Quantum Mechanics and Number Theory: an Introduction (preliminary version)

Giuseppe Mussardo
International School for Advanced Studies (SISSA)
via Beirut 2-4, 34014 Trieste, Italy
and
Piergiulio Tempesta
Departamento de Física Teórica II,
Métodos y modelos matemáticos,
Facultad de Físicas, Universidad Complutense,
28040 – Madrid, Spain

June 3th, 2010

PREFACE

These Lecture notes are a first version of a book in progress on Quantum Mechanics and Number Theory. This is a living book: the present version is still preliminary and will be periodically updated.

The figures will be provided in a separate file.

Contents

Part I

Quantum mechanics

Chapter 1

Mathematical Introduction

In this first Lecture, we will revise some basic aspects of Elementary Number Theory.

1.1 Formulas for π

1.1.1 Leibnitz formula

The following result, due to Leibnitz, holds:

$$\frac{\pi}{4} = 1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + ... = \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1}.$$

The proof is immediate, since

$$\frac{\pi}{4} = arctg1 = \int_0^1 \frac{dx}{1+x^2} = \sum_{n=0}^{\infty} \int_0^1 (-1)^n \, x^{2n} dx = \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1}.$$

The above formula is completely equivalent to the one of Lord Bronncker

$$\frac{4}{\pi} = 1 + \cfrac{1^2}{2 + \cfrac{3^2}{2 + \cfrac{5^2}{2 + \cfrac{7^2}{\ddots}}}}.$$

This remarkable formula links π with the integers in a far more striking way that does the decimal expansion of π, which appears to exhibit no regularity in the sequence of its digits.

The equivalence between the two formulas is based on the fact that a convergent infinite series of the form

$$\gamma_1 + \gamma_1\gamma_2 + \gamma_1\gamma_2\gamma_3 + \gamma_1\gamma_2\gamma_3\gamma_4 + ...$$

is equivalent to the continued fraction

$$\cfrac{\gamma_1}{1 - \cfrac{\gamma_2}{1+\gamma_2 - \cfrac{\gamma_3}{1+\gamma_3 -}}}.$$

Other remarkable continued fractions.

$$1 + \cfrac{1}{1 + \cfrac{1}{1+\cfrac{1}{1+\ddots}}} = \frac{\sqrt{5}+1}{2}.$$

$$\cfrac{1}{1 + \cfrac{e^{-2\pi}}{1+\cfrac{e^{-4\pi}}{1+\ddots}}} = \left(\sqrt{\frac{5+\sqrt{5}}{2}} - \frac{\sqrt{5}+1}{2}\right) e^{\frac{2\pi}{5}}.$$

The Leibnitz formula is however slowly convergent. Better formulas are, for instance

$$\frac{\pi^2}{6} = \sum_{n=1}^{\infty} \frac{1}{n^2}, \qquad \frac{\pi^4}{90} = \sum_{n=1}^{\infty} \frac{1}{n^4}.$$

As we will see, we also have the general formula

$$\xi(2k) = \sum_{n=1}^{\infty} \frac{1}{n^{2k}} = \frac{(2\pi)^{2k}}{2(2k!)} (-1)^{k-1} B_{2k},$$

where B_{2k} are the (even) Bernoulli numbers, defined as the coefficients of the expansion

$$\frac{x}{e^x - 1} = \sum_{n=0}^{\infty} B_n \frac{x^n}{n!}.$$

They satisfy the recursive equation

$$B_{n+1} = \sum_{k=0}^{n+1} \left(\begin{array}{c} n+1 \\ k \end{array} \right) B_k,$$

which is one of the ways for calculating them. Their first values are

$$B_0 = 1, \quad B_1 = -\frac{1}{2}, \quad B_2 = \frac{1}{6}, \quad B_4 = -\frac{1}{30}...$$

with $B_{2k+1} = 0$ for $k = 1, 2, 3, ...$

Exercise
Prove that

$$\frac{7\pi^4}{720} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n^4}.$$

Another relevant formula, due to Wallis, is

$$\frac{\pi}{4} = \frac{2}{3} \cdot \frac{4}{3} \cdot \frac{4}{5} \cdot \frac{6}{5} \cdot \frac{6}{7} \cdot \frac{8}{7} \cdot \frac{8}{9} \cdot ...$$

It can be proved in different ways.
1) The first proof is based on the infinite product expansion of $\sin x$

$$\sin x = x \prod_{k=1}^{\infty} \left[1 - \left(\frac{x}{k\pi}\right)^2\right].$$

Substituting $x = \frac{\pi}{2}$, we have

$$\frac{2}{\pi} = \frac{1 \cdot 3}{2 \cdot 2} \frac{3 \cdot 5}{4 \cdot 4} \frac{5 \cdot 7}{6 \cdot 6} ...$$

2) Another proof is based on the integral

$$I(n) = \int_0^1 \left(1 - x^2\right)^n dx.$$

It is easy to see that it satisfies the recursive equation

$$I(n) = \frac{2n}{2n+1} I(n-1).$$

Hence, if n is an integer, we have

$$I(1) = \frac{2}{3} I(0) = \frac{2}{3}, \qquad I(2) = \frac{4}{5} I(1) = \frac{2 \cdot 4}{3 \cdot 5},$$

$$...$$

$$I(n) = \frac{2 \cdot 4 \cdot 6 \cdot ... \cdot 2n}{3 \cdot 5 \cdot 7 \cdot ... \cdot (2n+1)}.$$

Consider now the sequence of $I(n)$ for half integers

$$n = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, ...$$

where

$$I\left(\frac{1}{2}\right)=\int_0^1\sqrt{1-x^2}dx=\frac{\pi}{4},$$

$$\dots$$

$$I\left(n-\frac{1}{2}\right)=\frac{1\cdot 3\cdot 5\dots(2n-1)}{2\cdot 4\cdot 6\dots 2n}\frac{\pi}{2}.$$

But it is easy to prove that

$$I(n)\leq I\left(n-\frac{1}{2}\right)\leq I(n+1),$$

i.e.

$$\frac{2\cdot 4\cdot 6\cdot\dots\cdot 2n}{3\cdot 5\cdot 7\cdot\dots\cdot(2n+1)}\leq\frac{1\cdot 3\cdot 5\dots(2n-1)}{2\cdot 4\cdot 6\dots 2n}\frac{\pi}{2}\leq\frac{2\cdot 4\cdot 6\cdot\dots\cdot(2n-2)}{3\cdot 5\cdot 7\cdot\dots\cdot(2n+1)},$$

so that one obtains Wallis' result for $n\to\infty$.

1.1.2 Viete's formula

Another beautiful formula is

$$\frac{2}{\pi}=\frac{\sqrt{2}}{2}\frac{\sqrt{2+\sqrt{2}}}{2}\frac{\sqrt{2+\sqrt{2+\sqrt{2}}}}{2}\dots$$

This formula was found by Viete (2540–160..) at the end of the 16th century. It is the first numerical formula for π and the first one expressed as an infinite product. The proof is based on the duplication formulas of trigonometric functions:

$$\sin\theta=2\sin\frac{\theta}{2}\cos\frac{\theta}{2}=4\sin\frac{\theta}{4}\cos\frac{\theta}{4}\cos\frac{\theta}{2}=\dots=2^n\sin\frac{\theta}{2^n}\cos\frac{\theta}{2}\cos\frac{\theta}{4}\dots\cos\frac{\theta}{2^n}.$$

Since

$$\lim_{n\to\infty}2^n\sin\frac{\theta}{2^n}=\theta,$$

taking $\theta=\frac{\pi}{2}$ and using the formula $\cos\frac{x}{2}=\sqrt{\frac{1}{2}(1+\cos x)}$, we arrive to Viete's formula.
Another proof is based on the recursive formula

$$a_{2n}=\sqrt{2-\sqrt{4-a_n^2}},$$

which relates the length a_n of the side of a regular n–gon inscribed in the unit circle to the side a_{2n} of the $2n$–gon.

1.1.3 Other formulas for π

In the formula

$$\pi = \sum_{n=0}^{\infty} \left[\frac{4}{8n+1} - \frac{2}{8n+4} - \frac{1}{8n+5} - \frac{1}{8n+6} \right] \left(\frac{1}{16} \right)^n$$

the factor $\frac{1}{16}$ appears. Since this turns out to be the anomalous dimension of the spin–field of the Ising Model, on would speculate on the field theoretical origin of this number.
The following surprising formula is due to Ramanujan:

$$\frac{1}{\pi} = \frac{\sqrt{8}}{9801} \sum_{n=0}^{\infty} \frac{(4n)! \left[1103 + 26390n\right]}{(n!)^4 \left(396\right)^{4n}}.$$

The fastest convergent formula is the one found by Gauss, and related to the arithmetic–geometric mean (AGM) of two numbers (a, b). This is defined as the common limit of the sequences

$$\begin{cases} a_{n+1} = \left(a_{n+b_n}\right)/2 & a_0 = a \\ b_{n+1} = \sqrt{a_n b_n} & b_0 = b \end{cases}.$$

It is easy to see that $\{a_n\}$ decreases whereas $\{b_n\}$ increases, as it comes from the inequalities

$$a_{n+1} - b_{n+1} = \frac{1}{2} \left(\sqrt{a_n} - \sqrt{b_n} \right)^2 \geq 0,$$

$$a_n - a_{n+1} = \frac{1}{2} \left(a_n - b_n \right) \geq 0,$$

$$b_{n+1} - b_n = \sqrt{b_n} \left(\sqrt{a_n} - \sqrt{b_n} \right) \geq 0.$$

Hence these sequences converge. From the first equality, we have in fact

$$a_n - b_n \leq 2^{-n},$$

i.e. the limit is reached exponentially fast. The AGM gives rise to the highly efficient method to compute π. Jonathan and Peter Borwein have found surprising formulas, like

$$\pi = 2 \left[AGM \left(\sqrt{2}, 1 \right) \right]^2 / \left(1 - \sum_n 2^n \varepsilon_n \right), \quad \varepsilon_n = a_n^2 - b_n^2.$$

There is also a formula which links π to the Fibonacci numbers, defined by

$$F_{n+2} = F_{n+1} + F_n, \qquad F_1 = F_2 = 1.$$

There is a close expression for these numbers given by the Binet formula:

$$F_n = \frac{1}{\sqrt{5}} \left[\left(\frac{\sqrt{5}+1}{2} \right)^n - \left(\frac{1-\sqrt{5}}{2} \right)^n \right],$$

simple to prove. In fact, from the ansatz $F_n = x^n$, the recursive equation gives

$$x^2 = x + 1 \Rightarrow x = \frac{1 \pm \sqrt{5}}{2},$$

hence

$$F_n = A x_+^n + B x_-^n,$$

where the two constants A and B can be fixed by the initial conditions: $A = -B = \frac{1}{\sqrt{5}}$.
The Fibonacci numbers are generated by

$$\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}^n = \begin{pmatrix} F_{n+1} & F_n \\ F_n & F_{n-1} \end{pmatrix},$$

from which we infer

$$F_{n-1} F_{n+1} - F_n^2 = (-1)^n .$$

Notice that the Fibonacci numbers admit a generating function, given by

$$\frac{x}{1 - x - x^2} = \sum_{n-1}^{\infty} F_n x^n$$

(Generating function of a partition

$$\prod_{n=1}^{\infty} \frac{1}{1 - q^n} = \sum_{n=0}^{\infty} P(n)\, q^n,$$

with $P(n) \simeq \frac{1}{4n\sqrt{3}} e^{\pi \sqrt{\frac{2n}{3}}}$. Finally, the formula connecting F_n with π is

$$\frac{\pi}{4} = \sum_{n=1}^{\infty} \arctan \frac{1}{F_{2n+1}}.$$

1.2 The quantum propagator

A basic quantity in Quantum Mechanics is given by the quantum propagator. This is defined as the amplitude for a particle that is in a position q_0 at the time t_0 to reach the point q at the time t:

$$K\left(q,t;q_0,t_0\right)=\left\langle qt\right|\left.q_0t_0\right\rangle .$$

In the following, we will treat for simplicity the one dimensional case, but the relevant formulas can be easily generalized to higher dimensions (as a matter of fact, they can be generalized to Quantum Field Theory as well). We will assume that at any given time, the coordinate operator $\widehat{q}$ possesses a complete set of eigenvalues, so that

$$\widehat{q}\left(t\right)\left|q,t\right\rangle =q\left|q,t\right\rangle ,$$

with the completeness condition

$$\int dq\left|q,t\right\rangle \left\langle q,t\right|=1.$$

There are two ways of expressing the quantum propagator. The first one employs wave functions, the second one the concept of *"path integral"*. First of all, the translation in time is dictated by the Hamiltonian, so that

$$K\left(q,t;q_0,t_0\right)=\left\langle q\right|e^{-\frac{i}{\hbar}H(t-t_0)}\left|q_0\right\rangle .$$

Inserting now a complete set $\{|E_n\rangle\}$of orthogonal eigenstates of H, we have

$$K\left(q,t;q_0,t_0\right)=\sum_{n,m}\left\langle q\right|\left.E_n\right\rangle \left\langle E_n\right|e^{-\frac{i}{\hbar}H(t-t_0)}\left|E_m\right\rangle \left\langle E_n\right|\left.q_0\right\rangle =$$

$$\sum_n\psi_n\left(q\right)\psi_n^*\left(q_0\right)e^{-\frac{i}{\hbar}E_n(t-t_0)},$$

where

$$\left\langle q\right|\left.E_n\right\rangle =\psi_n\left(q\right),\left\langle E_n\right|\left.q\right\rangle =\psi_n^*\left(q\right).$$

where we have used the orthogonality of the eigenstates. The above is the first expression of the quantum propagator. To get the other one, let's divide initially the time interval $T=(t-t_0)$ in n small intervals $(n\rightarrow\infty)$, and let's insert $(n-1)$ times the completeness relation:

$$\left\langle qt\right|\left.q_0t_0\right\rangle =\int dq_1...dq_n\left\langle qt\right|\left.q_{n-1}t_{n-1}\right\rangle \left\langle q_{n-1}t_{n-1}\right|\left.q_{n-2}t_{n-2}\right\rangle ...\left\langle q_1t_1\right|\left.q_0t_0\right\rangle . \tag{1.1}$$

Let us consider each term in this expression.

$$\langle q_k t_k|\ q_{k-1} t_{k-1}\rangle = \langle q_k|\, e^{-\frac{i\delta t}{\hbar} H}\, |q_{k-1}\rangle =$$

$$\int dp_{k-1}\, \langle q_k|\ p_{k-1}\rangle\, \langle p_{k-1}|\, e^{-\frac{i\delta t}{\hbar} H}\, |q_{k-1}\rangle\,, \tag{1.2}$$

where we have introduced a completeness relation in term of the momentum eigenstates:

$$\int dp\, |p\rangle\, \langle p| = 1.$$

Suppose that the Hamiltonian is given by

$$H = \frac{p^2}{2m} + V(q)\,.$$

Using the Baker–Campbell–Hausdorff formula at the leading order in δt, we have

$$\langle p_{k-1}|\, e^{-\frac{i\delta t}{\hbar} H}\, |q_{k-1}\rangle \simeq \langle p_{k-1}|\, e^{-\frac{i\delta t}{\hbar}\frac{p^2}{2m}} e^{-\frac{i\delta t}{\hbar} V(q)}\, |q_{k-1}\rangle =$$

$$\langle p_{k-1}|\ q_{k-1}\rangle\, e^{-\frac{i\delta t}{\hbar}\left[\frac{p^2}{2m} + V(q_{k-1})\right]}.$$

Since

$$\langle q|\ p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipq/\hbar}.$$

For the expression (1.2) we have

$$\langle q_k t_k|\ q_{k-1} t_{k-1}\rangle \simeq \frac{1}{2\pi\hbar}\int dp_{k-1} e^{-\frac{i\delta t}{\hbar}\frac{p_{k-1}^2}{2m} + \frac{i(q_k - q_{k-1})p_{k-1}}{\hbar}} e^{-\frac{i\delta t}{\hbar}}.$$

In the infinitesimal time δt, we may assume a constant velocity $\dot{q}_{k-1}$, such that $q_k - q_{k-1} \simeq \dot{q}_{k-1}\delta t$, and we can perform the Gaussian integral. The result is very simple:

$$\langle q_k t_k|\ q_{k-1} t_{k-1}\rangle = \sqrt{\frac{m}{2\pi i\hbar\delta t}}\exp\left[\frac{\delta t}{\hbar} L\left(q, \dot{q}\right)\right],$$

where $L\left(q, \dot{q}\right)$ is the Lagrangian of the theory:

$$L = \frac{m\dot{q}^2}{2} - V(q)\,.$$

Putting now this result into (1.1), we arrive to the interesting result for the quantum propagator:

$$k\left(q,t;q_0,t_0\right)=\int\mathcal{D}qe^{i/\hbar\int_{t_0}^{t}L\left(q,\dot{q}\right)d\tau}, \tag{1.3}$$

where the measure is formally defined by

$$\mathcal{D}q=\lim_{n\to\infty}\left(\frac{mn}{2\pi i\hbar T}\right)^{n/2}dq_1...dq_{n-1}.$$

The meaning of the above expression is obvious.. One can go from the point (q_0,t_0) to the point (q,t) by following all possible paths. These paths, however, are weighted with the oscillating phase of the action of these paths. In the semiclassical limit $\hbar\to 0$, the above integral can be evaluated in the saddle point approximation, i.e. there exists one path which dominates the expression. This is given by the condition

$$\delta\int_{t_0}^{t}L\left(q,\dot{q}\right)d\tau=0,$$

i.e.

$$\int_{t_0}^{t}\left[\frac{\partial L}{\partial q}\delta q+\frac{\partial L}{\partial\dot{q}}\delta\dot{q}\right]dt=\int_{t_0}^{t}\left[\frac{\partial L}{\partial q}-\frac{d}{dt}\frac{\partial L}{\partial\dot{q}}\right]\delta qdt+p\delta q\mid_{t_0}^{t}. \tag{1.4}$$

For variational paths which leave the end points fixed, the last term in (17) vanishes. Therefore we see that in the semiclassical limit the Lagrangian satisfies the classical equation of motion

$$\frac{\partial L}{\partial q}-\frac{d}{dt}\frac{\partial L}{\partial\dot{q}}=0.$$

It is now immediate to see that $K\left(q,t,q_0,t_0\right)$ is the Green function of the time–dependent Schrödinger operator, i.e. the propagator of the theory. In fact, from the time evolution of the states

$$\left|\psi\left(t\right)\right\rangle=e^{-\frac{i}{\hbar}H(t-t_0)}\left|\psi\left(t_0\right)\right\rangle$$

we can "sandwich" it with $\langle q|$, obtaining

$$\left\langle q\right|\left.\psi\left(t\right)\right\rangle=\psi\left(q,t\right)=\int dq^{'}\left\langle q_k\right|e^{-\frac{i}{\hbar}H(t-t_0)}\left|q^{'}\right\rangle\left\langle q^{'}\right|\left.\psi\right\rangle=\int dq^{'}K\left(q,t,q_0^{'},t_0^{'}\right)\psi\left(q^{'},t_0\right).$$

The function $K(q, q_0, t - t_0)$ satisfies the composition law

$$\left(q, q^{'}, t - t^{'}\right) = \int dq^{''} K\left(q, q^{''}, t - t^{''}\right) K\left(q^{''}, q^{'}, t^{''} - t^{'}\right),$$

and the differential equation

$$\left(-i\hbar\frac{\partial}{\partial t} + H\right) K\left(q, q^{'}, t - t^{'}\right) = -i\hbar\delta\left(q - q^{'}\right).$$

We want to consider now the density of states of the system. This is defined as

$$g(E) = \sum_n \delta(E - E_n) g_n,$$

where g_n is the degeneracy of the energy levels. We suppose $g_n = 1$. The integral of this expression is called the "number staircase function" $N(E)$ and counts the number of levels (including their degeneracy) up to a given energy E

$$N(E) = \int_0^E g(E) dE.$$

The density of states enters several important formulas and, as we will see immediately, is related to the quantum propagator. First of all, a Laplacian transform of $g(E)$ yields the canonical partition function $Z(\beta)$:

$$Z(\beta) = \mathcal{L}_\beta [g(E)] = \int_0^\infty e^{-\beta E} g(E) dE = \sum_n e^{-\beta E_n}.$$

In order to relate $g(E)$ to the propagator, let us consider initially the Fourier transform of K with respect to the time difference $t \equiv t^{'} - t$:

$$G\left(q, q^{'}, E\right) \equiv -\frac{i}{\hbar}\int_0^\infty K\left(q, q^{'}, t\right) e^{-\frac{i}{\hbar}Et} = -\frac{i}{\hbar}\sum_n \psi_n^*\left(q^{'}\right)\psi_n(q)\int_0^\infty e^{\frac{i}{\hbar}(E - E_n)t} dt.$$

Since the last integral oscillates and does not converge, we give a small imaginary part to the energy: $E \to E + i\varepsilon$, so that

$$G\left(q, q^{'}; E\right) = \sum_n \psi_n^*\left(q^{'}\right)\psi_n(q)\frac{1}{E - E_n + i\varepsilon}. \tag{1.5}$$

This Green function satisfies

$$(E - H) G\left(q, q^{'}, E\right) = \delta\left(q - q^{'}\right),$$

and for free theories it can be easily computed

$$D=1 \qquad G_0\left(q,q^{'},E\right)=-\left(\frac{2m}{\hbar^2}\right)\frac{i}{2k}\exp\left(-ik\left|q-q^{'}\right|\right),$$

$$D=2 \qquad G_0\left(q,q^{'},E\right)=-\left(\frac{2m}{\hbar^2}\right)\frac{i}{4}H_0^{+}\left(k\left|q-q^{'}\right|\right),$$

$$D=3 \qquad G_0\left(q,q^{'},E\right)=-\left(\frac{2m}{\hbar^2}\right)\frac{\exp\left[ik\left|q-q^{'}\right|\right]}{4\pi\left|q-q^{'}\right|},$$

where $k=\sqrt{2mE}$. If we now take the trace of (26), i.e.

$$trG=\int dqG\left(q,q^{'},E\right)=\sum_n\frac{1}{E-E_n+i\varepsilon}\equiv\widehat{G}\left(E\right)$$

by using the identity

$$\frac{1}{x+i\varepsilon}=P\left(\frac{1}{x}\right)-i\varepsilon\pi\delta\left(x\right),$$

we see that

$$g\left(E\right)=\sum_n\delta\left(E-E_n\right)=-\frac{1}{\pi}Im\widehat{G}\left(E+i\varepsilon\right)=-\frac{1}{\pi}\int ImG\left(q,q^{'},E+i\varepsilon\right)dq.$$

From the above relation between $g\left(E\right)$ and the canonical partition function, we also have that the density of states is given by the inverse Laplace transform of the latter function

$$g\left(E\right)=\mathcal{L}_E^{-1}\left[Z\left(\beta\right)\right]=\frac{1}{2\pi i}\int_{\varepsilon-i\infty}^{\varepsilon+i\infty}e^{\beta E}Z\left(\beta\right)d\beta,$$

where the integral is to be taken in the complex β–plane along a contour C which is parallel to the imaginary axis. The positive distance ε of the contour from the imaginary axis has to be chosen large enough so that all poles of the integrand lie to the left of the contour. If the integrand has isolated poles we can easily evaluate this integral by the residue theorem.

A very instructive example.

Let us consider the harmonic oscillator, with the spectrum given by $E_n = n$ (we will take care of the $\frac{1}{2}$ term later). For such system the partition function is easily done:

$$Z(\beta) = \sum_{n=0}^{\infty} e^{-\beta n} = \frac{1}{1-e^{-\beta}} = \frac{e^{\beta/2}}{2\sinh \beta/2}.$$

The poles of this function are all simple and all lying on the imaginary axis at the values

$$\beta_k = 2\pi i k, \qquad k = 0, \pm 1, \pm 2, ...$$

with residue $(-1)^k$. By choosing the contour as in the figure

FIGURE

summing up all residues, and taking into account the extra factors $\exp(\beta_k/2)$ as well as $\exp(E\beta_k)$ appearing in the inverse Laplacian transform, we have

$$g(E) = \sum_n \delta(E - E_n) = \sum_{k=-\infty}^{+\infty} e^{2\pi i k E}.$$

As we will see, this is equivalent to the Poisson resummation formula.
Since the spectrum is bounded by $E = 0$, only non–negative values of the energy are relevant. The above formula can be written

$$g(E) = \left\{ 1 + 2\sum_{k=1}^{\infty} \cos(2\pi k E) \right\}.$$

Note that the constant term, which corresponds to the average level density, comes from the pole at $\beta = 0$, whereas the other poles along the imaginary axis combine pairwise to make up all Fourier components of the oscillating part.
It is now trivial to restore the actual dependence $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$ of the energy levels. In fact, we have

$$g(E) = \frac{1}{\hbar\omega}\left\{ 1 + 2\sum_{k=1}^{\infty} \cos\left[2k\pi \left(\frac{E}{\hbar\omega} - \frac{1}{2} \right) \right] \right\} =$$

$$\frac{1}{\hbar\omega}\left\{ 1 + 2\sum_{k=1}^{\infty} (-1)^k \cos\left(\frac{2\pi k E}{\hbar\omega} \right) \right\}.$$

Comment.
Notice that $g(E)$ naturally splits into a smooth part $\widetilde{g}(E)$ and an oscillatory part $\delta g(E)$:

$$g(E) = \widetilde{g}(E) + \delta g(E).$$

The smooth part is, in the above example, just the constant $1/\hbar\omega$, namely there is one energy level per unit $\hbar\omega$. The oscillating part contains cosine functions with constant amplitudes; their arguments are multiples of $2\pi E/\hbar\omega$. This quantity is easily recognized as the classical action: in fact, taking the classical momentum $p(x) = \sqrt{2m(E - V(x))}$ and integrating between the two turning points

$$x_0 = \pm\frac{\sqrt{2E/m}}{\omega},$$

we obtain

$$S(E) = \oint p dx = 2\int_{-x_0}^{x} p(x)\, dx = \frac{2\pi E}{\omega}.$$

For the stair–case function the situation is as in the figure

FIGURE

The previous example is the simplest of a general theory. This states that the smooth part is simply given by the corresponding integral on the *classical phase space:*

$$g(E) = \frac{1}{(2\pi\hbar)^f}\int dq^f dp^f \delta(E - H(q,p)),$$

for a system of f degrees of freedom. This gives reason of the rule that the number of eigenstates with energy lass than E equals the number of cells less than E. Much more interesting is the oscillatory part, which is controlled by the so–called Gutzwiller trace formula. It reads

$$\delta g(E) = \sum_{\Gamma\in\{ppo\}}\sum_{k=1}^{\infty} A_{\Gamma_k}(E)\cos\left[\frac{k}{\hbar}S_\Gamma(E) - \sigma_{\Gamma_k}\frac{\pi}{4}\right],$$

where Γ counts classes of topologically distinct *primitive periodic orbits* (ppo) (with energy E as a parameter); k counts the repeated revolution around each primitive orbit which yields a series of harmonics; $S_\Gamma(E) = \oint p_\Gamma dq_\Gamma$ is the classical action integral along the orbit Γ; and σ_{Γ_k} is the "*Maslov index*" of the orbit.

Finally, the amplitudes A_{Γ_k} depend on energy, time period and stability of the orbits and their nature, being isolated or non–isolated. In the latter case, one must sum over all distinct families of degenerate orbits.
The trace formula represents a Fourier decomposition of the oscillating part of the level density. It gives the basis for many interesting interpretations of quantum phenomena in terms of classical orbits. The reason why classical periodic orbits are important can be understood by the path integral representation of the propagator. Suppose, in fact, that in the formula (1.3), we put $q_0 = q$ and integrate on q, in order to obtain the trace of the propagator

FIGURE

In this case the action is a function of the variable q. The paths which dominate the path integral are those for which $p_{in} = p_{fin}$, as it can be seen from eq. (1.4). Those are just the periodic orbits

1.3 General spectrum depending on one quantum number

It is simple to derive in full generality the previous result. Let us assume that the spectrum E_n is given by a function $f(n)$ and each level has a degeneracy $d_n = D(n)$

$$E_n = f(n); \qquad d_n = D(n), \qquad n = 0, 1, ..$$

We assume $f(n)$ to be a monotonic function with differentiable inverse $f^{-1}(x) \equiv F(x)$ so that

$$n = F(E_n).$$

Using the general properties of the δ..function, we have

$$\delta(E - E_n) = \delta(E - f(n)) = \delta(n - F(E)) \left|F'(E)\right|.$$

Further defining $D(E) = D[F(E)]$, we have then

$$g(E) = D(E) \left|F'(E)\right| \sum_{n=0}^{\infty} \delta(n - F(E)).$$

We can apply now the previous formula of the harmonic oscillator (i.e. Poisson resummation formula) and obtain

$$g(E) = D(E) \left|F'(E)\right| \left\{1 + 2\sum_{k=1}^{\infty} \cos[2\pi k F(E)]\right\}.$$

This formula can be applied to any system where the values of E_n and d_n are known explicitly. This is not restricted to one–dimensional problems: there exists in fact some high–dimensional potentials for which the spectrum can be written analytically in terms of one single quantum number n with known degeneracy. For all these systems the average level density is

$$\widetilde{g}(E) = D(E)\left|F'(E)\right|,$$

whereas the oscillating part is

$$\delta g(E) = 2D(E)\left|F'(E)\right|\sum_{k=1}^{\infty}\cos\left[2\pi kF(E)\right].$$

Within the periodic orbit theory, $2\pi\hbar F(E)$ is the classical action integrated along an elementary closed orbit. The number k corresponds to the number of revolutions around the orbit. If several distinct orbits exist, they have to be summed separately. The amplitudes of the oscillation depend, in these cases, on the chosen orbit and are, in general, much more difficult to obtain. In fact the Bohr–Sommerfeld quantization rule reads

$$S(E) = \oint pdx = 2\int_{x_1}^{x_2} p(x)\,dx = 2\pi\hbar n$$

(the eventual extra constant is irrelevant for the subsequent considerations). Hence, since $n = F(E_n)$, we see by construction that

$$F(E) = \frac{1}{2\pi\hbar}S(E).$$

Example 1. Particle in a box of length L.
The exact spectrum is given in this case by

$$E_n = E_0(n+1)^2, \qquad E_0 = \frac{\hbar^2\pi^2}{2mL^2}, \qquad (n = 0, 1...)$$

In the above notation $F(E) = \sqrt{\frac{E}{E_0}} - 1$, and therefore

$$g(E) = \frac{1}{2\sqrt{E_0 E}}\left\{1 + 2\sum_{k=1}^{\infty}\cos\left[2\pi k\sqrt{\frac{E}{E_0}}\right]\right\}.$$

Example 2. Spherical harmonic oscillator in D–dimensions.
For this system the energy levels are given by one quantum number n with a degeneracy d_n which is a polynomial of order $D-1$

(Example

$$D = 2 \qquad d_n = n + 1$$

$$D = 3 \qquad d_n = \frac{1}{2}(n+1)(n+2).$$

Through the previous formulas we easily obtain

$$g(E) = \frac{E}{(\hbar\omega)^2}\left\{1 + 2\sum_{k=1}^{\infty}\cos\left(2\pi k\frac{E}{\hbar\omega}\right)\right\},$$

for $D = 2$, and

$$g(E) = \frac{1}{2(\hbar\omega)^3}\left[E^2 - \frac{1}{4}(\hbar\omega)^2\right]\left\{1 + 2\sum_{k=1}^{\infty}(-1)^k\cos\left(2\pi k\frac{E}{\hbar\omega}\right)\right\}$$

for $D = 3$.

1.4 The Gamma Function

In this Section, some of the basic properties of the Gamma Function will be reviewed, due to its relevance in the subsequent considerations.

$\Gamma(z)$ is an analytic function of the complex variable z, defined, for $\mathbb{R}\mathrm{e}(z) \geq 0$, by the following integral

$$\Gamma(z) = \int_0^{\infty} dt e^{-t} t^{z-1} dt. \tag{1.6}$$

By making the change of variable $t \to t^2$, it can be equivalently expressed as

$$\Gamma(z) = 2\int_0^{\infty} dt e^{-t^2} t^{2z-1} dt.$$

When $z = \frac{1}{2}$,the above is nothing but the gaussian integral. Therefore

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}.$$

The analytic continuation of $\Gamma(z)$ can be achieved with many different techniques. First of all, it is easy to show that $\Gamma(z)$ has simple poles at $z = 0, -1, -2, ..., -n$. Let us write (1) as

$$\Gamma(z) = \int_0^1 dt e^{-t} t^{z-1} + \int_1^{\infty} dt e^{-t} t^{z-1}.$$

The second integral is convergent for all values of z in the complex plane. About the first one, for $\mathbb{R}\mathrm{e}(z) \geq 0$,where it converges uniformly, we can expand the exponential and integrate term by term so that

$$\Gamma(z) = \int_0^1 dt t^{z-1} \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} t^k + \widehat{\Gamma}(z) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \int_0^1 dt t^{z+k-1} + \widehat{\Gamma}(z)$$

$$= \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} \frac{1}{(z+k)} + \widehat{\Gamma}(z).$$

This expression clearly shows the poles at negative integer values of z. Nearby the poles we have

$$\Gamma(z) \simeq \frac{(-1)^k}{k!(z+k)}.$$

Another way of extending analytically its definition in the complex plane is by using its functional equation

$$\Gamma(z+1) = z\Gamma(z), \tag{1.7}$$

which is immediately obtained by integrating by parts eq. (1). By virtue of eq. (1.7), $\Gamma(z)$ can be interpreted as a generalization of the factorial function to complex numbers. Indeed, for integer positive values, we have

$$\Gamma(n) = (n-1)!$$

Moreover, eq. (1.7) can be used to extend the definition of $\Gamma(z)$ to other values of the complex plane. Since $\Gamma(z) = \frac{\Gamma(z+1)}{z}$, and $\Gamma(z+1)$ is defined for $\mathbb{R}\mathrm{e}(z) \geq -1$, we can use this relation to extend analytically the domain of $\Gamma(z)$ in the strip $-1 \leq \mathbb{R}\mathrm{e}(z) \leq 0$. Repeating the same argument, we can extend $\Gamma(z)$ to all values of the complex plane, except for $z = 0, -1, -2.....$

The Gamma function admits other interesting representations.

Infinite limit representation

$$\Gamma(z) = \lim_{n\to\infty} \frac{1 \cdot 2 \cdot 3 \cdot .. \cdot n}{z(z+1)(z+2)...(z+n)} n^z.$$

Infinite product representation

$$\frac{1}{\Gamma(z)} = ze^{\gamma z} \prod_{n=1}^{\infty} \left(1 + \frac{z}{n}\right)^{e^{-\frac{z}{n}}}.$$

To prove the first, let us introduce the function of two variables

$$F(z,u) = \int_0^n \left(1 - \frac{t}{n}\right)^n t^{z-1} dt.$$

Since

$$\lim_{n\to\infty} \left(1 - \frac{t}{n}\right)^n = e^{-t},$$

we have

$$\lim_{n\to\infty} F(z,u) = F(z,\infty) = \int_0^\infty e^{-t} t^{z-1} dt = \Gamma(z). \tag{1.8}$$

We can evaluate $F(z,u)$ in successive integrations by parts. Take $v \equiv \frac{t}{n}$, hence

$$F(z,u) = n^z \int_0^1 (1-v)^n v^{z-1} dv.$$

Integrating by parts, we get

$$\frac{F(z,u)}{n^z} = (1-v)^n \frac{v^z}{z} \,|_0^1 + \frac{n}{z} \int_0^1 (1-v)^{n-1} v^z dv.$$

The integrated part vanishes at both extremes. Repeating the procedure, we have

$$F(z,u) = n^z \frac{n(n-1)....1}{z(z+1)(z+2)...(z+n-1)} \int_0^1 v^{z+n-1} dv$$

$$= \frac{1 \cdot 2 \cdot 3 \cdot .. \cdot n}{z(z+1)(z+2)...(z+n)} n^z$$

and using eq. (1.8) we obtain Euler's result.
The Weierstrass result is particularly interesting for our aim: in fact, it resembles the spectral function for the Schrödinger problem! It can be easily obtained from Euler's limit form. Let us write it as

$$\Gamma(z) = \lim_{n\to\infty} \frac{1 \cdot 2 \cdot ... \cdot n}{z(z+1)...(z+n)} n^z = \lim_{n\to\infty} \frac{1}{z} \prod_{m=1}^{n} \left(1 + \frac{z}{m}\right)^{-1} n^z.$$

Inverting this expression and using the relation $n^{-z} = e^{-z \ln n}$, we obtain

$$\frac{1}{\Gamma(z)} = z \lim_{n\to\infty} e^{-z \ln n} \prod_{m=1}^{n} \left(1 + \frac{z}{m}\right).$$

Multiplying and dividing by

$$\exp\left[\left(1+\frac{1}{2}+\frac{1}{3}+...+\frac{1}{n}\right)z\right]=\prod_{m=1}^{n}e^{\frac{z}{m}}$$

we obtain

$$\frac{1}{\Gamma(z)}=z\lim_{n\to\infty}\exp\left[\left(1+\frac{1}{2}+\frac{1}{3}+...+\frac{1}{n}-\ln n\right)z\right]\cdot\lim_{n\to\infty}\prod_{m=1}^{n}\left(1+\frac{z}{m}\right)e^{-\frac{z}{m}}.$$

Since

$$\lim_{n\to\infty}\left(\sum_{k=1}^{\infty}\frac{1}{k}-\ln n\right)=\gamma$$

we finally obtain the Weierstrass result

$$\frac{1}{\Gamma(z)}=ze^{\gamma z}\prod_{n=1}^{\infty}\left(1+\frac{z}{n}\right)e^{-\frac{z}{n}}.$$

The Weierstrass definition shows that $\Gamma(z)$ has simple poles at $z=0,-1,-2,...$ and that $[\Gamma(z)]^{-1}$ has no poles in the finite complex plane.
This formula gives us the opportunity to discuss in general the (infinite) product representation of entire functions. They generalize the concept of polynomial expressions

$$P(z)=a_nz^n+....+a_0=A(z-z_1)(z-z_2)...(z-z_n)$$

which can be always decomposed in terms of the roots in the complex plane. A function analytic for all finite z is called and entire function of z. The logarithmic derivative f'/f is a meromorphic function with a pole expansion. If $f(z)$ has simple zeroes at $z=a_n$, we have

$$\frac{f'(z)}{f(z)}=\frac{f'(0)}{f(0)}+\sum_{n=1}^{\infty}\left[\frac{1}{a_n}+\frac{1}{za_n}\right]$$

and integrating both sizes,

$$\ln\frac{f'(z)}{f(z)}=z\frac{f'(0)}{f(0)}+\sum_{n=1}^{\infty}\left[\ln\left(1-\frac{z}{a_n}\right)+\frac{z}{a_n}\right].$$

Therefore, we arrive to the Weierstrass infinite product representation for entire functions

$$f(z)=f(0)\exp\left[z\frac{f'(0)}{f(0)}\right]\prod_{n=1}^{\infty}\left(1-\frac{z}{a_n}\right)e^{\frac{z}{a_n}}.$$

The Gamma function satisfies a series of remarkable identities. One of these is

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z}. \tag{1.9}$$

To prove it, notice that, by virtue of the functional equation, the function $\Phi(z) = \Gamma(z)\Gamma(1-z)$ is periodic with period equal to 2,

$$\Phi(z+2) = \Phi(z)$$

Moreover, it has simple poles at all points $z \in \mathbb{Z}$. Hence by multiplying it by

$$z \prod_{k=1}^{\infty} \left(1 - \frac{z^2}{k^2}\right)$$

we obtain a function without singularities in the complex plane, i.e. a constant equal to 1, as it can be checked by taking the limit $z \to 0$. But

$$z \prod_{k=1}^{\infty} \left(1 - \frac{z^2}{k^2}\right) = \frac{1}{\pi} \sin \pi z$$

and eq. (1.9) is proved.
Another important result, due to Legendre, is the so called duplication formula, relevant in the theory of the Riemann zeta function.

$$\Gamma(z)\Gamma\left(z + \frac{1}{2}\right) = \sqrt{\pi} 2^{1-2z} \Gamma(2z).$$

For future applications it is also useful to have the asymptotic expansion of the Gamma function. It can be obtained by a saddle point approximation. Performing the change of variable $t = xz$, we get

$$\Gamma(z+1) = z^{z+1} \int_0^{\infty} dx e^{z(\log x - x)}.$$

The function $\varphi(x) = \ln x - x$ goes to $-\infty$ both at $x \to 0$ and $x \to \infty$. It presents a unique maximum at $x = 1$. For $z \to \infty$, the above integral is dominated by the region nearby this maximum. Expanding $\varphi(x)$ in series near this point

$$\varphi(x) = -1 - \frac{(x-1)^2}{2} + ...$$

and substituting into (38) we have

$$\Gamma(z+1) = z^{z+1}e^{-z}\int_0^\infty e^{-z\frac{(x-1)^2}{2}}dx = \sqrt{2\pi}z^{z+\frac{1}{2}}e^{-z}.$$

Hence

$$\Gamma(z+1) = \sqrt{2\pi}z^{z+\frac{1}{2}}e^{-z}$$

$$\ln\Gamma(z+1) = \left(z+\frac{1}{2}\right)\ln z - z + \frac{1}{2}\ln 2\pi + O\left(\frac{1}{z}\right).$$

Let us mention also the integral representation

$$\int_C e^{-\eta}\eta^z d\eta = \left(e^{2\pi iz}-1\right)\Gamma(z+1)$$

where the contour is shown in the Figure

FIGURE

This is particularly useful when z is not an integer; in this case the origin is a branch point. The above equation can be easily verified by deforming the contour as in Figure

FIGURE

The integral from ∞ to the origin gives $-\Gamma(z+1)$, placing the phase of the logarithmic branch at the origin. The integral out of ∞ then yields $e^{2\pi iz}\Gamma(z+1)$, whereas the integral around the origin vanishes for $z > -1$. It is simple to extend the range to include all non–integral values of z: the integral exists in fact for $z < -1$, as far as we stay far from the origin. Second, integrating by parts, one gets the usual functional equation

1.5 Poisson summation formula

Let us deal now with a very interesting application of Fourier transform: the Poisson summation formula. Consider the function

$$S(x) = \sum_{n=-\infty}^{+\infty} f(x+nT)$$

where $f(x)$ is an arbitrary function. It is clear that $S(x)$ is periodical with period T:

$$S(x+T) = \sum_{n=-\infty}^{+\infty} f(x+(n+1)T) = \sum_{n=-\infty}^{+\infty} f(x+nT) = S(x).$$

Therefore $S(x)$ can be developed in Fourier series

$$S(x) = \sum_{k=-\infty}^{+\infty} C_k e^{\frac{2\pi ikx}{T}}$$

where the coefficients are given by

$$C_k = \frac{1}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} S(x)\, e^{-\frac{2\pi ikx}{T}} dx.$$

By substituting the expression for $S(x)$ we have

$$C_k = \frac{1}{T}\int_{-\frac{T}{2}}^{\frac{T}{2}} \sum_{n=-\infty}^{+\infty} f(x+nT)\, e^{-\frac{2\pi ikx}{T}} dx.$$

Making the change of variable $y = x + nT$, we get

$$C_k = \frac{1}{T}\sum_{n=-\infty}^{+\infty} \int_{n-\frac{T}{2}}^{n+\frac{T}{2}} f(y)\, e^{-\frac{2\pi iky}{T}} dy = \frac{1}{T}\int_{-\infty}^{+\infty} f(y)\, e^{-\frac{2\pi iky}{T}} dy.$$

The last term is the Fourier transform of the function $f(x)$ (let us denote it by $\widehat{f}(\omega)$), and then

$$C_k = \frac{2\pi}{T}\widehat{f}\left(\frac{2\pi k}{T}\right).$$

Finally, the function $S(x)$ can be rewritten as

$$S(x) = \sum_{n=-\infty}^{+\infty} f(x+nT) = \frac{2\pi}{T}\sum_{k=-\infty}^{+\infty} \widehat{f}\left(\frac{2\pi k}{T}\right) e^{\frac{2\pi ikx}{T}}.$$

This is the Poisson Summation Formula. Let us see some applications.

Example 1
Compute

$$S_0 = \sum_{n=0}^{+\infty} \frac{1}{a^2+n^2}.$$

This series can be written as

$$S_0 = \frac{1}{2a^2} + \frac{1}{2}\sum_{n=-\infty}^{+\infty} \frac{1}{a^2+n^2}.$$

Let us apply the PRF to the second term, where

$$f(v) = \frac{1}{a^2+v^2}, \quad T = 1, \quad x = 0.$$

The Fourier transform of $f(v)$ is

$$\widehat{f}(v) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{1}{a^2+v^2} e^{-iv\nu} dv.$$

This integral can be computed using the residue theorem.
a) $v < 0$. Close the contour as in figure..
The integral on the semicircle vanishes when the radius goes to infinity, so it remains the contribution of the residue:

$$I = iRes\left[\frac{1}{a^2+v^2}e^{-iv\nu}\right]_{v=ia} = \frac{1}{2a}e^{-a|v|}.$$

b) $v > 0$. we get again the same result. Consequently

$$S_0 = \frac{1}{2a^2} + \frac{\pi}{2a}\sum_{k=-\infty}^{+\infty} e^{-a|2\pi k|} = \frac{1}{2a^2} - \frac{\pi}{2a} + \frac{\pi}{a}\frac{1}{1-e^{-2\pi a}}.$$

Let us prove as an example the following identity

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}.$$

Notice that

$$S_0 = \sum_{n=0}^{\infty} \frac{1}{a^2+n^2} = \frac{1}{a^2} + \sum_{n=1}^{\infty} \frac{1}{a^2+n^2},$$

therefore

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \lim_{a\to 0}\left[S_0 - \frac{1}{a^2}\right].$$

Expanding in series S_0

$$S_0 \simeq \frac{1}{2a^2} - \frac{\pi}{2a} + \frac{\pi}{a}\frac{(1+2\pi a + \frac{(2\pi a)^2}{2} + ...)}{2\pi a(1+\frac{2\pi a}{2!} + \frac{(2\pi a)^2}{3!} + ...)} =$$

$$\frac{1}{2a^2}-\frac{\pi}{2a}+\frac{1}{2a^2}(1+2\pi a+\frac{(2\pi a)^2}{2}+...)(1-\frac{2\pi a}{2!}-\frac{(2\pi a)^2}{3!}+\left(\frac{2\pi a}{2!}\right)^2...)=$$

$$\frac{1}{2a^2}-\frac{\pi}{2a}+\frac{1}{2a^2}+\frac{\pi}{2a}+\frac{1}{2}\left[\pi^2-\frac{4\pi^2}{6}\right]=\frac{\pi^2}{6}+\frac{1}{a^2},$$

hence the result. The Poisson resummation formula is clearly useful from the point of view of numerical calculus.

Example 2
Consider the series

$$S(t)=\sum_{-\infty}^{+\infty}e^{-k^2t}.$$

Suppose that we want compute it at $t=0.01$. In this case, to have a precision of 10^{-10} we need ~ 50 terms. Using Poisson formula we have

$$S(t)=\sqrt{\frac{\pi}{t}}\sum_{-\infty}^{+\infty}e^{-\frac{\pi^2n^2}{t}}.$$

At $t=0.01$, we get

$$S=\sqrt{\frac{\pi}{0.01}}\left(1+2e^{-100\pi^2}+...\right)=\dots$$

Exercise 1
Show that

$$S_1=\sum_{n=0}^{\infty}\frac{1}{a^2+(2n+1)^2}=\frac{\pi}{4a}\frac{1-e^{-\pi a}}{1+e^{-\pi a}}.$$

Exercise 2
Show that

$$S_2=\sum_{n=0}^{\infty}\frac{(-1)^n}{a^2+n^2}=\frac{1}{2a^2}+\frac{\pi}{a}\frac{e^{-\pi a}}{1+e^{-2\pi a}}$$

Exercise 3
Prove that

$$\sum_{n=0}^{\infty}\frac{(-1)^n}{n^4}=-\frac{7\pi^4}{720}.$$

1.6 Spectral Functions

The previously introduced functions are some representatives of a large class of functions which deal with the spectrum of a system. They will be the object of our future study. To fix the ideas, let us take a one–dimensional system with Hamiltonian

$$H = \frac{p^2}{2m} + V(q), \qquad [p, q] = i\hbar \tag{1.10}$$

with the eigenvalues which goes like

$$E_n \cong n^\alpha \tag{1.11}$$

(we will see later how to compute these quantities). Let us define the following spectral functions

- Partition function

$$Z(t) = Tr \exp(-tH) = \sum_{n=0}^{\infty} e^{-tE_n}, \qquad Ret \geq 0$$

- Resolvent Trace

$$R(E) = Tr(H + E)^{-1} = \sum_{n=0}^{\infty} \frac{1}{E + E_n}, \qquad E \in \mathbb{C} - \{-\not\geq\} \tag{1.12}$$

- Fredholm determinant

$$\Delta(E) = \det\left(1 - EH^{-1}\right) = \prod_{n=0}^{\infty} \left(1 - \frac{E}{E_n}\right), \qquad E \in \mathbb{C}. \tag{1.13}$$

- Zeta function,

$$\xi(s) = TrH^{-s} = \sum_{n=0}^{\infty} \frac{1}{E_n^s}, \qquad Res > \frac{1}{a}. \tag{1.14}$$

- Mellin Transform of $R(E)$

$$M(s) = \int_0^\infty E^{-s} R(E) dE \tag{1.15}$$

Few comments

(i) Note that we have defined the resolvent trace with $(-E)$, comparing with the previous formula.

(ii) In the Fredholm determinant we assume the absence of Hadamard factors, i.e. we assume

$$\sum \frac{1}{E_n} < \infty.$$

This formula can be modified consequently if this condition of convergence is not satisfied.

It is easy to see that all these functions are related to each other, a result which is intuitive, since all of these are based on the spectrum $\{E_n\}$. We have

$$R(E) = \int_0^\infty Z(t)\, e^{-tE} dt$$

in the region where $Re\, E > 0$. Similarly

$$\Delta(-E) = \prod_{n=0}^{\infty} \left(1 + \frac{E}{E_n}\right) = \exp\left[\int_0^E n(\lambda)\, d\lambda\right], \qquad E \in \mathbb{C}. \tag{1.16}$$

Moreover,

$$\int_0^\infty Z(t)\, t^{s-1} dt = \sum_{n=0}^{\infty} \int_0^\infty e^{-tE_n} t^s \frac{dt}{t}$$

making the change of variables $tE_n = x$ we have

$$\int_0^\infty Z(t)\, t^{s-1} dt = \sum \frac{1}{E_n^s} \int_0^\infty dx e^{-x} x^{s-1} = \Gamma(s)\, \xi(s).$$

Finally

$$\xi(s) = \frac{1}{\pi} \sin \pi s M(s), \tag{1.17}$$

which can be proved as follows.

$$\sum_n \int_0^\infty E^{-s} \frac{1}{E + E_n} dE = \sum_n \int_0^\infty dE e^{-s \ln E} \frac{1}{E + E_n}.$$

In order to compute this integral, let us choose the contour as in the figure

FIGURE

In going to the lower branch II, the logarithmic function changes, since $E \to Ee^{2\pi i}$. Therefore, applying the theorem of residues to the above contour, with vanishing contribution from the external circle and the one near the origin, we have

$$I\left(1 - e^{-2\pi i s}\right) = 2\pi i e^{-i\pi s} \sum_n E_n^{-s}.$$

Hence we get formula (1.17).

Chapter 2

Semiclassical methods:WKB Approximation

2.1 Introduction

Consider the one dimensional Schrödinger equation

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}\left[E - V\left(x\right)\right]\Psi = 0. \tag{2.1}$$

If the potential doesn't have a simple form, solving the Schrödinger equation is usually a complicated problem, which requires the use of approximate or numerical methods, such as

1) Perturbation theory
2) Variational methods
3) Numerical diagonalization.

One particular method has found its greatest use in the case of one–dimensional systems. This is the so called WKB method (after Wentzel, Kramers and Brillouin).
The basic idea is very simple and it is similar to the eikonal expansion in optics.
Notice that if $V = const$, eq. (2.1) has the solutions $\Psi_{\pm} = e^{\pm ikx}$. This suggests to look for a solution of the form

$$\Psi = e^{iS(x)}.$$

Substituting into eq. (2.1), we get

$$iS^{''} - (S')^2 + \left[K\left(x\right)\right]^2 = 0,$$

where

$$K(x) = \begin{cases} \sqrt{\frac{2m}{\hbar}[E - V(x)]}, & E > V(x) \\ -i\sqrt{\frac{2m}{\hbar}[V(x) - E]} & E < V(x) \end{cases}$$

The above equation can be solved recursively, i.e. substituting the n–th approximation, for the $(n+a)$–th approximation we have

$$S_{n+1} = \pm \int^x \sqrt{K^2(x) + iS_n''(x)} + C_{n+1},$$

hence

$$S_0 = \pm \int^x K(x) + C_0,$$

$$S_1 = \pm \int^x \sqrt{K^2(x) \pm iK'(x)}dx + C_1.$$

Obviously, to make sense of this procedure, the next approximation should be close to the previous one, which for the above terms is equivalent to say

$$\left|K'(x)\right| \ll \left|K^2(x)\right| \tag{2.2}$$

In the above equations, both signs have to be chosen equal, since S_1 is supposed to be an improvement of S_0. Hence

$$S_1 = \pm \int^x K(x) \sqrt{1 \pm i\frac{K'}{K^2}}dx \simeq \pm \int^x \left[K(x) \pm i\frac{K'}{K}\right] dx =$$

$$\pm \int^x K(x) + \frac{i}{2}\log K(x) + C.$$

Therefore, at this level of approximation, for the wave function we have

$$\Psi(x) \simeq \frac{A}{\sqrt{K(x)}} \exp\left[\pm i \int^x K(t)\, dt\right].$$

The condition (2.2) has a very physical meaning. We can define, in the regions where $E > V(x)$, an effective wave length

$$\lambda(x) = \frac{2\pi}{k(x)}$$

and therefore eq. (2.2) can be written

$$\lambda(x)\left|\frac{dp}{dx}\right| \ll |p(x)|,$$

where $p(x) = \pm\hbar K(x)$ is the momentum of the particle. Hence, the range of the validity of the WKB approximation (at this order) is that the change of the momentum over a wavelength must be small compared to the square of its amplitude.

The method falls down if $K(x)$ vanishes or if $K(x)$ varies very rapidly. This certainly happens at the classical turning point for which

$$V(x) = E,$$

or whenever $V(x)$ has a very steep behaviour. In both cases a more accurate solution has to be found. Obviously, the WKB method would not be useful unless we find a way to analyze such situations.

2.2 The connection formulas

Consider a potential as in the figure

FIGURE

Let us consider initially the case $x \gg x_2$. In this region the classical momentum is imaginary and therefore one of the solutions blows up. Hence we have to consider only the exponentially decaying part, i.e.

$$\psi(x) = \frac{c}{\sqrt{|K(x)|}} \exp\left[-\int^x \left|K'(x)\right| dx'\right]. \tag{2.3}$$

In the region $x_1 < x < x_2$, on the other hand, far away from the turning points, we have

$$\psi(x) = \frac{A}{\sqrt{K(x)}} \exp\left[i\int^x K\left(x'\right) dx'\right] + \frac{B}{\sqrt{K(x)}} \exp\left[-i\int^x K\left(x'\right) dx'\right] \tag{2.4}$$

Let us consider now more closely the situation near one of the turning point, let's say $x = x_2$. Suppose that the potential is smooth and admits a series expansion. Keeping only the leading term we have

$$\frac{d^2\Psi}{dx^2} = \frac{2m}{\hbar^2}(x - x_2) V'(x_2)\Psi.$$

By posing

$$\frac{2m}{\hbar^2} V'(x_2) \equiv \alpha^3, \qquad y = \alpha x,$$

the above equation becomes

$$\frac{d^2\Psi}{dy^2} = y\,\Psi.$$

This is the differential equation of the Airy function (see later). Disregarding once again the exponential growing function, its solution is expressed by the so called Airy function $Ai\,(y)$,
defined by

$$Ai\,(y) = \frac{1}{\sqrt{\pi}}\int_0^\infty dv \cos\left(\frac{v^3}{3} + vy\right).$$

For negative y, corresponding to the interior of the potential, it is oscillatory, whereas for positive y is exponentially decaying. Its asymptotic expansions are

$$Ai\,(y) = \begin{cases} |y|^{-\frac{1}{4}} \sin\left(\frac{2}{3}\,|y|^{\frac{3}{2}} + \frac{\pi}{4}\right), & y \to -\infty \\ \frac{1}{2} y^{-\frac{1}{4}} \exp\left(-\frac{2}{3} y^{\frac{3}{2}}\right), & y \to -\infty \end{cases}.$$

We have to match this behaviour with our previous expressions. We have

$$B = -A = iCe^{i\frac{\pi}{4}},$$

and therefore for $x_1 < x < x_2$ we have now

$$\Psi = \frac{2C}{\sqrt{K\,(x)}} \sin\left[i\int_x^{x_2} K\left(x^{'}\right) dx^{'} + \frac{\pi}{4}\right]. \tag{2.5}$$

Inspecting the expressions (2.3) and (2.4), we see that a phase factor $\frac{\pi}{4}$ has been introduced in the wave function at the turning point of a smooth potential.
The WKB condition can be now obtained by demanding single–valuedness of the wave function. In fact, repeating now the analysis for the other turning point, we arrive to the expression

$$\Psi = \frac{2\widetilde{C}}{\sqrt{K\,(x)}} \sin\left[i\int_x^{x_2} K\left(x^{'}\right) dx^{'} + \frac{\pi}{4}\right]. \tag{2.6}$$

The two phase factors in eqs. (2.5) and (2.6) should be the same up to a negative sign, which can be absorbed in the overall function. So, with $\widetilde{C} = (-1)^n C$, we have

$$\int_{x_1}^{x} K\left(x^{'}\right) dx^{'} + \frac{\pi}{4} = -\int_{x_1}^{x_2} K\left(x^{'}\right) dx^{'} - \frac{\pi}{4} + (n-1)\,\pi,$$

i.e.

$$\int_{x_1}^{x_2} K(x)\,dx = \left(n+\frac{1}{2}\right)\pi, \qquad n = 0, 1, 2, ...$$

By extracting the $\hbar$ dependence, this becomes the familiar equation of quantization

$$2\int_{x_1}^{x_2} p(x)\,dx = \oint p(x)\,dx = \left(n+\frac{1}{2}\right)h.$$

The left–hand side of this equation is equal to the area enclosed by the curve representing the motion in phase space and it is called the *phase integral* I. On the other hand, it also measure the phase change which the oscillatory wave function $\Psi(x)$ undergoes between the turning points.

$$\int_{x_1}^{x_2} K(x)\,dx = \left(n+\frac{1}{2}\right)h.$$

Dividing this expression by 2π, we see that according to the WKB approximation

$$\frac{n}{2}+\frac{1}{4}$$

of quasi wavelengths fit between x_1 and x_2. Hence, n represents the number of modes of the wave function, a fact which helps in visualizing the elusive ψ. According to eq. (23), the area of the phase space between one bound state and the next one is equal to h. From this observation we see that it comes the statement often used in statistical mechanics, that each quantum state occupies a volume h in phase space.
In order to find the normalization of the semi–classical wave function, we assume that the contribution beyond the turning points is negligible, so

$$A_u^2\int_{x_1}^{x_2}\frac{dx}{p(x)}\sin^2\left(\int_{x_1}^{x} K\left(x'\right)dx' + \frac{\pi}{4}\right) \simeq \frac{A^2}{2}\int_{x_1}^{x_2}\frac{dx}{p(x)},$$

hence

$$A^2 = \frac{2}{\int_{x_1}^{x_2}\frac{dx}{p(x)}}.$$

With all the above quantities fixed, it is nice to check how the semi–classical wave functions match the exact ones. This check can be done easily for the harmonic oscillator. Obviously at the turning points the wave function blows up and one need the connecting formulas.

2.3 Infinite well

The quantization condition changes if one of the walls of the potential is an infinite step. In this case the wave function is zero at the boundary. Suppose then that we have two turning points, one x_2 with a smooth behaviour and x_1 with an infinite well. In this case, coming from right hand side of x_2, we have for the wave function

$$\Psi \sim \sin\left[\int_x^{x_2} K(x) + \frac{\pi}{4}\right].$$

But then we have to impose

$$\Psi(x_c) = 0.$$

Therefore we have the quantization condition

$$\int_{x_1}^{x_2} K(x)\,dx + \frac{\pi}{4} = (n+1)\,\pi$$

and therefore, in this case

$$\oint p(x)\,dx = \left(n + \frac{3}{4}\right) h.$$

Since $\frac{\pi}{4}$ of the phase of the right hand side of the above equation may be attributed as before to the turning point x_2, the extra phase factor $\pi/2$ has to be attributed to the step well.

2.4 Airy function

Consider the Schrödinger equation in a linear potential $V = Ax$,

$$\frac{d^2\Psi}{dx^2} = \frac{2m}{\hbar^2}\left[Ax - E\right]\Psi.$$

It is obvious that if we shift the variable

$$x \to x + \frac{E}{A},$$

we can absorb the eigenvalue E, so if we find a solution for one value, we find it for all other values. We write then

$$\frac{d^2\Psi}{dx^2} = \frac{2m}{\hbar^2} Ax\Psi.$$

Introduce the quantities

$$\alpha^3 = \left(\frac{2mA}{\hbar^2}\right),$$
$$y = \alpha x.$$

The above equation becomes

$$\frac{d^2\Psi}{dy^2} = y\Psi.$$

The Fourier transform of Ψ is

$$\Psi(y) = \int_{-\infty}^{+\infty} dp \Psi(p) e^{ipy}.$$

Then we have the differential equation

$$i\frac{d}{dp}\Psi(p) = p^2\Psi,$$

whose solution is

$$\Psi(p) = \exp\left[-i\frac{p^3}{3}\right].$$

Hence

$$\Psi(y) = \int_{-\infty}^{+\infty} dp \exp\left[i\left(py - \frac{p^3}{3}\right)\right] = 2\sqrt{\pi}\Phi(y),$$

with

$$\Phi(y) = \frac{1}{\sqrt{\pi}}\int_0^{\infty} \cos\left(yp + \frac{p^3}{3}\right) dp.$$

This function can be written in terms of Bessel functions

$$\Phi(y) = \begin{cases} \sqrt{\frac{y}{3\pi}} K_{\frac{1}{3}}\left(\frac{2}{3}y^{\frac{3}{2}}\right), & y > 0 \\ \frac{1}{3}\sqrt{\pi y}\left[J_{\frac{1}{3}}\left(\frac{2}{3}y^{\frac{3}{2}}\right) + J_{-\frac{1}{3}}\left(\frac{2}{3}y^{\frac{3}{2}}\right)\right], & y < 0 \end{cases}.$$

Hence, it goes exponentially to zero for $y \to +\infty$, whereas has an infinite number of zeros for $y < 0$. [Comments. Ideal spectral function! Up to Hadamard factors,

$$\Delta(E) = \prod_i \left(1 + \frac{E}{\lambda_i}\right),$$

with λ_i zeros of Airy function.

2.5 WKB for radial motion

The previous considerations can be easily extend to deal with quantum mechanical systems in a central potential. Let us consider first a two–dimensional problem

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2}\right]\Psi(r,\varphi)+V(r)\,\Psi(r,\varphi)=E\Psi(r,\varphi)\,.$$

The radial and angular eqs. are separable in this case. Furthermore, by dividing the radial wave function by $\sqrt{r}$, we obtain for it an eq. in the radial variable which is similar to the one–dimensional case, i.e.

$$\Psi(r,\varphi)=\sum_l \frac{v_l(r)}{\sqrt{r}}e^{il\varphi}$$

and

$$Q_l^2(r)=\frac{2m}{\hbar^2}\left[E-V(r)-\frac{\hbar^2}{2mr^2}\left(l^2-\frac{1}{4}\right)\right],$$

where $\hbar l$ is the eigenvalue of the angular momentum. The above formulas are indeed similar to the one dimensional case and we are tempted to write down analogous WKB expressions, with

$$\frac{p(x)}{\hbar}\to Q_l(x)\,.$$

To check if this procedure gives the correct asymptotic phase in the wave function, let's analyze a solvable case.

2.6 Square–well potential

Consider $V(r)$ to be a square–well potential of depth V_0 Let us also assume $l\neq 0$. The exact regular solution is $J_l(kr)$, where J_l is the Bessel function and the wave number

$$k^2=\frac{2m(E-V_0)}{\hbar^2}$$

is a constant. For large r, such that

$$kr\gg|l|\,,$$

$$J_l(kr)\simeq\sqrt{\frac{2}{\pi kr}}\cos\left(kr-\frac{l\pi}{2}-\frac{\pi}{4}\right).$$

Let us construct the WKB wave function for this problem. To match the asymptotic form let's do in Q_l^2 the replacement $\left(l^2 - \frac{1}{4}\right) \to s^2$, where s^2 is a parameter to be determined shortly.
Then, using the previous formulas, the WKB formula for v_l is

$$v_l(r) \simeq \frac{2}{\sqrt{\widetilde{Q}_l(r)}} \cos\left[\int_{r_1}^{r} \widetilde{Q}_c(r')\, dr' - \frac{\pi}{4}\right]$$

where

$$\widetilde{Q}_c(r) \equiv \frac{2m}{\hbar^2}\left[E - V_0 - \frac{\hbar^2}{2mr^2}s^2\right]$$

and r_1 is the turning point near the origin determined by the condition

$$k^2 r_1^2 - s^2 = 0.$$

The integral in (10) can be done explicitly

$$I = \int_{r_1}^{r} \left[k^2 r'^2 - s^2\right]^{1/2} \frac{dr'}{r'} = \sqrt{(kr)^2 - s^2} - s \arccos\left(\frac{s}{kr}\right).$$

In the asymptotic region $kr \gg s$, it is equal to

$$I \simeq kr - s\frac{\pi}{2}.$$

Comparing now with (8), we see that

$$s^2 = e^r,$$

in order to have a match of the phases. In turns out that this prescription is also valid in the more general case where $V(r)$ varies with r, i.e. we have to use the substitution

$$l^2 - \frac{1}{4} \to h^2.$$

This condition can be justified by the request that the angular part of the wave function is semi–classical as well.
We can now derive the WKB quantization condition for the bound states. Define initially the phases

$$\phi_l(r_1, r) \equiv \int_{r_1}^{r} \widetilde{Q}_l\left(r'\right) dr'$$

$$\phi_l(r_1, r_2) \equiv \int_{r_1}^{r_2} \widetilde{Q}_l\left(r'\right) dr'.$$

Since the WKB wave function at r may be written in terms of either one of them, it follows that

$$\cos\left(\phi_l\left(r_1,r\right)-\frac{\pi}{4}\right)=\pm\cos\left(\phi_l\left(r_1,r_2\right)-\frac{\pi}{4}\right),$$

and therefore we arrive to the quantization condition

$$\phi_l\left(r_1,r_2\right)=\int_r^{r_2}\widetilde{Q}_l\left(r\right)dr=\left(n_l+\frac{1}{2}\right)\pi.$$

Defining the action variable

$$I_r\equiv\frac{1}{2\pi}S_r=\frac{1}{2\pi}\oint p_r dr,$$

the quantization condition may be written in the generalized form

$$I_r=\left(n_r+\frac{\mu}{4}\right)\hbar,$$

where μ is called the *Maslov index*. In the above example μ counts the number of classical turning points, where the amplitude of the wave function diverges.
Note that in this case the WKB wave function over a complete cycle acquires a factor $\pm 2\pi\left(n_r+\frac{\mu}{4}\right)$.
In case the particle encounters a hard wall b times, the wave function goes to zero under Dirichel b.c. at every encounter and picks an extra phase $b\pi$ for the b reflections. The total acquired phase may be written then as

$$2\pi\left(n_r+\frac{\mu}{4}+\frac{b}{2}\right).$$

Under Neumann b.c., on the other hand, there is no change in the phase of the wave at the wall and $b=0$, in this case. Thus the above quantization condition may be written as

$$I_r=\left(n_r+\frac{\mu}{4}+\frac{b}{2}\right)\hbar.$$

This formula is important for obtaining Gutzwiller trace formula in the integrable cases, although it does not apply for the non–integrable ones.
Finally, in the 3–dimensional case, the semiclassical formalism is set up by the substitution

$$l\left(l+1\right)\rightarrow\left(l+\frac{1}{2}\right)^r,$$

obtained by the same request of semi–classical behaviour for the angular wave function.

2.7 Connection formulas for semiclassical wave functions

The previous analysis can be done in another way which is very instructive. This provides the connection formula between semi–classical wave functions in the allowed and forbidden classical region. Let us consider first a turning point in the right part, as in figure

FIGURE

In the region $I : x > a$, far away from the turning point we have

$$\Psi = \frac{C}{\sqrt{|p|}} \exp\left[-\frac{1}{\hbar}\int_a^x |p|\, dx\right] \tag{2.7}$$

whereas, in the region $II : x < a$, the wave function is given by a linear superposition of the two allowed solutions

$$\Psi = \frac{A}{\sqrt{p}} \exp\left[\frac{i}{\hbar}\int_a^x p dx\right] + \frac{B}{\sqrt{p}} \exp\left[-\frac{i}{\hbar}\int_a^x p dx\right]. \tag{2.8}$$

How can we determine the coefficients A and B ?
In the vicinity of the turning point we have

$$E - V(x) \simeq F_0 (x - a), \qquad F_0 = -\frac{dv}{dx} \mid_{x=a} < 0.$$

Suppose now that we can still use the semiclassical approximation sufficiently close to the turning point. In this case, in the region I we have

$$\Psi = \frac{C}{\sqrt{2m\,|F_0|}} \frac{1}{(x-a)^{1/4}} \exp\left[-\frac{1}{\hbar}\int_a^x \sqrt{2m\,|F|}\sqrt{x-a} dx\right]. \tag{2.9}$$

Consider now this function as a function of the *complex variable* x and the passage from positive to negative $(x - a)$ must be along a path which is always sufficiently far from the point $x = a$, so that the WKB is still valid. Let us consider first the variation of this function from right to left along a semicircle of radius ρ in the upper half–plane.

FIGURE

Along this semicircle

$$x-a=\rho e^{i\varphi}, \qquad \int_a^x \sqrt{t-a}dt=\frac{2}{3}z^{\frac{3}{2}}=\frac{2}{3}\rho^{\frac{3}{2}}\left(\cos\frac{3}{2}\varphi+i\sin\frac{3}{2}\varphi\right).$$

The exponential factor in (2.9), at the beginning $\left(0<\varphi<\frac{2}{3}\pi\right)$ increases in modulus and then decreases to modulus 1. At the end of the semicircle the exponent becomes purely imaginary and equal to

$$-\frac{i}{\hbar}\int_a^x \sqrt{2m\left|F_0\right|(a-x)}dx=-\frac{i}{\hbar}\int_a^x p\left(x\right)dx.$$

In the coefficient of the exponential, the change along the semicircle is

$$(x-a)^{-\frac{1}{4}}\rightarrow(a-x)^{-\frac{1}{4}}e^{-i\frac{\pi}{4}}.$$

Hence the function (2.7) has become the second term in (2.8) with

$$B=Ce^{-i\frac{\pi}{4}}.$$

Why is it possible to determine only the coefficient B passing in the upper complex plane? There is a simple explanation of this fact. Suppose we follow the variation of the function (2.8) along the same semicircle but in the opposite direction.

FIGURE

In this case we have, as before

$$\int_a^x \sqrt{(a-x)}dx=\frac{2}{3}\rho^{\frac{3}{2}}\left(\cos\frac{3}{2}\varphi+i\sin\frac{3}{2}\varphi\right).$$

Correspondingly, for the exponentials

$$A\exp\left[-\frac{2}{3}\rho^{\frac{2}{3}}\sin\frac{3}{2}\varphi\right]\exp\left[\frac{i}{\hbar}\frac{2}{3}\rho^{\frac{2}{3}}\cos\frac{3}{2}\rho\right]+$$

$$B\exp\left[\frac{2}{3}\rho^{\frac{2}{3}}\sin\frac{3}{2}\varphi\right]\exp\left[-\frac{i}{\hbar}\frac{2}{3}\rho^{\frac{2}{3}}\cos\frac{3}{2}\rho\right].$$

We see that at the very beginning of the path the first term becomes exponentially small with respect to the second and it must be discarded! So, in this way we have lost the information on A. In order to obtain A, we must continue the function (2.7) along a path in the lower half plane.

FIGURE

Repeating the exercise we find that along this path the exponential has become the one of the term in A, whereas its prefactor has become

$$(x-a)^{-\frac{1}{4}} \to (a-x)\, e^{i\frac{\pi}{4}}.$$

In this way we find

$$A = Ce^{i\frac{\pi}{4}}$$

and therefore the final solution is

$$\Psi = \left\{ \begin{array}{ll} \frac{C}{\sqrt{p}} \exp\left[-\frac{1}{\hbar}\int_a^x |p|\, dx\right], & x > a \\ \frac{2C}{\sqrt{p}} \cos\left[\frac{1}{\hbar}\int_a^x p dx + \frac{\pi}{4}\right], & x < a \end{array} \right| .$$

What has it been the connection formula for the divergent solution? Namely, suppose that in I we have

$$\Psi = \frac{C}{\sqrt{p}} \exp\left[\frac{1}{\hbar}\int_a^x |p|\, dx\right].$$

What is the analytic continuation in $x < a$? Repeating the calculations, coming from the path in the upper plane, we find this time

$$A = Ce^{-i\frac{\pi}{4}},$$

whereas, along the path in the lower plane

$$B = Ce^{i\frac{\pi}{4}}.$$

Hence

$$\frac{C}{\sqrt{p}} \exp\left[\frac{1}{\hbar}\int_a^x |p|\, dx\right] \to \frac{C}{\sqrt{p}} e^{i\frac{\pi}{2}} \exp\left[\frac{i}{\hbar}\int_a^x p dx + i\frac{\pi}{4}\right] + \frac{C}{\sqrt{p}} e^{-i\frac{\pi}{2}} \exp\left[-\frac{i}{\hbar}\int_a^x p dx - i\frac{\pi}{4}\right] =$$

$$-\frac{1}{\sqrt{p}} C \sin\left[\int_a^x p dx + \frac{\pi}{4}\right].$$

So, we have the connection formulas

$$\frac{1}{\sqrt{p}} \cos\left[\frac{1}{\hbar}\int_a^x p dx + \frac{\pi}{4}\right] \to -\frac{1}{\sqrt{p}} \exp\left[-\frac{i}{\hbar}\int_a^x |p|\, dx\right],$$

$$\frac{1}{\sqrt{p}} \sin\left[\frac{1}{\hbar}\int_a^x p dx + \frac{\pi}{4}\right] \to -\frac{1}{\sqrt{p}} \exp\left[\frac{1}{\hbar}\int_a^x |p|\, dx\right].$$

From these formulas we see that an "innocent" component $\sin\left[\frac{1}{\hbar}\int_a^x p dx + \frac{\pi}{4}\right]$ in the allowed region produces a dangerous component outside!

2.8 Transmission through a barrier

Suppose we have a barrier potential with a particle hitting from the left the barrier, with an energy E insufficient (classically) to pass on the right. We would like to compute semiclassically the transmission coefficient.

For the semiclassical solution, in the three regions, we have

$$\Psi = \left\{ \begin{array}{ll} \frac{A}{\sqrt{p}} \exp\left[i \int_a^x k dx\right] + \frac{B}{\sqrt{p}} \exp\left[-i \int_a^x k dx\right], & x < a \\ \frac{C}{\sqrt{p}} \exp\left[-\int_a^x |k|\, dx\right] + \frac{C}{\sqrt{p}} \exp\left[\int_a^x |k|\, dx\right], & a < x < b \\ \frac{F}{\sqrt{p}} \exp\left[i \int_b^x k dx\right] + \frac{G}{\sqrt{p}} \exp\left[-i \int_b^x k dx\right], & x > b \end{array} \right| .$$

Using the previous connection formula, we can easily establish the linear combination between the coefficients and the final result is very simple.

$$\left(\begin{array}{c} A \\ B \end{array} \right) = \frac{1}{2} \left(\begin{array}{cc} 2\theta + \frac{1}{2\theta} & i\left(2\theta - \frac{1}{2\theta}\right) \\ -i\left(2\theta - \frac{1}{2\theta}\right) & 2\theta + \frac{1}{2\theta} \end{array} \right) \left(\begin{array}{c} F \\ G \end{array} \right),$$

where

$$\theta \equiv \exp \int_a^b |p|\, dx.$$

This parameter measures the height and the thickness of the barrier. For the transmission coefficient, we have simply (assuming $G = 0$, i.e. no wave from the right)

$$T = \left| \frac{F}{A} \right|^2 = \frac{4}{\left(2\theta + \frac{1}{2\theta}\right)^2}.$$

For a high and broad barrier $\theta \gg 1$ and

$$T \simeq \frac{1}{\theta^2} = \exp\left[-\frac{2}{\hbar} \int_a^b |p|\, dx \right].$$

2.9 Metastable states

Consider now the same problem of computing the transmission amplitude for a potential as in the figure

FIGURE

i.e., a symmetric potential with respect to the origin and a deep well inside. Repeating the previous calculations, one obtains

$$T = \frac{4}{\left(4\theta^2 + \frac{1}{4\theta^2}\right) \cos^2 L + \sin^2 L},$$

where

$$\theta \equiv \exp \int_a^b |k| \, dx,$$

$$L \equiv \int_{-a}^{a} k(x) \, dx.$$

The above quantity reaches its maximum when $\cos L = 0$, i.e. when

$$L = \int_{-a}^{a} K(x) \, dx = \left(n + \frac{1}{2} \right) \pi,$$

the quantization condition for the bound states!

FIGURE

This is a very important observation. In fact, suppose we want to determine if a given number belongs or not to a given sequence $\{E_n\}$. If we are able to find a potential which has $\{E_n\}$ as a spectrum, the above question, of a mathematical nature, becomes a physical question. In fact, once such potential is constructed, we round it to make its eigenstates metastable and we perform a scattering experiment, with a beam of particles hitting the target with the energy equal to the number we want to probe. If the particle passes with probability 1, we have hit an eigenvalue! Obviously, once we round the potential, its eigenvalues acquire an imaginary part. In fact, there is now a probability to escape from the well and to go at infinity. We have a decay process

$$E_n \to E_n - \frac{1}{2} i \Gamma_n,$$

with

$$\Gamma_n \equiv \frac{1}{\theta^2 \left(\frac{\partial L}{\partial E} \right)_{E=E_n}}.$$

2.10 Potential $V(x) = \lambda |x|^a$

Consider the Schrödinger equation in one variable:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \Psi(x) + V(x) \Psi(x) = E \Psi(x).$$

We want to write initially the Schrödinger equation in homogeneous variable. To this aim, let us introduce the dimensionless quantity

$$\eta = \frac{x}{\xi},$$

where ξ is a length scale. We have

$$\left[-\frac{\hbar^2}{2m\xi^2}\frac{d^2}{d\eta^2} + \lambda\xi^a |\eta|^a\right]\psi = E\psi.$$

Hence

$$\widehat{E}_0\left[-\frac{1}{2}\frac{d^2}{d\eta^2} + b|\eta|^a\right]\psi = E\psi,$$

where

$$\widehat{E}_0 = \frac{\hbar^2}{m\xi^2}, \qquad b = \frac{m\lambda}{\hbar^2}\xi^{a+2}. \tag{2.10}$$

From now on, all the energies will be measured in units of $\widehat{E}_0$. Notice that b is a dimensionless parameter. It will be fixed through the WKB quantization.

2.10.1 WKB quantization of $V(x) = \lambda|x|^a$

Consider the following potential.

FIGURE

We have:

$$\oint p(x)\,dx = \left(n + \frac{1}{2}\right)h.$$

For the left–hand side we have

$$\oint p(x)\,dx = 4\int_0^{\overline{x}} \sqrt{2m\left(E - V(x)\right)}dx = 4\int_0^{\overline{x}} \sqrt{2m\left(E - \lambda|x|^a\right)}dx =$$

$$\sqrt{2m}4E^{1/2}4\int_0^{\overline{x}} \sqrt{1 - \frac{\lambda|x|^a}{E}}dx.$$

Making the change of variable $y^a = \left(\frac{\lambda^{1/a}x}{E^{1/a}}\right)^a$, the above integral becomes

$$4\sqrt{2m}\frac{E^{\frac{1}{2}+\frac{1}{a}}}{\lambda^{1/a}}\int_0^1 \sqrt{1 - y^a}dy.$$

Since

$$I(a) = \int_0^1 \sqrt{1-y^a}dy = \frac{\sqrt{\pi}}{2}\frac{\Gamma\left(1+\frac{1}{a}\right)}{\Gamma\left(\frac{3}{2}+\frac{1}{a}\right)},$$

we finally have for the LHS

$$\oint p(x)\,dx = 2\sqrt{2\pi m}\frac{\Gamma\left(1+\frac{1}{a}\right)}{\Gamma\left(\frac{3}{2}+\frac{1}{a}\right)}\frac{E^{\frac{a+2}{2a}}}{\lambda^{\frac{1}{a}}}.$$

Equating this formula to the RHS, we deduce the quantization of energy levels:

$$E_n = E_0\left(n+\frac{1}{2}\right)^{\frac{2a}{a+2}},$$

$$E_0 = \left[\frac{\hbar}{\sqrt{2m}}\frac{\lambda^{1/a}\Gamma\left(\frac{3}{2}+\frac{1}{a}\right)}{\Gamma\left(1+\frac{1}{a}\right)}\sqrt{\pi}\right]^{\frac{2a}{a+2}}.$$

In order to compare the two results we have to make equal the two energy scales, i.e. E_0 and $\widehat{E}_0$. One way of doing this consists in extracting initially ξ from the second of (2.10)

$$\xi = \left(\frac{\hbar^2 b}{m\lambda}\right)^{\frac{1}{a+2}},$$

and then substituting it into $\widehat{E}_0$, which becomes

$$\widehat{E}_0 = \left[\frac{\hbar\sqrt{2}}{\sqrt{2m}}\frac{\lambda^{\frac{1}{a}}}{b^{\frac{1}{a}}}\right]^{\frac{2a}{a+2}}.$$

Comparing now this expression with the corresponding one for the semiclassical expression, the two ones match if we choose

$$\widehat{E}_0 = \left[\sqrt{\frac{2}{\pi}}\frac{\Gamma\left(1+\frac{1}{a}\right)}{\Gamma\left(\frac{3}{2}+\frac{1}{a}\right)}\right]^a.$$

2.11 Harmonic oscillator: semiclassical estimate of $\langle x^\alpha \rangle_n$

There is a beautiful application of the semiclassical formula. This consists in the semiclassical estimate of

$$\langle n|\, x^\alpha \,|n\rangle \equiv \int_{-\infty}^{+\infty} dx x^\alpha \psi_n(x)\,\psi_n(x)\,dx,$$

where

$$\psi_n(x) = \left(\frac{1}{\pi}\right)^{\frac{1}{4}} \frac{1}{2^{n/2}} \frac{1}{\sqrt{n!}} e^{-\frac{x^2}{2}} H_n(x).$$

The difficulty of the problem consists in the lacking of suitable approximation of the Hermite polynomials with respect to the variable n. We can get around this problem by using the semiclassical approximation. Before doing that, we have to fix a convenient notation. In the units where $m = \omega = \hbar = 1$, the exact energy levels (and the semiclassical ones) are $E_n = n + \frac{1}{2}$. The position of the inversion points a_n

FIGURE

is given by the condition

$$V(a_n) = E_n,$$

i.e.

$$\frac{1}{2}a_n^2 = n + \frac{1}{2},$$

and therefore

$$a_n = \sqrt{2n+1}.$$

The momentum $p(x)$ is given by

$$p(x) = \sqrt{2m(E - V(x))} = \sqrt{a_n^2 - x^2}.$$

With the above notation the semiclassical wave function in the allowed region $-a < x < a$ ($|x| > a$ is supposed to give a negligible contribution to all the following computation) is represented by

$$\psi_n(x) \simeq \frac{A_n}{\sqrt{p}} \cos\left[\int_{-a}^{x} p(t)\,dt - \frac{\pi}{4}\right].$$

The normalization constant A_n is easily fixed. In fact

$$\int_{-a}^{a} \psi_n^2 dx = A_n^2 \int_{-a}^{a} \frac{dx}{p(x)} \cos^2\left[\int_{-a}^{x} p(t)\,dt - \frac{\pi}{4}\right] \simeq \frac{A^2}{2} \int_{-a}^{a} \frac{dx}{p(x)}.$$

Here we have taken the average $\frac{1}{2}$ of the rapid oscillating trigonometric function. Since

$$\int_{-a}^{a} \frac{dx}{p(x)} = 2\int_{-a}^{a} \frac{dx}{\sqrt{a^2 - x^2}} = 2\int_{0}^{1} \frac{dt}{\sqrt{1 - t^2}} = \pi,$$

for the normalization constant A we have

$$A=\sqrt{\frac{2}{\pi}}.$$

Last observation. We can write the wave function as

$$\psi_n=\frac{A}{a_n^{\frac{1}{2}}\left[1-\left(\frac{x}{a_n}\right)^2\right]^{\frac{1}{4}}}\cos\left[2a_n^2\int_{-1}^{x/a_n}\sqrt{1-t^2}dt-\frac{\pi}{4}\right],$$

i.e.

$$\psi_n=\frac{A}{a_n^{\frac{1}{2}}\left[1-\eta^2\right]^{\frac{1}{4}}}\cos\left[a_n^2 f\left(\eta\right)\right],$$

where $\eta\equiv\frac{x}{a_n}$. By using the above formula is now easy to compute the average of x^{α}. We have

$$\langle x^{\alpha}\rangle=\int_{-a_n}^{a_n}x^{\alpha}\psi_n\left(x\right)\psi_n\left(x\right)dx=\frac{A^2}{a_n}\int_{-a_n}^{a_n}x^{\alpha}\frac{1}{\sqrt{1-\eta^2}}\cos^2\left[a_n^2 f\left(\eta\right)\right]dx.$$

By making the change of variable $x\rightarrow x/a_n$ and taking the average of the rapid oscillating function, we have

$$\langle x^{\alpha}\rangle=A^2a_n^{\alpha}\int_0^1 dt\frac{t^{\alpha}}{\sqrt{1-t^2}}.$$

For the last integral we obtain

$$I\left(\alpha\right)\equiv\int_0^1 dt\frac{t^{\alpha}}{\sqrt{1-t^2}}=\frac{\sqrt{\pi}}{\alpha}\frac{\Gamma\left(\frac{1+\alpha}{2}\right)}{\Gamma\left(\frac{\alpha}{2}\right)},$$

i.e.

$$\langle n|\,x^{\alpha}\,|n\rangle=\frac{2}{\sqrt{\pi}}\frac{1}{\alpha}\frac{\Gamma\left(\frac{1+\alpha}{2}\right)}{\Gamma\left(\frac{\alpha}{2}\right)}\left(2n+1\right)^{\frac{\alpha}{2}}.$$

Simple checks of the above formula are obtained by taking

$\alpha=2$

$$\left\langle x^2\right\rangle=\frac{2}{\sqrt{\pi}}\frac{1}{2}\frac{\Gamma\left(\frac{3}{2}\right)}{\Gamma\left(\frac{1}{2}\right)}\left(2n+1\right)=\frac{1}{2}\left(2n+1\right)=n+\frac{1}{2},$$

which coincides with the exact result.

$\alpha = 4$

$$\left\langle x^4 \right\rangle = \frac{2}{\sqrt{\pi}} \frac{1}{4} \frac{\Gamma\left(\frac{5}{2}\right)}{\Gamma(2)} (2n+1)^2 .$$

Since $\Gamma\left(\frac{5}{2}\right) = \frac{3}{4}\sqrt{\pi}$,

$$\left\langle x^4 \right\rangle = \frac{3}{4}\left(2n^2 + 2n + \frac{1}{2}\right),$$

whereas the exact result seems to be (according to Landau)

$$\left\langle x^4 \right\rangle_{ex} = \frac{3}{4}\left(2n^2 + 2n + 1\right).$$

2.12 Exact WKB quantization

The WKB quantization condition can be actually converted into an algebraic form, which can be used to calculate the eigenvalues to any order. The method is due to Dunham and brought to its full glory by Bender, Olanssem and Way.
In the following we will use their notation.
Starting from the Schrödinger equation written as

$$\left[-\frac{d^2}{dx^2} + V(x) - E\right]\psi = 0, \qquad \psi(\pm\infty) = 0$$

we introduce a small parameter ε and consider the eigenvalue problem

$$\varepsilon^2 \psi'' = Q(x)\,\psi, \qquad Q(x) = V(x) - E. \tag{2.11}$$

The parameter ε helps in organizing the WKB series and it os obviously related to $\hbar$. The WKB solution is expressed as

$$\psi(x) = \exp\left[\frac{1}{\varepsilon}\sum_{n=0}^{\infty} \varepsilon^n s_n(x)\right].$$

Substituting this expression into (2.11) and comparing the equal powers of ε, we obtain

$$S'(0) = -\left[a(x)\right]^{1/2},$$

$$2S_0' S_n' + \sum_{j=1}^{n-1} S_j' S_{n-j}' + S_{n-1}'' = 0, \qquad n \geq 1. \tag{2.12}$$

The recursion equation in (2.12) is, as a matter of fact, a simple algebraic rule for computing $S_n'(x)$ from $s_j^{'}$ for $j<n$. Straightforward computations give

$$S_1^{'}(x)=-\frac{Q'(x)}{4Q(x)},$$

$$S_2^{'}(x)=\frac{5\left[Q'(x)\right]^2}{32\left[Q(x)\right]^{\frac{5}{2}}}-\frac{Q''(x)}{8\left[Q(x)\right]^{\frac{3}{2}}},$$

$$S_3^{'}(x)=-\frac{15\left[Q'(x)\right]^3}{64\left[Q(x)\right]^4}+\frac{9Q'(x)Q''(x)}{32\left[Q(x)\right]^3}-\frac{Q'''(x)}{16\left[Q(x)\right]^2},$$

and so on. Once the S_n' have been found, there is a simple formula which is a generalization of the well–known formula of the WKB quantization

$$\int_{x_1}^{x_2}\left[E-V(x)\right]^{\frac{1}{2}}dx=\left(k+\frac{1}{2}\right)\pi,$$

which states the *exact* quantization of the eigenvalues. This formula is simply

$$\frac{1}{2\pi i}\oint\sum_{n=0}^{\infty}S_n'(x)=k\qquad k=0,1,2... \tag{2.13}$$

and it expresses, through the logarithmic derivative of the wave function, the fact that this solution possesses k zeros. It is easy to see that the above formula reduces to the usual one at the leading order. The leading WKB formula takes into account both $S_0(x)$ and $S_1(x)$ substituting $S_0^{'}(x)$ into (2.13) and making $\left[Q(x)\right]^{\frac{1}{2}}$ single valued by joining the turning points x_1 and x_2 by a branch cut, we have

$$-\frac{1}{2\pi i}\oint\left[V(x)-E\right]^{\frac{1}{2}}dx=\int_{x_1}^{x_2}\sqrt{E-V(x)}dx,$$

for the term coming from S_0, whereas for the term coming from $S_1^{'}(x)$

$$-\frac{1}{2\pi i}\oint\frac{Q'(x)}{4Q(x)}dx=-\frac{1}{8\pi i}\ln Q(z)\mid_C=-\frac{1}{8\pi i}4\pi i=-\frac{1}{2}, \tag{2.14}$$

Here $\ln Q(z)$ has been evaluated once around the contour (it gives $4\pi i$ because the contour encircles two simple poles of $Q(x)$).
Then, one reproduces the well–known formula

$$\int_{x_1}^{x_2}\sqrt{E-V(x)}=k+\frac{1}{2}.$$

An important comment is in order. It is remarkable that the above formula (2.13) takes into account only the basic property of the wave function, i.e. the number of nodes. Any reference, for instance, to the Airy function has disappeared. Moreover, there is no reference to $\psi(x)$ or to its boundary conditions. The construction is *purely algebraic*; it involves differentiation and not integration. It is necessary though to use complex contour integration instead of ordinary integration along the real axis between x_1 and x_2. This because all the functions $S_i^{'}(x)$ are singular at the turning points.
There is an interesting open question. Since the integrals in (2.13) involve closed contours, it is possible to add total derivatives to $S_n'(z)$ under the integral without altering the value of the integral. Hence, S_n' as generated by the recursion equation (2.12) is but one element of a large equivalence class which we denote by F_n. The elements of F_n are all different but their contour integral are always the same. Is it possible that for *all* n there is some elements of F_n which is so simple that the indicate sum in (2.13) may be evaluated in close form? This possibility seems quite remote. Nevertheless, there are some interesting results.

(i) One element of F_{2n+1} is always zero (for $n \geq 1$), because $S_{2n+1}^{'}$ is itself a total derivative. For example, $S_3^{'}(x)$ can be written

$$S_3^{'}(x) = \frac{d}{dx}\left[\frac{5\left[Q^{'}(x)\right]^2}{64\left[Q(x)\right]^3} - \frac{Q^{''}(x)}{16\left[Q(x)\right]^2}\right],$$

which vanishes once integrated along the close contour. This can be understood by a simple argument. The quantization condition (2.14) is a constraint on the phase of $\psi(x)$. $S_{2n+1}^{'}(x)$ $(n \geq 1)$ is always real because it contains no fractional powers of $(V-E)$ and therefore cannot contribute to the phase of $\psi(x)$. It is S_{2n}' instead that becomes imaginary as x crosses into a classically allowed region and causes the wave function to become oscillatory. Hence it is no longer surprising that $S_{2n+1}^{'}$ $(n \geq 1)$ drops from the quantization condition.

(ii) The even terms $S_{2n}'(z)$, the only ones which survive, can be drastically simplified by adding and subtracting total derivatives. For instance

$$S_2^{'}(x) = -\frac{Q^{''}(x)}{48\left[a(x)\right]^{\frac{3}{2}}} - \frac{d}{dx}\left[\frac{5Q^{'}(x)}{48\left[a(x)\right]^{\frac{3}{2}}}\right].$$

(iii) There is a close parallelism between the search of the simplest element of F_{2n} and the construction of the conserved quantities for the non–

linear wave equation like the KdV

$$\dot{u} = u''' - 6uu'.$$

For this equation, the conserved quantities are derived from the Miura transformation

$$u(x) = -v^2(x) - v'.$$

They satisfy a recursive equation, similar to (2.12).

The recursion equation for the elements S'_n of the WKB expansion may be derived from the Miura transformation if we put $u = v/\varepsilon$ and let $v = \sum \varepsilon^n S'_n$.

The Miura transformation if nothing but the Riccati equivalent of the Schrödinger equation.

2.12.1 Some "numerology"

Let us analyze the potential $V = x^N$, with N even. For such potential, the WKB series is a power series in inverse fractional powers of the energy E, i.e.

$$E^{\frac{1}{N}+\frac{1}{2}} \sum_{n=0}^{\infty} E^{-n\left(1+\frac{2}{N}\right)} a_n(N) = \left(k + \frac{1}{2}\right)\pi.$$

The coefficients $a_n(N)$ have the form

$$a_n(N) = \frac{2\sqrt{\pi}\Gamma\left(1+\frac{1-2n}{N}\right)}{\Gamma\left(\frac{3-2n}{2}+\frac{1-2n}{N}\right)} \frac{P_n(N)(-1)^n}{(2n+2)!2^n},$$

where $P_n(N)$ is a polynomial in N:

$$P_0(N) = 1$$

$$P_1(N) = 2(N-1)$$

$$P_2(N) = (N-3)(N-1)(2N+3)$$

$$P_3(n) = \frac{4}{9}(N-1)(N-5)\left(24N^3 + 22N^2 - 117N - 139\right)$$

$$\vdots$$

All these polynomials contain $(N-1)$ as a factor, and this explains why for the harmonic oscillator the WKB quantization is *exact*.

One should keep in mind that the above series is an asymptotic series. Like the Stirling series for the Γ function, the coefficients get smaller for a while but eventually grow without bound. This means that for any given value of k, successive approximations to $E^{(k)}$, obtained by truncating the series, improve to some maximal accuracy and then become worse. Also, since E increases with k, more terms in the series should be required to reach maximal accuracy as k increases, and the accuracy should also increase with k. This is precisely what happens. For instance, with $V = x^4$,

$$E^0_{exact} = 1.060362090$$

$$(WKB)_1 = 0.87$$

$$(WKB)_2 = 0.98$$

$$(WKB)_4 = 0.95$$

$$(WKB)_6 = 0.78$$

$$(WKB)_8 = 1.13$$

$$(WKB)_{10} = 1.40,$$

$$E^8_{exact} = 37.923001027033$$

$$(WKB)_1 = 37.904471845068$$

$$(WKB)_2 = 37.923021140528$$

$$\vdots$$

$$(WKB)_{10} = 37.923001027043 \qquad \left(10^{-14}!\right).$$

2.13 Estimate of the ground state energy

In the following we will discuss some useful tools which allows us to estimate the ground state energy, i.e. to have upper and lower bounds for this quantity.

Variational principle

The Hamiltonian can be decomposed as

$$H = \sum_n E_n \left|\psi_n\right\rangle \left\langle\psi_n\right|. \tag{2.15}$$

In the following we assume to have an increasing sequence of eigenvalues and, for simplicity, to have no degeneracy. Taking the expectation value of (2.15) on a state $|\psi\rangle$, we have

$$\langle\psi| H |\psi\rangle = \sum_n E_n |\langle\psi| \psi_n\rangle|^2 \geq E_0 \sum_n E_n |\langle\psi_n| \psi\rangle|^2 = E_0 \langle\psi| \psi\rangle , \quad (2.16)$$

i.e.

$$E_0 \leq \frac{\langle\psi| H |\psi\rangle}{\langle\psi| \psi\rangle}. \quad (2.17)$$

If the state depends on a parameter, i.e. $|\psi\rangle = |\psi(\beta)\rangle$ and it has the same qualitative features of the ground state wave function (i.e. it has no nodes and decreases sufficiently rapidly at infinity), we can obtain an estimate of E_0 by computing (2.17) and determining the value minimizing this quantity.

Example

$$H = \frac{p^2}{2m} + \lambda |x|^a = \varepsilon_0 \left[\frac{\widehat{p}^2}{2} + b |\eta|^a\right], \quad (2.18)$$

where we have chosen the natural units, previously introduced, which match the semiclassical expression. Let us take now, as a trial wave function,

$$\psi_\beta(\eta) = \sqrt{\frac{\beta}{\sqrt{\pi}}} \exp\left(-\frac{\beta^2\eta^2}{2}\right).$$

By using the formula

$$I(n) = \int_{-\infty}^{+\infty} |x|^n e^{-\alpha^2 x^2} dx = \left(\frac{1}{\alpha}\right)^{n+1} \Gamma\left(\frac{n+1}{2}\right),$$

it is easy to obtain the expectation value of the Hamiltonian. In fact, we have,

$$\psi' = -\beta^2\eta\psi; \qquad \psi'' = \beta^4\eta^2\psi - \beta^2\psi.$$

Therefore, for the kinetic term we get

$$\langle\psi| \frac{p^2}{2} |\psi\rangle = -\frac{1}{2} \langle\psi| \psi''\rangle = \frac{\beta^2}{2} - \frac{\beta^4}{2} \langle\psi| \eta^2 |\psi\rangle =$$

$$\frac{\beta^2}{2} - \frac{\beta^2}{4} = \frac{\beta^2}{4},$$

whereas for the potential term we have

$$\langle\psi| V |\psi\rangle = b \langle\psi| |\eta|^a |\psi\rangle = \frac{b}{\beta} \frac{\Gamma\left(\frac{a+1}{2}\right)}{\sqrt{\pi}} = \frac{B}{\beta},$$

where

$$B = \frac{b(a)}{\sqrt{\pi}}\Gamma\left(\frac{a+1}{2}\right).$$

Hence

$$\langle\psi| H |\psi\rangle = \varepsilon_0 \left[\frac{\beta^2}{4} + \frac{B}{\beta^a}\right]. \tag{2.19}$$

Minimizing with respect to β, we have

$$\frac{\partial}{\partial\beta}\langle\psi| H |\psi\rangle = \varepsilon_0 \left[\frac{\beta}{2} - a\frac{B}{\beta^{a+1}}\right] = 0,$$

i.e.

$$\beta_{op} = (2aB)^{\frac{1}{a+2}}.$$

Substituting now into (2.19), we have

$$E_0 \leq \varepsilon_0 \left[\frac{1}{4}(2aB)^{\frac{2}{a+2}} + \frac{B}{(2aB)^{\frac{1}{a+2}}}\right] = \varepsilon_0 \left(\frac{2aB}{4} + B\right)\frac{1}{(2aB)^{\frac{1}{a+2}}} =$$

$$\varepsilon_0 \left(\frac{a+2}{4a}\right)(2aB)^{\frac{2}{a+2}} = \varepsilon_0 \left(\frac{a+2}{4a}\right)\left[\frac{2ab(a)}{\sqrt{\pi}}\Gamma\left(\frac{a+1}{2}\right)\right]^{\frac{2}{a+2}},$$

so, finally

$$E_0 \leq \varepsilon_0 \left(\frac{a+2}{4a}\right)\left[\frac{2ab(a)}{\sqrt{\pi}}\Gamma\left(\frac{a+1}{2}\right)\right]^{\frac{2}{a+2}}.$$

For $a = 2$, we get correctly $E_0 = \frac{\varepsilon_0}{2}$.
The variational principle can be used to establish the following general result: *an attractive potential, i.e. a potential $V(x) < 0$, has always at least a bound state.*

2.14 Uncertainty relation and lower bound

The previous variational principle permits to obtain an upper bound for the ground state energy E_0. In order to obtain a lower bound, we rely on Heisenberg's uncertainty relation

$$\Delta p \Delta q \geq \frac{\hbar}{2}.$$

For an Hamiltonian as the one in (2.18), we have

$$E_0 \geq \varepsilon_0 \left[\frac{1}{8}\left(\frac{1}{\Delta q}\right)^2 + b|\eta|^a\right].$$

Requiring that Δq is of the order of 2η we have

$$E_0 \geq \varepsilon_0 \left[\frac{1}{32} \left(\frac{2}{\Delta q} \right)^2 + b \left(\frac{\Delta q}{2} \right)^a \right] \equiv$$

$$\varepsilon_0 \left[\frac{1}{32} \left(\frac{1}{x} \right)^2 + b x^a \right], \tag{2.20}$$

where $x \equiv \frac{\Delta q}{2}$. Computing the extremum of the above quantity w.r.t. x we have

$$-\frac{1}{16} \left(\frac{1}{x} \right)^3 + abx^{a-1} = 0, \qquad \Rightarrow x_{op} = \left(\frac{1}{16ab} \right)^{\frac{1}{a+2}}.$$

Substituting this value into (2.20), we have, after some manipulations

$$E_0 \geq \varepsilon_0 \left(\frac{a+2}{32a} \right) (16ab)^{\frac{2}{a+2}}.$$

For the ratio of the uncertainty bound and the one of the variational principle we have

$$\frac{E_{un}}{E_{var}} = \frac{1}{8} \left(\frac{8\sqrt{\pi}}{\Gamma\left(\frac{a+1}{2}\right)} \right)^{\frac{2}{a+2}},$$

and this quantity is correctly always less than 1.

Chapter 3

Thermodynamic Bethe Ansatz and Ordinary Differential Equations

3.1 Spectral determinant

In this section we will come back to the problem of the spectral determinant of the Schrödinger equation. We will see that for a particular class of potentials this function satisfies a nonlinear functional equation which, as a matter of fact, is equal to the Bethe Ansatz equations for integrable models in Statistical Mechanics! Consider the Schrödinger equation

$$\left(-\frac{d^2}{dx^2}+P\left(x\right)\right)\psi\left(x\right)=0 \tag{3.1}$$

for arbitrary complex values of x, with

$$P\left(x\right)=x^{2M}-E+\frac{l\left(l-1\right)}{x^2}.$$

For non integer values of M we have a branch cut at the origin. Using the results of the analysis by Sibuya in [**?**], we state that (3.1) admits a solution $y=y\left(x,E,l\right)$, such that

(i) y is an entire function of x, E, where due to the branch point at $x=0$, x must be in general considered to live on a suitable cover of the punctured complex plane;

(ii) y and $y^{'}$ admit the asymptotic expressions

$$y\sim x^{-\frac{M}{2}}\exp\left[-\frac{1}{M+1}x^{M+1}\right] \tag{3.2}$$

$$y \sim -x^{\frac{M}{2}} \exp\left[-\frac{1}{M+1}x^{M+1}\right], \tag{3.3}$$

as x goes to infinity in any closed sector satisfying

$$|\arg x| < \frac{3\pi}{2M+2}.$$

(**Remark**. Extra terms appear though for $0 < M \leq 1$).

(iii) Furthermore, the solution y is uniquely identified by the above information. From WKB theory, we know that eq. (3.1) has two solutions $\Phi_\pm$ given by

$$\Phi_\pm(x) = [P(x)]^{-\frac{1}{4}} \exp\left[\pm \int_{x_0}^{x} \sqrt{P(x)}dx\right].$$

It is then easy to see that the asymptotic (ii) is, up to a normalization constant N, the large x limit of Φ_-:

$$y(x,E) \simeq N\Phi_-(x,E)$$

with $x = \rho e^{i\theta}$ we have

$$\Phi_\pm(\rho,\theta) \simeq x^{-\frac{\pi}{2}} \exp\left[\pm\frac{\rho M+1}{M+1}e^{i\theta(M+1)}\right].$$

Let us fix now some terminology. A solution tending to zero for large ρ in the sector

$$a < \theta < b$$

is called *subdominant* in that sector. A solution growing for large ρ in the sector

$$a' < \theta' < b'$$

is called *dominant* in this sector.
Let us denote by S_k the sector

$$\left|\theta - \frac{2k\pi}{2M+2}\right| < \frac{\pi}{2M+2}.$$

We see then

(i) in S_0, $y \simeq N\Phi_- \to 0$, i.e. y is subdominant in S_0;
(ii) at $\theta = \pm\frac{\pi}{2M+2}$ it decays algebraically;
(iii) in $S_{\pm 1}$, $y \simeq N\Phi_- \to \infty$, i.e. y is dominant in these sectors.
FIGURE

Note that in $S_{\pm 1}$, with some coefficients $C(E)$

$$y(x) = y_-(x) + C(E)\, y_+(x)$$

and that exactly at $\theta \geq \frac{3\pi}{2M+2}$ we have lost control of the exponential asymptotic behaviour of y. This is the reason of the above restriction

$$|\theta| = |\arg x| < \frac{3\pi}{2M+2}.$$

To find subdominant solutions on other sectors, we can use the following technique. Consider $\widehat{y}(x) = y(ax, E, l)$ for any constant a. This function satisfies the differential eq.

$$\left[-\frac{d^2}{dx^2} + a^{2M+2}x^{2M} - a^2 E + \frac{l(l+1)}{x^2}\right]\widehat{y}(x) = 0.$$

Thus, if $a^{2M+2} = 1$, $P\left(y\left(ax, a^{-2}E, l\right)\right)$ is another solution of (3.1). Setting

$$\omega = e^{i\pi/M+1},$$

we have therefore the set of solutions

$$y_k \equiv y_k(x, E, l) = \omega^{\frac{k}{2}} y\left(\omega^{-k}x, \omega^{2k}E, l\right) \tag{3.4}$$

with y_k subdominant in S_k and dominant in $S_{k\pm 1}$ (the prefactor $\omega^{\frac{k}{2}}$ is for later convenience). The first conclusion of the above analysis is that each pair

$$\{y_k, y_{k+1}\}$$

of functions provides a set of linearly independent solutions of (3.1) and any other solution can be expressed in terms of them. In particular

$$y_{k-1}(x, E, l) = C_k(E, l)\, y_k(x, E, l) + \widetilde{C}_k(E, l)\, y_{k+1}(x, E, l). \tag{3.5}$$

The functions C_k and $\widetilde{C_k}$ are called the Stokes multipliers for y_{k-1} w.r.t. y_k and y_{k+1}. Clearly, from (3.4), we have

$$C_k(E, l) = C_{k-1}\left(\omega^2 E, l\right)$$

$$\widetilde{C_k}(E, l) = \widetilde{C_{k-1}}\left(\omega^2 E, l\right).$$

From now on, we denote C_0 and $\widetilde{C_0}$ by C and $\widetilde{C}$. The second result is that the Stokes multipliers can be expressed in terms of the Wronskians.

Definition 1. *The Wronskian $W[f,g]$ of two functions is defined by*

$$W(f,g) = fg' - f'g.$$

If f and g are both solutions of the Schrödinger equation (3.1), their Wronskian is a constant, independent of x. In fact

$$W'(f,g) = f'g' + fg'' - f''g - f'g' = fg'' - f''g = -P(x,E,l)(fg - gf) = 0.$$

Consider the Wronskian of (3.5) (with $k=0$) with respect to the functions y_1 and y_0:

$$y_{-1} = C_0 y_0 + \widetilde{C_0} y_1$$

$$W[y_{-1}, y_1] \equiv W_{-1,1} = C_0 W[y_0, y_1] = C_0 W_{01}$$

$$W[y_{-1}, y_0] \equiv W_{-1,0} = \widetilde{C_0} W\left[y_1, y_0 = \widetilde{C_0} W_{1,0} = -\widetilde{C_0} W_{01}\right],$$

i.e.

$$C = \frac{W_{-1,1}}{W_{01}}; \qquad \widetilde{C} = -\frac{W_{-1,0}}{W_{0,1}}. \tag{3.6}$$

These Wronskians are entire functions of E and l (since the same holds for the functions y_k). Since y_0 and y_1 are linearly independent, W never vanishes. Therefore C and $\widetilde{C}$ are also entire functions. As a matter of fact, all $\widetilde{C_k}$ are identically equal to -1,

$$\widetilde{C_k} = -1.$$

This result follows from the relations

$$W_{k_1+1,k_2+1} = W_{k_1 k_2}\left(\omega^2 E, l\right)$$

$$W_{0,1}(E,l) = 2i.$$

The last condition is obtained by evaluating $W_{0,1}$ as $x \to \infty$ in the sectors S_0 or S_1, where the asymptotic behaviours of y_0 and y_1 (and their derivatives) are determined by eqs. (3.2)–(3.3). Since $y_{-1}(x,E,l) = y_1(x^*, E^*, l^*)$ it also follows from (3.6) that $C(E,l)$ is real whenever E and l are real.
Finally, the basic Stokes relation (3.5) at $k=0$ can be written in the form

$$C(E,l)\, y_0(x,E,l) = y_{-1}(x,E,l) + y_1(x,E,l)$$

$$C(E,l) = \frac{1}{2i} W_{-1,1}(E,l), \tag{3.7}$$

i.e.

$$C(E,l)\,y(x,E,l) = \omega^{-\frac{1}{2}} y\left(\omega x, \omega^{-2}E, l\right) + \omega^{\frac{1}{2}} y\left(\omega^{-1}x, \omega^{2}E, l\right).$$

Let us analyze this equation. Any solution of (3.1) can be written in terms of another basis of functions

$$\{\psi_+, \psi_-\}$$

where $\psi_+(x)$ is the solution which for $x \to 0$ goes as

$$\psi_+ \sim x^{l+1} \tag{3.8}$$

whereas $\psi_-(x)$ behaves as

$$\psi_- \sim x^{-l}.$$

Notice that both of them vanish if $l(l+1) < 0$, whereas one of the two diverges if $l(l+1) > 0$.
Since l enters eq. (3.1) only in the combination $l(l+1)$, we can decide to fix $\psi_+(x)$ as the solution which behaves as (3.8) and to define $\psi_-(x)$ by its analytic continuation, i.e.

$$\psi_-(x,E,l) \equiv \psi_+(x,E,-1-l).$$

In analogy with what done previously, we define the shifted solutions $\psi_k^{\pm}$

$$\psi_k^{\pm} = \psi_k^{\pm}(x,E,l) = \omega^{\frac{k}{2}} \psi^{\pm}\left(\omega^{-k}x, \omega^{2k}E, l\right).$$

They also solve the original problem (3.1). By considering the limit $x \to 0$, it is easily seen that

$$\psi_k^{\pm}(x,E,l) = \omega^{\mp k\left(l+\frac{1}{2}\right)} \psi^{\pm}(x,E,l).$$

We also have

$$W\left[y_{k+1}, \psi_{k_2+1}^{\pm}\right](E,l) = W\left[y_{k+1}, \psi_{k_2+1}^{\pm}\right]\left(\omega^2 E, l\right)$$

and therefore

$$W\left[y_k, \psi^{\pm}\right](E,l) = \omega^{\pm k\left(l+\frac{1}{2}\right)} W\left[y_k, \psi^{\pm}\right](E,l) =$$

$$\omega^{\pm k\left(l+\frac{1}{2}\right)} W\left[y, \psi^{\pm}\right]\left(\omega^{2k}E, l\right). \tag{3.9}$$

We can now take the Wronskian of both sides of (3.7) with $\psi^{\pm}$. Defining

$$D^{\mp}(E,l) \equiv W\left[y(x,E,l), \psi^{\pm}(x,E,l)\right]$$

and using (3.9), the Stokes eq. (3.7) becomes

$$C(E,l)\,D^{\mp}(E,l) = \omega^{\mp\left(l+\frac{1}{2}\right)} D^{\mp}\left(\omega^{-2}E,l\right) + \omega^{\pm\left(l+\frac{1}{2}\right)} DD^{\mp}\left(\omega^{2}E,l\right). \quad (3.10)$$

We will discover soon the meaning and the beauty of this functional equation.
First of all, notice that expressing

$$y = \alpha\psi^{+} + \beta\psi^{-},$$

the coefficients of this linear combination are given by the above Wronskians. In fact, using

$$W\left[\psi^{-},\psi^{+}\right] = x^{-l}(l+1)\,x^{l} + lx^{-l-1}x^{l+1} = 2l+1,$$

we have

$$W\left[y,\psi^{+}\right] \equiv D^{-} = \beta(2l+1)$$
$$W\left[y,\psi^{-}\right] \equiv D^{+} = -\alpha(2l+1),$$

i.e.

$$(2l+1)\,y = D^{-}(E,l)\,\psi^{-} - D^{+}(E,l)\,\psi^{+}.$$

Moreover, from the relation

$$\psi^{-}(x,E,l) = \psi^{+}(x,E,-1-l)$$

we deduce

$$D(E,l) \equiv D^{-}(E,l) = D^{+}(E,-1-l).$$

Requiring a non–singular behaviour at the origin for $y(x)$ restricts E to the set of eigenvalues $\{E_n\}$ of the spectral problem, i.e.

$$D(E,l)\mid_{E=E_n} = 0, \qquad l > -\frac{1}{2}.$$

Therefore we arrive at the following remarkable conclusion: $D(E,l)$ is an entire function which has zeros on the real positive axis, in correspondence with the eigenvalues E_M of the Schrödinger equation. This because the solution y vanishes at infinity $(x \to \infty)$ and it is regular as $x \to 0$. Hence $D^{\pm}(E,l)$ *are the Fredholm determinants*. We have the following properties.

(i) C and D^{-} are entire functions of E, since the functions entering their definition are entire.

(ii) If l is real and larger than $-\frac{1}{2}$, then the zeros of D^{-} all lie on the positive real axis of the complex plane E. In fact, we have already commented

that a zero of $D^{-}(E,l)$ signals the existence of a proper eigenfunction. The Hermitian nature of the problem for $l > -\frac{1}{2}$ then ensures the reality of these zeros.. Moreover, for $l > 0$ the potential is everywhere positive. Therefore, by multiplying for ψ^{*} and integrating from $(0,\infty)$ shows that all eigenvalues E_M must be positive.

(iii) When $M > 1$, $D^{-}(E,l)$ has the following large E asymptotic

$$\ln D^{-}(E,l) \simeq \frac{a_0}{2}(-E)^{\mu}, \qquad |E| \to \infty, \qquad |\arg(-E)| < \pi, \tag{3.11}$$

where

$$a_0 = -\frac{1}{\sqrt{\pi}}\Gamma\left(-\frac{1}{2} - \frac{1}{2M}\right)\Gamma\left(1 + \frac{1}{2M}\right), \qquad \mu = \frac{M+1}{2M}.$$

(iv) If $E = 0$, then

$$D^{-}(0,l) = -\frac{1}{\sqrt{\pi}}\Gamma\left(1 + \frac{2l+1}{2M+2}\right)(2M+2)^{\frac{2l+1}{2M+2}+\frac{1}{2}}.$$

Notice that at $l = 0$, we simply have

$$D^{-}(E,0) \equiv y(x,E)\,|_{x=0}, D^{+}(E,0) \equiv y'(x,E)\,|_{x=0}\,.$$

In this case, the problem reduces to an ordinary Schrödinger equation, but on a half line. WE can choose Dirichlet b.c. for the solution, i.e.

$$y(x,E)\,|_{x=0} = 0,$$

or Neumann b.c.

$$y^{'}(x,E)\,|_{x=0} = 0.$$

The first one are those appropriate for the wave function in the odd–parity sector, as for instance

FIGURE

whereas the second one refers to the even–parity sector, as

FIGURE

In this case $D^{-}(E,0)$ will have zeroes in correspondence of the energy levels E_n^{-} with odd parity, whereas $D^{+}(E,0)$ will have zeros in correspondence of E_n^{+}. This is equivalent, in fact, to choose the proper combination which expresses y in this case.

For $l = 0$, it is simple to establish the formula (3.11). In this case, in fact, $D^{-}(E,0) \equiv y(x,E) \mid_{x=0} = 0$, so we have to find the value of this function at the origin. When $E \to \infty$, we have

$$\frac{P'(x,E)}{P(x,E)} \to 0,$$

and therefore we can rely on WKB. We have, in fact

$$y(x,E) \simeq N\phi_{-}(x,E)$$

and therefore

$$\ln \frac{y}{N} \cong \int_{x}^{x_0} \left(E^{2M} - E\right)^{\frac{1}{2}} dE \underset{x,x_0 \gg 0}{\simeq} \frac{x_0^{M+1}}{M+1} - \frac{x^{M+1}}{M+1}.$$

We can drop the first term by choosing

$$\ln N = -\int_{0}^{x_0} t^M dt.$$

Sending now $x_0 \to \infty$, we end up with

$$\ln y \mid_{\substack{x=0 \\ .E \gg 0}} \sim \int_{0}^{\infty} \left[\left(t^{2M} - E\right)^{\frac{1}{2}} - t^M\right] dt = a_0 (-E)^M,$$

where

$$a_0 = \int_{0}^{\infty} \left(\left[t^{2M} + 1\right]^{\frac{1}{2}} - t^M\right) dt = -\frac{1}{\sqrt{\pi}} \Gamma\left(-\frac{M+1}{2M}\right) \Gamma\left(1 + \frac{1}{2M}\right),$$

with

$$\mu = \frac{M+1}{2M}.$$

The same result can be shown to hold also for $l \neq 0$. We can now use the *Hadamard factorization theorem.*

3.2 Hadamard Factorization Theorem

An entire function $f(z)$ is said to be of finite order if there is a positive number A such that

$$|f(z)| = O\left(e^{|z|^A}\right), \qquad |z| \to \infty.$$

The lower bound δ of the numbers A for which this is true is called the order of $f(z)$. In our specific example,

$$\ln D(E,l) \mid_{-E\gg 0} \sim a_0 (-E)^M$$

which is valid everywhere except for $\arg(E) = 0$, i.e. the real axis, where the growth of D is not greater than for $\arg(E) \neq 0$. Hence

$$order[D] = \mu = \frac{M+1}{2M} < 1, \qquad M > 1.$$

The celebrated Hadamard theorem can be stated as follows.

Theorem 1. *An entire function f(z) of finite order δ admits a factorization over his zeros $\{z_n\}$ of the form*

$$f(z) = e^{Q(z)} \prod_{n=0}^{\infty} K\left(\frac{z}{z_n}, P\right),$$

where

$$K(v,0) = 1 - v; \qquad K(v,p) = (1-v)^{v+\frac{v^2}{2}+\ldots+\frac{v^p}{p}}$$

are called "primary factors" and $Q(z)$ is a polynomial of order not greater than δ. If δ is not an integer, then $p = Int[\delta]$. Consequently, for $M > 1$,

$$\delta = \mu = \frac{M+1}{2M}, \qquad p = 0$$

and

$$D(E,l) = D(0,l) \prod_{n=0}^{\infty} \left(1 - \frac{E}{E_n}\right).$$

For $M \leq 1$ things are complicated by the possibility of nontrivial $Q(z)$. Exactly at $M = 1$,

$$D(E,l) = D(0,l) \prod_{n=0}^{\infty} \left(1 - \frac{E}{E_n}\right) e^{\frac{E}{E_n}}.$$

3.3 Bethe Ansatz Equations

The functional eq. (3.10) can be used to derive the energy levels of the considered quantum mechanical problem. Let us consider the one for $D^- \equiv D$

$$C\left(E,l\right)D\left(E,l\right)=\omega^{-\left(l+\frac{1}{2}\right)}D\left(\omega^{-2}E,l\right)+\omega^{\left(l+\frac{1}{2}\right)}D\left(\omega^{2}E,l\right).$$

Setting $E=E_i$ the left–hand side vanishes and we are led to the equation

$$-1=\omega^{2l+1}\frac{D\left(\omega^{2}E_i,l\right)}{D\left(\omega^{-2}E_i,l\right)};\qquad \omega\equiv e^{i\pi/M+1}.$$

For $M>1$, we can use the Hadamard factorization theorem and write

$$-1=\omega^{2l+1}\prod_{n=0}^{\infty}\left(\frac{E_n-E_i\omega^2}{E_n-E_i\omega^{-2}}\right).$$

This is an equation for the energy levels, equivalent to the Bethe Ansatz equation in Statistical Mechanics! This equation can be converted into an integral nonlinear equation, which can be solved very fast numerically. To this aim, let us define

$$a\left(E,l\right)\omega^{-2l-1}=\frac{D\left(E\omega^{2}\right)}{D\left(E\omega^{-2}\right)}=\prod_{n=0}^{\infty}\left(\frac{E_n-E\omega^2}{E_n-E\omega^{-2}}\right). \tag{3.12}$$

When $a\left(E,l\right)=-1$, we get the quantization condition for the energy levels. From eq. (3.12), taking the logarithm we have

$$\ln Q\left(E,l\right)=i\frac{2l+1}{M+1}\pi+\sum_{n=0}^{\infty}F\left(\frac{E}{E_n}\right),$$

with

$$F\left(E\right)=\ln\frac{1-\omega^2E}{1-\omega^{-2}E}.$$

Assuming that all E_n lie on the positive real axis, and that these are the only points in some strip about this axis for which $a\left(E,l\right)=-1$. By Cauchy's theorem we have

$$\ln a\left(E,l\right)=i\frac{2l+1}{M+1}\pi+\int_C\frac{dE'}{2\pi i}F\left(\frac{E}{E'}\right)\partial_{E'}\ln\left(1+a\left(E',l\right)\right).$$

FIGURE

since

$$\partial_{E'} \ln\left(1 + a\left(E', l\right)\right) = \frac{a'\left(E'\right)}{1 + a\left(E'\right)}$$

and then apply the residue theorem. We make the change of variables

$$E = e^{\frac{\theta}{\mu}}$$

and integrate by parts. We get

$$\ln a\left(\theta\right) = i\frac{2l+1}{M+1}\pi + \int_C d\theta' R\left(\theta - \theta'\right) \ln\left(1 + a\left(\theta'\right)\right) +$$

$$- \int_C d\theta' R\left(\theta - \theta'\right) \ln\left(1 + a\left(\theta'\right)\right),$$

where the contour C_1 and C_2 run from $-\infty$ to $+\infty$, infinitesimally below and above the real axis, and

$$R\left(\theta\right) \equiv \frac{i}{2\pi}\frac{d}{d\theta} F\left(e^{\frac{\theta}{\mu}}\right).$$

FIGURE

Using the fact that $i \ln a$ is a real analytic function for which

$$\left[a\left(\theta\right)\right]^* = \left[a\left(\theta^*\right)\right]^{-1},$$

and pushing C_1 and C_2 toward the real axis, we have

$$\ln a\left(\theta\right) = i\frac{2l+1}{M+1}\pi + \int_{-\infty}^{+\infty} d\theta' R\left(\theta - \theta'\right) \left\{\ln\left[1 + a\left(\theta' - i\varepsilon\right)^{-1}\right]^* - \ln\left(1 + a\left(\theta' - i\varepsilon\right)\right)\right\}$$

$$= i\frac{2l+1}{M+1}\pi + \int_{-\infty}^{+\infty} d\theta' R\left(\theta - \theta'\right) \left[\ln a\left(\theta'\right) - 2iIm \ln\left(1 + a\left(\theta' - i\varepsilon\right)\right)\right].$$

Let us define the Fourier transform

$$\widetilde{f}\left(k\right) = F\left(f\right)\left(k\right) = \int_{-\infty}^{+\infty} f\left(\theta\right) e^{-ik\theta} d\theta$$

$$f\left(\theta\right) = F^{-1}\left[\widetilde{f}\right]\left(\theta\right) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \widetilde{f}\left(k\right) e^{i\theta k} dk,$$

and taking the Fourier transform of the above equation

$$\left[1-\widetilde{R}\left(k\right)\right]F\left[\ln a\right]\left(k\right)=\frac{2i\pi\left(2l+1\right)}{M+1}\delta\left(k\right)-2i\widetilde{R}\left(k\right)ImF\left[\ln\left(1+a\right)\right]\left(k\right).$$

Transforming back and restoring the integrations over C_1 and C_2, we have

$$\ln a\left(\theta\right)=i\pi\left(l+\frac{1}{2}\right)-ib_0e^{\theta}+$$

$$+\int_{C_1}d\theta^{'}\varphi\left(\theta-\theta'\right)\ln\left(1+a\left(\theta'\right)\right)-\int_{C_2}d\theta^{'}\varphi\left(\theta-\theta'\right)\ln\left(1+a^{-1}\left(\theta'\right)\right),$$

with

$$\varphi\left(\theta\right)\equiv\int_{-\infty}^{+\infty}\frac{dk}{2\pi}e^{ik\theta}\frac{sh\frac{\pi}{2}\left(\xi-1\right)k}{2sh\frac{\pi}{2}\xi kch\frac{\pi k}{2}},\qquad\xi=\frac{1}{M}.$$

$$b_0=2\cos\frac{\pi}{2M}a_0.$$

The driving force ib_0e^{θ} of the above equation arises from a zero mode, which can be traced to the zero of

$$1-\widetilde{R}\left(k\right)\qquad at\qquad K=i.$$

Its value can be fixed by the WKB result

$$D\left(E,l\right)\underset{E\rightarrow-\infty}{\simeq}a_0\left(-E\right)^n=a_0\left(-e^{\frac{\theta}{\mu}}\right)^n$$

and from the definition

$$a\left(E,l\right)=\omega^{2l+1}\frac{D\left(E\omega^2,l\right)}{D\left(E\omega^{-2},l\right)}.$$

A first consistency check of this equation is immediate in the large θ limit, the driving term dominates and therefore

$$a\left(\theta,l\right)=-1$$

at the points θ_n, with

$$b_0e^{\theta_n}\simeq\pi\left(l+\frac{1}{2}\right)+\left(2n+1\right)\pi,\qquad n=0,1,\ldots$$

giving

$$E_n\simeq\left[\frac{\pi}{2b_0}\left(4n+2l+3\right)\right]^{\frac{1}{n}},\qquad n=0,1,\ldots$$

which at $M=1$, a potential can be solved exactly, coincides with the exact result!

Part II

Analytic Number Theory: an Introduction

Chapter 4

Prime numbers

4.1 Introduction

Number theory is one of the most fascinating areas of Mathematics. There are many unproved results and conjectures. The most amazing aspect is that there are problems which can be stated in a very simple way, but very difficult to prove.
Example: $(3n+1)$ Problem.
Take a number N. If it is even divide it by 2, otherwise multiply it by 3 and add 1.

$$N \to \left\{ \begin{array}{ll} N/2, & N \ even \\ 3N+1, & N \ odd \end{array} \right| .$$

Iterate the operation. Does the numbers always end to 1?
(Argument based on random walk).
Number theory has deep overlaps with calculus and also with geometry.
Example: Pitagoric triple.

$$a^2 + b^2 = c^2, \qquad a, b, c \in \mathbb{N}.$$

$$\begin{array}{rcl} a & = & 3, b = 4, c = 5, \\ a & = & 5, b = 12, c = 13, \\ a & = & 8, b = 15, c = 17, \\ & \vdots & \quad \vdots \qquad \vdots \end{array}$$

There is an infinite number of them. Geometrically, the problem consists in finding all rational points on a circle

$$\left(\frac{a}{c}\right)^2 + \left(\frac{b}{c}\right)^2 = 1.$$

FIGURE

This happens when the slope is rational! The generalization of this problem consists in finding rational points on an elliptic curve. According to the recent proof of Fermat's last theorem, there are no integer solutions to the equation

$$a^n + b^n = c^n, \qquad n > 2.$$

Another classical connection between Number Theory and Geometry is about the possibility to construct regular polygons by rule and compass. According to the proof by Gauss, this is possible for all those polygons of n sides when n is a product of different Fermat primes and powers of 2:

$$F_n = 2^{2^n} + 1.$$

At present, only 5 such primes are known for $n = 0, 1, 2, \ldots$, i.e.

$$F_0 = 3, \quad F_1 = 5, \quad F_2 = 17, \quad F_3 = 257, \quad F_4 = 65537.$$

So, regular polygons with

$$n = 2, 3, 4, 5, 6, 8, 10, 12, 15, 17, 20, 24, 30, \ldots$$

sides are constructible while those with

$$n = 7, 9, 11, 13, 14, 18, 19, 21, 22, 23, 25, \ldots$$

cannot be constructed.
In these lectures, we will cover only a small set of topics of this large subject. In the first lecture we will discuss some beautiful identities, collected and presented almost in a random order. The other two lectures will deal with one of the most fascinating and mysterious functions of Mathematics, i.e. the Riemann zeta function. We will discuss its main properties and its relationship with prime numbers.

4.2 Induction

One of the strongest properties of integers is their inductive nature: if the assumption that some law holds for n implies that holds for $n+1$ as well (and it is proved true for $n=1$), then it is always true.
A typical result that can be easily proven by induction is

$$\sum_{k=1}^{n} k = \frac{n\,(n+1)}{2}.$$

Another, less well known, is the derivation by Newton of the infinite expansion of the series

$$(1+x)^{-2} = 1 - 2x + 3x^2 - 4x^3 + 5x^4 + ...$$

$$(1+x)^{-3} = 1 - 3x + 6x^2 - 10x^3 + 15x^4 + ...$$

Consider the Tartaglia triangle for the binomial expression $(1+x)^n$, with n nonnegative integer:

$$\begin{array}{rccccccc} n=0 & & & 1 & & & & \\ n=1 & & 1 & & 1 & & & \\ n=2 & & 1 & 2 & 1 & & & \\ n=3 & 1 & & 3 & & 3 & & 1 \\ n=4 & & 1 & & 4 & & 6 & \\ & & & & & & & \end{array}$$

Of course, each number is the sum of the two numbers above it, i.e.

$$\left(\begin{array}{c} n+1 \\ k \end{array} \right) = \left(\begin{array}{c} n \\ k-1 \end{array} \right) + \left(\begin{array}{c} n \\ k \end{array} \right).$$

By applying this rule back–forward, we get

$$\begin{array}{rccccccc} n=-3 & & & 1 & & -3 & & 6 \\ n=-2 & & 1 & & -2 & & 3 & \\ n=-1 & 1 & & -1 & & 1 & & -1 \\ n=0 & & 1 & & 0 & & 0 & \\ & & & & & & & \end{array} \qquad \begin{array}{rccccc} & & -10 & & 15 & \\ & -4 & & 5 & & -6 \\ 1 & & -1 & & 1 & \\ & 0 & & 0 & & \end{array}$$

Let us consider now some limiting formulas

$$\sqrt{1+\sqrt{1+\sqrt{1+...}}} \to \frac{1+\sqrt{5}}{2}$$

$$\sqrt{7+\sqrt{7+\sqrt{7+...}}} \to \frac{1+\sqrt{29}}{2}$$

$$\sqrt{1+2\sqrt{1+3\sqrt{1+4\sqrt{...}}}} \to 3$$

$$\sqrt{1+\sqrt{2+\sqrt{3+\sqrt{4+...}}}} \to \sqrt{3}$$

$$\sqrt{1+\sqrt{2+\sqrt{...\sqrt{p_n+}...}}} \to 1.8507...$$

4.3 Prime Numbers

Let us consider now the Prime Numbers p_i, the building blocks of Number Theory. The first primes are

$$p_i = 1, 2, 3, 5, 7, 11, 13, 17, 19, 23, 29, ...$$

There are infinitely many prime numbers. Several proofs of this fact are known; the oldest and simplest one is due to Euclid.

Euclid's proof. Assume that there are only k primes $p_1, ..., p_k$. Consider the number $N = p_1 \cdot ... \cdot p_k + 1$. It is not divisible for any p_i, so either it is a prime or it has a prime divisor larger than all $p_1, ..., p_k$.

The basic theorem of Arithmetic states that any natural number n either is a prime or admits an unique decomposition in terms of the primes, i.e.:

$$n = p_1^{\alpha_1} \cdot ... \cdot p_k^{\alpha_k}.$$

The mathematical problem of identifying a prime number or to determine its prime decomposition is one of the most challenging of Mathematics.

Let us discuss briefly the *Primality Problem*. The crucial point is that it doesn't exist a formula which determines all and only the primes, i.e. a relation of the type $P_n = f(n)$. There are several formulas providing an answer to the primality problem, but in practice almost useless.

Example. Wilson formula

$$f(n) = \sin\left[\pi \frac{(n-1)! + 1}{n}\right].$$

One can prove that this function is zero if and only if n is a prime. Unfortunately, this primality test is of no practical advantage, because calculating $f(n)$ takes longer than the ordinary Eratosthenes's sieve.

Example: $101! \simeq 10^{160}$.

4.4 Measure of Complexity

Consider an algorithm which applies to a problem made of N data. The complexity of the problem can be related to the time of elaboration, in particular how this time scales with N. The problem has a polynomial complexity if the time of elaboration scales as a power law of N:

$$\tau_{poly} \sim N^{\alpha}.$$

These are the "easy" problems of mathematics. On the other hand, the problem is said to have an exponential complexity if the time scales faster than any power of N

$$\tau_{\exp} \sim \exp\left[\beta N^{\gamma}\right].$$

These are the "toughest" problems of mathematics. Among them:

- the problem of salesman,
- the determination of the vacuum states in random systems.

Consider now a number A, expressed, say, in the usual decimal basis. The number of its digits is about $\log_{10} A$. In this context, a polynomial algorithm scales as

$$\tau_{poly} \sim (\log_{10} A)^{\alpha},$$

whereas an exponential algorithm scales as the number A itself, since

$$\tau_{\exp} \sim \exp\left[\beta \log A\right] \sim A^{\beta}.$$

Let us discuss then the primality test. In its simplest version it consists in the Eratosthenes's sieve. This means, in practice, testing the divisibility of the number A for all numbers $B \leq \sqrt{A}$, hence

$$\tau \simeq A^{1/2},$$

and we have an exponential algorithm! Only recently, it has been proved by Agrawal et al. that there exists a primality test with polynomial complexity. The same story happens for the factorization problem. In fact, is its naive implementation, the factorization algorithm scales as well as $\tau \simeq A^{1/2}$. Until now, it doesn't still exist a factorization algorithm with polynomial complexity.
Let us see how Quantum Mechanics may help in this respect.

4.5 A Primality Test in Quantum Mechanics

Suppose we have constructed a potential $V(x)$ which has as eigenvalues the prime numbers sequence (this can be reasonably done in a semi–classical approximation). We can construct an algorithm for a primality test with zero complexity, i.e. it does not scale or depend on the number of digits of the number A under check!

FIGURE

Let us denote by G (in honour of Gauss) the device furnishing the primality test. If a wave of energy $E = \hbar\omega A$ is transmitted, A is a prime. Otherwise, it is composite, and it remains the problem of determining its factors : $A = p_1 \cdot ... \cdot p_k$.
For simplicity, assume they are all different; the following discussion can be easily generalized. The question is: how Quantum Mechanics does solve the factorization problem?

4.6 Factorization Problem in Quantum Mechanics

Quantum Mechanics works well with sums of numbers rather than with products. Hence take initially the logarithm of the numbers under check and promote them to energies. From the unique factorization theorem, we know that any number can be written in an unique way as a product of primes: $A = p_1 \cdot ... \cdot p_k$, so

$$\log A = \sum_{i=1}^{k} \log p_i.$$

In the last expression, single out one term (any of them), and write

$$\log A = \log \widehat{p}_j + \sum_{i \neq j}^{k} \log p_i \equiv \log \widehat{p}_j + \log \widehat{N}_j,$$

where $\widehat{N}_j = A/p_j$.
Let us construct now (by the inversion formula) a potential $V_{\log p}(x)$ which possesses as eigenvalues all and only the logarithms of primes. Let us construct also another potential $W_{\ln N}(y)$ whose eigenvalues, instead, are all

the logarithms of the integer numbers. Consider now the 2–dimensional Hamiltonian

$$H(x,y) = \frac{1}{2m}\left[p_x^2 + p_y^2\right] + V(x) + W(y).$$

With respect to this Hamiltonian, the eigenvalues associated with a number A of k prime factors is k–times degenerate. This is obvious since one can choose any term $\ln \widehat{p}_j$ in the previous decomposition. Denote the k–th element of the basis of this degenerate level as

$$|\widehat{p}_j\rangle \left|\widehat{N}_j\right\rangle.$$

Suppose that we switch on an energy precisely equally to $\log A$ into the system. According to Von Neumann's theorem, the system immediately after will be in a linear combination of these k states:

$$|\psi(t)\rangle = \sum_{j=1}^{k} c_j \,|p_j, N_j; t\rangle.$$

This state, under time evolution, remains always in the original degenerate subspace.
Suppose now that we send on the system an electromagnetic wave, polarized precisely along the y–axis. In a dipole approximation the system couples to the operator $\widehat{y}$. This operator induces a transition among the levels of the $W(y)$ potential, in particular the most important ones are between the next neighborhoods

$$|\ln N\rangle \begin{array}{c} \nearrow \\ \\ \searrow \end{array} \begin{array}{l} |\ln N + 1\rangle \\ \\ |\ln N + 1\rangle \end{array}$$

and the spectrum of emission/absorption of the system becomes the one of k multiplets.

FIGURE

If the original system was an harmonic oscillator, the splitting of these multiplets would be always the same, since the energy levels of the harmonic oscillator are equally spaced.

FIGURE

But is this case the potential along y has eigenvalues which are $\log N$, hence

$$\Delta E_{\pm} = \ln \frac{(N \pm 1)}{N} \simeq \pm \frac{1}{N},$$

i.e. the separation of the energy levels contains information on the level. In this way, we have two basic informations.

1. How many factors the number A is made of, since it is equal to the number of multiplets,

2. From their splittings we can derive $1/\widehat{N}_i$, taken the largest one (i.e. the one associated to the smallest $\widehat{N}_i$), one determines $\widehat{N}_i$. Dividing the original number by $\widehat{N}_i$, one extracts $\widehat{p}_i$ and the problem has reduced its difficulty to a step less.

Continuing in this way, in k measurements one ends up with a complete factorization of the original number A.

4.7 Elementary facts about prime numbers

- Each odd prime number is always of the form

$$4n \pm 1.$$

- All prime numbers of the form $4n + 1$ can be written as sum of two squares, while the other ones cannot.

4.8 Fermat's little theorem

This is a famous result in elementary number theory.

Theorem 2. *If a is any integer and p is a prime, then $a^p - a$ is divisible by p, or*

$$a^{p-1} \equiv 1 \qquad (mod p)\,.$$

This theorem has been generalized by Euler. He introduced the function $\phi\,(m)$, called *Euler's ϕ function* or *totient function*. It counts the number of positive integers r smaller than m that are coprime to m.
Example. $m = 10$, $r = 1, 3, 7, 9$, $\phi\,(10) = 4$.

For a prime number p, each of the previous $r = 1, 2, ..., p-1$ is coprime to p, hence

$$\phi(p) = p - 1.$$

It is easy to prove that

$$\phi(p^\alpha) = (p-1)\, p^{\alpha-1} = p^\alpha \left(1 - \frac{1}{p}\right).$$

In fact, among the p^α numbers less than the number $\phi(p^\alpha)$, $p^{\alpha-1}$ are divisible by p, hence the result.
The Euler function is a multiplicative function, i.e.

$$\phi(n \cdot m) = \phi(n)\,\phi(m) \qquad \text{if } (n, m) = 1.$$

Therefore, it is easy to calculate for any number $m = \prod_i p_i^{\varepsilon_i}$

$$\phi(m) = \prod_i \phi(p_i^{\varepsilon_i}) = \prod_i (p_i - 1)\, p_i^{\varepsilon_i - 1} = m \prod_i \left(1 - \frac{1}{p_i}\right).$$

Notice that this function depends on the multiplicative properties of the considered number so, it has wild jumps

$$\phi(n) = 1, 1, 2, 2, 4, 2, 6, 4, 6, 4, 10, 4, 12, 6, 8, 8, 16, ...$$

$$n = \quad 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17...$$

With the above definitions, the Euler theorem states that

$$b^{\phi(m)} \equiv 1 \qquad (mod m) \qquad if \qquad (b, m) = 1.$$

We will estimate later on the behaviour of $\phi(m)$ and its average properties. Note that

$$\frac{\phi(n)}{n} = \prod_{p_i | n} \left(1 - \frac{1}{p_i}\right).$$

We can convert this product over primes dividing n into a product over all primes by a probabilistic argument. Indeed, the probability that any "old" prime will divide n is $1/p_i$ and the probability that it will not is $1 - 1/p_i$. In the latter case, the prime p_i "contributes" the factor 1 to the product. Hence

$$\prod_{p_i | n} \left(1 - \frac{1}{p_i}\right) \simeq \prod_{p_i} \left[\left(1 - \frac{1}{p_i}\right)\frac{1}{p_i} + 1 \cdot \left(1 - \frac{1}{p_i}\right)\right] = \prod_{p_i} \left(1 - \frac{1}{p_i^2}\right).$$

Hence $\langle \phi(n)/n \rangle \simeq \left(\sum_n \frac{1}{n^2}\right)^{-1} = \frac{6}{\pi^2}$.

4.9 Prime numbers and polynomials

We mentioned before that it does not exists a close formula for the value of prime numbers. However, there is, first of all, an excellent estimate of the n–th prime, given by

$$p_n \simeq n \log n + n (\log \log n - 1) + O\left(\frac{n \log \log n}{\ln n}\right).$$

This expression can be derived by knowing the function $\prod (x)$ which counts the primes $\leq x$.
It is also interesting to notice that there is a remarkable number of polynomial formulas which furnish prime numbers for long sequences of consecutive integers. Such is, for example, the polynomial

$$P(x) = x^2 + x + 41,$$

(Euler!) . $P(x)$ is prime for the 40 consecutive values $x = 0, 1, 2, ..., 39$!
Observe that

Lemma 1. *A polynomial with integer coefficients cannot take on prime values for all integral values of the argument.*

Proof. Suppose to the contrary that $P(n)$ is prime for every n. Let α be an arbitrary positive integer and put $\beta = P(\alpha)$. Consider now the sequence

$$P(\alpha + \beta); P(\alpha + 2\beta); P(\alpha + 3\beta) ...$$

By virtue of the binomial theorem, for each $n \in \mathbb{N}$

$$P(\alpha + n\beta) - P(\alpha) = \text{integral multiple of } \beta.$$

Hence $P(\alpha + n\beta)$ is also an integral multiple of β and, since this value must be a prime, it can be only β. Thus

$$P(\alpha + n\beta) - P(\alpha) = P(\alpha + n\beta) - \beta = 0$$

for every positive integer n, contradicting the fact that a polynomial can only have finitely many roots.
Other remarkable polynomial expressions are

$$P(n) = n^2 - 79n + 1601,$$

with $P(n)$ prime for $n = 1, 2, ...79$.

$$P(n) = n^2 + n + 17$$

prime for $n = 0, ..., 16$,

$$P(n) = 2n^2 + 29,$$

prime for $n = 0, 1, ..., 28$.
These quadratic expressions plotted on a spiral lattice (square spiral) produce straight lines!

16	15	14	13
5	4	3	12
6	1	2	11
7	8	9	10

.

What happens on a triangular spiral lattice?

4.10 Distribution of prime numbers

How are prime numbers distribute among the integer ones? This question was posed for the first time by Gauss and it has given rise to extraordinary developments in analytic number theory, culminating with the work of Riemann and the prime number theorem by Chebyshev, de la Vallée–Poussin and Hadamard. The Gauss's contribution was almost empirical, i.e. he took the table of primes known at that time and he simply counted the relative frequency of primes among the integers. It should be noticed that

(i) the primes become rarer and rarer, larger they get

(ii) apart a certain regularity in their mean density, their distribution seems rather irregular.

In few words, prime numbers resemble the behaviour of statistical mechanics, i.e. smooth properties of the ensemble can be rather irregular for and particular representative.
The determination of $\pi(x)$ by Riemann will be the topic of the future lectures. Here we will present a simple argument which permits to derive the correct asymptotic estimate

$$\pi(x) \simeq \frac{x}{\ln x}$$

It should be noticed that the close formula for the n–th prime number could be obtained if one knew how to invert the function $\pi(x)$, i.e.

$$p_n = \pi^{-1}(n).$$

FIGURE

The simple proof is based on the observation that the probability that an arbitrary integer is divisible by the prime p_i is $1/p_i$. Said in another way, one number over p_i is precisely divisible by it (Eratosthenes's sieve!). Thus, the probability that it is not divisible by p_i is $(1-1/p_i)$. Assuming now that divisibility by different primes is not correlated (we will see that, actually, it is not the case), the probability that a number x is not divisible by any prime below it is expressed as

$$W(x) \simeq \left(1-\frac{1}{2}\right)\left(1-\frac{1}{3}\right)\left(1-\frac{1}{5}\right)...\simeq \prod_{p_i\leq x}\left(1-\frac{1}{p_i}\right).$$

If x is not divisible by any prime below it, it is of course a prime. Taking the logarithm of both terms and expanding it for small $1/p_i$, we have

$$\ln W(x) \simeq \sum_{p_i<x} \ln\left(1-\frac{1}{p_i}\right) \simeq \sum_i \frac{1}{p_i}.$$

The last sum on primes can be expressed as a sum on integers by using the same function $W(x)$. In fact,

$$\sum_i \frac{1}{p_i} \simeq \sum_n \frac{W(n)}{n} \simeq \int_1^n \frac{W(t)}{t}dt.$$

Hence, we arrive to the expression

$$\log W(x) \simeq -\int_1^x \frac{W(t)}{t}dt.$$

Deriving both terms we obtain the differential equation

$$\frac{1}{W^2(x)}\frac{dW}{dx} = -\frac{1}{x},$$

whose solution is

$$W(x) \simeq \frac{1}{\log x}.$$

This function expresses the probability that an integer x is a prime. Their number up to x is then

$$\Pi(x) = \int_1^x dtW(t) \simeq \int_1^x \frac{dt}{\ln t} \equiv Li(x) \simeq \frac{x}{\ln x},$$

i.e., the result by Gauss.
We will say that the exact expression for the smooth part of $\Pi(x)$ will be given by

$$\Pi(x) \equiv R(x) = Li(x) - \frac{1}{2}Li\left(\sqrt{x}\right) - \frac{1}{3}Li\left(\sqrt[3]{x}\right) + ...$$

$$\equiv \sum_{n=1}^{\infty} \frac{\mu(n)}{n} Li\left(x^{\frac{1}{n}}\right),$$

where $\mu(n)$,$n = p_1...p_k$ is the Moebius coefficient, defined by

$$\mu(n) = \begin{cases} 1 & n = 1 \\ 0 & ... \\ (-1)^k & otherwise \end{cases}.$$

More surprising is the fact that there exists a close exact formula for $\Pi(x)$, able to follow also its jumps. This formula involves the nontrivial zeros of the Riemann zeta function. Indeed

$$\Pi(x) = \lim_{k\to\infty} R_k(x),$$

where

$$R_k(x) \equiv R(x) + \sum_{l=-k}^{k} R(x^{\rho_l}),$$

and ρ_l is the l–th zero of the Riemann zeta function

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}.$$

The first nontrivial zeros have all real part equal to $1/2$, whereas their imaginary part is given by

TABLE

4.11 Probabilistic methods

By using the previous result on the distribution of primes, we can have a fair estimate of several questions in number theory. In the following we will discuss some of them.

$$\sum_i \frac{1}{p_i} \to \infty$$

since

$$\sum_i \frac{1}{p_i} \simeq \sum_n \frac{W(n)}{n} \simeq \int_1^\Lambda \frac{dn}{n \ln n} \simeq \log\log\Lambda.$$

4.11.1 Coprime probability

What is the probability that two numbers (a, b) randomly chosen are co–primes?

The probability that one of them is divisible by p_i is $\frac{1}{p_i}$ and the probability that both are divisible by the same prime, assuming no correlations, is $1/p_i^2$. Hence the probability that they are not both divisible by p_i is

$$P = \prod_i \left(1 - \frac{1}{p_i^2}\right) = \frac{6}{\pi^2}.$$

Since

$$\prod_i \left(1 - \frac{1}{p_i^2}\right)^{-1} = \prod_i \left(1 + \frac{1}{p_i^2} + \frac{1}{p_i^4} + ...\right) = \sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}.$$

4.11.2 Square–free probability

What is the probability that a randomly chosen integer n is square free (i.e. not divisible by a square)? The probability is equal to the above one, i.e.

$$P = \frac{6}{\pi^2} = 0.608...$$

In fact, if an integer is square free, it must not be divisible for the same prime p_i more than once. Hence, either it is not divisible by p_i or, if it is, it is not divisible again. Thus

$$P_i \simeq \left(1 - \frac{1}{p_i}\right) + \frac{1}{p_i}\left(1 - \frac{1}{p_i}\right) = 1 - \frac{1}{p_i^2},$$

and taking the product on all i, we obtain the above result.

4.11.3 Merten's formula

The previous estimate of the product on primes can be refined as

$$\prod_{p_i<x}\left(1-\frac{1}{p_i}\right)\simeq\frac{e^{-\gamma}}{\ln x},$$

where γ is the Euler–Mascheroni constant

$$\gamma=0.57721..., \qquad e^{-\gamma}=0.5614...$$

The above number gives, somehow, an estimate of the correlation among prime numbers. This means that in the previous derivation of the "prime number theorem", we should take the product on the primes not less than x (this would be excessive any way), but

$$\prod_{p_i<x^{\exp(-\gamma)}}\left(1-\frac{1}{p_i}\right)\simeq\frac{1}{\ln x}.$$

4.12 Mersenne numbers

These are the primes of the form

$$M_p=2^p-1,$$

where p is a prime (observe that if p were not a prime, say $p=n\cdot m$, we would have

$$2^{n\cdot m}-1=(2^n-1)\left(2^{n(m-1)}+2^{n(m-2)}+...1\right),$$

i.e. the number is composite). Moreover, not for any prime p is 2^p-1 a prime number.
Notice that any Mersenne number has as a companion a perfect even number, i.e. a number equal to the sum of its divisors:

$$P=M_p2^{p-1}.$$

The above formula is a necessary and sufficient condition in order for an even number to be perfect. It is still an open question whether there exist odd perfect numbers.

There exists a remarkable conjecture, due to Wagstaff, concerning these numbers. Given a number of the form $2^p - 1$, the probability that it is prime is about

$$\frac{1}{\ln(2^p - 1)} \simeq \frac{1}{p \ln 2}.$$

Among the numbers of this form, the Mersenne's ones are quite special. Indeed, it can be shown that if a prime q divides $2^p - 1$, then q must be of the form $q = kp + 1$ for some $k \in \mathbb{N}$. So, no "small" primes can divide a number of the form $2^p - 1$. Qualitatively, this implies that such numbers have a bigger probability of being primes than the "prime theorem" estimate. To quantify it, we will argue on the reverse, namely, the fact that for each prime $q < p$, the probability that q divides $2^p - 1$ is zero. This increases the probability of $2^p - 1$ to be a prime by $\left(1 - \frac{1}{q}\right)^{-1}$. Therefore, for all primes less than p, we have

$$\prod_{q<p} \left(1 - \frac{1}{q}\right)^{-1} \simeq e^{\gamma} \ln p.$$

Combining now the two probabilities, together with the one that p is a prime, we obtain for the probability that $2^p - 1$ is prime,

$$\frac{e^{\gamma} \ln p}{\ln p \ln(2^p - 1)} \simeq \frac{e^{\gamma}}{\ln 2p}.$$

Therefore, for the total number of Mersenne primes less than x we have

$$\prod Mers(x) \simeq \frac{e^{\gamma}}{\ln 2} \sum_{p<\ln x} \frac{1}{p} = \frac{e^{\gamma}}{\ln 2} \ln \ln x.$$

There is a remarkable fit of this formula. This can also be expressed as follows: If x is the n–th Mersenne number, so that

$$n = \prod Mers(x),$$

Then

$$\log \log x \simeq \frac{\ln 2}{e^{\gamma}} n.$$

This conjecture in turn implies, since $\log \log x \to \infty$, that there exist infinitely many Mersenne primes. But the quantity of Mersenne numbers less than x os approximately $\pi(\log x)$, i.e. the quantity of primes less than $\log x$ (because $\log_2 x$ differs only by a constant factor $\log 2$ from $\log x$). Since

$$\pi(\log x) \simeq \frac{\log x}{\log \log x}$$

is much bigger than $\log\log x$, the Wagstaff conjecture implies also that there are infinitely many composite Mersenne numbers.

4.13 Arithmetical functions

Sequences of real or complex numbers play a major role in number theory. They are called arithmetical functions.

Definition 2. *An arithmetical function is a function f:* $\mathbb{N} \to \mathbb{R}$ *or* $\mathbb{C}$.

There are many classical examples of arithmetical functions.

Definition 3. *An arithmetical function* $f(n)$ *is said to be multiplicative if*

$$f(n \cdot m) = f(n) \cdot f(m), \qquad (n, m) = 1.$$

The multiplicative function $f(n)$ *is said to be completely multiplicative if*

$$f(n \cdot m) = f(n) \cdot f(m), \qquad for\ all\ n, m \in \mathbb{N}.$$

4.14 Dirichlet characters

There are also *periodic arithmetical functions*, which are sequences of real of complex numbers, periodic with period T:

$$f(n + T) = f(n).$$

The most important example is provided by the Dirichlet characters.

Definition 4. *A Dirichlet character of the conductor* T *is a function* $\chi(n)$ *satisfying the following axioms:*
1) periodicity: $\chi(n + T) = \chi(n)$
2)multiplicativity: $\chi(nm) = \chi(n)\chi(m)$
3) $\chi(n) = 0$, *if* $(n, T) \neq 1$.

The *principal character* χ_T of conductor T is given by

$$\chi_T(n) = \begin{cases} 1 & if \quad (n, T) = 1 \\ 0 & if \quad (n, T) \neq 1 \end{cases}.$$

This definition is motivated by the role played by Dirichet characters in group theory.

Chapter 5

The Riemann ζ function

The Riemann $\zeta(s)$ function is defined for $\mathbb{R}es \geq 1$ by the following relation

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}. \tag{5.1}$$

The series is absolutely convergent for $\sigma > 1$, where $s = \sigma + it$. The following result holds:

$$\sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_{p_i} \frac{1}{\left(1 - \frac{1}{p_i^s}\right)}. \tag{5.2}$$

Expanding the factor $\left(1 - \frac{1}{p_i^s}\right)^{-1}$ in the domain $\sigma > 1$, we have

$$\prod_{p_i} \frac{1}{\left(1 - \frac{1}{p_i^s}\right)} = \prod_i \left[1 + \frac{1}{p_i^s} + \frac{1}{p_i^{2s}} + \frac{1}{p_i^{3s}} + ...\right] =$$

$$1 + \left(\frac{1}{p_1^s} + ... + \frac{1}{p_k^s}\right) + \left(\frac{1}{p_1^s p_2^s} + ...\right) + ...$$

Each term of the product is an integer, due to the unique factorization theorem, hence one obtains eq. (5.2). The above formula (as well as the others which we will discuss below) is actually a particular example of a more general formula involving multiplicative functions.
For these functions we have

$$f\left(p_1^{\alpha_1} p_2^{\alpha_2} ... p_k^{\alpha_k}\right) = f\left(p_1^{\alpha_1}\right) f\left(p_2^{\alpha_2}\right) ... f\left(p_k^{\alpha_k}\right)$$

and the general identity

$$\sum_{n=1}^{\infty}\frac{f(n)}{n^s}=\prod_{p_i}\left[1+\frac{f(p_i)}{p_i^s}+\frac{f\left(p_i^2\right)}{p_i^{2s}}+\frac{f\left(p_i^3\right)}{p_i^{3s}}+...\right].$$

The identity (5.1) was already established by Euler, but it was Riemann who had the idea of studying the ζ function in terms of the complex variable s. It is easy to see that $\zeta(s)$ has no zeroes for $\sigma>1$. In fact, for $\sigma>1$, we can use its product representation of this function and we have

$$\left(1-\frac{1}{2^s}\right)\left(1-\frac{1}{3^s}\right)\left(1-\frac{1}{4^s}\right)\cdot...\cdot\left(1-\frac{1}{p^s}\right)\zeta(s)=1+\frac{1}{m_1^s}+\frac{1}{m_2^s}+...$$

where m_1, m_2,... are all integers whose prime factors exceed P. Hence

$$\left|\left(1-\frac{1}{2^s}\right)\left(1-\frac{1}{3^s}\right)\left(1-\frac{1}{4^s}\right)\cdot...\cdot\left(1-\frac{1}{p^s}\right)\zeta(s)\right|\geq\rightarrow 1-\frac{1}{(p+1)^{\sigma}}-...-\frac{1}{(p+k)^{\sigma}}>0$$

if P is large enough. Therefore $|\zeta(s)|>0$.
Said in another way, a product can vanish if and only if at least one of the factors vanishes. Since the general expression is

$$\frac{p_i^s}{p_i^s-1}=\frac{e^{s\ln p_i}}{e^{s\ln p_i}-1}=\frac{e^{\sigma\ln p}\left[\cos(t\ln p)+i\sin(t\ln p)\right]}{e^{\sigma\ln p}\left[\cos(t\ln p)+i\sin(t\ln p)\right]-1},$$

we see that the generic term never vanishes. On the other hand, the point $s=1$ is singular for $\zeta(s)$.

5.1 Relation between $\zeta(s)$ and $\prod(x)$

There is a deep relation between the behaviour of $\zeta(s)$ and the function $\pi(x)$, which counts the primes less than x. It can be seen as follows. For $\sigma>1$ (where Euler's formula is valid), we have

$$\log\zeta(s)=-\sum_{p}\ln\left(1-\frac{1}{p^s}\right)=-\sum_{n=2}^{\infty}\left[\pi(n)-\pi(n-1)\right]\ln\left(1-\frac{1}{n^s}\right)=$$

$$-\sum_{n=2}^{\infty}\pi(n)\left[\ln\left(1-\frac{1}{n^s}\right)-\ln\left(1-\frac{1}{(n+1)^s}\right)\right]=$$

$$\sum_{n=2}^{\infty}\pi(n)\int_n^{n+1}\frac{s}{x\left(x^s-1\right)}dx=s\int_2^{\infty}\frac{\pi(x)\,dx}{x\left(x^s-1\right)},$$

i.e.

$$\ln\zeta(s)=s\int_2^{\infty}\frac{\pi(x)\,dx}{x\left(x^s-1\right)}.$$

5.2 Moebius function

For $\sigma > 1$, we define

$$Z_M(s) = \frac{1}{\zeta(s)} = \prod_p \left(1 - \frac{1}{p^s}\right) = \sum_{n=1}^{\infty} \frac{\mu(n)}{n^s}, \tag{5.3}$$

where

$$\mu(n) = \begin{cases} 1 & n = 1 \\ (-1)^k & n = p_1 ... p_k, \quad p_i \neq p_j \\ 0 & n = p_1^2 ... \end{cases},$$

i.e. $\mu(n)$ is zero each time that the number n contains more than once the same factor p_i. From this respect, prime numbers appear as "fermionic" particles!
The arithmetic function $\mu(n)$ is known as the Moebius function. It plays a fundamental role in analytic number theory, since it rules the convolution of series. Let us study its main properties.
First of all

$$\sum_{d|q} \mu(d) = \begin{cases} 1 & q = 1 \\ 0 & q > 1 \end{cases},$$

This identity follows from the relations

$$1 = Z_M(s)\,\zeta(s) = \sum_{m=1}^{\infty} \frac{1}{m^s} \sum_{n=1}^{\infty} \frac{\mu(n)}{n^s} = \sum_{q=1}^{\infty} \frac{1}{q^s} \sum_{d|q} \mu(d).$$

The Moebius function enters the so called inversion formulas, i.e.

$$g(q) = \sum_{d|q} f(d)$$

$$\Downarrow$$

$$f(d) = \sum_{d|q} \mu\left(\frac{q}{d}\right) g(d).$$

The above formula can be written in a variety of ways:

$$g(x) = \sum_{n=1}^{\infty} f\left(\frac{x}{n}\right) \leftrightarrow f(x) = \sum_{n=1}^{\infty} \mu(n)\, g\left(\frac{x}{n}\right), \tag{5.4}$$

$$H(x) = \sum_{n=1}^{\infty} h(nx) \leftrightarrow h(x) = \sum_{n=1}^{\infty} \mu(n)\, H(nx). \tag{5.5}$$

Let us see the proof of (5.4). Making the change of variable $x = t/m$ and summing on m, we get

$$\sum_{m=1}^{\infty} f\left(\frac{t}{m}\right) = \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} \mu(n)\, g\left(\frac{t}{nm}\right) = \sum_{q} g\left(\frac{t}{q}\right) \sum_{d|q} \mu(d) = g(x),$$

since $\sum_{d|q} \mu(d) = \delta_{q,1}$.

5.3 The Mangoldt function $\Lambda(n)$

Taking the logarithm and differentiating eq. (5.2), we have for $\sigma > 1$

$$\frac{\zeta'(s)}{\zeta(s)} = -\sum_{p} \frac{\ln p}{p^s}\left(1 - \frac{1}{p^s}\right)^{-1} = -\sum_{p} \ln p \sum_{m=1}^{\infty} \frac{1}{p^{ms}} =$$

$$= -\sum_{n=2}^{\infty} \frac{\Lambda(n)}{n^s},$$

where

$$\Lambda(n) = \begin{cases} \log p & \text{if } n = p \text{ or a power of } f \\ 0 & \text{otherwise} \end{cases}.$$

Integrating we have

$$\log \zeta(s) = \sum_{n=2}^{\infty} \frac{\Lambda_1(n)}{n^s},$$

where $\Lambda_1(n) = \Lambda(n)/\ln n$.
The Riemann function enters a variety of identities. For instance,

$$\frac{\zeta(s-1)}{\zeta(s)} = \sum_{n=1}^{\infty} \frac{\phi(n)}{n^s} \qquad \sigma > 2,$$

where $\phi(n)$ is the Euler function. In fact

$$\frac{\zeta(s-1)}{\zeta(s)} = \prod_{p}\left(\frac{1-p^{-s}}{1-p^{1-s}}\right) = \prod_{p}\left\{\left(1-\frac{1}{p^s}\right)\left(1+\frac{p}{p^s}+\frac{p^2}{p^{2s}}+...\right)\right\} =$$

$$\prod_{p}\left\{1+\left(1-\frac{1}{p}\right)\left(\frac{p}{p^s}+\frac{p^2}{p^{2s}}+...\right)\right\}.$$

Observe that, if $n = p_1^{\alpha_1}...p_k^{\alpha_k}$

$$\phi(n) = n\left(1 - \frac{1}{p_1}\right)...\left(1 - \frac{1}{p_k}\right).$$

Hence we obtain the above formula.
We also have

$$\sum_p \frac{1}{p^s} = \sum_{n=1}^{\infty} \frac{\mu(n)}{n} \log \zeta(ns).$$

To prove it, notice that

$$\log \zeta(s) = \sum_m \sum_p \frac{1}{mp^{ms}} = \sum_{m=1}^{\infty} \frac{P(ms)}{m},$$

with $P(s) = \sum_p p^{-s}$.
Hence

$$\sum_{n=1}^{\infty} \frac{\mu(n)}{n} \log \zeta(ns) = \sum_{n=1}^{\infty} \frac{\mu(n)}{n} \sum_{m=1}^{\infty} \frac{P(mns)}{m} =$$

$$\sum_{r=2}^{\infty} \frac{P(rs)}{r} \sum_{n|2} \mu(n) = P(s).$$

Exercise. Prove that

$$\prod_{p=2}^{\infty} \frac{p^2+1}{p^2-1} = \frac{5}{2}.$$

5.4 Analyticity properties of $\zeta(s)$ and its functional equation

The function $\zeta(s)$ is regular for all values of s except $s = 1$, where there is a simple pole with residue 1. It satisfies the functional equation

$$\zeta(s) = 2^s \pi^{s-1} \sin \frac{\pi s}{2} \Gamma(1-s) \zeta(1-s).$$

This equation can be written in a more symmetric way: introducing the function

$$\phi(s) \equiv \frac{1}{2} s(s-1) \pi^{-\frac{s}{2}} \Gamma\left(\frac{s}{2}\right) \zeta(s)$$

we have

$$\phi(s) = \phi(1-s).$$

We know that $\zeta(s)$ is defined for $Res > 1$. How can we extend analytically its definition to the complex plane? Consider the Γ function: $\Gamma(s) = \int_0^\infty dx x^{s-1} e^{-x}$. With the substitution $x \to nx$, we have

$$\Gamma(s) = n^s \int_0^\infty dx x^{s-1} e^{-nx},$$

hence

$$\frac{\Gamma(s)}{n^s} = \int_0^\infty dx x^{s-1} e^{-nx}.$$

Summing now on n, we have

$$\Gamma(s)\zeta(s) = \int_0^\infty dx \frac{x^{s-1}}{e^x - 1}.$$

Consider now the integral

$$I(s) = \int_C \frac{z^{s-1}}{e^z - 1} dz,$$

where the contour C starts at infinity on the positive axis, encircles the origin once in the positive direction excluding the points $\pm 2\pi i$, $\pm 4\pi i, \ldots$ and returns to the positive axis again.

FIGURE

If $Res > 1$, we can shrink the circle around the origin to zero, so that

$$I(s) = -\int_0^\infty \frac{x^{s-1}}{e^x - 1} dx + \int_0^\infty \frac{\left(xe^{2\pi i}\right)^{s-1}}{e^x - 1} dx =$$

$$\left(e^{2\pi i s} - 1\right) \int_0^\infty \frac{x^{s-1}}{e^x - 1} dx = \left(e^{2\pi i s} - 1\right) \Gamma(s)\zeta(s) = \frac{2\pi i e^{i\pi s}}{\Gamma(1-s)} \zeta(s).$$

Since $\Gamma(s)\Gamma(1-s) = \frac{\pi}{\sin \pi s}$, we obtain

$$\zeta(s) = \frac{e^{-i\pi s}\Gamma(1-s)}{2\pi i} \int_C \frac{z^{s-1}}{e^z - 1} dz.$$

This formula has been proved for $Res > 1$. However, the integral is uniformly convergent in any finite region of the s–plane and so it is an integral

function of s. Hence, it defines the analytic continuation of $\zeta(s)$ for all values of s. The only possible singularities are the poles of $\Gamma(1-s)$, i.e. $s = 1, 2, 3, ...$ We know already that $\zeta(s)$ is regular at $s = 2, 3, 4...$ and this follows immediately from Cauchy theorem (the contour, in these cases, does not encircle any singularities).
The only possible singularity is a simple pole at $s = 1$. In this case

$$I(1) = \int_C \frac{dz}{e^z - 1} = 2\pi i,$$

$$\Gamma(1-s) = -\frac{1}{s-1} + ...$$

Therefore

$$\zeta(s) \simeq \frac{1}{s-1}, \qquad s \to 1.$$

Notice that if s is any integer (negative or null), the integrand in $I(s)$ is one–valued, and $I(s)$ can be evaluated by the theorem of residues. Since

$$\frac{x}{e^x - 1} = \sum_{n=0}^{\infty} B_n \frac{x^n}{n!},$$

we have

$$\zeta(0) = -\frac{1}{2}, \qquad \zeta(-2m) = 0,$$

$$\zeta(1-2m) = (-1)^m \frac{B_{2m}}{2m}.$$

In order to derive the functional equation of $\zeta(s)$, consider the integral along the contour C_M

FIGURE

Inside the contour there are now poles at

$$\pm 2\pi i, \pm 4\pi i, ..., \pm 2n\pi i.$$

The residues at $2m\pi i$ and $-2m\pi i$ are together

$$\left(2m\pi e^{\frac{i\pi}{2}}\right)^{s-1} + \left(2m\pi e^{\frac{3i\pi}{2}}\right)^{s-1} = (2m\pi)^{s-1} e^{i\pi(s-1)} 2\cos\frac{\pi(s-1)}{2} =$$

$$-2(2m\pi)^{s-1} e^{i\pi s} \sin\frac{\pi s}{2}.$$

Hence

$$I(s) = \int_{C_M} \frac{z^{s-1}}{e^z - 1} dz + 4\pi i e^{i\pi s} \sin\frac{\pi s}{2} \sum_{m=1}^{n} (2m\pi)^{s-1}.$$

Consider now $Res < 0$, and $n \to \infty$. The function $1/(e^x - 1)$ is bounded on the contour C and $z^{s-1} = 0\left(|z|^{s-1}\right)$, hence $\int_{C_M} \to 0$, i.e.

$$I(s) = 4\pi i e^{i\pi s} \sin\frac{\pi s}{2} \sum_{m=1}^{\infty} (2m\pi)^{s-1} = 4\pi i e^{i\pi s} \sin\frac{\pi s}{2} (2\pi)^{s-1} \zeta(1-s),$$

from which one derives the functional equation.

5.4.1 Consequences of the functional equation

- Link with the Bernoulli numbers:

$$\zeta(2m) = 2^{2m-1}\pi^{2m}\frac{B_{2m}}{(2m)!}$$

- For the derivative at zero:

$$\zeta'(0) = -\frac{1}{2}\ln 2\pi.$$

From the functional equation,

$$-\frac{\zeta'(1-s)}{\zeta(1-s)} = -\ln 2\pi - \frac{1}{2}\pi\tan\frac{\pi s}{2} + \frac{\Gamma'(s)}{\Gamma(s)} + \frac{\zeta'(s)}{\zeta(s)}.$$

Near $s \simeq 1$, $\frac{1}{2}\pi\tan\frac{\pi s}{2} \simeq -\frac{1}{s-1}$, and $\frac{\Gamma'(s)}{\Gamma(s)} = -\gamma$, so

$$\frac{\zeta'(s)}{\zeta(s)} = \frac{-\frac{1}{(s-1)^2} + A + ...}{\frac{1}{(s-1)} + \gamma + A(s-1)} = -\frac{1}{s-1} + \gamma.$$

Hence

$$-\frac{\zeta'(0)}{\zeta(0)} = -\ln 2\pi.$$

The functional equation for the Riemann function can be derived in many different ways. One is, for instance, to use the Poisson resummation formula

$$\sum_{-\infty}^{+\infty} f(n) = \sum_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(x)\cos 2\pi n x dx.$$

Let us sketch the original proof by Riemann.
Make the change of variable $x \to n^2 \pi x$ in the Γ function $\Gamma\left(\frac{s}{2}\right)$:

$$\int_0^\infty x^{\frac{s-1}{2}} e^{-n^2 \pi x} dx = \frac{\Gamma\left(\frac{s}{2}\right)}{n^s \pi^{\frac{s}{2}}}.$$

For $Res > 1$, summing on n, we have

$$\frac{\Gamma\left(\frac{s}{2}\right)\zeta(s)}{\pi^{\frac{s}{2}}} = \int_0^\infty x^{\frac{s}{2}-1} \psi(x)\, dx$$

$$\psi(x) \equiv \sum_{n=1}^{\infty} e^{-n^2 \pi x}.$$

This function is a Jacobi θ–function. It satisfies the basic functional identities

$$\sum_{-\infty}^{+\infty} e^{-n^2 \pi x} = \frac{1}{\sqrt{x}} \sum_{-\infty}^{+\infty} e^{-n^2 \frac{\pi}{x}},$$

$$2\psi(x) + 1 = \frac{1}{\sqrt{x}} \left[2\psi\left(\frac{1}{x}\right) + 1\right].$$

After some manipulations, we get

$$\Gamma\left(\frac{s}{2}\right)\zeta(s)\,\pi^{-\frac{s}{2}} = \int_0^1 x^{\frac{s}{2}-1} \psi(x)\, dx + \int_1^\infty x^{\frac{s}{2}-1} \psi(x)\, dx =$$

$$\frac{1}{s(s-1)} + \int_1^\infty \left[x^{-\frac{s}{2}-1} + x^{\frac{s}{2}-1}\right] \psi(x)\, dx.$$

The last integral is convergent for all values of s and therefore this formula remains true, by analytic continuation, for all values of s. But the right hand side is invariant under the substitution $s \to 1 - s$. Hence

$$\pi^{-\frac{s}{2}} \Gamma\left(\frac{s}{2}\right) \zeta(s) = \pi^{-\frac{1}{2}+\frac{s}{2}} \Gamma\left(\frac{1-s}{2}\right) \zeta(1-s).$$

5.5 Some consequences of Euler's formula

The Euler's formula reads

$$\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s} = \prod_p \left(1 - \frac{1}{p^s}\right)^{-1}.$$

The relation with the function $\pi(x)$:

$$\ln\zeta(s) = -\sum_p \ln\left(1-\frac{1}{p^s}\right) = -\sum_{n=2}^{\infty}\left[\pi(n)-\pi(n-1)\right]\ln\left(1-\frac{1}{n^s}\right) =$$

$$-\sum_{n=2}^{\infty}\pi(n)\left[\ln\left(1-\frac{1}{n^s}\right)-\ln\left(1-\frac{1}{(n+1)^s}\right)\right] =$$

$$=\sum_{n=2}^{\infty}\pi(n)\int_n^{n+1}\frac{s}{x\left(x^s-1\right)}dx = s\int_2^{\infty}\frac{\pi(x)\,dx}{x\left(x^s-1\right)}.$$

Also,

$$\frac{1}{\zeta(s)} = \prod_p\left(1-\frac{1}{p^s}\right) = \sum_{n=1}^{\infty}\frac{\mu(n)}{n^s}.$$

The Moebius function has the property

$$\sum_{d|q}\mu(d) = \delta_{q,1}.$$

It is easy to prove:

$$1 = \sum_{m=1}^{\infty}\frac{1}{m^s}\sum_{n=1}^{\infty}\frac{\mu(n)}{n^s} = \sum_{q=1}^{\infty}\frac{1}{q^s}\sum_{d|q}\mu(d).$$

Moebius inversion formula:

$$g(x) = \sum_{n=1}^{\infty} f\left(\frac{x}{n}\right)$$

$$f(x) = \sum_{n=1}^{\infty}\mu(n)\,g\left(\frac{x}{n}\right).$$

Indeed:

$$f\left(\frac{x}{m}\right) = \sum_{n=1}^{\infty}\mu(n)\,g\left(\frac{x}{mn}\right);$$

$$\sum_m f\left(\frac{x}{m}\right) = \sum_{m.n}\mu(n)\,g\left(\frac{x}{mn}\right) = \sum_q\sum_{d|q}\mu(q)\,g\left(\frac{x}{q}\right) = g\left(\frac{x}{1}\right) = g(x).$$

Finally, observe that

$$\sum_p \frac{1}{p^s} = \sum_{n=1}^{\infty} \frac{\mu(n)}{n} \log \zeta(ns),$$

with

$$\ln \zeta(s) = \sum_m \sum_p \frac{1}{m p^{ms}} = \sum_{m=1}^{\infty} \frac{F(ms)}{m},$$

where $F(s) = \sum \frac{1}{p^s}$.
Hence,

$$\sum \frac{\mu(n)}{n} \ln \zeta(ns) = \sum_{n,m} \frac{\mu(n)}{nm} F(mns) = \sum_{r=1}^{\infty} \frac{\Gamma(rs)}{s} \sum_{n|r} \mu(r) = \Gamma(s).$$

5.6 Dirichlet series

Dirichlet series are one of the most relevant and classical topics in analytic number theory. Here we will follow strictly the book by J.–P. Serre [10].
Let $a(n)$ be a complex–valued arithmetic function.

Definition 5. *A Dirichlet series with exponents $\{\lambda_n\}$ is a series of the form*

$$\sum_{n=1}^{\infty} a(n) e^{-\lambda_n z}, \tag{5.6}$$

where $\{\lambda_n\}$ is a sequence of real numbers tending to infinity, and $z \in \mathbb{C}$.

The simplest example is when $\lambda_n = n$ for all n. Then, putting $e^{-z} = t$, the series (5.6) is a power series in t.
Another nontrivial case is $\lambda_n = \log n$. This reduces the series (5.6) to an ordinary Dirichlet series.
We remind that, if the coefficients $a(n)$ are bounded, then $\varphi(s)$ is absolutely convergent for $Re(s) > 1$.

Definition 6. *An (ordinary) Dirichlet series with coefficients $a(n)$ is a series of the form*

$$\varphi(s) = \sum_{n=1}^{\infty} \frac{a(n)}{n^s}.$$

The most known examples of Dirichlet series are the Riemann zeta function $\zeta(s) = \sum_{n=1}^{\infty} \frac{1}{n^s}$ and the L–series

$$L(s,\chi) = \sum_{n=1}^{\infty} \frac{\chi(n)}{n^s},$$

corresponding to a Dirichlet character χ of conductor T. Other interesting example are

$$\frac{\zeta(s-1)}{\zeta(s)} = \sum_{n=1}^{\infty} \frac{\phi(n)}{n^s},$$

where $\phi(n)$ is the totient function, and

$$\zeta(s)\zeta(s-a) = \sum_{n=1}^{\infty} \frac{\sigma_a(n)}{n^s},$$

where $\sigma_a(n)$ is the divisor function. Also, the logarithm of the zeta function is expressed, for $Re(s) > 1$, by the Dirichlet series

$$\log\zeta(s) = \sum_{n=2}^{\infty} \frac{\Lambda(n)}{\log(n)} \frac{1}{n^s},$$

where $\Lambda(n)$ is the von Mangoldt function. A very simple result holds for the logarithmic derivative of a Dirichlet series $\Phi(s) = \sum_{n=1}^{\infty} \frac{f(n)}{n^s}$, corresponding to a completely multiplicative function $f(n)$:

$$\frac{\Phi'(s)}{\Phi(s)} = -\sum_{n=1}^{\infty} \frac{f(n)\Lambda(n)}{n^s}.$$

Chapter 6

Numerical Spectral Methods

Most of the times, the Schrödinger equation cannot be solved exactly. In order to determine the energy spectrum, one has to rely on some numerical methods. Here we will discuss, in particular, two different approaches. Each of them has certain advantages and disadvantages.
The first of them is the truncated Hilbert space method, the second one the tight–binding method. Before starting the discussion, it is useful to remind some basic formulas concerning the harmonic oscillator.

6.1 Basic formulas for the quantum harmonic oscillator

The Hamiltonian is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 q^2 =$$

$$\frac{m\omega^2}{2}\left(q + i\frac{p}{m\omega}\right)\left(q - i\frac{p}{m\omega}\right) - \frac{\hbar\omega}{2},$$

with

$$[q, p] = i\hbar.$$

Introducing

$$a = \sqrt{\frac{m\omega}{2\hbar}}\left(q + i\frac{p}{m\omega}\right), \qquad a^+ = \sqrt{\frac{m\omega}{2\hbar}}\left(q - i\frac{p}{m\omega}\right)$$

we get

$$\left[a, a^+\right] = 1.$$

Hence

$$q = \sqrt{\frac{\hbar}{2m\omega}}\left(a + a^{+}\right) = \frac{l}{\sqrt{2}}\left(a + a^{+}\right),$$
$$p = i\sqrt{\frac{m\omega\hbar}{2}}\left(a^{+} - a\right) = \frac{i\hbar}{l}\frac{1}{\sqrt{2}}\left(a^{+} - a\right),$$

where l is the basic length

$$l = \sqrt{\frac{\hbar}{m\omega}}.$$

In terms of a and a^{+}, the Hamiltonian can be written as

$$H = \hbar\omega\left(a^{+}a + \frac{1}{2}\right).$$

Denoting by $|n\rangle$ the n–th eigenvector of this Hamiltonian, we have

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle,$$
$$a^{+}\,|n\rangle = \sqrt{n+1}\,|n+1\rangle,$$

The Hilbert space of physical states is finitely generated, since it can be obtained from the vacuum state via the formula

$$|n\rangle = \frac{1}{\sqrt{n!}}\left(a^{+}\right)^{n}|0\rangle.$$

The occupation number operator is defined by

$$N = a^{+}a,$$

and for its eigenstates we have

$$N\,|n\rangle = n\,|n\rangle.$$

Finally, we recall that the Schrödinger representation is defined by

$$a\psi_0(q) = \left(q + \frac{\hbar}{m\omega}\frac{d}{dq}\right)\psi_0(q) = 0,$$

i.e.

$$\psi_0(q) = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}\exp\left(-\frac{m\omega q^2}{2\hbar}\right).$$

The excited states are expressed by

$$\psi_n(q) = \sqrt{\frac{1}{2^n n!}}\left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}q^2} H_n\left(\sqrt{\frac{m\omega}{\hbar}}q\right), \tag{6.1}$$

where the operator

$$H_n(x) = (-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}$$

is the generator of the classical Hermite polynomials.

6.2 Truncated Hilbert space method

Let us assume for simplicity that the potential $V(x)$ entering the Schrödinger equation is an even function, unbounded at infinity

FIGURE

The problem is to find the eigenvalues and the eigenvectors of the Hamiltonian

$$H = \frac{p^2}{2m} + V(x).$$

The THSM, first of all, amounts to choosing a basis $|\psi_n\rangle$ in the Hilbert space and computing the matrix elements

$$\langle\psi_n| H |\psi_m\rangle \equiv H_{n,m}.$$

Second, one has to truncate the above basis at a certain level N and to consider the finite–dimensional Hamiltonian

$$H_N = H_{n,m} \qquad n, m = 0, 1, ..., N$$

which can be diagonalized numerically. A practical way of implementing the algorithm consists of using the harmonic oscillator basis (6.1). Its vectors depend on the free parameter ω. The strategy then is the following.

(i) Use the variational principle on the ground state wave function to identify the optimal value of ω, say $\overline{\omega}$, and use this value to construct the remaining vectors of the basis.

(ii) Compute separately the matrix elements of the kinetic term $T = \frac{p^2}{2m}$ and of the potential term $V(x)$.

(iii) On the harmonic oscillator basis, T has matrix elements on the diagonal, and along the next main diagonals only

$$T = \begin{bmatrix} \ddots & \ddots & & & & \\ \ddots & \ddots & \ddots & & 0 & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & 0 & & \ddots & \ddots & \ddots \\ & & & & \ddots & \ddots \end{bmatrix}$$

as evident from the representation p.

(iv) The potential $V(x)$, in general, has sparse matrix elements, given by all the overlapping integrals

$$V_{nm} = \int dx \psi_n(x) V(x) \psi_m.$$

The main advantages of the method are:

1) It is easy to implement.

2) It furnishes reasonable estimates of the first eigenvalues.

The main disadvantages are:

1) The integrals V_{nm} can be only poorly estimated for large values of the quantum numbers n and m, due to the oscillatory nature of the Hermite polynomials (the same is true for any other basis).

2) The final form of the truncated Hamiltonian H_N, as mentioned above, in general possesses nonzero matrix elements in all entries. For large values of N this may represent a problem for a fast and sufficiently accurate numerical diagonalization of this matrix.

However, for polynomial potentials, one can overcome at least the first of the mentioned disadvantages, since the algebraic expressions of the matrix elements can be computed without performing the numerical integration. Let's see how this is possible.

Consider the Hamiltonian

$$H = \frac{p^2}{2m} + \lambda |x|^n,$$

where n is an integer. First of all, we can identify the optimal choice of ω for this Hamiltonian and, correspondingly, the harmonic oscillator length

$$l = \sqrt{\frac{\hbar}{m\omega}}.$$

The related representation of the operators x and p reads

$$x = \frac{l}{\sqrt{2}} \left(a + a^+\right),$$

$$p = \frac{i\hbar}{l} \frac{1}{\sqrt{2}} \left(a^+ - a\right).$$

On the other hand, the above Hamiltonian can be put into and a–dimensionless form by using the intrinsic length scale of the problem

$$\xi = \left(\frac{\hbar^2}{m\lambda} b(n)\right)^{\frac{1}{n+2}},$$

where the function $b(n)$, as before, is chosen so that the energy levels match, for large values of the quantum numbers, with their semi–classical expressions.
We are led to compute the universal ration of the two scales

$$R = \frac{l}{\xi},$$

and by substituting the value of the optimal choice of ω,

$$\omega_{op} = \left(\frac{2n\Gamma\left(\frac{n+1}{2}\right)\lambda\hbar^{\frac{n-2}{2}}}{\sqrt{\pi}m^{\frac{n}{2}}} \right)^{\frac{2}{n+2}},$$

we obtain

$$R = \left(\frac{\sqrt{\pi}}{2nb(n)\Gamma\left(\frac{n+1}{2}\right)} \right)^{\frac{1}{n+2}}.$$

The Hamiltonian can be written as

$$H = \xi_0 \left[-\frac{1}{4}\frac{1}{R^2}\left(a^+ - a\right)^2 + \frac{bR^n}{2^{\frac{n}{2}}}\left(a + a^+\right)^n \right]. \tag{6.2}$$

The operators a and a^+ can be easily computed, since

$$a = \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & \cdots & \\ 0 & 0 & \sqrt{2} & 0 & & \\ 0 & 0 & 0 & \sqrt{3} & 0 & \\ 0 & 0 & 0 & 0 & \sqrt{4} & \\ 0 & 0 & 0 & 0 & 0 & \ddots \\ & & & & & \end{bmatrix}$$

$$a^+ = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots & \\ \sqrt{1} & 0 & 0 & 0 & & \\ 0 & \sqrt{2} & 0 & 0 & 0 & \\ 0 & 0 & \sqrt{3} & 0 & 0 & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & & & & \ddots \end{bmatrix}.$$

Obviously, the truncated matrices $a_{(N)}$ and $a^+_{(N)}$ do not satisfy the usual commutation relation

$$\left[a, a^+\right] = \mathbb{I}.$$

Instead, they satisfy the relation

$$\left[a_{(N)}, a^{+}_{(N)}\right] = \mathbb{I}_N - (N+1)\,\delta_{N,N},$$

i.e.

$$\left[a_{(N)}, a^{+}_{(N)}\right] = \begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & & \ddots & \\ & & & & & -N \end{bmatrix},$$

so that the trace of the commutator vanishes, as it happens for any finite dimensional representation. Even with this drawback, it is however evident the algebraic advantage of the expression (6.2). In fact, the matrix elements of this matrix can be computed just by sum and matrix multiplication of the known matrices a_N and a^{+}_{N}.
It still remains the computational problem of diagonalizing a sparse matrix. This problem can be attacked by using a different method, the so–called Tight–Binding Method.

6.3 Tight–Binding Method

This method reduces the problem of finding the eigenvalues and the eigenvectors of the Schrödinger Hamiltonian to the one of diagonalizing numerically a matrix with non–vanishing matrix elements only along the main diagonal and the upper and lower ones. However, a certain care is needed in order to interpret correctly the results. To this aim, it is useful to discuss preliminarily the problem of a particle in a box.

6.3.1 Particle in a box

Consider the Schrödinger problem for a free particle in a box of length L:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi = E\psi,$$

$$\psi\,(0) = \psi\,(L) = 0.$$

FIGURE

The solution of the problem is well known. We have

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}E\psi,$$

with

$$\psi = A\sin\left(\sqrt{\frac{2mE}{\hbar^2}}x + \varphi\right).$$

By imposing the boundary conditions, we end up with $\varphi = 0$ and $\sin\left(\sqrt{\frac{2mE}{\hbar^2}}L\right) = 0$, i.e.

$$\sqrt{\frac{2mE}{\hbar^2}}L = n\pi \qquad (n = \pm 1, \pm 2, ...)$$

$$E_n = \frac{\hbar^2\pi^2}{2mL^2}n^2, \qquad n = 1, 2, ... \tag{6.3}$$

The (normalized) wave functions are given by

$$\psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right).$$

Notice that ψ_n and ψ_{-n} describe the same physical vector. Suppose now that we discretize the previous equation, i.e. first we divide the interval $(0, L)$ in N steps, as in figure

FIGURE

with lattice space

$$\varepsilon \equiv \frac{L}{N}.$$

The wave functions take now values only on the discrete points $p_n \equiv n\varepsilon$, with $\psi_0 = \psi_N = 0$. The discrete version of the second derivative term is

$$\frac{d^2\psi(x)}{dx^2} \to \frac{\psi_{m+1} + \psi_{m-1} - 2\psi_m}{\varepsilon^2}.$$

In this way we are led to find the eigenvalues and eigenvectors of the following linear problem

$$\psi_{m+1} + \psi_{m-1} - 2\psi_m = \left(-\frac{2m\varepsilon^2}{\hbar^2}\right)E\psi_m. \tag{6.4}$$

This problem can be easily solved by expressing ψ_m as

$$\psi_m = \sum_k e^{ikm\varepsilon}\widehat{\psi}_k,$$

where the range of k will be clear from the subsequent considerations.

Substituting this expression into (6.4), we have

$$2\cos(k\varepsilon - 1)\,\widehat{\psi}_k = -\frac{2m\varepsilon^2}{\hbar^2}E\widehat{\psi}_k,$$

i.e.

$$E(k) = \frac{\hbar^2}{m}\frac{1}{\varepsilon^2}(1 - \cos k\varepsilon). \tag{6.5}$$

For an infinitesimal value of ε we shall recover the previous result: expanding the right hand side of (6.5) we have

$$E(k) \simeq \frac{\hbar^2}{m}\frac{k^2}{2}, \tag{6.6}$$

and comparing with (6.3) we obtain the discrete values of k:

$$k_n = \frac{\pi n}{L}, \qquad n = 0, \pm 1, ...$$

Since $L = n\varepsilon$, the only relevant values are

$$k_n = \frac{\pi n}{n\varepsilon}, \qquad n = 0, \pm 1, ... \pm (N-1).$$

However, due to the parity of the expression (6.5) for $k \to -k$, and taking into account the boundary conditions

$$\psi_0 = \psi_N = 0,$$

we can restrict the attention to the values

$$k_n = \frac{\pi n}{L}, \qquad n = 0, 1, ..., N-1,$$

so that, finally we get

$$E_n = \frac{\hbar^2}{m}\frac{N^2}{L^2}\left(1 - \cos\frac{\pi n}{N}\right), \qquad n = 1, 2, ..., N-1.$$

For the corresponding wave functions we have

$$\psi^{(n)}_{m\varepsilon} = \sum_{p=0}^{n-1} \sin\left[\frac{\pi pm}{N}\right]\widehat{\psi}^{(n)}_p,$$

where

$$\widehat{\psi}_p^{(n)} = \sqrt{\frac{2}{N\varepsilon}}\delta_{n,p}.$$

The important thing to notice is that now the spectrum of the discrete Schrödinger equation has additional features, namely the lowest part of the spectrum is similar to the actual Schrödinger equation, whereas the higher part of the spectrum is dominated by the lattice effects and it shows the typical form of the case

FIGURE

Consider now the discrete version of the Schrödinger equation in the presence of a potential

$$-\frac{\hbar^2}{2m}\frac{1}{\varepsilon^2}\left(\psi_{m+1} + \psi_{m-1} - 2\psi_m\right) + V_m\psi_m = E\psi_m.$$

For studying the problem, we have to cut the potential on a finite interval $(0, L)$. This introduces new aspects in the problem: with boundary conditions

$$\psi_0 = \psi_L = 0.$$

The effective potential felt by the particle is $V(x)$ inside the box, but $V = \infty$ at $x = 0$ and $x = L$.

FIGURE

It is obvious that if we discretize the Schrödinger equation in terms of N points, we will obtain N different energy levels.
However, not all of them are those relative to the potential V! Only those which take values

$$E > V_0 = V_L$$

may have some resemblance to the actual eigenvalues. The higher ones, in fact, come just from the infinite well problem, further masked by the lattice effects. So, typically the spectrum obtained in this way has three different behaviours, as shown in figure

FIGURE

The region I, the lowest part of the spectrum, probes the potential and gives an approximation of the true eigenvalues. The region II, where the

eigenvalues are larger that the value of the potential at the edge of the interval, is simply the spectrum of the infinite well potential, for values of the discrete index n which allows the expansion (6.6). The region III is, instead, just a lattice artifact of the spectrum.

In order to separate the above region one has to perform a finite size scaling, i.e. follow the evolution of the eigenvalues by changing the value of L (increasing correspondingly the number N of discrete points), the "true" eigenvalues are those which do not change by varying L.

FIGURE

In conclusion, the tight binding method provides an Hamiltonian which is relatively simple and fast to diagonalize numerically, given its (almost) diagonal form

$$\begin{bmatrix} \ddots & \ddots & & & & \\ \ddots & \ddots & \ddots & & 0 & \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & 0 & & \ddots & \ddots & \ddots \\ & & & & \ddots & \ddots \end{bmatrix}$$

The potential is treated in a local way and it is not necessary to compute the overlapping integrals. However, it is necessary to have certain care in interpreting the result and in identifying the "true" eigenvalues of the problem.

Bibliography

[1] T. M. Apostol, *Introduction to analytic Number Theory*, Springer–Verlag, Berlin, 1976.

[2] C.M. Bender, S. A. Orszag, *Advanced mathematical methods for scientists and engineers*. Springer, Berlin, 1999.

[3] C. Cohen–Tanoudji, B. Diu, F. Laloë, *Quantum Mechanics*, John Wiley and Sons, New York, 2005.

[4] P. Erdos, J. Surányi, *Topics in the Theory of Numbers*, Springer, Berlin, 2003.

[5] L. D. Landau, E. M. Lifschitz, *Quantum Mechanics: non–relativistic theory*, Oxford : Butterworth-Heinemann, 2002.

[6] G. Mussardo, *Il modello di Ising : introduzione alla teoria dei campi e delle transizioni di fase*, Boringhieri, Torino, 2007.

[7] G. Mussardo, *Statistical Field Theory: An introduction to exactly solved models in Statistical Physics*, Oxford Graduate Texts, 2009.

[8] A. Ogg, *Modular Forms and Dirichlet Series*, Mathematics Lecture Note Series, W. A. Benjamin, Inc. 1969.

[9] J. J. Sakurai, *Advanced Quantum Mechanics*, Addison-Wesley, 1967.

[10] J.–P. Serre, *A course in Arithmetic*, Springer–Verlag, Berlin, 1973.

[11] *Frontiers in Number Theory, Physics and Geometry*, P. cartier, B. Julia, P. Moussa and P. Vanhove Editors, Springer–Verlag, vol. I, 2006 and vol. II, 2007.

[12] *From Number Theory to Physics*, M. Waldschmidt, P. Moussa, J.–M. Luck and C. Itzykson Editors, Springer–Verlag, Berlin, 1995.