmost curve gives the total states density.

Other exact relations are:

$$\omega(1,1,m) = m \,, \tag{6.16a}$$

$$\omega(2,2,m) = (m-1)((m-1)^2/3 - 5/6 + (-)^m/2)/8 \,, \qquad A_{2,2}=1 \,, \tag{6.16b}$$

$$\begin{aligned}\omega(3,3,m) = (m-3)\Big[&(m-3)^4 - 70(m-3)^2/3 + 503/6 + (-)^{m-3}135/2 + \lambda_3 z_3^{-m} + \\ &+ \lambda_3^* z_4^{-m}\Big]/4320 \,, \qquad A_{3,3} = 3 \,,\end{aligned} \tag{6.16c}$$

where $\lambda_3=(13^2+i53/\sqrt{3})/3$ and $z_3=z_4^*=\exp(2\pi i/3)$. We have obtained many other exact expressions but we stop here to save space.

An interesting result arises, which can only be seen clearly after the exact formulae have been worked out. Namely, the states densities with fixed particles and holes numbers are composed of two parts. The first is a smooth (polynomial) function and the second is a fluctuating contribution $\delta\omega$ of increasing complexity as the exciton number grows. In the above exact relations, eq.(6.16b) and eq(6.16c), we have explicitely:

$$\delta\omega(2,1,m) = (-)^m/8 \,, \tag{6.20a}$$

$$\delta\omega(3,2,m) = \frac{(m-3/2)}{32}(1,-1)\,\mathrm{circ}\,2_m + \left(\frac{53}{512}, \frac{-35}{4608}\ \frac{-35}{4608}\right)\mathrm{circ}\,3_m \,, \tag{6.20b}$$

and similarly for the other densities. In general, the fluctuating contributions grow also polynomially (although slowlyer) with the excitation energy. In other words, in this most simple case the fluctuations of the state densities are not the same at all excitation energies .

6.2 Formula for n Kinds of Fermions

If we choose to consider now n kinds of Fermions, then the generalization of the preceding lines is not very difficult, although laborious. We must simply multiply the corresponding partition functions of the form given in eq.(6.5), viz.:

$$\prod_{k=1}^{n} \frac{q^{p_k h_k}}{(q)_{p_k}(q)_{h_k}} = \sum_{m\geq o} \omega(p_1,\ldots,p_n,h_1,\ldots,h_n,\, m)\, q^m \,, \tag{6.17}$$

here $\omega(p_1, \ldots, p_n, h_1, \ldots, h_n, m)$ will be the states density at excitation energy m with fixed numbers of particles and holes of types 1 to n. The application of the same method leads to:

$$\omega(p,h,U)= \frac{(U-A)^{p+h-1}}{(p+h-1)!\,\prod_k p_k!\, h_k!} \quad , \ p=\sum p_k \ , \ h=\sum h_k \ , \tag{6.18}$$

where the energy shift A is given by:

$$A(p,h) = \sum_k p_k h_k - \frac{1}{4}\sum_k \left(p_k(p_k+1) + h_k(h_k+1)\right) . \tag{6.19}$$

This quantity is again symmetric in p_k and h_k .

6.3 Pairing Correlations

The effect of pairing correlations has also been studied since the first contribution to this subject by V. Strutinsky (1958) for Boltzmann particles. Using our method we can easily extend his result to Fermi particles for the case of different number of particles and holes. We consider only the case where the pairing correlations can be approximated by a gap Δ in the constant single particle just above the Fermi level at the ground state configuration. Firstly consider $p \geq h$. If we follow now the same method we applied before, we find the generating function :

$$\frac{q^{ph+\Delta h}(1-q^{p-h+1})\cdots(1-q^{p-h+\Delta})}{(q)_h\,(q)_{p+\Delta}} = \sum_{m\geq 0} \omega_\Delta(p,h,m)\, q^m \ , \tag{6.21}$$

where we assumed that Δ is measured in units of the single particle spacing, here equal to one. In this problem the generating function is not symmetric in h and p, since their spectra are clearly different because of the presence of the gap in only one of them. The procedure is completely analogous and we obtain for the largest order contribution :

$$\omega_\Delta(p,h,m) = \frac{(m-A_\Delta)^{p+h-1}(h+\Delta)!}{(h)!^2(p+\Delta)!(p+h-1)!} + O((m-A_\Delta)^{p+h-3}) \ , \tag{6.22}$$

where the Pauli correction is now :

$$A_\Delta(p\geq h) = ph - \frac{1}{4}(p(p+1)+h(h+1)) + \frac{\Delta(\Delta+1)}{4} + \frac{3}{2}\Delta p - \frac{1}{2}\Delta h \ . \tag{6.23}$$

For $\Delta=0$ we obtain of course again the results without pairing. This relation is not symmetric in h and p , if we interchange p and h we find the relation for $h \geq p$. Further correction terms can be computed as well as exact expressions for low h and p. A system with n kinds of Fermions could also be easily analysed in a similar way.

CHAPTER SEVEN

RELATION WITH OTHER TOPICS OF MATHEMATICAL AND THEORETICAL PHYSICS

During this work we have mentioned that our formalism is related to some other problems of modern Mathematical and Theoretical Physics. In this chapter we would like to give examples of such relations. It is actually very easy to find such similitudes because the counting problems we have studied can also be understood in different ways outside the Nuclear Physics problem. These similitudes are not only of combinatorial character but are also analytical. This occurs in an analogous way as the original identities of Euler were first only formal (infinite) series or products which contained, as found later, a deeper analytical meaning.

The relation to other fields of Mathematical Physics is expected to be fruitful in both directions. **First**, as we have shown, the application of our method leads to results which can be confronted succesfully with experimental data of the level density shell effects problem in Nuclear Physics. Thus, we could expect to be amused to see what occurs with the most relevant mathematical concepts, with sound physical meaning, in at least formally similar problems. **Secondly**, in the inverse direction, there are many beautiful results in other research fields, with or without clear physical interpretation (reads: experimentally tested), which could lead to a better foundation of our understanding in Nuclear Physics.

The relation to other branches of Physics is of great importance. The consequence is a clearer physical understanding of natural phenomena and a better foundation of the involved branches.

In the **first part** of this chapter, the important result of H. Rademacher and H. Zuckermann (1938) is sketched. It concerns the **Fourier series** expansion of **modular forms** and is a generalization of the exact representation of the number of partitions p(n) of a positive integer n in terms of sums of positive integers. The purpose is to motivate the possibility to obtain correction terms (the expressions of Rademacher and Zuckerman contain **all contributions** in a convergent series) beyond the saddle point approximation considered in this work. The **second topic** in this chapter is directed towards the relation between modular forms and the **infinite**

dimensional Lie algebras of V. Kac (1967 and 1985) and R.V. Moody (1967). The connections with Analytic Number Theory are multiple and some methods are identical. Again, here the objective is to estimulate further work, relating the classification of nuclear spectra with the representations theory of infinite dimensional Lie algebras.

The **last topic** of this chapter will be physically more motivated. It regards recent results in nuclear, atomic and molecular **clusters** [see contributions in M. Brenner et al., Eds. (1992)]. For example, interesting experimental results with small metallic particles show shell structure effects akin with those effects we studied here. Our mathematical framework can also be applied in some cases and new results are presented.

7.1 Fourier Series of Modular Forms

As mentioned in chapter two, it is, at least in principle, possible to compute the next order contributions to the saddle point approximation given there. Although the method is relatively clear, no such calculation exists presently, as far as we know, in our Nuclear Physics application. The method of the steepest descent applied to the **Partitio Numerorum** problems [first studied deeply by L. Euler (1750)] has its roots in the important work of G.H. Hardy and S. Ramanujan (1918), where these authors obtained an **asymptotic** (divergent) **series** for the number of unrestricted partitions p(n) of integer numbers n expressed as sums of smaller ones. As pointed out by S. Goudsmit (1937), the level density $\rho(N,E)$ for a system of N **Fermions** of only one kind in a spectrum consisting of equidistant energy levels and total energy $E = M + \frac{1}{2}N(N+1)$ is equal to the number of partitions $p_N(M)$ of the integer M in parts not exceeding N [we have $p(M) = p_N(M)$ for $M \leq N$]. In chapter 6 we denoted $p_N(M)$ by $\omega_N(M)$ in eq.(6.4) to be in better agreement with the literature cited there. Thus, for a degenerated system the level density is given by the coefficients p(n) in the Fourier series for the Dedekind η function :

$$e^{-\pi i\tau/12}\sum_{n\geq 0} p(n)e^{2\pi i n\tau} = \frac{1}{\eta(\tau)} = \frac{e^{-\pi i\tau/12}}{\prod_{k>0}(1-\exp(2\pi i k\tau))} .$$

As noticed by C. van Lier and G.E. Uhlenbeck (1937), $p_N(M)$ gives the number of states either of a system of N **Bosons** in a spectrum of equidistant levels, or alternatively a system of **Bosons** with an undetermined number of particles in a spectrum of only N equidistant levels, both with a total energy

M.

Ramanujan conjectured further the existence of an **exact relation** for p(n), which indeed was found later by H. Rademacher in 1937 refining the same method. A little later the method was applied by Rademacher (1938) to find again an exact expression for the Fourier coefficients of the **modular invariant:**

$$12^3\ J(\tau) = \frac{(\vartheta_2^8 + \vartheta_3^8 + \vartheta_0^8)^3}{\eta(\tau)^{24}} = q^{-1} + \sum_{n \geq o} a_n q^n\ , \quad q = e^{2\pi i\tau}, \tag{7.1}$$

The Fourier coefficients a_n are integer numbers (e.g. $a_o=744$, $a_1=196884$, $a_2= 21493760$, etc.). This function satisfies : $J((a\tau+b)/(c\tau+d))= J(\tau)$, for a, b, c, d, integers and ad-cb=1, i.e. $J(\tau)$ is invariant with respect to the transformations of the full modular group. The Fourier expansion of Rademacher for $J(\tau)$ was, however, obtained earlier by H. Petersson (1932) by very different methods, applicable only for negative or zero dimensions (see below).

Finally 1938, the method was applied succesfully by H. Rademacher and H. Zuckerman to homogeneous **modular forms of positive dimension** and invariant with respect to the full modular group. Afterwards, the result was extended to include also modular forms invariant with respect to **subgroups of the modular group**. For example, for the level-N principal congruence subgroup $\Gamma(N)$, given by matrices with: $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ mod N , see H. Zuckerman (1939).

Let us quote now the result of Rademacher and Zuckerman (1938) :

Let $F(\tau)$ be an **entire modular form** of **positive dimension** r and **multiplier system** ε**(a,b,c,d)**, i.e.: $F(\tau)$ is analytic in the upper half-plane and :

$$F(\tfrac{a\tau+b}{c\tau+d}) = \varepsilon(a,b,c,d)(-i(c\tau+d))^{-r}\ F(\tau)\ ,\quad c>0,\ |\varepsilon|=1\ , \tag{7.2a}$$

$$F(\tau+1)= e^{2\pi i\alpha}\ F(\tau)\ ,\quad 0\leq\alpha<1\ . \tag{7.2b}$$

If further, its Fourier series contains only a finite number of terms with negative exponents (i.e. finite order pole at q=0) :

$$F(\tau)= e^{2\pi i\tau\alpha}\sum_{m\geq-\mu} a_m\, e^{2\pi i m\tau} , \qquad (7.3)$$

where the coefficients are given by:

$$a_m= \frac{1}{2\pi i}\int_C d\tau\; e^{-2\pi i\alpha\tau}\, F(\tau)\; \tau^{-m-1} , \qquad (7.4)$$

and the contour C lies inside the unit circle, then, for $m\geq0$:

$$a_m=2\pi\sum_{\nu=1}^{\mu} a_{-\nu}\sum_{k\geq1}\frac{1}{k}A_{k,\nu}(m)\left(\frac{\nu-\alpha}{m+\alpha}\right)^{(r+1)/2} I_{r+1}(4\pi(\nu-\alpha)^{1/2}(m+\alpha)^{1/2}/k) , \qquad (7.5)$$

with:

$$A_{k,\nu}(m)=\sum_{\substack{0\leq h\leq k\\ (h,k)=1}} \varepsilon(h', -(hh'+1)/k, k, -h)^{-1} \exp\{(-2\pi i/k)((\nu-\alpha)h'+(m+\alpha)h)\} , \qquad (7.6)$$

where $I_{r+1}(z)$ is a Bessel function of the third kind. □

The key of the proof is the subdivision of the integration path into smaller paths near the "rational points" of the unit circle. The transformation relation eq.(7.2a) allows then the reduction of the resulting integrals into an infinite sum of integrals of the same kind around the unity. The remaining integrals can be evaluated exactly. All contributions resulting from the paths around the "irrational points" of the unit circle can be shown to be zero.

The most simple example is the convergent series of Rademacher for unrestricted partitions, as we mentioned before, for which: $r=1/2$, $\mu=1$, $\alpha=23/24$, $F(\tau)=1/\eta(\tau)$ and the numbers $A_{k,\nu}$ has been expressed by Selberg as [see A.L. Whitemann(1956)] :

$$A_{k,\nu} = (k/3)^{1/2}\sum_{(3j^2+j)/2\equiv-\nu \bmod(k)} (-)^{j} \cos \frac{6j+1}{6k}\pi , \quad A_{1,1}=1 . \qquad (7.7)$$

The argument of the Bessel function in eq.(7.5) is $4\pi((1/24)^{1/2}(n-1/24)^{1/2}/k)$ with $n=m+\mu$ in this case. Now, since $I_{r+1}(z) \sim (2\pi z)^{-1/2}\exp(z)$ for large z, the asymptotic form to which the exact result reduces is precisely the Hardy-Ramanujan expression: $p(n)\sim (4n)^{-1}3^{-1/2}\exp(\pi\sqrt{2(n-1/24)/3})$.

In relation (7.5), we recognize a "shell effect" given by $\mu-\alpha$, since the number of partitions in eq.(7.3) is shifted by $-\alpha$. This means that the "level density" $a_{m-\mu}$ is given in terms of the "excitation energy" m shifted by an amount equal to $\mu-\alpha$. The leading term for high excitation energies is of the form $\exp\{4\pi(\mu-\alpha)^{1/2}[m-(\mu-\alpha)]^{1/2}\}$, where the numbers α and μ are fixed respectively by the transformation given by eq.(7.2b) and by the pole order in eq.(7.3).

From these results of Rademacher and Zuckerman, we see that, at least for many products in one variable, it is possible not only to obtain additional correction terms, but astonishingly to find an exact expression. In our work we have studied products depending on one variable for each nucleon number and one for the excitation energy, but as we mentioned, we considered only degenerated systems. With this last assumption we simplified sufficiently the problem to obtain the lowest order term using the saddle point method. It could be very interesting to try to obtain further correction terms, if not an exact relation, for general spectra and degenerated systems using similar methods.

An interesting generating function appearing in the theory of infinite dimensional Lie algebras [see V. Kac and D. Peterson (1984) and V. Kac (1985)] is the following:

$$f(\tau) = q^{\xi} \prod_{n>o} (1 - q^{n/N})^{-a_n} \qquad , \; a=\sum_{n=1}^{N} a_n \quad , \tag{7.9}$$

with $q=\exp(2\pi i\tau)$ and where the sequence a_n is periodic with period N with $a_j=a_{N-j}$. The constant ξ is :

$$\xi = \frac{-a}{24} + \frac{1}{4N^2} \sum_{n=1}^{N} n(N - n)\, a_n \, . \tag{7.10}$$

The function $f(\tau)$ is a modular form with respect to some subgroup of the modular group, depending on the integers a_n and provided $a_j=a_{N-j}$, see eq.(4.2.2) with $N=p$. Let us observe now that, from our point of view, we can associate a Dirichlet series to any product of the type $q^{-\xi}f(\tau)$ as we did in chapter three for more general products :

$$\ln q^{-\xi} f(\tau) = \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} ds\, \Gamma(s)\, \zeta(s+1)\, D(s)\, \tau^{-s} \, , \qquad \sigma>1 \, , \tag{7.11}$$

with :

$$D(s) \;=\; \sum_{j=1}^{N} a_j\, \zeta(s,\, j/N)\ , \tag{7.12}$$

which has a simple pole at $s=1$ with residue a . This is exactly the same series as for the periodic spectrum we studied in section 4.2 with $a_j = a_{N-j}$. The values at the negative integers can be readily computed, in particular, we find :

$$-D(-1)\ \zeta(0) = -\frac{a}{24} \quad + \frac{1}{4N^2} \sum_{n=1}^{N} n(N\ -\ n)\ a_n\ , \tag{7.13}$$

which is interestingly equal to the constant ξ given by eq.(7.10). We find the following expansion :

$$\ln\, q^{-\xi}\ f(\tau) \;=\; \tau^{-1} 4\pi^2\, a/24\ + D'(0)\ -\ \tau\zeta(0) D(-1)\ +\ R(\tau)\ \ , \tag{7.14}$$

where we have have written the coefficient of the first term in such a form to make clear its relation with the first term in eq.(7.13). The remaining contribution $R(\tau)$ can also be calculated explicitly using the functional relation eq.(4.2.4) for the Hurwitz ζ-function. We find :

$$R(s) = \frac{1}{2\pi i N} \int_{\sigma - i\infty}^{\sigma + i\infty} ds\ \Gamma(s)\ \zeta(s)\ D_c(s+1)\ \ (4\pi^2 N/\tau)^{-s}, \qquad \sigma > 1\ , \tag{7.15}$$

The Dirichlet series $D_c(s)$ is obtained as in eq.(4.2.5) after the substitution of the numbers a_n by the finite Fourier cosine transforms given in eq.(4.2.5a). From eqs.(7.14) and (7.15) it is possible to obtain many identities for the function $f(\tau)$. In particular the simplest application corresponds to the Dedekind η-function and the immediate result of eq.(7.14) is the transformation formula eq.(3.5.4e). If we proceed now as we did in chapter 3 and analyse the q-series associated here with the function $f(\tau)$, we equally find a number of identities under modular transformations. We have still not compared all our results with the large number of available relations on this topic, but it could be an interesting task, which we cannot cover here.

It is simple to obtain the asymptotic form of the leading term of the Fourier coefficients of the infinite product in $f(\tau)$. We can use the steepest descent method and find the first term of the Rademacher and Zuckerman relation as a power of n times $\exp\{4\pi(a(n+\xi)/24)^{1/2}\}$. Thus, the constant ξ appearing in the definition of the function $f(\tau)$ [cf. eq.(7.9)] will be related to the analogue of the "shell effect" in the level density problem [see for example eq.(5.4)].

The transformation properties of the function $f(\tau)$ play an important role in the theory of affine Kac-Moody algebras [cf. V.G. Kac (1967,1985) and R.V. Moody (1967)]. In particular, the relevant relations known as Macdonald's identities [cf. I.G. Macdonald (1972)] can be proved using the fact that the function $f(\tau)$ is a modular form. The mentioned identities relate infinite products with theta series associated with root lattices. As is well known, the theta series have excellent convergence properties, which makes very desirable to reduce or rewrite partition functions in terms of similar functions for explicit numerical evaluations.

7.2 On Kac-Moody algebras

One way to initiate the study Kac-Moody algebras consists in starting from a $n \times n$ matrix A of rank ℓ, called the (generalized) **Cartan matrix**, whose elements satisfy: $a_{ii}=2$; $a_{ij}<0$ for $i \neq j$; $a_{ij}=0$ implies $a_{ji}=0$. Next, consider the algebra $\tilde{\mathfrak{g}}$, whose generators satisfy :

$$\begin{aligned} &[h,h']=0, && [e_i,f_j]=\delta_{ij}\alpha_i^{\vee}, \\ &[h,e_i]=<\alpha_i,h>e_i \;, && [h,f_i]= -<\alpha_i,h>f_i \;, \end{aligned} \tag{7.16}$$

with $i,j=1, \ldots , n$; $h,h' \in \mathfrak{h}$ a complex vector space of dimension $2n-\ell$. And $<\alpha_i^{\vee},\alpha_j> =a_{ij}$, $\alpha_i \in \mathfrak{h}^*$, $\alpha_j^{\vee} \in \mathfrak{h}$. The algebra $\mathfrak{g}(A)=\tilde{\mathfrak{g}}/I$ is called a **Kac-Moody algebra**, where I is the maximal ideal in $\tilde{\mathfrak{g}}$, which intersects the **Cartan subalgebra** $\mathfrak{h}$ trivially. The α_i are called simple roots and the center of $\mathfrak{g}(A)$ is $\mathfrak{c}=\{h \in \mathfrak{h} \mid <\alpha_i,h>=0,\ i=1, \ldots ,n\}$. Kac-Moody algebras are classified into three classes: i) **Finite** iff all principal minors of A are positive; ii) **Affine** iff all proper principal minors are positive; iii) **Indefinite** if there exist $u>0$ such that $Au<0$ and if $Av>0$ and $v \geq 0$ implies $v=0$. To each matrix A there is associated a **Dynkin diagram** S(A) whose vertices i and j are connected by $|a_{ij}|$ lines (with an arrow toward i if $|a_{ij}|>1$) if $a_{ij}a_{ji}<4$ and $|a_{ij}|>|a_{ji}|$; but are connected by a bold face line equiped with an ordered pair of integers $|a_{ij}|$, $|a_{ji}|$ if $a_{ij}a_{ji}>4$. For affine A the diagram S(A) has labels a_i which are the coordinates of a vector $\delta=(a_o,a_1, \ldots ,a_\ell)$ such that $A\delta=0$. The labels of $S(A^t)$ are denoted by $a_i^{\vee}$. The Cartan matrix A is called symmetrizable if there exists an invertible diagonal matrix $D=\mathrm{diag}(\varepsilon_1, \ldots , \varepsilon_n)$ and a symmetric matrix B such that $A=DB$. A symmetric bilinear $\mathbb{C}$-valued form $(\cdot|\cdot)$ on $\mathfrak{h}$ is defined by $(\alpha_i^\vee|h)=<\alpha_i,h>\varepsilon_i$, $(h'|h'')=0$, for $h,h',h''\in\mathfrak{h}$, $i=1, \ldots ,n$.

A fundamental result of the representation theory of Kac-Moody algebras with symmetrizable Cartan matrix is the **Weyl-Kac character formula** for an integrable highest weight modul L (with highest weight Λ) :

$$\mathrm{ch}\ L(\Lambda)=\sum_{\lambda}\mathrm{mult}_\Lambda(\lambda)e^\lambda = \frac{\sum_{w\in W}\det(w)\exp[w(\Lambda+\rho)-\rho]}{\prod_{\alpha\in\Delta_+}[1-\exp(-\alpha)]^{\mathrm{mult}(\alpha)}} . \tag{7.17}$$

The first sum is over all distinct weights of the representation. Δ_+ is the set of all positive roots; $\rho\in\mathfrak{h}^*$ is such that $<\rho,\alpha_i^\vee>=1$; mult $\alpha=$ dim $\mathfrak{g}_\alpha$; $\mathfrak{g}_\alpha=\{x\in\mathfrak{g}(A)|[h,x]=\alpha(h)$ for all $h\in\mathfrak{h}\}$ is the root space attached to α. The Weyl group W is generated by the reflexions $r_i(\lambda)=\lambda-<\lambda,\alpha_i^\vee>\alpha_i$ with $\lambda\in\mathfrak{h}^*$. The character formula can be rewritten in terms of multivariable ϑ-functions with characteristics and string functions. This leads to a direct relation with the theory of modular forms. A famous example for the character formula is the level one character for $E_8^{(1)}$ given by $12(qJ(\tau))^{1/3}$ [cf. eq.(7.1) to the power 1/3] which is modular invariant and whose Fourier coefficients are thus dimensions of certain weight modules. The modular invariant itself is related with the "Monstrous Moonshine" [cf. I.B. Frenkel, J. Lepowsky and A. Meurman (1983)].

The irreducible representation with highest weight $\Lambda=0$ is the trivial one dimensional representation with ch $L(0)=1$. Thus the character formula leads to the **denominator formula** :

$$\prod_{\alpha\in\Delta_+}[1-\exp(-\alpha)]^{\mathrm{mult}\ \alpha} = \sum_{w\in W}\det(w)\ \exp[w(\rho)-\rho] . \tag{7.18}$$

However, this formula has only formal meaning, since for a general Kac-Moody algebra its explicit form is unknown. Only certain cases have been worked out in detail.

In particular, for **affine** algebras the denominator formula is a generalization of the Macdonald's identities and of Weyl's (polynomial) denominator formula for the **finite** algebras. The infinite sum can be expressed as a ϑ-series. The most simple examples of the Macdonald's identities are the Jacobi relations eqs.(3.5.1a-d) resulting from the $A_1^{(1)}$ root lattice, as well as the positive integer powers of the Dedekind's η-function expressed as infinite series convergent in the upper half plane. Some of these relations were independently found by F. Dyson (1972).

To establish a first contact with the possible applications we have in mind for **periodic single particle spectra** in Nuclear Physics, introduce now the following **gradation of type s**. Consider a non-zero sequence of non-negative integers $s=\{s_o, \dots, s_\ell\}$ and set $m=k\sum \alpha_i s_i$, $i=0,\dots,\ell$; and $k=1,2,3$ is the order of a diagram automorphism μ of the finite dimensional simple Lie algebra $\mathfrak{g}$ of type X_N. Then, $\mathfrak{g}=\mathfrak{g}_{\bar{0}}\oplus\mathfrak{g}_{\bar{1}}$ if $k=2$ and $\mathfrak{g}=\mathfrak{g}_{\bar{0}}\oplus\mathfrak{g}_{\bar{1}}\oplus\mathfrak{g}_{\bar{2}}$ for $k=3$. Let $\Delta_{\bar{0}}$ be the root system of $\mathfrak{g}_{\bar{0}}$ (fixed point set of μ on $\mathfrak{g}$) and $\Delta_{\bar{0}+}$ be a subset of positive roots for which $\alpha_1, \dots, \alpha_\ell \in \mathfrak{h}_o{}^*$ are simple roots. Let $\mathfrak{g}= \oplus_j \mathfrak{g}_j$ be the associated $\mathbb{Z}/k\mathbb{Z}$ gradation. Let furthermore ρ_o be the half sum of elements from $\Delta_{\bar{0}+}$; $\gamma_s \in \mathfrak{h}_o^*$ be defined through $(\gamma_s|\alpha_i)=ks_i/m$, $i=1,\dots,\ell$. For $s_i > 0$, the sequence s defines a homomorphism $F : \mathbb{C}[[\exp(-\alpha_1), \dots, \exp(-\alpha_\ell)]] \rightarrow \mathbb{C}[[q]]$ by $F(\exp(-\alpha))=q^{<h^s,\alpha>}$, $h^s \in \mathfrak{h}$, $<h^s,\alpha_i>=s_i$. This map is called a **specialization of type s**. Then, the denominator formula can be written as:

$$q^{-\frac{m}{2gk}|\rho_o-g\gamma_s|^2}\prod_{j\geq 1}(1-q^j)^{-d_{j \bmod(m)}}=\sum_{w\in W_o^s}\varepsilon(w)\sum_{\alpha\in M}D_s(w(\rho_o)+g\alpha)q^{-\frac{m}{2gk}|w(\rho_o)+g\alpha-g\gamma_s|^2}, \tag{7.19}$$

for the **affine Lie algebras** of type $X_N{}^{(k)}$ with $\mathbb{Z}$-gradation of type s: $\mathfrak{g}(A)= \oplus_{j\in\mathbb{Z}}\, \mathfrak{g}_j(s)$, $\dim\, \mathfrak{g}_j(s)= d_{j \bmod(m)}$. In Eq. (7.19):

$$D_s(\lambda)= \prod_{\alpha\in\Delta_{s+}} (\lambda|\alpha)/(\rho_s|\alpha)\ , \quad \text{for } \lambda\in\mathfrak{h}_o^*\ ,$$

where Δ_{s+} is the subset of roots of $\mathfrak{g}_{\bar{0}}$ which are linear combinations with non-negative coefficients of the roots from the set $\{\alpha_i|s_i=0,\ i=0,1, \dots ,\ell\}$ and ρ_s is the half-sum of the roots from Δ_{s+}. And where $W_{o,s}$ is the subgroup of the Weyl group W_o of $\Delta_{\bar{0}}$ generated by reflexions in the roots from Δ_s and W_o^s a set of representations of right cosets in W_o for the subgroup W_s (generated by r_α, $\alpha\in\Delta_{s+}$) so that $W_o=W_{o,s}W_o^s$. The lattice $M\subset\mathfrak{h}_o^*$ is spanned over $\mathbb{Z}$ by elements $W_o\cdot\theta_o$ (resp. $W_o\cdot\theta_o/2$) if $X_N{}^{(k)}\neq A_{2\ell}^{(k)}$ (resp. $=A_{2\ell}^{(k)}$). The element $\theta_o\in\mathfrak{h}_o^*$ is called the highest weight and has the decomposition $\theta_o=\sum a_j\alpha_j$; the dual Coxeter number g is given by $g=\sum a_i^\vee$, $i=0,1, \dots ,\ell$.

Now, since the right hand side of eq.(7.19) is a modular form (essentially a theta series, from other considerations), the following "very

strange formula" results :

$$\frac{1}{2gk}|\rho_o-g\gamma_s|^2=\frac{1}{24}\dim \mathfrak{g}_\sigma-\frac{1}{4m^2}\sum_{j=1}^{m} j(m-j)d_j(s,k)\ . \tag{7.20}$$

This equation relates the "degeneracies" $d_{j\ \mathrm{mod}(m)}$ of the periodic spectrum with important quantities of the affine Lie algebra $\mathfrak{g}(A)$. Let us remark again that the right hand side of eq.(7.20) [cf. eq.(7.10) with $\dim \mathfrak{g}_\sigma = a$, $m=N$], are related to the analogues of the experimentally measurable ground state shell correction in the Nuclear Physics problem.

With an affine Lie algebra of type $X_N^{(k)}$ there is associated a **realization of type s** given by: $\sum_{j\in\mathbb{Z}} t^j\otimes\mathfrak{g}_{j\ \mathrm{mod}(m)}(s;k) \oplus \mathbb{C}c \oplus \mathbb{C}d$, with the Lie algebra structure:

$$[P\otimes x\oplus\lambda c\oplus\mu d, Q\otimes y\oplus\lambda' c\oplus\mu' d]=[x,y](PQ+\mu\partial Q-\mu'\partial P)\oplus\tfrac{k}{m}\mathrm{Res}(P\partial Q)(x|y)c$$

here $\lambda,\mu,\lambda',\mu'\in\mathbb{C}$; $x,y,\in\mathfrak{g}$; $P,Q\in\mathbb{C}[t,t^{-1}]$, the algebra of Laurent polynomials in t; $\partial=d/dt$; $(\cdot|\cdot)$ a normalized invariant bilinear form. Also: $(d|d)=0$; $(c|c)=0$; $[d,c]=0$; $d(P\otimes x)=t\partial P\otimes x$; $(\mathbb{C}c+\mathbb{C}d|P\otimes x)=0$; $(c|d)=m/k$; $(P\otimes x|Q\otimes y)=\mathrm{Res}(t^{-1}PQ)(x|y)$. Finally, consider an interesting fact, noticed by Kac and Peterson after observation of the related **Virasoro algebra** given by:

$$[L_i\ ,\ L_j\ ]\ =\ (i\ -\ j)\ L_{i+j}\ +\ (\tfrac{a}{12}i^3\ +\ 2i\xi\ )\ \delta_{i+j,o}\ ,\ i,j\ \in\mathbb{Z}, \tag{7.21}$$

here a and ξ are the **same constants** as above [cf. eq.(7.10)]. This is a centrally extended algebra of meromorphic vector fields on the Riemann sphere and singular at most at 0 or at ∞. A realization of the centerless algebra is given by the generators $z^{i+1}\partial$. As we see, the constants appearing in the central term are connected in a simple way with the constants appearing in the asymptotic behaviour of the Fourier coefficients of the function $f(\tau)$ [see eq.(7.9) and second paragraph after eq.(7.15)], as well as in the very strange formula, eq.(7.20). This coincidence has not been yet fully clarified.

We have performed calculations also for more general algebras of differential operators on Riemann surfaces with punctures. In particular, algebras of vector fields and their central extensions has been studied. However, the extension of the calculations leads us to publicate these results sepparately [cf. A. Anzaldo-Meneses (1992)].

The kind of relations appearing in the nuclear level density problem have analogous counterparts in the theory of **affine** Kac-Moody algebras only for **periodic single particle** spectra. And as shown in chapters four and five, periodic single particle spectra permit a good description of experimental data of the nuclear level density. It is therefore desirable at this stage, to systematize or classify the most relevant physical parameters (for example the shell widths W) in a clear way. But also from the point of view of the explicit evaluation of the level densities it is important to study more in detail the appearing partition functions. These facts are enough motivation to see how the results of the representation theory of affine Kac-Moody algebras can be used to clarify further the nuclear level density problem and related matters.

Now, in the **general nuclear level density problem**, modular transformations play also an outstanding role and this occurrs not only for the simple infinite products of periodic single particle spectra, of the same type as those for the modular forms of eq.(7.19), but for the more general products studied in chapter three. Some relations, that we have obtained in chapter three, do not seem to have a counterpart in the theory of affine Kac-Moody algebras. However, it would not be surprising when the **indefinite** Kac-Moody algebras would lead to formulas containing polynomials of the index number, instead of periodic constants for mult α in eq. (7.18). We think that these topics are worth to be studied more in detail.

7.3 Shell Effects in Clusters and Mesoscopic Systems.

Shell structure occurs in nuclei in a subtil way. It is certainly related to the symmetries of the finite system constituted by the strongly interacting nucleons. In the way in which we have studied the shell structure, the validity of the shell model was assumed and the question about its origin was not stated. We preferred simply to consider general kinds of single particle spectra and to distribute non-interacting nucleons on them. The discrete spectra had a form manageable with the methods of Analytic Number Theory. It was shown how to proceed to calculate some quantities to be confronted with experiments and to select parameters associated with the most adequate spectra.

Atomic clusters or sufficiently **small metal particles** are other physical systems which can be studied using discrete single particle spectra on which Fermions or Bosons are distributed [see for example J. Perenboom et al. (1981)]. In the last years, methods of Nuclear Physics have been applied succesfully to these systems. Both aspects have been considered: The methods of random matrices and the shell model. The first has been applied not only to the level spacing distributions as in Nuclear Physics, but also to the theory of conductance in small conductors (see B.L. Altshuler et al., 1991). However, this important and vast field is not a topic of this work and will not be contemplated here. Rather, the second aspect concerning shell effects is of relevance for us.

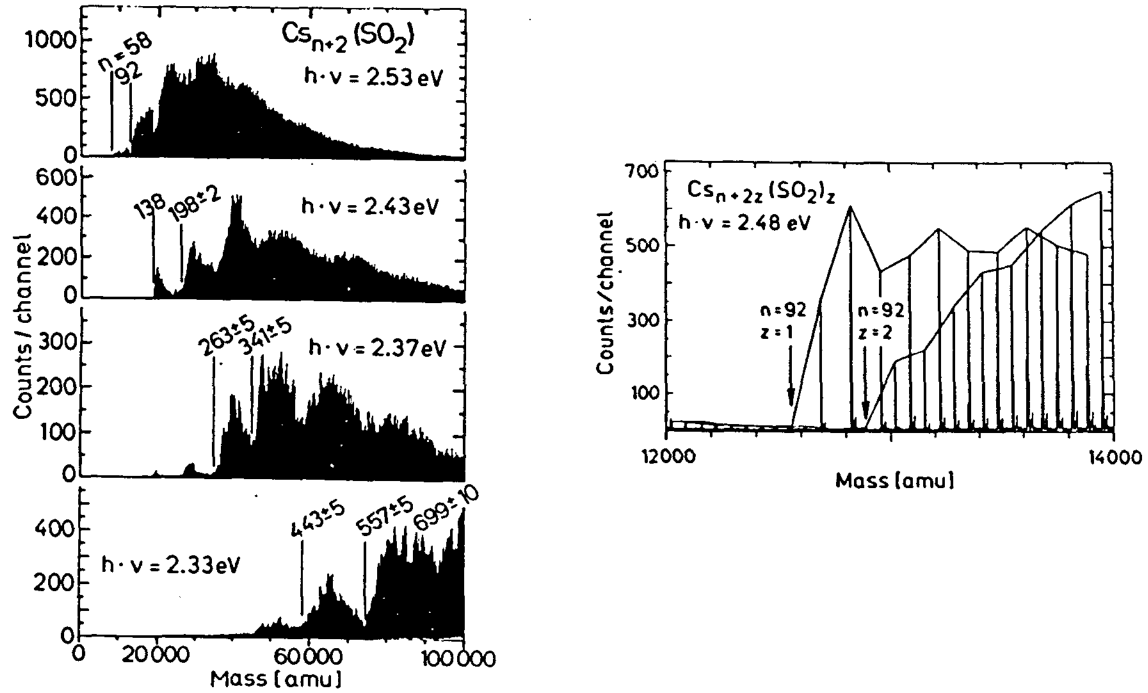


Figure 7.1 Mass spectra of $Cs_{n+2}(SO_2)$. The selected values of n, are magic numbers. Taken from Göhlich et al. (1990).

Electronic shell structure in metal clusters is a field of intensive research [see for example M. Brenner et al., Eds. (1992)]. Generally, a large (but finite) number of delocalized electrons is assumed to move in a finite space region. This region is given by a cluster or "small particle" of few up to thousands of atoms or molecules. In Fig. 7.1, the mass spectrum of $Cs_{n+2}(SO_2)$ clusters [cf. H. Göhlich et al. (1990)] clearly shows a shell structure as an abrupt increase or decrease of the intensity peaks. Ionizing laser photon energies of 2.33 eV to 2.53 eV are displayed. The values of n are also given at shell closures, i.e. at the **magic numbers**. A simple explanation of this mass spectra given by Göhlich et al. is the following. The delocalized electrons move freely in the cluster and occupy subshells of equal angular momentum. Therefore, the clusters will not appear in the mass spectra when one of these subshells is closed and the laser photon energy is smaller than the ionization energy. Also numerical shell model calculations have been performed by Göhlich et al. supporting this approach.

The arrangement of atoms in a cluster depends on many factors, for example their preparation and their size. The possible kinds of discrete spectra are very diverse and thus our general method could be also of help here to classify spectra according to a small number of mathematical quantities.

As early as 1937, H. Fröhlich considered small metallic particles using methods for a bulk metal and studied quantum size effects on the electronic specific heat. The most important observation was that the mean spacing between levels decreases with increasing particle size. In fact, the average level separation δ near the Fermi level ε_F is $\delta=2/\rho(\varepsilon_F)$, where $\rho(\varepsilon_F)$ is the density of states evaluated at ε_F. For a system of N conduction electrons in a small particle it follows that δ is of order ε_F/N. Thus, for a small metallic particle of size of order 10^{-8}m and containing about 10^5 conduction electrons it would correspond $\delta\sim0.1$ meV or equivalently a temperature of $\delta/k_B\sim1^oK$. Fröhlich considered a **constant single particle spectrum**, but R. Kubo (1962) replaced it by a **random spectrum** (with Poisson spacings distribution) and included additionally the important distinction between an even and an odd number of electrons. Finally, L.P. Gor'kov and G.M. Eliashberg (1965) pointed out the possibility to use the more general distributions used in Nuclear Physics. These considerations are of importance for the low temperature behaviour of the specific heat averaged over the size and shape distributions of all particles in a sample.

But here our point of view departs towards the study of general single particle spectra and the degree of "bunching" of the single particle levels into shells. These aspects are necessary to understand the mass spectra of clusters and phenomena like the density of excited states of individual clusters or also of colloids, gases and plasmas containing them.

R. Denton et al. (1971, 1973) based on the studies of Fröhlich and

Kubo considered a system of N electrons in a magnetic field H allocated in a single particle spectrum with energy levels ε_n . To calculate the heat capacity and the spin susceptibility they studied the canonical partition function:

$$Q(N,\beta)=\frac{1}{2\pi i}\int_C dy\ y^{-N-1} \prod_{\substack{n=o\\ s=\pm 1}} [1+y\exp(sh-\beta\varepsilon_n)], \quad \beta=1/k_BT, \tag{7.22}$$

where $y=\exp(\beta\mu)$ is the fugacity and $h=\beta g\mu_B H/2$. The integration contour C encloses the origin. The ground state energy is given by:

$$E_o(N)= 2\sum_{n=1}^{f-1}\varepsilon_n + x\varepsilon_f\ . \tag{7.23}$$

Here, ε_f is the topmost occupied level and contains $x=1$ or 2 electrons. Denton et al. considered next the constant spectrum studied by Fröhlich and showed that $Q(N,\beta)$ can be given in a closed form for $\beta(\varepsilon_f-\varepsilon_o)\gg 1$ using Jacobi theta functions. But the most important part and goal of their calculation was to study the low temperature behaviour of the specific heat averaging single particle level spacings. They followed the statistical description of the random matrix models of Nuclear Physics. Since they were not interested on shell structure effects, they analyzed only the constant single particle spectrum.

This is precisely the point where our method could be applied. The spectrum involved in eq.(7.22) can be assumed to be of the kind studied in preceding chapters of this work. For example, we have an explicit expression for the logarithm of the above infinite product [cf. eq.(3.3.20)]. Also for periodic spectra with shell structure, we could use the results of chapter four.

We will generalize now the result of Denton et al. for the canonical partition function. Instead of a constant single particle spectrum (with only twofold degenerated levels) we consider now a **periodic single particle spectrum.** Let us use the notation of section 4.2 and write for a system of N electrons the **grand canonical partition function:**

$$Z(\alpha,\beta)= \sum Q(N,\beta)\ y^N \quad , y=\exp(\alpha), \tag{7.24a}$$

with the **canonical partition function** given by:

$$Q(N,\beta)=\frac{1}{2\pi i}\int_C dy\, y^{-N-1}\prod_{j=1}^{e}\prod_{n\geq o}\left(1+y\,e^{-\beta\delta n-\beta\delta\nu_j}\right), \tag{7.24b}$$

where the energy levels are $\varepsilon_{nj}=\delta(n+\nu_j)$, $n=0,1,\ldots$; $j=1,\ldots,e$; e is the degeneracy of each shell, δ the spacing between adjacent shells. Now we divide the infinite product in two parts according whether the single particle levels are smaller or larger than the topmost occupied energy level $\varepsilon_f=\delta(f+\nu_f)$, f integer. After rearranging terms and changing the variable $y \to ze^{\beta\delta f}$, it follows:

$$Q(N,\beta)=\frac{\exp(-\beta E_1)}{\prod_{n>o}(1-e^{-\beta\delta n})^e}\;\frac{1}{2\pi i}\int_C dz\; z^{-1-ex+e/2}\prod_{j=1}^{e}\Big[(z^{1/2}e^{-\beta\delta\nu_j/2}+z^{-1/2}e^{\beta\delta\nu_j/2})\cdot$$

$$\cdot\prod_{m=1}^{f}(1+z^{-1}e^{\beta\delta\nu_j}\,e^{-\beta\delta m})\cdot\prod_{n>o}(1-e^{-\beta\delta n})(1+ze^{-\beta\delta\nu_j}\,e^{-\beta\delta n})\Big], \tag{7.25}$$

where $E_1=\ \delta ef(f-1)/2+\ \delta ef\langle\nu\rangle+\ \delta exf+\ 3\delta e\langle\nu\rangle/2+\ \delta e/8$, $\langle\nu\rangle=\sum_j \nu_j/e$. Also $N=\ ef+ex$, i.e. x is the filled fraction of the last shell. Now, we assume thermal degeneracy $\beta\delta f\gg 1$ and extend the upper limit f in the finite product to infinity. Define: $q^2=\exp(2\pi i\tau)=\exp(-\beta\delta)$, set $z\exp(-\beta\delta\nu_j)=\exp(2\pi i z_j)$ and look at the infinite product representation of the Jacobi ϑ_2-function given in eq.(3.5.1c). The canonical partition function will read:

$$Q(N,\beta)\approx\frac{\exp(-\beta E_1-\beta\delta e/24)}{\eta(\tau)^e}\;\frac{1}{2\pi i}\int_C dz\; z^{-1-ex+e/2}\prod_{j=1}^{e}\vartheta_2(z_j|\tau), \tag{7.26}$$

where we used also the infinite product representation eq.(3.5.2) for the Dedekind η-function. To integrate the product of theta functions, remember their infinite series representation eq.(3.5.1c) and write:

$$Q(N,\beta)\approx\frac{\exp(-\beta E_1-\beta\delta e/24+\beta e\langle\nu\rangle)}{\eta(\tau)^e}\sum_{\{n_1,\ldots,n_e\}}\alpha_1\cdots\alpha_e\int_C\frac{dz}{2\pi i}\,z^{\Sigma n_j-ex-1}, \tag{7.27}$$

where the sums are over the $n_i\in\mathbb{Z}$ and $\alpha_j=\exp[-\beta\delta(n_j-1/2)^2/2\ -\ \beta\delta n_j\nu_j]$. The integration is now immediate and leads to:

$$Q(N,\beta)\approx\eta(\tau)^{-e}\exp(-\beta E_2)\sum_{\{n_1,\ldots,n_{e-1}\}}\exp\{-\beta\delta\sum{}'[n_i^2-(ex+\nu_e-\nu_i)n_i]-\beta\delta\sum_{i<j}{}'n_in_j\}\ . \tag{7.28}$$

The primed sums run over $i,j=1,\ldots,e-1$ and $E_2=\delta ef(f-1)/2+\delta ef\langle\nu\rangle\ +$ $+\delta efx\ +\delta ex(ex-1)/2\ +\delta e/24\ +\delta ex\nu_e$.

To transform the infinite multiple sum in eq.(7.28) into known functions, consider the following symmetric bilinear form:

$$\langle \mathbf{n}+\mathbf{a},\mathbf{n}+\mathbf{a}\rangle = (\mathbf{n}+\mathbf{a})^t\ \Omega\ (\mathbf{n}+\mathbf{a}), \tag{7.29}$$

where **n** and **a** are the (e−1) dimensional vectors $(n_1, \dots, n_{e-1})$ and $(a_1, \dots, a_{e-1})$ with $a_i = \nu_i - \langle\nu\rangle - x$. The $(e-1)\times(e-1)$ matrix Ω has components $\Omega_{ii}=2$ and $\Omega_{ik}=1$ for $i \neq k$. Explicitly, it follows:

$$\tfrac{1}{2}\langle \mathbf{n}+\mathbf{a},\mathbf{n}+\mathbf{a}\rangle = \sum{}'(n_i^2 + a_i^2) + \sum_{i<j}{}'(n_in_j+a_ia_j) + 2\sum{}' n_ia_i + \sum_{i<j}{}'(a_in_j+n_ia_j) =$$

$$= \sum{}'(n_i{}^2+a_i{}^2) + \sum{}'(\nu_i-\nu_e-ex)n_i + \sum_{i<j}{}'(n_in_j+a_ia_j)\ , \tag{7.30}$$

where we have used: $\sum{}'_{i<j}(a_in_j+n_ia_j) = \sum{}' n_j\left(\sum{}' a_i - a_j\right)$ and $a_i + \sum{}' a_j = \nu_i - \nu_e - ex$. The only terms in the inner product which are not in the exponential of eq.(7.28) are:

$$\sum{}' a_i{}^2 + \sum{}' a_ia_j = \tfrac{1}{2}e(e-1)x^2 - ex\langle\nu\rangle + \tfrac{e}{2}(\langle\nu^2\rangle - \langle\nu\rangle^2) + ex\nu_e\ . \tag{7.31}$$

But this constant can be allied to the constant E_2 yielding the **final result:**

$$Q(N,\beta) \approx \exp(-2\pi i\tau\widetilde{E}_0/\delta)\ \theta_{\mathbf{a}}(0|\tau)/\eta^e(\tau)\ , \quad \text{with } 2\pi i\tau = -\beta\delta, \tag{7.32}$$

where $\widetilde{E}_0$ is precisely the **smooth ground state energy:**

$$\widetilde{E}_0/\delta = e(f+x+\langle\nu\rangle-1/2)^2/2 - e/12 + e\langle\nu\rangle/2 - e\langle\nu^2\rangle/2, \tag{7.33}$$

as given by eq.(4.2.14), setting $N = ef+ex$ and $\delta = \hbar\omega$. We introduced further the **θ-function** (with characteristic **a**) in (e−1) variables [see for example V. Kac (1985)] defined by:

$$\theta_{\mathbf{a}}(z|\tau) = \sum_{\mathbf{n}} \exp(\ \pi i\tau\langle \mathbf{n}+\mathbf{a},\mathbf{n}+\mathbf{a}\rangle - 2\pi i z\cdot(\mathbf{n}+\mathbf{a}))\ , \quad \mathbf{n} \in \mathbb{Z}^{e-1}, \tag{7.34}$$

In our case only **z=0** is needed.

With relation eq.(7.32) we arrived at a closed expression. The most interesting observation is that (for rational **a**) the canonical partition function is given by the product of the modular form $\theta_{\mathbf{a}}(0|\tau)/\eta^e(\tau)$ and the exponential factor $\exp(2\pi i\tau\widetilde{E}_0/\delta)$ containing only the smooth ground state energy. Note also the Bosonic partition function $1/\eta^e(\tau)$. Since $-\beta\delta = 2\pi i\tau$, eq.(7.32) is given in terms of the inverse of the temperature. The obtained analytic form allows also the application of the methods of Analytic Number Theory developed in chapter four.

From eqs. (7.24a), (7.32) and (7.33), the grand partition function is:

$$Z(\alpha,\beta)= q^{-4\xi} y^{e/2-e\langle\nu\rangle} \eta^{-e}(\tau) \sum_{xe=0}^{e-1} \theta_a(0|\tau)\vartheta_\alpha(ez|e\tau), \tag{7.35a}$$

where the "anomaly" $\xi = -e/24+e\langle\nu\rangle/4-e\langle\nu^2\rangle/4$ is again the same constant appearing in eq.(7.10) and in the central term of the Virasoro algebra, eq.(7.21) [Set there a=e and parametrize the (rational) ν_i with the numbers a_n.] Here we used the ϑ-function in **one variable** ϑ_α with characteristic $\alpha = xe+e\langle\nu\rangle-e/2$, [cf. eq.(4.2.20)].

Further, note that the assumption of "thermal degeneracy" $\beta\delta f\gg 1$ before eq.(7.26) is equivalent to take as grand canonical partition function the infinite product:

$$Z(\alpha,\beta)=\prod_{i=1}^{e} \prod_{n\geq 0}(1+q^{2n}\, e^{2\pi i(z+\tau\nu_i)})(1+q^{2n+2}\, e^{-2\pi i(z+\tau\nu_i)}). \tag{7.35b}$$

Using now the ϑ-functions in one variable with characteristics $\nu_i-1/2$, it follows:

$$Z(\alpha,\beta)= q^{-4\xi} y^{e/2-e\langle\nu\rangle} \eta^{-e}(\tau) \prod_{i=1}^{e} \vartheta_{\nu_i-1/2}(z|\tau) . \tag{7.35c}$$

In other words, we found two equivalent expressions for $Z(\alpha,\beta)$. Therefore, we arrive at the identity:

$$\prod_{i=1}^{e}\vartheta_{\nu_i-1/2}(z|\tau) = \sum_{xe=0}^{e-1} \theta_a(0|\tau)\vartheta_\alpha(ez|e\tau) . \tag{7.36}$$

Using the same method we have derived many other identities which include also θ-functions in several variables of higher levels. Identities of this kind are the result of the underlying **ring structure** of the θ-functions.

The particular case e=1 of eq.(7.32) yields the result of Goudsmit mentioned at the beginning of this chapter:

$$Q(N,\beta)\approx \exp(2\pi i\tau\widetilde{E}_0/\delta)/\eta(\tau), \tag{7.37}$$

with $\tilde{E}_0/\delta = f(f-1)/2 + {}^1/_{24}$ and $\langle\nu\rangle = 0$.

The next particular case e=2 reduces to the result of Denton et al. (1973) taking $\langle\nu\rangle = 0$, $\nu_2 = -\nu_1 = g\mu_B H/2$, $a = \nu_1 - x$ and the two values $x = 0$, ${}^1/_2$. The two corresponding relations are:

$$Q_{even} \approx \exp[2\pi i\tau(\tilde{E}_{0,even}/\delta + g^2\mu_B^2 H^2/4)]\ \vartheta_3(-\tau g\mu_B H|2\tau)/\eta^2(\tau)\ ,\ \text{for } x = 0, \quad (7.38)$$

with $\tilde{E}_{0,even}/\delta = f(f-1) + {}^1/_{12} - g^2\mu_B^2 H^2/2$. And the second leads to:

$$Q_{odd} \approx \exp[2\pi i\tau(\tilde{E}_{0,odd}/\delta + g^2\mu_B^2 H^2/4)]\ \vartheta_2(-\tau g\mu_B H|2\tau)/\eta^2(\tau),\ \text{for } x = {}^1/_2\ , \quad (7.39)$$

with $\tilde{E}_{0,odd}/\delta = f^2 - {}^1/_6 - g^2\mu_B^2 H^2/4$. Here we have written the background magnetic field dependence in the z-argument of the ϑ-functions.

The transformation formulas given by eqs.(3.5.4a-e) can be used to express $Q_{even,odd}$ in terms of $k_B T = -\delta/2\pi i\tau$. Also for the general result eq.(7.32) holds a similar modular transformation. These transformations permit us to find expressions with better convergence properties for large temperatures.

Remember now the first section of this chapter. We mentioned that for a given modular form (defined with respect to a certain subgroup of the modular group) it is possible to obtain the **exact** Fourier coefficients. In other words, from eq.(7.32) we can assert that (for rational ν_i) it is possible to obtain the **exact** Fourier coefficients of the canonical partition function for a system of Fermions in a periodic single particle spectrum. Here we can return to the nuclear level density problem of section 4.2. Note that the Fourier coefficients of the canonical partition function are nothing else but the nuclear level density itself. Thus, we have found a way to solve exactly the calculation of the nuclear level density for (rational) periodic single particle spectra and not too high excitation energies.

Whether the new expression for the canonical partition function leads to a better understanding of concrete physical problems needs to be studied more in detail. Let us remark that eq.(7.32) and eq.(7.35) lead us naturally to the consideration of some **affine Kac-Moody algebras**. The Weyl-Kac character formula eq.(7.17) has a similar form. In the numerator it contains a θ-function and in the denominator infinite products related with Dedekind's η-function. This can be shown more clearly for particular affine cases. Of course, the mere definition of a character [first equality in eq.(7.17)] is the origin of the analogies. However, we will make here only some general observations.

Most important in the classification of the affine Kac-Moody algebras are the (generalized) **Cartan matrices.** As mentioned in the last section they are linked with the definition of a symmetric bilinear form. It is therefore appealing to try to interpret the bilinear form given by eq.(7.29) as a bilinear form associated with a Kac-Moody algebra. The simplest possibility could be that Ω would be itself a Cartan matrix of finite type. However, the nondiagonal elements are not negative as required. This can be solved easily by a simple matrix transformation. We obtain directly the $\ell \times \ell$ Cartan matrix for a finite algebra A_ℓ with $\ell = e-1$:

$$A = \begin{bmatrix} 2 & -1 & 0 & 0 & \cdots & & 0 \\ -1 & 2 & -1 & 0 & \cdots & & 0 \\ 0 & -1 & 2 & -1 & \cdots & & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdots & & \cdots & -1 & 2 & -1 \\ 0 & \cdots & & \cdots & 0 & -1 & 2 \end{bmatrix} . \tag{7.40}$$

This Cartan matrix is related to Ω by $A = V\Omega V^t$ with:

$$V = \begin{bmatrix} 1 & -1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & -1 & 0 & \cdots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdots & 0 & 1 & & 0 \\ 0 & \cdots & 0 & 0 & & -1 \end{bmatrix} , \quad V^{-1} = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 & 0 \\ 0 & 1 & 1 & \cdots & 1 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdots & & 0 & 1 & 0 \\ 0 & \cdots & & 0 & 0 & -1 \end{bmatrix} .$$

The quadratic form of the lattice is thus $\mathbf{x}^t A \mathbf{x}$ with ℓ-dimensional vectors $\mathbf{x}$. The Cartan matrix A can be written as $A = GG^t$ where G is constructed with the basis vectors of the lattice and is called the **generator matrix.** For the lattice A_ℓ, we can take for example one of the $\ell \times (\ell+1)$ matrices:

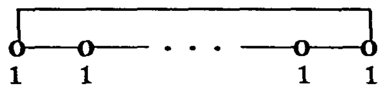
$$G = \begin{bmatrix} -1 & 1 & 0 & 0 & \cdots & & 0 \\ 0 & -1 & 1 & 0 & \cdots & & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdots & & -1 & 1 & & 0 \\ 0 & \cdots & & 0 & -1 & & 1 \end{bmatrix} , \quad G' = \begin{bmatrix} -1 & 0 & 0 & \cdots & 1 & 0 \\ 0 & -1 & 0 & \cdots & 1 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & \cdots & & -1 & 1 & 0 \\ 0 & \cdots & & 0 & 1 & -1 \end{bmatrix} .$$

The first leads to A and the second to Ω. Clearly, the lattice is given by

$\{(x_0,\cdots,x_\ell)\in\mathbb{Z}^{\ell+1}|\ x_0+\cdots+x_\ell=0\}$. The **Dynkin diagram** of A_ℓ is:

(7.41)

and has ℓ vertices, each corresponding to the square of a coordinate in the quadratic form and a line for each cross term in the corresponding variables: $\frac{1}{2}x^tAx=x_1^2-x_1x_2+x_2^2-x_2x_3+\cdots-x_{\ell-1}x_\ell+x_\ell^2$. The **Dynkin diagram** of the **affine** Lie algebra $A_\ell^{(1)}$ (for $\ell\geq2$) is:



(7.42)

This diagram has $\ell+1$ vertices. The extra vertex is related to the imaginary roots, which lead to the infinite sets of roots Δ_+ in the Weyl-Kac character formula and in the denominator identity [cf. eqs.(7.17-18)].

Equation (7.37) for the nondegenerated single particle levels corresponds to the trivial lattice. For zero magnetic field eqs.(7.38-39) correspond to the lattice $A_1\cong\mathbb{Z}$. In general, for the e-fold degenerated single particle levels, the lattices (and their translates) associated with the affine algebras $\widehat{su}(e)$ will arise.

More general bilinear forms could be introduced by starting with the single particle energy levels: $\varepsilon_{njk}=\delta_k n+\mu_j$; $n=0,\ 1,\ \ldots$; $j=1,\ \cdots,\ e$; $k=1,\cdots,\ f$; for positive integers δ_k, e, f and $\mu_j\in\{0,1,\cdots,\delta_k-1\}$. Although the corresponding single particle spectra could also be understood using the original levels (i.e. all $\delta_i=\delta$ and μ_j rational), the underlying number theoretical symmetries would become more apparent.

The θ-function in the expression for the canonical partition function, eq. (7.32), contains additionally to Ω the characteristic **a**. Accordingly, the associated mathematical structures become richer. For example, the elements a_i could be identified with the gradation of type s referred just before eq.(7.19). The **very strange formula** [eq. (7.20)] seems to bear a more important and clearer role for the study of periodic single particle spectra in Nuclear and Clusters Physics.

Here we want to conclude this chapter. We leave open the possible developments of the obtained new relations.

CHAPTER EIGHT

COMPLEX ANALYSIS AND GRAPH THEORY

The functions we have considered in this work were sometimes well known functions of Analytic Number Theory and in other occasions we could not found references about them. Nevertheless in both cases it is difficult to have a clear picture of them, since, involving infinite series and products, they are quite complicated. The simplest (and certainly the most fundamental) function of this kind, the Riemann ζ-function, keeps still hidden some secrets like for example its zeros distribution. We were very interested to "see" somehow all the considered functions and after some attempts we came to a very simple and interesting method, which we like to expose shortly here.

We try now to give a graphical meaning to each analytic function we considered. We have stressed many times our interest not on the particular values that a function attains but rather on the understanding of its most relevant characteristics in terms of as few parameters as posssible. For an analytic function, we look after its singularities and after its transformation properties. Similarly, if we like to have a clear graphical representation for a given function, we do not look for its particular values but mainly for a graphical representation for its singularities and its transformation properties. We try therefore to introduce concepts from the Theory of Functions into Graph Theory, i.e. a kind of "analytic Graph Theory". Needless to say that our considerations are very modest since both mentioned theories are very developed and the author's knowledge on them scarse. An introduction to Graph Theory can be found in B. Bollobás "Graph Theory", (1979).

We start with some definitions to settle ideas. A **graph** G is an ordered pair of disjoint sets **(E,V)** such that the set of **edges E** is a subset of the set of unordered pairs of **vertices V**. An edge vw with endpoints $v,w \in V$ is said to join the vertices v and w. Two vertices joined by an edge are called **adjacent**. If v coincides with w we call the edge a **loop**. If two edges have the same endvertices they are called **multiple**. Any edge has at least one vertex but the vertices can exist isolated. The **order** of a graph is its number of vertices. The **degree** of a vertex is the number of its adjacent vertices. We will consider only graphs without loops and with vertices of order at least two. Further restrictions will appear in the sequel, although extensions of our considerations to more general graphs will often be possible.

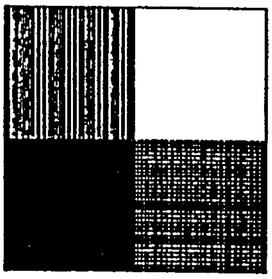
Let us now follow first a path from Complex Analysis towards Graph Theory. Later, we shall make some comments concerning the inverse path. For a given single valued function f(z) of one complex variable z in certain domain $U \subset \mathbb{C}$, we associate a graph G_f in the following way. We define a four colorable graph assigning to each point in U a label ("color") according to the following scheme:

Color	Re f	Im f
1	>0	>0
2	>0	<0
3	<0	<0
4	<0	>0

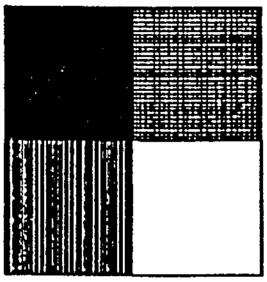
This labeling is of course arbitrary and the resulting tessellation, tiling or parketing is a natural extension of the old well known two coloring : color 1 (2) for the upper (lower) half plane, for complex maps.

The set of points for which we cannot assign a single color are, besides the singularities (say poles, zeros, saddle points, essential singularities, cuts, etc.), the points at which Re f=0 or at which Im f=0. This set of points constitutes the edges of the graph G_f with vertices at the singularities. Multiply valued functions can be considered assigning a set of graphs depending on the number of branches.

Clearly, at a simple pole and at a simple zero we have the following local behaviour :



Near a simple zero



Near a simple pole

Re<0 Im>0 4	1 Re>0 Im>0
Re<0 3 Im<0	2 Re>0 Im<0

Near a simple zero

Re<0 Im<0 3	2 Re>0 Im<0
Re<0 4 Im>0	1 Re>0 Im>0

Near a simple pole

We have in this way associated a positive (counterclockwise) direction for the colors around a pole and a negative (clockwise) direction around a zero. In general for poles (zeros) of order n we will have 4n sectors of $\pi/2n$, in positive (negative) direction. It can futher occur near a saddle point the following picture:

Color a	Color b
Color b	Color a

That is, a vertex with only two contiguous colors: $a \equiv (b \pm 1) \bmod 4$. But this will not happen in general. For the moment this fact is immaterial.

We notice also the following eight possible permutations after the displayed mappings :

(1, 2, 3, 4) (2, 3, 4, 1)	f(z) -if(z)	(4, 3, 2, 1) (3, 2, 1, 4)	-1/f(z) -i/f(z)
(3, 4, 1, 2) (4, 1, 2, 3)	-f(z) if(z)	(2, 1, 4, 3) (1, 4, 3, 2)	1/f(z) if(z)

In all these transformations the number of vertices, edges and regions are conserved, only the orientation of the colors around vertices is changed or/and their relative positions are changed.

The corresponding maps for the complex conjugated functions are also easily recognized since $1/f = f^*/|f|^2$. The missing combinations can be achieved including also branch cuts.

If we consider first only **rational functions** then the above considerations are enough. We obtain a tiling of the Riemann sphere and the corresponding graph satisfies **Euler's equation** :

$$\chi = 2 - 2g = V - E + F , \qquad (8.1)$$

were g is the genus (for the sphere $g=0$), V the number of vertices, E the number of edges and F the number of faces. The number χ is called the Euler-Poincaré characteristic. We show in **Figure 8.1** and **Figures 8.2** examples for rational functions.

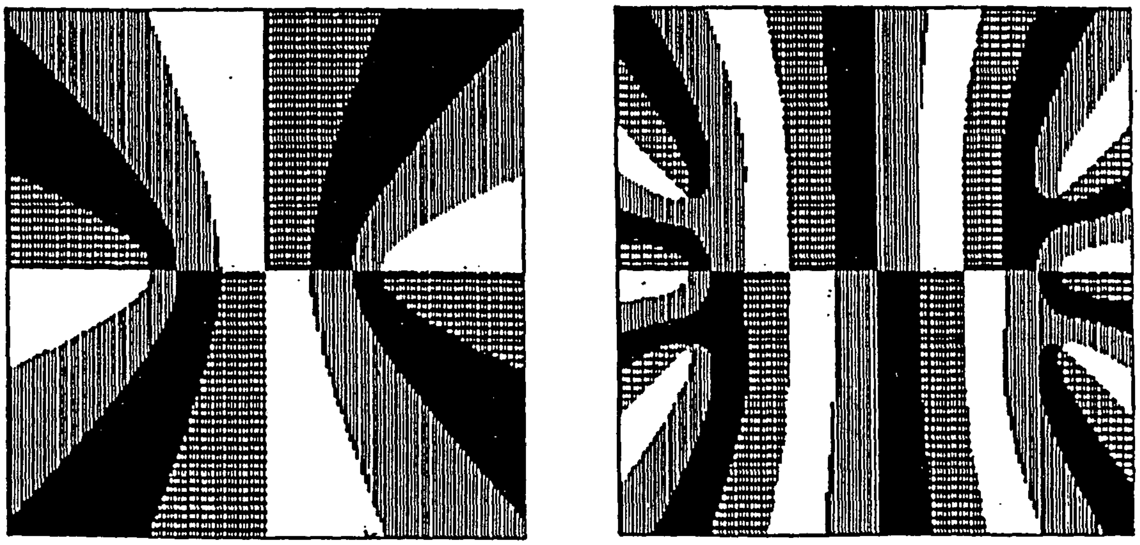


Figure 8.1 Bernoulli polynomials $B_4(z)$and $B_{10}(z)$.
For $Re(z) \in (-1,2)$ and $Im(z) \in (-1.5,1.5)$.

The set of **Figures 8.2** shows automorphic functions of the sphere. An automorphic function is an analytic function that takes the same values at points which are equivalent under a discrete group of linear fractional transformations (cf. eq.(3.5.4)), i.e. a subgroup of the modular group. The left figure corresponds to the tetrahedral function $f_{tetr.}(z) = 12i\sqrt{3}\ u^2/v^3$ and $u = z(z^4-1)$, $v = z^4 + 2i\sqrt{3}\ z^2 + 1$. The right figure represents the icosahedral function $f_{icos.}(z) = u^2/1728\ v^5$ with $u = z^{30} + 522\ z^{25} - 10005\ z^{10} - 522\ z^5 + 1$ and $v = z^5(z^{10} + 11\ z^5 - 1)$. We recognize easily the circles associated with the Möbius transformations forming the groups. The additional feature not present in the well known two colored tesselations (see for example W. Magnus, "Noneuclidean Tesselations and their Groups", Acad.Press, N.Y., 1974) are the non-circular curves, which among other things, provide us the distinction between poles, zeros and saddle points. With respect to these new curves we could also define groups of reflexions.

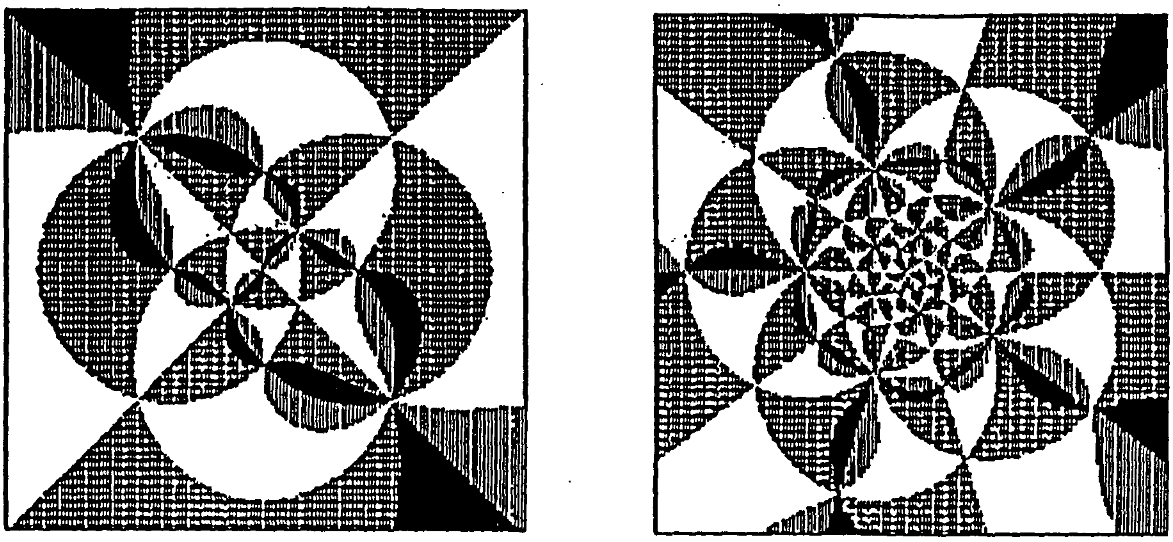
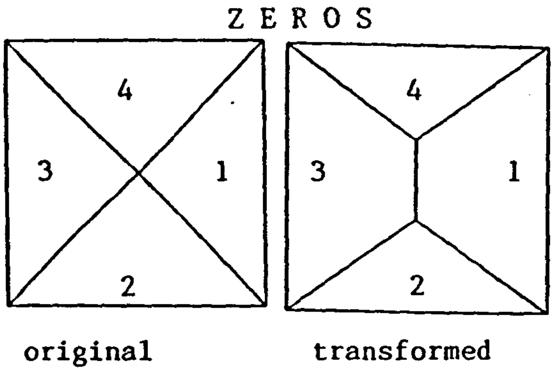
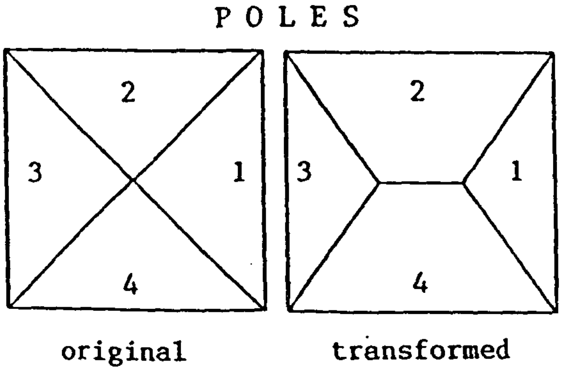


Figure 8.2 Automorphic functions of the sphere.

At first it appears, that we have obtained just a two colorable graph, since the colors 2 (3) and 4 (1) do not touch each other along any edge. But it is easy to find a four colorable graph by means of the following deformation usual in Graph Theory. We add a small circle around each vertex and give to the enclosed area one of the surrounding colors. This leads to a graph with vertices of valence three, this procedure is equivalent to the following reductions :



and



We have selected the color 1 for vertices corresponding to zeros and the color 2 for poles. The simplest example corresponds to f(z)=z and leads to a four colored tetrahedron.

As next we consider also the presence of **essential singularities.** In general such functions lead us to higher genus surfaces with punctures. The resulting graphs can be infinite and non-planar. In **Figure 8.3** we display graphs for the Γ-function and for the Riemann ζ-function, both with one essential singularity at infinity. For the first: Re $z\in(-4,1)$, Im $z\in(-2.5,2.5)$ and for the second: Re $z\in(-10,3)$, Im $z\in(-1,22)$.

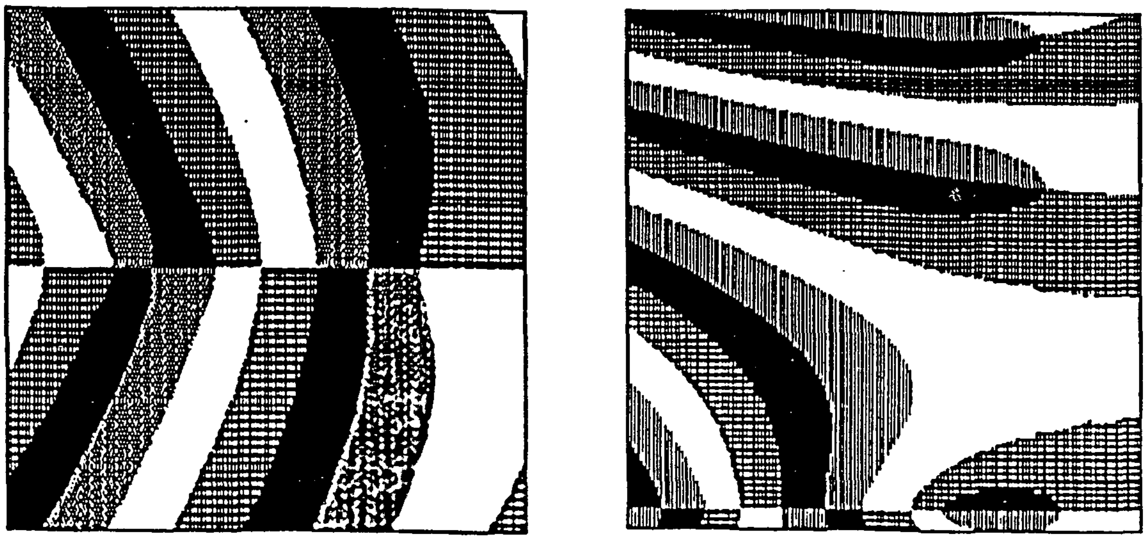


Figure 8.3 The Γ-function and the Riemann ζ-function
For the last we can recognize two non-trivial zeros at
$z= 0.5+i\,14.135$ and $z= 0.5+i\,21.022$

The series of graphs of **Figure 8.4** show a Jacobi function $\vartheta(z|\tau)$ as a function of z. We show also a quotient of these functions, in this case it is an elliptic function (i.e. a doubly periodic meromorphic function). A fundamental region of the doubly periodic tiling yields a single cover of the torus and a double cover of the sphere.

Functions with **natural** boundaries are also well known and good examples are the partitions functions of statistical physics. These functions cannot be analytically continued across a boundary on which they are in general singular, say at all "rational points". Examples are the Jacobi $\vartheta(z|\tau)$ functions as functions of τ as well as rational functions on them. We take $z=0$ and the natural boundary is in this case the real line and τ must be on the upper half plane.

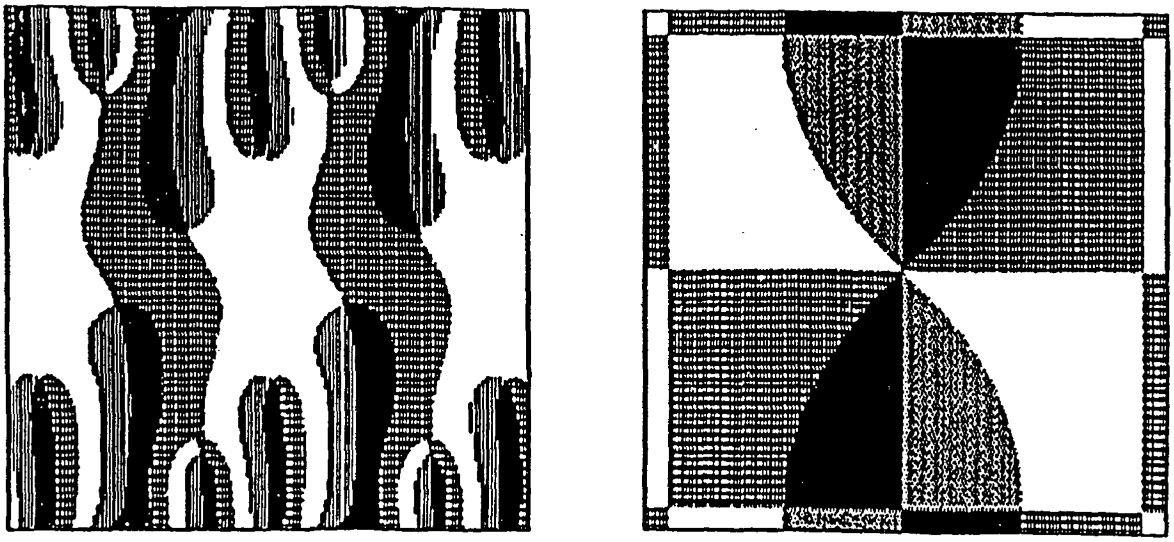


Figure 8.4 A Jacobi ϑ-function and the quotient $\vartheta_2^2(z)/\vartheta_1^2(z)$. For the last we can visualize easily a fundamental region with corners at four-fold vertices.

In Figure 8.5 we show some examples. We display pictures for Klein's modular invariant $J(\tau)$ and for the elliptic modular function $\lambda(\tau)$.

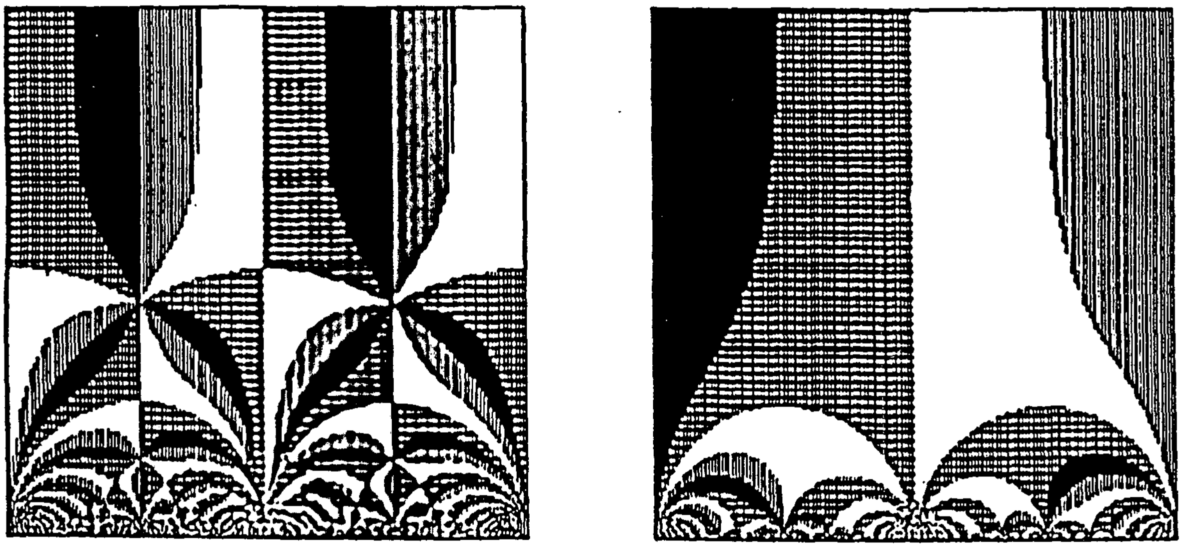


Figure 8.5 Modular invariant $J(\tau)$ and elliptic modular function $\lambda(\tau)$. For the first we see twice the fundamental region (and a corner at ∞). For the second once the fundamental region (and a corner at ∞).

The resulting graphs are infinite and planar, but if we consider quotients by certain discrete groups or identify equivalent edges, we can obtain again tessellations of the sphere. Both functions are **automorphic functions**, the first with respect to the full modular group, the second with respect to the congruence subgroup of level 2 ($a \equiv d \equiv \pm 1 \bmod 2$, $b \equiv c \equiv 0 \bmod 2$) .

The above graphical representation of functions can be extended further to higher genera and to non-differentiable boundaries, but such considerations are not important now.

Let us observe that the above 4 coloring results from the selection of two curves from a **vector field** with sources and sinks defined on the defining domain of the complex function f. Thus, we could also select other pairs of different curves and find essentially the same tilings. If we map the set of curves we recognize the vector field with critical points at zeros, poles and saddle points (for single valued functions). The resulting graph is the union of **two dual graphs** on the surface. One graph, say G_f , has regions with vertices at the zeros (resp. poles for the dual G_f') and centered at the poles (resp. zeros for the dual G_f') . In **Figure 8.6** we show examples of the associated direction fields using a set of narrow bands (bounded by two integral curves of the field) connecting poles with zeros and sometimes with saddle points. In both cases we show elliptic functions. The left is the same function as the right function of Fig.8.4. The right function of Fig.8.6 shows $\vartheta_2^2(z)/\vartheta_1^2(z)$ plus a constant.

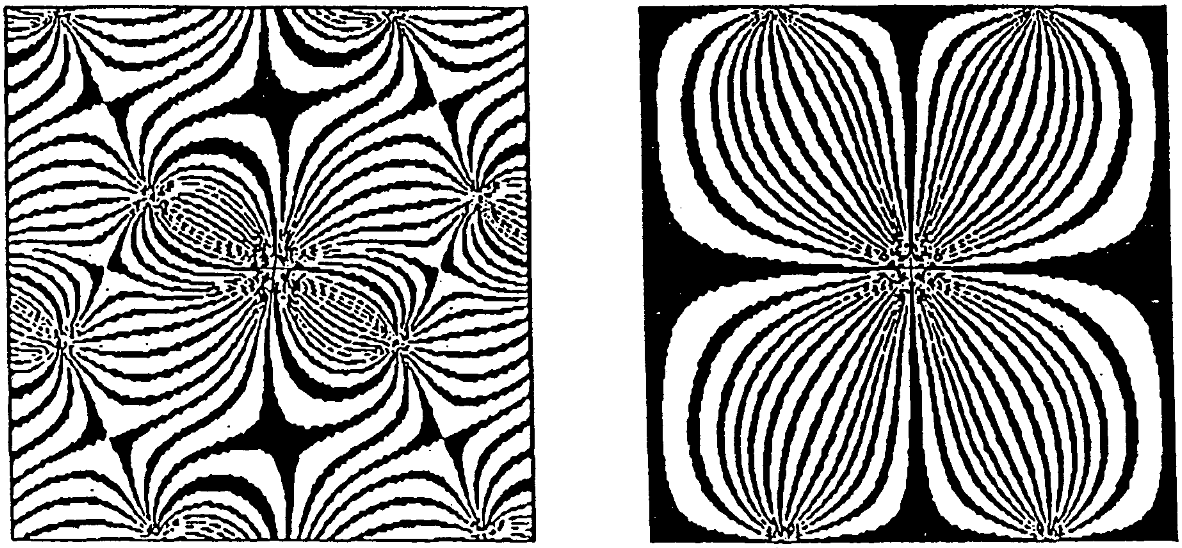


Figure 8.6 Direction fields

For orientable compact surfaces the **index theorem** of H. Poincaré(1885) establishes that the sum of indices of the critical points for a given vector field with V sources, each of index 1, E saddle points, each of index - k (according to their multiplicity), and F sinks, each of index 1, satisfies Euler's equation eq.(8.1). It is easy to verify that the presented fields in Figures 8.6 and 8.8 correspond to genus one. Most important is the fact that the graph with vertices at the zeros (resp. poles) and edges formed by integral curves avoiding the poles (resp. zeros) provides a **cell decomposition** of the enveloping surface. Each cell is completely covered by fibres (integral curves) joining poles with zeros.

In **Figure 8.7** we display the corresponding decompositions provided by Fig.8.6. The (shifted) horizontal foliation of the left figure can be easily computed using the Green's function for the square, but the foliation of the right is only pictorical. Both foliations can be thought as horizontal foliations of half infinite cylinders joined at the cells edges. The graphs formed by the edges of the cell decomposition are called **fat graphs**, when the edges are thickened slightly into bands. Let us add, that the number of colors necessary to assign a different color to any two adjacent cells for genus one is equal to seven, whereas for genus zero remains equal to four.

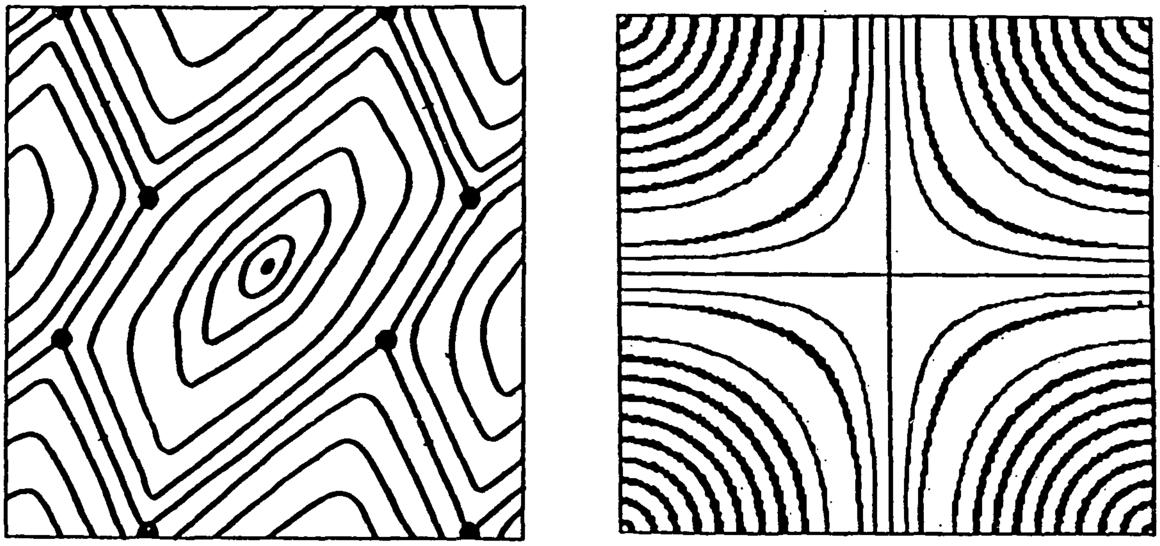


Figure 8.7 Cell decomposition and foliations for Fig.8.6 .

We can associate an **orthogonal vector field** after a carefull observation of the vector fields above. We find out that the field given by the absolute value of the function f, i.e. |f(z)|, leads us to a vector field consisting of concentric deformed circles around the zeros and poles, whereas near the saddle points the field lines look similar as for the original field but rotated by π/2. We ascribe an orientation to the displayed direction fields giving a positive (clockwise) orientation near poles and a negative near poles. In

Figure 8.8 we can see an example of this kind.

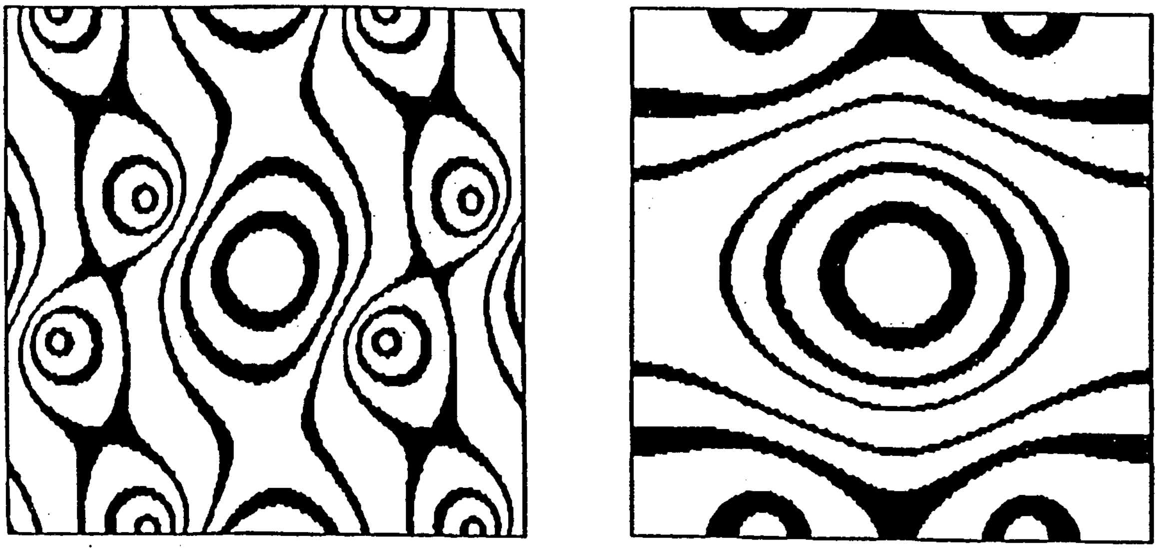


Figure 8.8 Orthogonal direction fields to figure 8.6

In **Figure 8.9** we can see a projection of a three dimensional embedding for two elliptic functions with a double pole and two simple zeros at different positions.

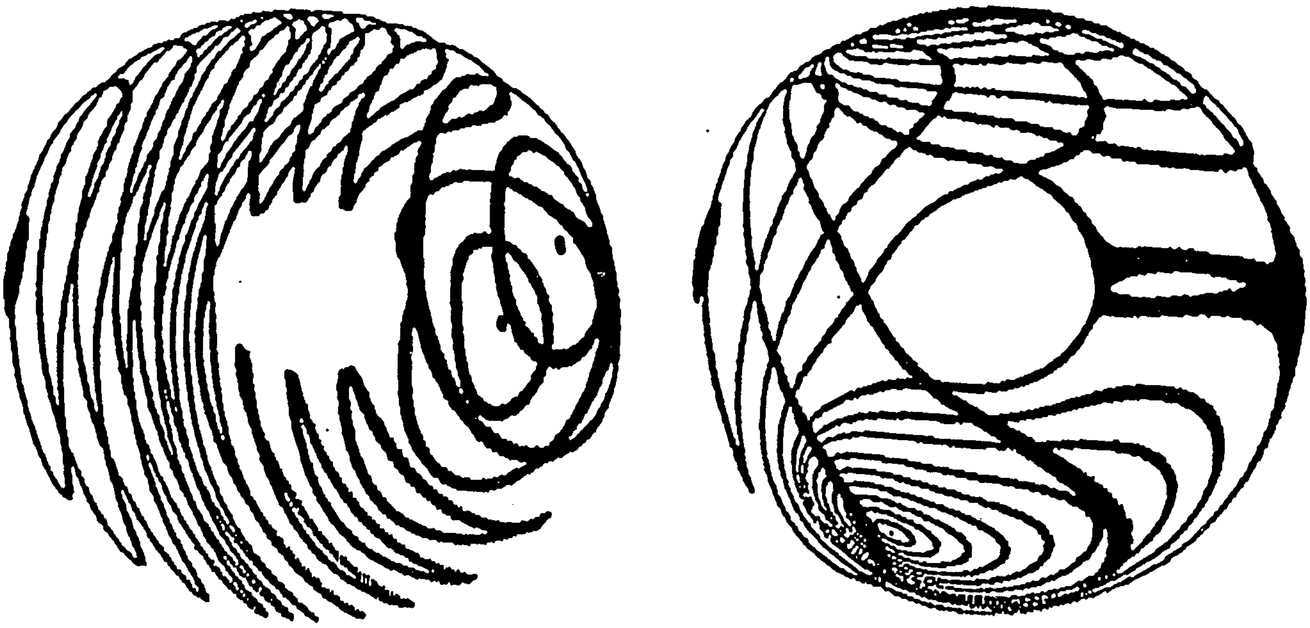


Figure 8.9 Three dimensional embedding for elliptic functions.

In these computations we recognize the foliation of the surface of the three torus by "closed strings" or deformed circular trajectories joining and splitting at 3 "interaction points" located at the middle horizontal axis. It is important to notice that the presented embedding is rather arbitrary, since before we join two equivalent edges of the fundamental region, we could twist them by any multiple of 2π. This situation is a result of the freedom we have to define the fundamental region by any "rectangle" of unit area, bound by two pairs of congruent curves and with vertices at four equivalent points. We can also understand this symmetry as an invariance under modular transformations of the quotient of both lattice periods. In **Figure 8.10** we display the foliations of the type of Figure 8.6 for an elliptic function, with a double pole and a double zero in the fundamental region, under the area preserving map: $x'=x+y$, $y'=x+2y$, or equivalently, under the modular transformation: $\tau'=(\tau+1)/(\tau+2)$.

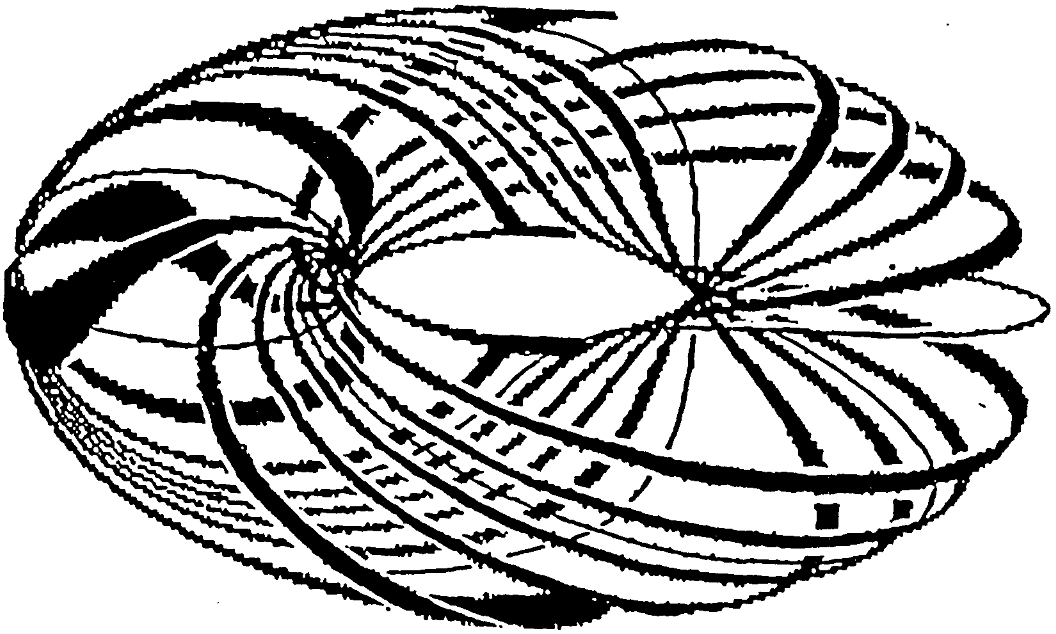


Figure 8.10 Three dimensional embedding for a direction field under a modular transformation.

CONCLUSIONS

In conclusion we like to stress the following results:

1) We have shown a consistent method to study and include the most relevant characteristics of an adopted single particle spectra for the explicit calculation of the nuclear level density. This includes the "smooth" behaviour as well as the shell energy corrections and their excitation energy dependency.

2) Only the consideration of an energy dependent chemical potential can lead to a correct description of the shell effects in the nuclear level density. This follows from the discontinuous character of the infinite sums as a whole. Instead of taking only few terms of a given series, it is necessary to understand them as analytic functions and to study their transformation properties.

3) All other analytic attempts in the current literature (to our best knowledge) on nuclear level densities can be seen as particular cases of the presented method. This is also true for those investigations which assume a smooth single particle level density given by a power series or by a Fourier series. A large class of single particle spectra was considered additionally.

4) The presented method is not only of academic interest but provides us with a useful tool for applications as our calculations in chapter five clearly show. We were able to reproduce experimental results introducing a minimum of physical assumptions (periodic spectra). The consideration of more "realistic" spectra, e.g. of the Nilsson or Woods-Saxon types, is also possible in principle.

5) As we have shown, in particular in chapters six and seven, the methods of Analytic Number Theory can also be applied successfully in related problems in Nuclear Physics or in other fields of Mathematical and Theoretical Physics in a similar way as we have done here. Some new results were obtained for the particle-hole state density in chapter six. A new expression for the canonical partition function for a system of Fermions in a periodic spectrum was found in chapter seven. The theories of modular forms and of Kac-Moody algebras were shown to be related to the study of partition functions in Nuclear and in Clusters Physics.

6) We introduced additionally, to improve our understanding of the involved analytical functions, a simple graphical method (cf. chapter eigth) which is applicable in a more general context.

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