

# MOKA<sup>1</sup> - Many Body Physics

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September 27, 2007

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# Chapter 1

## Equilibrium thermodynamics

### 1.1 Basic concepts

We assume that the reader is familiar with the basics of statistical mechanics and this first section is intended to be a recapitulation of fundamental concepts and formulas.

Although the problems of many body physics are varied and appear in many guises, at the fundamental level they all reduce to the study of the partition function  $Z$ , which is the sum over all possible states<sup>1</sup>:

$$Z = e^{-\beta F} = \text{Tr} e^{-\beta H} = \sum_{\text{n=all states}} e^{-\beta E_n}, \quad \beta \equiv \frac{1}{T}, \quad (1.1)$$

from which one can compute the statistical expectation values of the operators  $\mathcal{O}$

$$\langle \mathcal{O} \rangle = Z^{-1} \text{Tr} \mathcal{O} e^{-\beta H} \equiv \text{Tr} \mathcal{O} \rho. \quad (1.2)$$

In field theories with their infinite number of degrees of freedom one reformulates the sum Eq. (1.1) as a path integral, which is the sum over all field configurations:

$$Z = e^{-\beta F} = \text{Tr} e^{-\beta H} \Rightarrow \int \mathcal{D}\Phi e^{-S[\Phi]}, \quad (1.3)$$

where  $\Phi$  is a set of fields. The measure  $\mathcal{D}\Phi = \prod \mathcal{D}\Phi_i$  is the infinite product of all independent field configurations, while  $S[\Phi]$  is the Euclidean action of the theory governing the dynamics of the fields  $\Phi$ . Since it is a function of the configurations, which are functions,  $S[\Phi]$  is a functional. The N-point correlators of the field configurations are then given as the expectation values

$$\langle \Phi_1 \Phi_2 \dots \Phi_N \rangle = Z^{-1} \int \mathcal{D}\Phi \Phi_1 \Phi_2 \dots \Phi_N e^{-S[\Phi]}, \quad (1.4)$$

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<sup>1</sup>Our units are discussed in an Appendix. In particular, we always set the Boltzmann constant  $k_B = 1$ , a natural unit of temperature is energy. Also, we frequently set  $\hbar = 1$  or  $c = 1$ .

where  $|\rangle$  is the appropriate (quantum) state. We shall discuss path integrals in detail in Ch. 2.

**Note: trace and determinant.** In terms of eigenvalues  $a_n$  of a matrix  $A$ ,  $\text{Tr}A = a_1 + a_2 + \dots + a_N$ ,  $\det A = a_1 a_2 \dots a_N = \exp(\log a_1 + \log a_2 + \dots + \log a_N) = \exp(\text{Tr} \log A)$ . This relation holds also for a general non-diagonal matrix since both  $\text{Tr}$  and  $\det$  are invariant under  $A \rightarrow UAU^{-1}$ . From here one can further derive how much the determinant changes if the matrix is changed by a small matrix  $\delta A$ :  $\delta \det A = \det A \text{Tr}(A^{-1} \delta A)$ .

The practical difference between Eqs. (1.1) and (1.3) is that of the difference between quantum mechanics and quantum field theory. In the latter the sum is over all possible field configurations, not just over all the discrete states. The Euclidean action  $S[\Phi]$  gives a weight also to the configurations that do not obey the classical equations of motion and hence takes into account all possible quantum fluctuations (such as virtual particles).

The word "partition" refers to the way the fundamental degrees of freedom of the system are arranged into the available states. It could be argued that partition is a more fundamental concept than, say, thermal equilibrium, which corresponds to a very special partitioning. Indeed, "partition" and "correlation" may be considered as describing the fundamental properties of the system while "entropy" and "temperature" are derived concepts.

To demonstrate this, let us consider a system that is divided up in  $j$  subsystems consisting of  $N_j$  identical particles. Each subsystem contains  $G_j$  states and each state has the energy  $E_j$ . For any given state, the occupation probability is the same. Let us further impose a global constraint: there can be only one particle per state. Then we have a problem which is identical to the combinatorial problem of putting  $N_j$  balls into  $G_j$  slots. Each ball should be delivered into a slot independently, i.e. without any correlation to past or future. This can be done in  $Z_j = G_j(G_j - 1) \dots (G_j - N_j + 1)/N_j!$  ways so that the number of possible ways to partition balls into slots in the subsystem is  $Z_j = G_j!/N_j!(G_j - N_j)!$  while the total number of the partitions for the whole system is

$$Z = \prod_j Z_j . \quad (1.5)$$

If we now define entropy as  $S = \log Z$  it is clear that entropy is just a measure of the number of partitions. Using  $\log x! = x \log x/e$  for  $x \gg 1$  we find

$$S = - \sum_j G_j [\bar{n}_j \log \bar{n}_j + (1 - \bar{n}_j) \log(1 - \bar{n}_j)] \quad (1.6)$$

where we have defined the mean occupation number as  $\bar{n}_j \equiv N_j/G_j$ .

Let us consider a system whose total energy and total particle number is fixed:  $N = \sum_j N_j = \text{const.}$ ,  $E = \sum_j E_j N_j = \text{const.}$  What is the most probable partition? We maximize  $S$  subject to the energy and particle number constraint, writing

$$\frac{\partial}{\partial \bar{n}_j} (S - \alpha N - \beta E) = 0 , \quad (1.7)$$

where  $\alpha$  and  $\beta$  are Lagrange multipliers. We then find that the most probable occupation number is given by the Fermi-Dirac distribution

$$\bar{n}_j = \frac{1}{e^{\alpha + \beta E_j} + 1} , \quad (1.8)$$

identifying  $\alpha \equiv -\mu/T$ ,  $\beta \equiv 1/T$ . (Had we allowed many particles to occupy the same state, we would have obtained the Bose-Einstein distribution.) Thus thermal equilibrium is seen to correspond to the maximum entropy state or to the likeliest partition of completely uncorrelated degrees of freedom. If all other things are kept equal, adding correlations (i.e. interactions) will decrease the number of available partitions and hence entropy.

Note that if  $G_j \gg N_j$  we could argue that when partitioning particles into the available states, there is a very small probability to hit a state that is already occupied so that we could write just  $Z_j \approx G_j^N/N!$ ; the resulting most probable partition would then correspond to the Maxwell-Boltzmann distribution.

A similar line of argument can be carried over to quantum mechanics, where instead of classical energies one has to deal with operators. Recall that in quantum mechanics

$$E = \langle H \rangle = \text{Tr} \rho H , \quad (1.9)$$

where  $H$  is the Hamiltonian of any quantum system,  $\rho$  is the density matrix, and the expectation value is taken in a general quantum state  $|\Psi\rangle$ . The expression for entropy can then be written as

$$S = - \sum p_n \log p_n = -\text{Tr} (\rho \log \rho) . \quad (1.10)$$

Let us now vary  $S$  by requiring that  $E = \text{const}$  and  $\text{Tr} \rho = 1$ . Then

$$\begin{aligned} 0 &= \delta(S - \beta \langle H \rangle - \alpha \text{Tr} \rho) \\ &= \text{Tr} \delta \rho (-\log \rho - I - \beta H - \alpha) . \end{aligned} \quad (1.11)$$

Here again  $\beta$  and  $\alpha$  are Lagrange multipliers. Eq. (1.11) should hold for arbitrary variation so that we find the solution (taking now  $\alpha = 0$ )

$$\rho = \text{const} \times e^{-\beta H} \equiv Z^{-1} e^{-\beta H} , \quad (1.12)$$

which, recalling that  $\text{Tr} \rho = 1$ , reproduces Eq. (1.1).

**Reminder: density matrix.** Assume we have a quantum mechanical state  $|\psi\rangle = \sum_i c_i |\psi_i\rangle$ , where  $|\psi_i\rangle$  is some complete set of states. The density matrix of this pure state is

$$\rho = |\psi\rangle\langle\psi| = \sum_{ij} c_i c_j^* |\psi_i\rangle\langle\psi_j| , \quad (1.13)$$

the density matrix of a mixed state would be

$$\rho = \sum_i |c_i|^2 |\psi_i\rangle\langle\psi_i| , \quad (1.14)$$

where  $|c_i|^2$  is the probability of state  $i$ . Always  $\text{Tr} \rho = 1$  and  $\text{Tr} \rho^2 \leq \text{Tr} \rho$ ; equality for a pure state. Since  $\rho$  is Hermitian with positive matrix elements it can be diagonalised with positive normalised eigenvalues  $0 \leq \lambda_i \leq 1$  and the entropy is defined as  $S = - \sum_i \lambda_i \log \lambda_i$ . A thermal density matrix has  $\lambda_i \sim e^{-\beta E_i}$ . *Decoherence* means a time dependent disappearance of the off-diagonal terms in (1.13). *Entanglement entropy* is entropy contained in a reduced density matrix obtained by "tracing over" a subsystem, i.e.,  $\rho_r = \sum_a \langle a | \rho | a \rangle$ ,  $a$  contains only part of the degrees of freedom of the system. Even though  $\rho$  is a pure state and leads to  $S = 0$ ,  $\rho_r$  will have  $S \geq 0$ .

Thermodynamics proper is defined only in the limit where the number of degrees of freedom and the volume are infinite. However, in physics infinity is just given by a dimensionless number  $\gg 1$ , so that for practical purposes a system is infinite if the system size  $\gg$  relevant length scale, which could be some correlation length  $\xi$  or some mean free path  $\lambda \approx 1/(n\sigma)$ . Here  $n$  = number density and  $\sigma$  = cross section. Alternatively temporal infinity would mean system life time  $\gg$  relevant dynamical time scale, which could be the combination  $\xi/v_{\text{sound}}$  or the collision time  $\tau_{\text{coll}} = \lambda/v_{\text{thermal}}$ .

**Estimate: mean free part, collision time.** Why is  $\lambda \approx 1/(n\sigma)$  a good estimate of a mean free path and  $\tau_{\text{coll}} = \lambda/v_{\text{thermal}}$  of collision time? Check dimensions.

Theoretically one can study a homogenous infinite system (say,  $T = \text{constant}$  everywhere), but in practice there are always some gradients (say,  $T = T(x)$  varies as a function of one spatial coordinate  $x$ ). Nevertheless, there may exist *local* thermal equilibrium if the range in space or time within which  $T$  varies is  $\gg$  some microscopic scale.

Formally, one could write the conditions for local equilibrium as  $\lambda_{\text{free}} \cdot \nabla \ll 1$  or  $\tau_{\text{coll}} \partial_t \ll 1$  (small  $\lambda_{\text{free}}$  or frequent collisions thermalise the system locally). Dynamically, this also induces hydrodynamics ( $\nabla p \Rightarrow \text{flow} = \mathbf{v}(t, \mathbf{x})$ ). The smaller the above dimensionless variables are, the better the assumption of an ideal, i.e. adiabatic, i.e. entropy conserving, i.e. isentropic motion. As we shall see in Ch. 5, this dynamics is built in the Euler equations. Corrections of  $\mathcal{O}(\lambda_{\text{free}} \nabla)$  then give rise to dissipation ( $\Delta S > 0$ ), viscosities, and heat conductivity in the Navier-Stokes equations.

## 1.2 Microcanonical ensemble

Let us now recapitulate some of the formal aspects of thermodynamics from a pragmatic angle. We may define various equilibrium ensembles such as microcanonical, canonical, or grand canonical, which are all described by the minima of a given thermodynamical potential. The values of the potentials at the minima are unspecified (this is the cosmological constant problem!), but the partial derivatives of the potentials are related to real and measurable physical quantities.

The simplest case is the microcanonical ensemble, where the potential  $E$  depends only on *extensive* variables, which are proportional to the size of the system. The conjugates of the extensive variables are *intensive*. We use capital letters for the extensive variables and small letters for intensive ones (for historical reasons, this does not work for temperature  $T$  and the magnetic field  $H$ ). Thus we write  $E = E(S, V, A, B, N, \dots)$ . The variables, together with their conjugate intensive variables, are listed in Table 1.1.

The microcanonical potential  $E$  is explicitly given by

$$\begin{aligned} E &= TS - pV + \mu N + \sigma A + V\mathbf{H} \cdot \mathbf{B} + \dots \\ &= T(S, V, A, B, N)S - p(S, V, A, B, N)V + \mu(S, V, A, B, N)N + \dots \end{aligned} \quad (1.15)$$

We shall often use the intensive *densities*  $\epsilon = E/V$ ,  $s = S/V$  and  $n = N/V$ . In the non-relativistic cases  $\epsilon \rightarrow \rho = mc^2 n$ .

Note that the combination  $V\mathbf{H} \cdot \mathbf{B}$  is somewhat special. It should really be written as  $L\mathbf{H} \cdot \mathbf{AB}$  with  $V = LA$  and  $\mathbf{AB}$  symbolising the magnetic flux  $\Phi_B$ .

Extensive		Intensive	
S	entropy	T	temperature
V	volume	p	pressure
A	area	$\sigma$	interface tension
B	magnetic flux density	H	magnetic field
N	conserved particle number	$\mu$	chemical potential.

Extensive and intensive variables.

Differentiating Eq.(1.15) with respect to its variables gives

$$\begin{aligned} dE &= \frac{\partial E}{\partial S}dS + \frac{\partial E}{\partial V}dV + \frac{\partial E}{\partial N}dN + \dots \\ &= TdS - pdV + \mu dN + \dots \end{aligned} \quad (1.16)$$

From this one can find the partial derivatives of E which are physical and measurable: 1st derivatives yield  $T, -p, \mu, \dots$  while the 2nd derivatives can be used to define the heat capacities  $C_v$  and  $C_p$  as well as the speed of sound  $v_{\text{sound}}^2$ . There are many useful relations between the partial derivatives; for instance,

$$\left. \frac{\partial u}{\partial x} \right|_y = \frac{\partial(u, y)}{\partial(x, y)} = \frac{\frac{\partial(u, y)}{\partial(z, \omega)}}{\frac{\partial(x, y)}{\partial(z, \omega)}} = \left| \begin{array}{cc} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} \\ \frac{\partial y}{\partial x} & \frac{\partial y}{\partial y} \end{array} \right| \quad (1.17)$$

which, choosing  $z, \omega$  suitably, finds many applications in thermodynamics.

Starting from the microcanonical potential  $E$ , more potentials with various (and sometimes confusing) names can be defined by interchanging extensive and intensive variables by a Legendre transformation. A prototype Legendre transformation is the one encountered in Hamiltonian mechanics, where one obtains the Hamiltonian from the Lagrange function  $L(q, \dot{q}) = T - V$  as

$$H(p, q) = p\dot{q} - L(q, \dot{q}), \quad p = \frac{\partial L}{\partial \dot{q}}. \quad (1.18)$$

Equally, starting from any  $f(x, y)$  and defining  $z = \partial f / \partial y$  one can find the Legendre transform  $g(x, z)$  as

$$g(x, z) = f(x, y) - yz \quad (1.19)$$

which satisfies the relations

$$dg = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy - ydz - zdy = \frac{\partial f}{\partial x}dx - ydz = \frac{\partial g}{\partial x}dx + \frac{\partial g}{\partial z}dz \quad (1.20)$$

since  $\frac{\partial f}{\partial y}dy - zdy$  cancels.

## 1.3 Canonical Ensemble

For physical systems it is difficult to fix the total energy and, moreover, it is usually easier to measure the temperature than the entropy of the system. Thus it makes sense to take

$E = TS - pV + \mu N = E(S, V, N)$  (we omit possible other variables) and trade extensive  $S$  with intensive  $T$  by inverting  $T = \partial E / \partial S$  to obtain  $S = S(T, \dots)$ . Such an operation yields the canonical potential, or the free energy  $F$ , as

$$F(T, V, N) = E - TS = -p(T, V, N)V + \mu(T, V, N)N \quad (1.21)$$

which has the differential

$$\begin{aligned} dF &= \frac{\partial F}{\partial T} dT + \frac{\partial F}{\partial V} dV + \frac{\partial F}{\partial N} dN \\ &= -S dT - p dV + \mu dN. \end{aligned} \quad (1.22)$$

The first derivatives yield entropy, pressure and the chemical potential:

$$\frac{\partial F}{\partial T} = -S, \quad \frac{\partial F}{\partial V} = -p, \quad \frac{\partial F}{\partial N} = \mu. \quad (1.23)$$

For the pair  $T, V$  there are three second derivatives, which, using Eq. (1.17), can be expressed in terms of three measurable quantities. These are the two specific heats and the sound velocity  $v_s$  (here  $\rho = mn$  is the mass density):

$$F_{TT} = -S_T = -\frac{1}{T}C_V, \quad VF_{VV} = \rho \frac{C_V}{C_p} v_s^2, \quad F_{TV}^2 = \frac{\rho}{TV} C_V^2 v_s^2 \left( \frac{1}{C_V} - \frac{1}{C_p} \right).$$

**Special case:**  $p = nT$ -gas. An important special case is that of  $p = nT$ -gas, ideal gas of particles in Maxwell-Boltzmann statistics. Let us recapitulate the appropriate formulas for the NR case  $m \gg T$ ; for arbitrary mass, see Grand Canonical ensemble below.

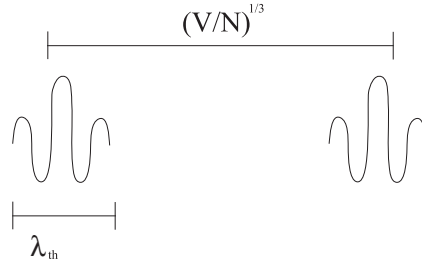


Figure 1.1: Particle wave packets should not overlap for MB statistics to be valid

From the definition of  $Z$  one obtains for  $N$  identical independent particles – which gives rise to the factor  $1/N!$  –

$$Z(T, V, N) = \sum_i e^{-\beta E_i} = \frac{1}{N!} \left( \frac{V}{\lambda_{\text{th}}^3} \right)^N = \frac{1}{N!} Z(1)^N \quad (1.24)$$

where

$$Z(1) = \int \frac{d^3 p d^3 x}{h^3} e^{-p^2 / (2mT)} = \frac{V}{\lambda_{\text{th}}^3} \quad (1.25)$$

and

$$\lambda_{\text{th}} = \hbar \sqrt{\frac{2\pi}{mT}} \quad (1.26)$$

is the thermal Compton wave length. In Eq. (1.25) one has applied the semiclassical rule that the volume  $dx dp$  in phase space should be divided by  $h$ , Planck's constant. The rule is derived in Eq. (1.79) below. This statistics is valid if the distance between particles,  $(V/N)^{1/3}$  is much greater than the size of wave packets,  $\lambda_{\text{th}}$ . From Eq. (1.24), using the Stirling approximation  $N! \approx (N/e)^N$ , we find

$$F(T, V, N) = -NT[1 + \log(Z(1)/N)] = -NT \left( 1 + \log \frac{V/N}{\lambda_{\text{th}}^3} \right) \quad (1.27)$$

so that the validity criterion implies that the log here and below is a number of order 10 (logs are never really very big). What remains is just a mechanical application of the formulas given above.

We thus have three first derivatives

$$S = -\frac{\partial F}{\partial T} = N \left( \frac{5}{2} + \log \frac{V/N}{\lambda_{\text{th}}^3} \right), \quad (1.28)$$

$$p = -\frac{\partial F}{\partial V} = \frac{NT}{V}, \quad (1.29)$$

$$\mu = -\frac{\partial F}{\partial N} = -T \log \frac{V/N}{\lambda_{\text{th}}^3}. \quad (1.30)$$

Inserting these back to Eq. (1.27) one sees that  $F = -NT + \mu N = -pV + \mu N = E - TS$ ,  $E = \frac{3}{2}NT$ . For the second derivatives in the  $T, V$  space one finds  $F_{TT} = -3N/2T$ ,  $F_{TV} = -N/V$ ,  $F_{VV} = NT/V^2$ , compatible with  $\gamma = C_p/C_V = 5/3$  and the sound speed of  $v_s^2 = \gamma T/m$ . We shall rederive these expressions in the fully relativistic case from the complete Bose-Einstein and Fermi-Dirac statistics. As a quantitative application, let us quote the experimental result for Argon:

$$\frac{S(\text{Argon})}{N} = 18.4 + \log \left[ \frac{V}{22.41} \cdot \left( \frac{T}{273\text{K}} \right)^{3/2} \right].$$

The formulas discussed above illustrate the following properties of the entropy  $S$ :

- $S$  is a pure number = (number of order 1)· $N$ .
- $S$  is additive (depends on  $V/N$ ).
- $S(T = 0)$  is so far undefined; it can be meaningfully discussed only in true Fermi-Dirac or Bose-Einstein statistics.

One difference between a physicist and a chemist is that the former counts particles microscopically and simply writes  $pV = NT$  or even more simpler  $p = nT$ . The latter measures amounts of gas of atomic number  $A$  by weighing macroscopically and thus has to convert mass to number by (g=gram)

$$N = \frac{M}{Am_p} \equiv \frac{M}{Ag} N_A, \quad m_p \equiv \frac{1}{N_A} \text{g} \quad (1.31)$$

so that the gas law becomes  $pV = (M/(Ag))N_A T \equiv RT$ , where  $R$  is the universal gas constant. Actually  $m_p$  is here replaced by mass of a  $^{12}\text{C}$  atom divided by 12. The dimensionless number  $M/(Ag)$  is called the number of moles of the gas.

**Estimate: distance between molecules.** Check that (room temperature/pressure) $^{1/3}$  gives the average distance between molecules in the air  $\approx 3$  nm.

**Modification: Tsallis statistics.** The exponential function  $e^x$  permeates statistical physics, but as with most things mathematical, one can think of many generalizations. The so-called Tsallis statistics<sup>2</sup> is one such phenomenological generalization. It starts from the observation that  $e^x = \lim_{n \rightarrow \infty} (1 + x/n)^n$  and introduces a parameter  $q$  by defining

$$e_q(x) = \left( 1 + \frac{x}{n} \right)^n, \quad n \equiv \frac{1}{1-q}. \quad (1.32)$$

<sup>2</sup>see, e.g., <http://www.ccsem.infn.it/issp2006/docs/Tsallis.pdf> or <http://tsallis.cat.cbpf.br/biblio.htm>

The inverse of  $e_q(x)$  defines a  $q$ -logarithm

$$\log_q(x) \equiv n(x^{1/n} - 1) = \frac{x^{1-q} - 1}{1 - q}. \quad (1.33)$$

The usual functional relations satisfied by log and exp are thus modified:

$$\log_q(xy) = \log_q(x) + \log_q(y) + (1 - q) \log_q(x) \log_q(y). \quad (1.34)$$

Entropy will now be defined by

$$S_q(p) = \frac{1}{q-1} \left( 1 - \sum_{i=1}^N p_i^q \right), \quad \sum_i p_i = 1. \quad (1.35)$$

It satisfies the relation  $S_q(p_i q_j) = S_q(p_i) + S_q(q_j) + (1 - q) S_q(p_i) S_q(q_j)$ ; hence in Tsallis statistics entropy is a non-extensive quantity. Proceeding from this one can develop  $q$ -thermodynamics with some interesting  $q$ -mathematics. The physical motivation for Tsallis statistics is that in Nature there are many phenomena with non-equilibrium stationary states; biological systems would be one example. Then, instead of exponential distributions, one typically has power-laws. These can often be fitted with some value of  $q$ . Effectively one writes

$$e^{-E/T} \Rightarrow \frac{1}{(1 + E/T_0)^{(T_0/T)}} \quad (1.36)$$

and fits the measured  $E$ -distribution. Note that one can write

$$e_q(x)^{-1} = \frac{1}{(1 + x/n)^n} = \frac{1}{\Gamma(n)} \int_0^\infty dt t^{n-1} e^{-t} e^{-xt/n}, \quad (1.37)$$

which describes the  $q$ -exponential as a weighted integral over exponentials.

## 1.4 Grand Canonical ensemble

Going from microcanonical to canonical ensemble is accomplished by replacing  $E = TS - pV + \mu N \Rightarrow F = -pV + \mu N$ . Now we clearly have two alternatives: either we trade  $N$  for  $\mu$  to obtain  $\Omega = -pV = -Vp(T, \mu)$ ; this defines the *grand canonical* ensemble. The other option is to trade  $V$  for  $p$  to obtain  $G = \mu N = N\mu(T, p)$  or the *Gibbs* ensemble. Chemists like to use the Gibbs ensemble. We shall however focus on the grand potential  $\Omega$  because in physics we often have some conserved particle number  $N$ .

The partition function for the grand canonical ensemble is then

$$\mathcal{Z}(T, V, \mu) = e^{-\beta\Omega} = \text{Tr} e^{-\beta(H - \mu N)} = \sum_{N=0}^{\infty} (e^{\beta\mu})^N Z(T, V, N), \quad (1.38)$$

where the conservation of the particle number means that the corresponding operator commutes with the Hamiltonian:

$$[H, N] = 0. \quad (1.39)$$

The partition function in Eq. (1.38) can also be called "the generating function of multiplicity moments" since  $\mathcal{Z} = \sum_{N=0}^{\infty} z^N Z(N)$ , where  $z = e^{\beta\mu}$  is sometimes called *fugacity*. Since the grand potential  $\Omega$  is extensive and  $V$  is the only extensive variable, we must have

$$\Omega = -Vp(T, \mu). \quad (1.40)$$

The basic thermodynamical equations are

$$d\Omega = -SdT - pdV - Nd\mu, \quad S = -\frac{\partial\Omega(T, \mu)}{\partial T}, \quad N = -\frac{\partial\Omega(T, \mu)}{\partial\mu}, \quad (1.41)$$

which we write in terms of entropy and number densities as

$$s(T, \mu) = +\frac{\partial p(T, \mu)}{\partial T}, \quad n(T, \mu) = \frac{\partial p(T, \mu)}{\partial\mu} = \frac{N}{V}. \quad (1.42)$$

Here the first derivatives give averages while the second derivatives yield fluctuations about the averages. For instance,

$$\langle N^2 \rangle - \langle N \rangle^2 = -T \frac{\partial^2 \Omega}{\mu^2} = TV \frac{\partial^2 p}{\partial \mu^2}. \quad (1.43)$$

Thus pressure is the fundamental quantity. It gives both  $s$  and  $n$  as well as the energy density  $\epsilon$  through

$$\epsilon = Ts - p + \mu n. \quad (1.44)$$

In thermal equilibrium,  $\Omega$  is minimised and hence  $p$  is maximised. In particular, if the system has several different minima of  $\Omega$ , the true stable ground state is the one with minimal  $\Omega$  (maximal pressure); the other ones are metastable states. This is a very common situation.

**Application:  $p = nT$ -gas in grand canonical ensemble** The usefulness of the grand canonical ensemble is obvious if one tries to work out the thermodynamics of a Maxwell-Boltzmann ideal gas. Keep  $m/T$  arbitrary and take  $\hbar = c = 1$ ,  $E = \sqrt{p^2 + m^2}$ . Then

$$Z(1) = V \int \frac{d^3p}{(2\pi)^3} e^{-\beta\sqrt{p^2+m^2}} = \frac{VTm^2}{2\pi^2} K_2\left(\frac{m}{T}\right), \quad (1.45)$$

where the Bessel function  $K_2(z) \rightarrow 2/z^2$  when  $z \rightarrow 0$  and  $\rightarrow \sqrt{\pi/(2z)}e^{-z}$  when  $z \rightarrow \infty$ . For the canonical free energy one obtains  $F(T, V, N) = -TN[1 + \log(Z(1)/N)]$ . However, for the grand potential the series (1.38) exponentiates and by taking the log and using (1.40) one obtains

$$p(T, \mu) = \frac{T^2 m^2}{2\pi^2} e^{\beta\mu} K_2\left(\frac{m}{T}\right). \quad (1.46)$$

Using the formulas above this further gives

$$s = \frac{m^3}{2\pi^2} e^{\beta\mu} \left[ K_1\left(\frac{m}{T}\right) + \frac{4T}{m} K_2\left(\frac{m}{T}\right) - \frac{\mu}{m} K_2\left(\frac{m}{T}\right) \right], \quad (1.47)$$

$$n = p/T, \quad (1.48)$$

$$\epsilon = \frac{m^2 T}{2\pi^2} e^{\beta\mu} \left[ K_1\left(\frac{m}{T}\right) + \frac{3T}{m} K_2\left(\frac{m}{T}\right) \right]. \quad (1.49)$$

From here one can see the role played by the chemical potential. In the NR limit  $T \ll m$  the number density becomes

$$n = \left(\frac{mT}{2\pi}\right)^{3/2} e^{\beta(\mu-m)} \equiv \frac{1}{\lambda_{\text{th}}^3} e^{\beta\mu}. \quad (1.50)$$

Since here  $m$  is an unnecessary constant one replaces  $\mu - m \rightarrow \mu$  and sees the role on  $\mu$ : it fixes the number density and one expects its value to be negative, to satisfy the conditions of validity of Maxwell-Boltzmann statistics.

**Application: ideal Fermi-Dirac and Bose-Einstein gases.** The term "ideal gas" denotes a collection of free particles within a system with known energy levels  $E_1, E_2, \dots$ . For example, if the system is a box of volume  $V = L^d$  (usually  $d = 3$ ) with periodic boundary conditions and if the particles satisfy the dispersion relation  $E^2(k) = (\hbar ck)^2 + (mc^2)^2 \equiv \mathbf{k}^2 + m^2$  the energy spectrum is

$$\begin{aligned} \mathbf{k} &= (k_1, k_2, k_3) = \frac{2\pi}{L}(n_1, n_2, n_3), \quad n_i = 0, \pm 1, \pm 2, \dots, \\ E^2(k) &= \frac{4\pi^2}{L^2}(n_1^2 + n_2^2 + n_3^2) + m^2 \end{aligned} \quad (1.51)$$

and each set of  $n_i$  corresponds to a state of the system. A second example is free particles in a 3d harmonic oscillator potential with  $E(\mathbf{n}) = \hbar\omega(n_1 + n_2 + n_3 + 3/2)$ .

The crucial assumption is then the following: each state is occupied with equal probability, given by the usual FD or BE statistics. This is easy to implement formally (and the standard steps are reproduced below), but leaves completely open the dynamical issue of how this kind of state is actually attained, i.e. how the system thermalises. Paradoxically, as will be discussed in Ch. XXXXX, the stronger the interactions are, the faster and more efficiently they thermalise the system; however, at the same time the interactions should be weak enough so that the system is perturbatively close to the non-interaction ideal system. Therefore, in reality ideal gas system is not a collection of free particles even if confined in a box!

Let us assume that the occupation number of each of the energy levels  $E_i$  is  $N_i$ . From the definition of grand canonical partition function  $\mathcal{Z}$  we find that

$$\mathcal{Z}(T, V, \mu) \equiv \sum_{N=0}^{\infty} z^N Z(T, V, N) = \sum_{N=0}^{\infty} (e^{\frac{\mu}{T}})^N \sum_{\{N_1, N_2, \dots\}} e^{-\frac{1}{T}(N_1 E_1 + N_2 E_2 + \dots)}. \quad (1.52)$$

Because of the condition  $\sum N_i = N$ , the summation in  $Z(T, V, N)$  is hard to perform. Note however that the

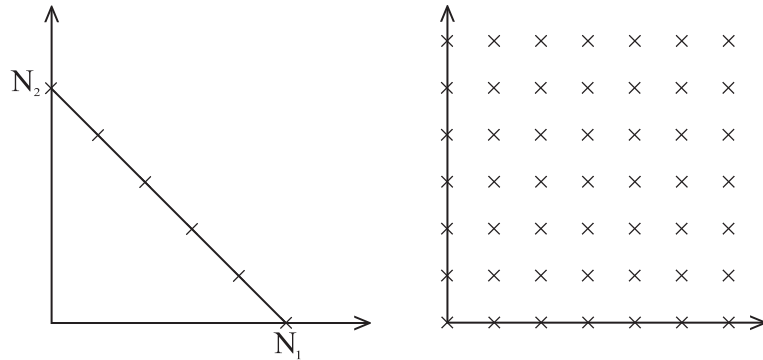


Figure 1.2:  $Z$  to the left and  $\mathcal{Z}$  to the right.

sum in  $\mathcal{Z}$  goes over all accessible states, as depicted in Fig. 1.2. Therefore, by rearranging the order of the summation we may write:

$$\begin{aligned} \mathcal{Z} &= \sum_{\{N_1, N_2, \dots=0\}}^{\infty} e^{\frac{\mu}{T} N_1} e^{\frac{\mu}{T} N_2} \dots (e^{-\frac{1}{T} E_1})^{N_1} (e^{-\frac{1}{T} E_2})^{N_2} \dots \\ &= \sum_{\{N_1, N_2, \dots=0\}}^{\infty} (e^{\frac{1}{T}(\mu - E_1)})^{N_1} (e^{\frac{1}{T}(\mu - E_2)})^{N_2} \dots \\ &= \sum_{N_1=0}^{\infty} (e^{\frac{1}{T}(\mu - E_1)})^{N_1} \sum_{N_2=0}^{\infty} (e^{\frac{1}{T}(\mu - E_2)})^{N_2} \dots, \end{aligned} \quad (1.53)$$

where the sums are now simple to evaluate:

$$\sum_{N=0}^{\infty} x^N = \begin{cases} 1+x & \text{FD} \\ \frac{1}{1-x} & \text{BE} \end{cases} . \quad (1.54)$$

Thus for FD we find

$$\mathcal{Z} = \prod_k [1 + e^{\frac{1}{T}(\mu - E_k)}], \quad \Omega = -Vp(T, \mu) = -T \sum_k \log[1 + e^{\frac{1}{T}(\mu - E_k)}], \quad (1.55)$$

whereas for BE

$$\mathcal{Z} = \prod_k \frac{1}{1 - e^{\frac{1}{T}(\mu - E_k)}}, \quad \Omega = -Vp(T, \mu) = T \sum_k \log[1 - e^{\frac{1}{T}(\mu - E_k)}], \quad (1.56)$$

From here one further derives, using  $s(T, \mu) = \partial p / \partial T = S/V$ ,  $n(T, \mu) = \partial p / \partial \mu = N/V$  and  $\epsilon = Ts - p + \mu n = E/V$  that

$$N(T, \mu) = \sum_k n_k, \quad (1.57)$$

$$S(T, \mu) = \sum_k [-(1 - n_k) \log(1 - n_k) - n_k \log n_k] \quad \text{FD}, \quad (1.58)$$

$$S(T, \mu) = \sum_k [(1 + n_k) \log(1 + n_k) - n_k \log n_k] \quad \text{BE}, \quad (1.59)$$

$$E(T, \mu) = \sum_k E_k n_k, \quad (1.60)$$

where the average occupation number of the level  $k$  is

$$n_k = \frac{1}{e^{\frac{1}{T}(E_k - \mu)} \pm 1} \begin{cases} \text{FD} \\ \text{BE} \end{cases} . \quad (1.61)$$

The above is valid for any set of energy levels  $E_k$ . If we further take our free particles in a box, the energy levels are indexed by  $E_k \equiv \sqrt{\mathbf{k}^2 + m^2}$  and the sums can be changed to integrals using the continuum limit of the density of states of particles in a 3d box (see below):

$$\sum_k \rightarrow \frac{V}{(2\pi)^3} \int d^3k. \quad (1.62)$$

Then for FD the pressure reads as

$$p(T, \mu) = \frac{T}{(2\pi)^3} \int d^3k \log[1 + e^{\frac{1}{T}(\mu - E_k)}] \quad (1.63)$$

while for BE

$$p(T, \mu) = -\frac{T}{(2\pi)^3} \int d^3k \log[1 - e^{\frac{1}{T}(\mu - E_k)}]. \quad (1.64)$$

These expressions should be multiplied by  $g$ , the degeneracy of the momentum level  $k$ ;  $g$  counts the internal degrees of freedom such as spin, colour, etc. One should also add the contribution of antiparticles. Since particles and antiparticles can annihilate, in equilibrium their chemical potentials are opposite and terms where  $\mu \rightarrow -\mu$  should be added to Eqs. (1.63) and (3.12). Non-relativistically, however, their contribution is exponentially suppressed by the Boltzmann factor  $\exp(-2\beta m)$  and thus negligible. To see this, write  $E(k) = \sqrt{m^2 + \mathbf{k}^2} = \sqrt{(mc^2)^2 + (\hbar ck)^2} \approx mc^2 + \frac{\hbar^2 \mathbf{k}^2}{2m}$ ; then in the combination  $\mu - E_k$  the rest energy  $mc^2$  has to be combined with  $\mu$  so that the chemical potential can be redefined as  $\mu \rightarrow \mu' = \mu - mc^2$ , which implies that the antiparticle occupation number goes like  $1/(\exp(\beta(2m + \mu' + E_{\text{kin}})))$ .

Partial integration, writing  $d^3k = 4\pi d(k^3/3)$ , permits one to eliminate the logarithm from the expressions (1.63) and (3.12) for  $p$ . The result is

$$p(T, \mu) = \frac{(\hbar c)^2}{(2\pi)^3} \int d^3k \frac{k^2}{3E(k)} \frac{1}{e^{\frac{1}{T}(E-\mu)} \pm 1} \equiv \frac{(\hbar c)^2}{(2\pi)^3} \int d^3k \frac{k^2}{3E(k)} n_0(k). \quad (1.65)$$

with

$$n_0(k) = \frac{1}{e^{\frac{1}{T}(E(k)-\mu)} \pm 1} \begin{cases} FD \\ BE \end{cases}.$$

From here one further derives, using  $s(T, \mu) = \partial p / \partial T = S/V$ ,  $n(T, \mu) = \partial p / \partial \mu = N/V$  and  $\epsilon = Ts - p + \mu n = E/V$  that

$$n(T, \mu) = \frac{1}{(2\pi)^3} \int d^3k n_0(k) \quad (1.66)$$

$$s(T, \mu) = \frac{1}{(2\pi)^3} \int d^3k \left[ (1 - n_0) \log \frac{1}{1 - n_0} + n_0 \log \frac{1}{n_0} \right] \quad FD \quad (1.67)$$

$$s(T, \mu) = \frac{1}{(2\pi)^3} \int d^3k \left[ -(1 + n_0) \log \frac{1}{1 + n_0} + n_0 \log \frac{1}{n_0} \right] \quad BE \quad (1.68)$$

$$\epsilon(T, \mu) = \frac{1}{(2\pi)^3} \int d^3k E n_0(k). \quad (1.69)$$

## 1.5 Black hole thermodynamics

The notion of thermal equilibrium can also be extended to gravitating systems, most famously to black holes. What really is happening here is one of the most fundamental questions of physics today and is connected with how classical Einsteinian gravity and quantum theory should be united. We shall here list without derivation a number of relevant and very suggestive formulas and compare them with what usual thermodynamics would say.<sup>3</sup>

The entropy of a black hole is proportional to the area of the event horizon  $A = 4\pi r_s^2$ , where  $r_s = 2GM/c^2$  is the Schwarzschild radius (for these values of mass and radius the escape velocity from a surface of a spherical object is that of light). The result is

$$S_{\text{BH}} = \frac{4\pi GM^2}{\hbar c} \equiv 4\pi \frac{M^2}{M_{\text{Pl}}^2} = \frac{c^3}{\hbar G} \frac{A}{4} \equiv \frac{A}{8\pi L_{\text{Pl}}^2}, \quad (1.70)$$

where  $M$  is the black hole mass. For a ball of gas like the Sun the entropy is essentially just the number of nucleons in it,  $S_{\text{sun}} \sim N \sim nV \sim M/m_p \sim 10^{57}$  since in the Sun there are about  $(M_{\text{Pl}}/m_p)^3 = 10^{57}$  ( $m_p =$  proton mass) nucleons. This number one has to derive from equations of stellar equilibrium, which balance gravitation pulling inwards and gas pressure pushing outwards. For a black hole with the same mass

$$S_{\text{BH}}(M = M_{\text{sun}} = m_p \left(\frac{M_{\text{Pl}}}{m_p}\right)^3) = 4\pi \left(\frac{M_{\text{Pl}}}{m_p}\right)^4 \approx 10^{77}. \quad (1.71)$$

Therefore the entropy of a solar mass black hole wins that of the Sun by a factor  $\sim 10^{20}$ ; collapse increases  $S$  tremendously. Similarly, the entropy of a single million solar mass black

<sup>3</sup>See, for example, Sean M. Carroll, Spacetime and geometry, Addison Wesley 2004

hole in the center of a galaxy equals the entropy of the entire cosmic background radiation. Given that entropy can only decrease, these considerations would imply that the ultimate destiny of a gravitating system is to become a collection of black holes. However, as shown by Hawking in the 1970's, black holes are not completely black but, because of quantum effects, radiate<sup>4</sup>.

Actually, even for a black hole entropy the entropy can be regarded as essentially the number of constituents,  $S \sim N$ , but  $N$  is now the number of quanta in the Hawking radiation emitted by the black hole. If the temperature of the radiation is  $T = T_{\text{Hawk}}$ , the energy of each quantum is  $\sim T_{\text{Hawk}}$  and hence one may argue that their number is

$$N \sim Mc^2/T_{\text{Hawk}} \sim S \sim (M/M_{\text{Pl}})^2 \quad (1.72)$$

so that (with correct factors inserted)

$$T_{\text{Hawk}} = \frac{\hbar\kappa}{2\pi c} = \frac{\hbar c}{4\pi r_s} = \frac{\hbar c^3}{8\pi GM} = \frac{M_{\text{Pl}}^2 c^2}{8\pi M}. \quad (1.73)$$

Here  $\kappa$  is the surface gravity  $\kappa = GM/r_s^2 = c^2/(2r_s)$ . Many alternative expressions were given here.

Let us parametrically estimate the lifetime of a radiating black hole. The radiation luminosity in  $\text{J/m}^2/\text{s}$  is  $\sim T^4$  (as will be derived later) so that the total power equals the mass loss, given by

$$\frac{dM}{dt} \sim -r_s^2 T_{\text{Hawk}}^4 \sim -\frac{1}{r_s^2} \sim -\frac{M_{\text{Pl}}^4}{M^2}. \quad (1.74)$$

Integration leads to  $M^3(t) = M^3(0) - 3M_{\text{Pl}}^2 t$  and the mass is gone when

$$t \sim \left( \frac{M(0)}{M_{\text{Pl}}} \right)^3 \frac{1}{M_{\text{Pl}}}. \quad (1.75)$$

A black hole of mass  $10^{12}\text{kg}$  would live as long as the present universe and radiate initially with a temperature of  $\sim 10 \text{ MeV}$ .

The key element leading to the existence of a temperature for a black hole is the existence of a horizon, region of space excluded from causal contact with observers outside it. A proper derivation of all the formulas - which so far have not been empirically confirmed - thus requires both a theory of space-time, general relativity, and field theory in curved space. The entropy of a black hole may seem a rather puzzling notion considering that a black hole in our space can only have three parameters, mass, charge and angular momentum. From a (classical) statistical perspective, it should not have entropy any more than, say, a single electron. However, perhaps a black hole has a substructure? The key question then is, what exactly are the microscopic degrees of freedom that give rise to the entropy of a black hole? This is one of the deepest questions of today's physics. The answer suggested by string theory is that black holes are just certain configurations in extra dimensional spaces. That this works has been verified for some theoretically defined black holes, but nobody has any idea of what those configurations would be for black holes in our world.

<sup>4</sup>S. Hawking, Commun. Math. Phys. 43:199,1975; Erratum, ibid. 46:206,1976.

## 1.6 Density of states

The basic definition of the partition function, Eq. (1.1), can, by normalising  $E \geq 0$ , be written in the form

$$Z = \sum_{n=\text{all states}} e^{-\beta E_n} = \int_0^\infty dE \frac{dN}{dE} e^{-\beta E}, \quad (1.76)$$

where

$$\frac{dN}{dE} \equiv \rho(E) \equiv \rho(E, N) \quad (1.77)$$

is the density of states, i.e. the number of states of the system per unit  $E$ . The relation (1.76) implies that  $Z(\beta)$  and  $\rho(E)$  are Laplace transforms of each other. Both are as good in giving the full thermodynamics. The notion of the density of states is of great practical interest since it arises naturally both in numerical simulations and in analytical treatments of various simple physical systems.

**Example: Ising model.** We shall later define the d-dimensional Ising model. It is a simple statistical model where one can numerically compute the exact numbers of states corresponding to a fixed total energy of the system. A concrete example for the 2d Ising model on a  $10 \times 10$  lattice is shown in Table 1.1. Here each of the 100 lattice points can have either spin up (+) or spin down (-); thus the total number of states is  $2^{100} \approx 1.267 \cdot 10^{39}$ . There are 200 links in the lattice and if the end points of a link have the same(different) spin one may define the energy to be  $-1(+1)$ . The total energy then is an integer between  $-200$  and  $+200$ ; the Table gives the exact number of states<sup>5</sup> corresponding to each value of  $E$ ; the sum of the entries is  $2^{100}$ .

One of the simplest possible physical systems is particle(s) in a box. This trivial case is indeed a cornerstone in understanding the density of states. Let us assume a periodic 3d box and neglect any surface effects. Then the allowed values of the wave number  $\mathbf{k}$  are

$$\mathbf{k} = \frac{2\pi}{L}(n_1, n_2, n_3), \quad n_i = 0, \pm 1, \pm 2, \dots \quad (1.78)$$

so that with  $E^2 = k^2 + m^2$  we find the sum over states as

$$\sum_i = \int d^3n = \frac{V}{(2\pi)^3} \int d^3k = \int_m^\infty dE \frac{V}{2\pi^2} E \sqrt{E^2 - m^2}. \quad (1.79)$$

Note that now we have derived the classical result Eq. (1.25):

$$\sum_i = \int \frac{V d^3k}{(2\pi)^3} = \int \frac{d^3x d^3p}{h^3} \quad (1.80)$$

since  $p = \hbar k$ . In the ultrarelativistic (UR) limit, where  $m \ll E$ , and in the non-relativistic (NR) limits we thus obtain the expressions

$$\rho_{\text{UR}}(E) = \frac{1}{2E} \frac{VE^3}{\pi^2}, \quad \rho_{\text{NR}}(E) = \frac{V}{2\pi^2} m \sqrt{2mE}. \quad (1.81)$$

**Modification: particles in a harmonic potential.** Instead of a box we can also have a smoother confinement such as a harmonic oscillator potential  $V = \frac{1}{2}m\omega^2 \mathbf{x}^2$ . This case will be important when discussing

<sup>5</sup>For even larger numbers, see Paul D. Biele, Phys. Rev. Letters 76, 78, 1996 or F. Wang and D.P.Landau, Phys. Rev. E64, 056101, 2001.

$E$	$N(E) = \log S(E)$	$E$	$N(E) = \log S(E)$
-200	1	0	108804232426376087683496097815
-196	0	4	127615138775266749696010320050
-192	100	8	138682226083589753382353631155
-188	190	12	139467535997338317070747513220
-184	5390	16	129673265537564086898449474485
-180	19920	20	111398087687361442602934363604
-176	226185	24	88394194656000609637107306835
-172	1123330	28	64789735278060885125545778420
-168	8441545	32	43882526876091406802688842040
-164	46439270	36	27484620182084875609413209920
-160	288232165	40	15934677821408488316923097025
-156	1596503840	44	8562769731912107647661352420
-152	9008597790	48	4271377195758556988860024315
-148	48530806690	52	1981325557749994784540426400
-144	258919598835	56	856247175668720270761391354
-140	1348085135068	60	345440085480687517414714344
-136	6918375532625	64	130373941135805243213306725
-132	34921952998720	68	46131131663242989983156880
-128	173864285141465	72	15336949736067657882440975
-124	853528946161100	76	4801625511818556981759340
-120	4131702217991006	80	1418746354667950902604900
-116	19598116107747500	84	396504230728933768862650
-112	92337394182797240	88	105044804469611713155910
-108	424635096183933970	92	26439076355718752657610
-104	1910993686546702565	96	6336775057494900296995
-100	8394325581182421100	100	1449347253869825330984
-96	35900636024138056610	104	317184792213120157975
-92	149134699701274540190	108	66590745159525686410
-88	600434187444808042305	112	13450173814318534170
-84	2338237484656296289710	116	2621824707749641960
-80	8790991827530811266845	120	494837291835094171
-76	31852806882802872810510	124	90726699739843320
-72	111039862678342970767760	128	16209249292505960
-68	371793726574328382611580	132	2829255985524290
-64	1193670523583033542771745	136	483344637121035
-60	3668437423804485582262430	140	80889449574800
-56	10772807184138254585743365	144	13259776474415
-52	30174747119602748554894980	148	2126884521530
-48	80467250627920555722255415	152	333319272600
-44	203904785227407787528278180	156	50912615760
-40	490026517327332203099130689	160	7565408818
-36	1114622254786255520262613920	164	1088231770
-32	2974787743912498152267010800	168	151489010
-28	4849969799910449080522379200	172	20119550
-24	9239228193366464362451697155	176	2579540
-20	16521328755364544210468233924	180	303762
-16	27673114057688890670065067455	184	35230
-12	43328960149817735987320787580	188	3340
-8	63289600282274727602148469440	192	350
-4	86076254527328476831763676120	196	20
		200	2

Table 1.1: The density of states for the Ising model on a 10 by 10 lattice (Stodolsky-Wosiek, Nucl.Phys. B413(1994) 817)

Bose-Einstein condensation. The energy spectrum of the 3d harmonic oscillator is (assuming a symmetric oscillator with  $\omega_i = \omega$ )

$$E = \hbar\omega(n_1 + n_2 + n_3 + \frac{3}{2}), \quad n_i = 0, 1, 2, \dots \quad (1.82)$$

and we may write, assuming that the  $n_i$  are so large that the constant 3/2 can be neglected,

$$\sum_{\text{states}} = \int d^3n = \int dE \int d^3n \delta(E - \hbar\omega(n_1 + n_2 + n_3)) \equiv dE \rho(E), \quad (1.83)$$

so that, integrating first over  $n_3$  and then imposing the condition  $n_3 > 0$ , we find

$$\rho(E) = \frac{1}{\hbar\omega} \int_0^\infty dn_1 dn_2 \Theta\left(\frac{E}{\hbar\omega} - n_1 - n_2\right) = \frac{E^2}{2(\hbar\omega)^3}. \quad (1.84)$$

More generally, in  $d$  dimensions,

$$\rho(E) = \frac{E^{d-1}}{(d-1)! \prod \hbar\omega_i}. \quad (1.85)$$

But what if we have  $N$  Maxwell-Boltzmann particles in a box? Then by just counting the states one has

$$\rho(E, N) = \frac{1}{N!} \int \delta(E - \sum_i E_i) \prod_1^N \frac{V}{(2\pi)^3} \int d^3k_i, \quad (1.86)$$

which one can evaluate by introducing a Fourier representation for the  $\delta$ -function and using the method of steepest descent, to be discussed in the next Section. But let us here compute  $\rho(E, N)$  by inverting the Laplace transformation:

$$\rho(E, N) = \frac{1}{2\pi i} \int_{-i\infty+\beta_c}^{i\infty+\beta_c} d\beta Z(\beta, N). \quad (1.87)$$

To simplify put  $m = 0$  and  $\hbar = c = 1$ . In this UR case we may evaluate from (1.25) by putting there  $E = cp = p$

$$Z(\beta, N) = \frac{1}{N!} \left(\frac{VT^3}{\pi^2}\right)^N. \quad (1.88)$$

A saddle point evaluation leading to  $\beta_c = 3N/E$  gives

$$\rho(E, N) = \frac{1}{N! (3N-1)!} \frac{1}{E} \left(\frac{VE^3}{\pi^2}\right)^N, \quad (1.89)$$

a powerlike behaviour. Remember, though, that the exponent can be gigantic.

However, if one carries out the same steps with the grand potential  $\Omega(T, \mu)$ , using

$$Z(T, z) = \sum_{N=0}^{\infty} z^N Z(T, N) = \int_0^\infty dE \rho(E, z) e^{-\beta E} = \exp(zVT^3/\pi^2), \quad z = e^{\beta\mu}, \quad (1.90)$$

together with Eq. (1.87) in the saddle point approximation (with  $\beta_c^4 = 3zV/(\pi^2 E)$ ), one finds

$$\rho(E, z) = \frac{1}{\sqrt{8\pi}} \left(\frac{3zV}{\pi^2}\right)^{\frac{1}{8}} E^{-\frac{5}{8}} \exp\left[\frac{4}{3} \left(\frac{3zV}{\pi^2}\right)^{\frac{1}{4}} E^{\frac{3}{4}}\right], \quad (1.91)$$

an exponential of a fractional power.

In the NR case one obtains, similarly,

$$\rho(E, N) = \frac{1}{N! \Gamma(\frac{3}{2}N)} \frac{1}{E} \left( \frac{V^{2/3} m E}{2\pi} \right)^{\frac{3}{2}N}. \quad (1.92)$$

**Example: Hagedorn temperature.** Conceptually, the notion of the density of states is very important. For instance, if the density of states is exponential, there is a singularity in the partition function which may signal a phase transition from weakly to strongly interacting theory. A well-known example is string theory, but a singularity was encountered already before strings in the bootstrap model of hadrons, which was in favor in the 1960's. The number of new hadron states seemed then to grow almost without a limit. Thus, one could consider the gas of interacting hadrons to consist of a large number of resonances with a grand canonical partition function for each species  $i$  as given by Eq. (1.38) with  $E^2 = p^2 + m_i^2$ . The total partition function of the hadron gas would then be

$$\ln \mathcal{Z}(T, V) = \sum_i \rho(m_i) \ln \mathcal{Z}(T, V, m_i), \quad (1.93)$$

where the sum begins with the ground state  $m_0$  and then includes all the possible resonances.

The bootstrap assumption was then imposed on the density of states  $\rho$ : "fireballs consist of fireballs, which consist of fireballs ...", or in other words, resonance formation and decay follow a self-similar pattern<sup>6</sup> with

$$\rho(m, V) = \delta(m - m_0) + \sum_N \frac{1}{N!} \left( \frac{V}{(2\pi)^3} \right)^N \int \prod_{i=1}^N d^3 p_i dm_i \rho(m_i) \delta(\sum p_i - p), \quad (1.94)$$

which was solved analytically to yield

$$\rho(m, V) = \text{const.} \times m^{-3} \exp(-M/T_H). \quad (1.95)$$

Here  $T_H$  is the Hagedorn temperature, which can be determined in terms of  $V$  and  $m_0$ . The volume factor  $V$  specifies the range  $r$  of strong interactions and is thus given by  $V \sim r^3 \sim 1/m_\pi^3$  with  $r \sim 1$  fm. In the limit  $m_0 \rightarrow 0$  the Hagedorn temperature is found to be  $T_H \sim 200$  MeV.

Replacing the sum with an integral and inserting the exponentially increasing density of states into the partition function we find

$$\ln \mathcal{Z}(T, V) \sim V \left( \frac{T}{2\pi} \right)^{3/2} \int dm m^{-3/2} \exp(-m(\frac{1}{T} - \frac{1}{T_H})). \quad (1.96)$$

Thus there is a divergence for all  $T > T_H$  so that the Hagedorn temperature was suggested to be the ultimate temperature for hadronic matter. What, in reality, happens is a transition to a new phase, quark-gluon plasma.

## 1.7 Method of steepest descent

Let us now try to evaluate the expression Eq. (1.76) in a convenient approximation. Since  $\rho(E)$  increases extremely fast and thence  $e^{-\beta E}$  decreases fast, the method of choice is the saddle

<sup>6</sup>See e.g. Ph. Blanchard, S. Fortunato and H. Satz, hep-ph/0401103.

point "semi-classical" approximation, where we expand the action about some background value:

$$\begin{aligned}
\int_{-\infty}^{\infty} dx e^{-\frac{1}{\hbar}S(x)} &= \int_{-\infty}^{\infty} dx \exp\left\{-\frac{1}{\hbar}[S(\bar{x}) + S'(\bar{x})(x - \bar{x}) + \frac{1}{2}S''(\bar{x})(x - \bar{x})^2 + \frac{1}{6}S'''(\bar{x})(x - \bar{x})^3 + \right. \\
&\quad \left. + \frac{1}{24}S''''(\bar{x})(x - \bar{x})^4 + \dots]\right\} \\
&= e^{-\frac{1}{\hbar}S(\bar{x})} \int_{-\infty}^{\infty} dx \exp\left[-\frac{1}{2\hbar}\bar{S}''(x - \bar{x})^2 - \frac{1}{6\hbar}\bar{S}'''(x - \bar{x})^3 - \frac{1}{24\hbar}\bar{S}''''(x - \bar{x})^4 + \dots\right] \\
&= e^{-\frac{1}{\hbar}S(\bar{x})} \sqrt{\frac{2\hbar}{\bar{S}''}} \int_{-\infty}^{\infty} dy e^{-y^2} \left[1 - \frac{\hbar}{6} \frac{\bar{S}''''}{(\bar{S}'')^2} y^4 + \frac{\hbar}{9} \frac{(\bar{S}''')^2}{(\bar{S}'')^3} y^6 \dots\right] \\
&= e^{-\frac{1}{\hbar}S(\bar{x})} \sqrt{\frac{2\pi\hbar}{\bar{S}''}} \left\{1 - \hbar \left[\frac{\bar{S}''''}{8(\bar{S}'')^2} - \frac{5}{24} \frac{(\bar{S}''')^2}{(\bar{S}'')^3}\right] + \mathcal{O}(\hbar^2)\right\} \tag{1.97}
\end{aligned}$$

Although the expansion above is mathematically simplistic in that almost always the action  $S$  is a functional, not a simple function, it nevertheless serves to illustrate several important physical features found in more realistic cases:

- We have introduced  $\hbar$  as a formal parameter so that one may appreciate the fact that the outcome is an expansion in  $\hbar$ .
- We have expanded the integrand around some point  $\bar{x}$  and chosen this point such that  $S'(\bar{x}) = 0$  (the name saddle point fits better when this is done in the complex domain or with more than one degree of freedom). This is the analogue of finding classical equations of motion by extremizing the action;  $S(x)$  is the action and  $\bar{x}$  is the analogue of the solution of classical equations of motion.
- For the solution to be a stable minimum, we must require  $\bar{S}'' \equiv S''(\bar{x}) > 0$ . Then we may take  $y = \sqrt{\bar{S}''/2\hbar}(x - \bar{x})$  as a new variable, expand in  $\sqrt{\hbar}$  and perform the  $y$  integral. The odd terms vanish and the result becomes an expansion in  $\hbar$ .
- The first term in the final result in Eq. (1.97) has, in various connections, the names classical, tree level, or mean field approximation. Its evaluation is relatively simple. One just finds the "classical field"  $\bar{x}$  and finds the value of the action for this field. The importance of the second term lies in the fact that it gives the correct dimensions (those of  $x$ ) to the integral. It is called the fluctuation, Gaussian, or one-loop term, and its evaluation is often possible - it comes from a Gaussian integration - but may nevertheless be technically very complicated. The remaining corrections are called loop corrections. For the harmonic oscillator they vanish.

To apply Eq. (1.97), we write the partition function Eq. (1.76) as

$$Z = \int_{-\infty}^{\infty} dE \frac{dN}{dE} e^{-\beta E} \equiv \int_{-\infty}^{\infty} dE \frac{1}{T} e^{S(E) - \beta E}. \tag{1.98}$$

Here we have inserted a prefactor  $1/T$  in order to keep  $Z$  dimensionless and have extended the lower limit to  $-\infty$ ; this is allowed for from a physical perspective since just small region around the saddle point gives a non-negligible contribution to the integral.

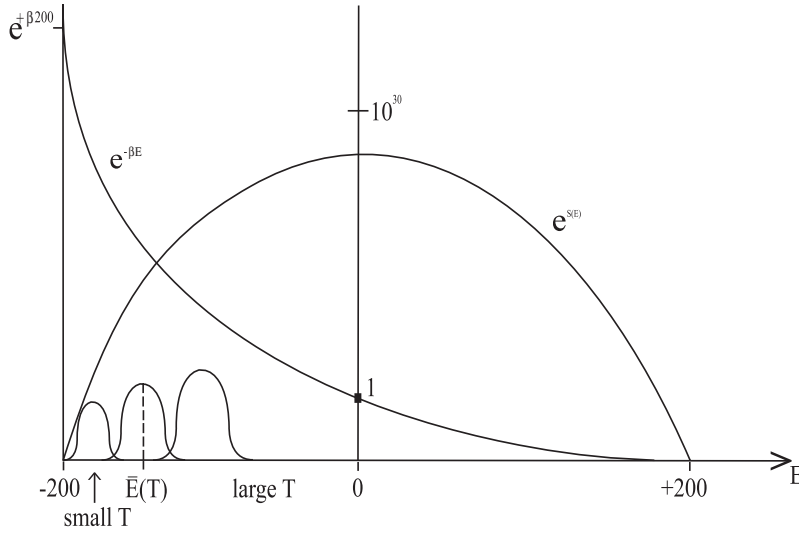


Figure 1.3: Competition between  $E$  (wants to be smaller) and  $S$  (wants to be larger) schematically. The net result is a Gaussian centered around some  $\bar{E}$ .

In the saddle point approximation one solves  $\bar{E}$  from  $S'(\bar{E}) = \beta$  and expands the integrand around  $\bar{E}$ . Neglecting higher order terms

$$S(E) - \beta E = S(\bar{E}) - \beta \bar{E} + \underbrace{S'(\bar{E}) - \beta}_{=0} + \frac{1}{2}(E - \bar{E})^2 S''(\bar{E}) \quad (1.99)$$

and we find

$$\begin{aligned} Z &= \frac{1}{T} e^{S(\bar{E}) - \beta \bar{E}} \int_{-\infty}^{\infty} dE e^{-\frac{1}{2} S''(\bar{E})(E - \bar{E})^2} \\ &= e^{S(\bar{E}) - \beta \bar{E}} \sqrt{\frac{2\pi}{-T^2 S''(\bar{E})}} = e^{-\beta F}. \end{aligned} \quad (1.100)$$

What is happening here is sketched in Fig. 1.7: rapidly increasing and decreasing terms combine to give together a Gaussian. The saddle point equation further gives  $S''(\bar{E}) \cdot d\bar{E}/dT = -1/T^2$  so that the specific heat is given by

$$C_V = d\bar{E}/dT = -1/T^2 S''(\bar{E}). \quad (1.101)$$

From the above we can then read

$$F(T) = \bar{E}(T) - TS(\bar{E}(T)) - \frac{1}{2} T \log C_V \approx \bar{E}(T) - TS(\bar{E}(T)), \quad (1.102)$$

since  $T \log C_V$  is tiny and can be neglected.

Neglecting  $N, \mu$ , thermodynamics is again found from the derivatives of  $F(T)$  in a simple manner:

$$\begin{cases} F'(T) = \bar{E}'(T) - S(\bar{E}(T)) - TS'(E) \cdot \frac{d\bar{E}}{dT} = -S(\bar{E}(T)), \\ F''(T) = -S'(\bar{E}) \cdot \frac{d\bar{E}}{dT} = -\frac{1}{T} C_V. \end{cases}$$

The probability for a configuration with a fixed  $E$  is given by the Boltzmann factor · density of states, together with a proper normalization, and reads

$$P(E) = \frac{1}{Z} \frac{dN}{dE} e^{-\beta E} \approx \sqrt{\frac{-S''}{2\pi}} e^{-\frac{(-S'')}{2}(E-\bar{E})^2} . \quad (1.103)$$

Thus the factor  $(-S'')$  represents the fluctuations in energy:  $\langle (E - \bar{E})^2 \rangle = 1/\sqrt{-S''} = T\sqrt{C_V}$ .

**Example: negative temperature.** The competition between entropy and energy is manifest also for negative temperatures. (When finding the most likely partition, temperature is just a Lagrange multiplier that can be either positive or negative, see Eq. (1.7).) Negative temperature requires that there is a finite upper limit in the energy spectrum; otherwise the Boltzmann factor, i.e. the occupation probability,  $e^{-\beta E}$  would grow without limit for  $\beta < 0$ .

Consider a 2-state spin system in an external magnetic field  $\mathbf{B}$  with

$$H = -\boldsymbol{\mu} \cdot \mathbf{B} = \begin{cases} +\mu B \equiv +E_0 & \text{spin } \downarrow \\ -\mu B \equiv -E_0 & \text{spin } \uparrow \end{cases} \quad (1.104)$$

For fixed particle number  $N$ , the total energy and entropy can then be written as

$$\begin{aligned} E &= -n_1 E_0 + (N - n_1) E_0, \\ S &= -n_1 \log n_1 - (N - n_1) \log (N - n_1), \end{aligned} \quad (1.105)$$

where  $n_1$  is the occupation number of the spin  $\uparrow$  level.

Since  $F = S - \beta E$ , as  $\beta \rightarrow 0_+$  the free energy is extremized by  $S$ , and  $dS/dn_1 = 0$  implies  $n_1 = N/2 = n_2$ , a fully disordered state. The same holds when  $\beta \rightarrow 0_-$ . For  $\beta \rightarrow \infty$ , when  $F$  is extremized by  $E$ , we would find  $n_1 = N, n_2 = 0$  so that at zero temperature the system is at its ground state. However, when  $\beta \rightarrow -\infty$ , we find  $n_2 = N, n_1 = 0$  so that the system finds itself in the excited state.

Since the disordered state corresponds to both  $T = \infty$  and  $T = -\infty$ , one can say that the jump from positive to negative temperatures goes by way of infinity. "Negative temperatures", i.e. certain partitions, have been observed in well isolated systems of e.g. silver and rhodium atoms<sup>7</sup>.

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<sup>7</sup>See P.Hakonen and O.Lounasmaa, Science 265 (1994) 1821.

## Chapter 2

# Partition function as path integral: quantum mechanics

In the previous section we discussed how all the equilibrium thermodynamics can be computed from the partition function, defined by

$$Z = e^{-\beta F} = e^{-\beta E + S} = \text{Tr} e^{-\beta H} = \sum_{\text{states}} e^{-\beta E_i}, \quad (2.1)$$

where the sum goes over all the eigenstates  $i$  of the *Hamiltonian* of the system.

Now comes a very important technical step: we write the fundamental formula for the partition function as a path integral containing the *Lagrangian* of the system. Symbolically,

$$Z = e^{-\beta F} = \text{Tr} e^{-\beta H} \Rightarrow \int \mathcal{D}\Phi e^{-S[\Phi]/\hbar}, \quad (2.2)$$

where  $\Phi$  is a set of degrees of freedom defining the system,  $\mathcal{L}[\Phi]$  is the Lagrangian density of the theory governing the dynamics of the degrees of freedom  $\Phi$  and  $S[\Phi] = \int d\tau d^3x \mathcal{L}[\Phi]$  is the *Euclidean* action. We shall see that thermodynamics leads to Euclidean spacetime with imaginary time which we shall, conventionally, define as  $\tau = it$ . The measure  $\mathcal{D}\Phi \equiv \prod d\Phi$  is defined so that in the path integral one is integrating over all possible field configurations  $\Phi(\mathbf{x}, \tau)$  (which are functions). To get a proper Minkowskian quantum (field) theory, we need to Wick rotate  $\tau \rightarrow it$  to obtain  $e^{-S_E[\Phi]/\hbar} \rightarrow e^{iS_M[\Phi]/\hbar}$ . (For rules of going from Minkowski to Euclidian space, see end of Section 2.2.)

The relation between quantum mechanics and field theory should be appreciated at this stage. In the simplest quantum mechanical case, particle in one dimension  $x$ ,  $\Phi = x$  so that one integrates over all possible paths  $x(t)$  of the particle. This is straightforward to generalise first into one particle in many dimensions,  $\Phi = \mathbf{x}$ , then to  $N$  particles in many dimensions,  $\Phi = \mathbf{x}_i$ ,  $i = 1, \dots, N$ , in just adds more indices.  $N$  can be arbitrarily large but it always obtains discrete values. However, in quantum field theory the index  $i$  corresponds to the value of some field  $\phi$  (possibly with many components  $\phi_a$ ) in the spatial point  $\mathbf{x}$ ,  $\phi(t, \mathbf{x}) \equiv \phi_{i=\mathbf{x}}(t)$  so that effectivly  $N \rightarrow \text{continuum } \infty$ . Then sums become integrals,  $\sum_{i=1}^N \rightarrow \int d^d x$ , functions of coordinates  $\mathbf{x}_i$  become functionals of fields  $\phi(t, \mathbf{x})$ , etc.

The partition function is a powerful tool in many fields of physics and writing it in path integral form is an exercise one will never regret. All the correlators – and hence all physics – can be constructed as expectation values from the probability distribution defined by  $Z$ :

$$\langle \Phi_1 \Phi_2 \dots \Phi_N \rangle = Z^{-1} \int \mathcal{D}\Phi \Phi_1 \Phi_2 \dots \Phi_N e^{-S[\Phi]/\hbar}. \quad (2.3)$$

To compute them, one introduces the *generating functional*

$$Z[J] = e^{-W[J]} = \int \mathcal{D}\Phi e^{-S[\Phi] - \int dx J\Phi}, \quad (2.4)$$

where  $dx$  stands for  $d\tau$  or  $d\tau d^n x$ , depending on the case at hand. One then takes (functional) derivatives with respect to  $J$  to obtain

$$\langle \Phi_1 \Phi_2 \dots \Phi_N \rangle = (-1)^{N-1} \frac{\delta^N Z[J]}{\delta J(x_1) \delta J(x_2) \dots \delta J(x_N)} \Big|_{J=0}. \quad (2.5)$$

**A reminder: Functional differentiation.** Let  $E[f]$  be a functional of  $f(x)$  (e.g.  $E = \int dx f(x)$  etc.). Then functional derivation is defined as

$$\frac{\delta E[f(x)]}{\delta f(y)} = \lim_{\epsilon \rightarrow 0} \frac{E[f(x) + \epsilon \delta(x-y)] - E[f(x)]}{\epsilon}. \quad (2.6)$$

The chain rule

$$\frac{\delta E}{\delta f(y)} = \int dx' \frac{\delta E}{\delta F(x')} \frac{\delta F(x')}{\delta f(y)} \quad (2.7)$$

holds and so on. The functional Taylor series is defined by

$$E[f] = \sum_{n=0}^{\infty} \frac{1}{n!} \int dx_1 \dots dx_n f(x_1) \dots f(x_n) \frac{\delta^n E[f]}{\delta f(x_1) \dots \delta f(x_n)} \Big|_{f=0}. \quad (2.8)$$

As a concrete example, let us consider the functional  $E[J] = \int dx dy J(x) K(x-y) J(y)$ ; this is a functional of the function  $J$ , and  $K$  is a fixed *kernel function*. Then the functional derivative is

$$\begin{aligned} \frac{\delta E}{\delta J(z)} &= \int dx dy \underbrace{\frac{\delta J(x)}{\delta J(z)}}_{\delta(x-z)} K(x-y) J(y) + \dots \\ &= \int dy K(z-y) J(y) + \int dx K(x-z) J(x) \\ &= 2 \int dx K(z-y) J(y). \end{aligned}$$

Likewise, the second functional derivative is found to be

$$\frac{\delta^2 E}{\delta J(z) \delta J(u)} = 2 \int dx K(z-y) \underbrace{\frac{\delta J(y)}{\delta J(u)}}_{\delta(y-u)} = 2K(z-u). \quad (2.9)$$

A practical way to approach functional derivation is to think of the function  $f(x)$  as a variable  $f$  with an index  $x$ , never minding what the mathematicians say.

## 2.1 Partition function of a particle in a potential as a path integral

What is important and perhaps surprising in the path integral formulation is that the Lagrangian (or its integral, the action) appears, not the Hamiltonian. This is a great simplification at least when Lorentz covariance is needed. So let us first collect some simple Hamiltonian mechanics formulas relating  $L(x, \dot{x})$  and  $H(x, p)$  for a particle in a potential  $V(x)$  in 1+1 dimensions (e.g.,  $V = \frac{1}{2}m\omega^2x^2$ ):

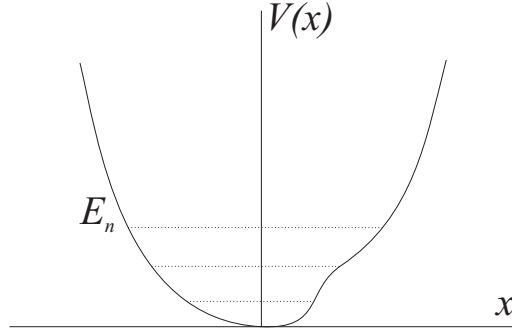


Figure 2.1: Particle in potential  $V(x)$ ; discrete energy levels are known.

Classically, the Lagrangian is

$$L(x, \dot{x}) = T - V = \frac{1}{2}m\dot{x}^2 - V(x) \quad (2.10)$$

leading to the equation of motion (the solutions of which give the extrema of the action  $\int dtL$ )

$$\frac{\partial L}{\partial x} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = -V'(x) - m\ddot{x} = 0 \quad \Rightarrow \quad m\ddot{x} = -V'(x) = F(x). \quad (2.11)$$

The Hamiltonian is obtained as the Legendre transform:

$$H = H(x, p) = p\dot{x} - L(x, \dot{x}) = \frac{p^2}{2m} + V(x), \quad p = \frac{\partial L}{\partial \dot{x}} = m\dot{x} \quad (2.12)$$

so that

$$dH = \frac{\partial H}{\partial x} dx + \frac{\partial H}{\partial p} dp = \dot{x} dp + p d\dot{x} - \frac{\partial L}{\partial x} dx - \frac{\partial L}{\partial \dot{x}} d\dot{x} \quad (2.13)$$

from which follow the Hamiltonian equations of motion

$$\dot{p} = -\frac{\partial H}{\partial x}, \quad \dot{x} = \frac{\partial H}{\partial p} \quad (2.14)$$

(and possibly  $\partial L/\partial t = \partial H/\partial t$ ). In quantum mechanics  $p \rightarrow -i\hbar\partial_x$  and  $E \rightarrow i\hbar\partial_t$ :

$$i\hbar\partial_t\Psi(x, t) = H\Psi(x, t) = \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right] \Psi(x, t) = E_n\Psi(x, t) \quad (2.15)$$

$$\Psi(x, t) = e^{-\frac{i}{\hbar} E_n t} \Psi(x) \tag{2.16}$$

so that the evolution operator is

$$U(t, 0) = e^{-iHt/\hbar} \tag{2.17}$$

and the amplitude for an infinitesimal step from  $x_1$  to  $x_2$  is given by

$$\langle x_2(t + \Delta t) | x_1(t) \rangle = \langle x_2 | e^{-iH\Delta t/\hbar} | x_1 \rangle . \tag{2.18}$$

We observe that the Boltzmann factor is obtained from the evolution operator by taking  $t = -i\hbar\beta$ :

$$U(t = -i\hbar\beta, 0) = e^{-\beta H} . \tag{2.19}$$

This hints at a the connection between imaginary time and thermodynamics (remember that there is no real time in equilibrium thermodynamics!) as well as at a connection between thermal averages and real-time amplitudes represented as sums over all possible paths.

In quantum mechanics, in important quantity is the matrix element  $\langle x_b t_b | x_a t_a \rangle$ , the propagator from point  $x_a$  at time  $t_a$  to point  $x_b$  at time  $t_b$ . This can be evaluated exactly for the harmonic oscillator. First, for a free particle the result, evaluated below in (2.31), is

$$\langle x_b t_b | x_a t_a \rangle = \sqrt{\frac{m}{2\pi i \hbar (t_b - t_a)}} \exp\left[\frac{i}{\hbar} \overbrace{\frac{m}{2} \frac{(x_b - x_a)^2}{t_b - t_a}}^{\text{class. action}}\right] \tag{2.20}$$

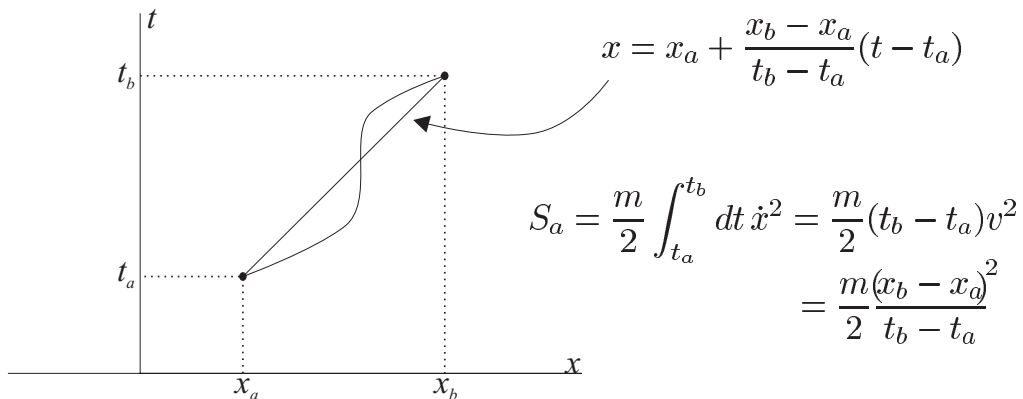


Figure 2.2: Free particle with classical path and action.

For the harmonic oscillator,  $V = \frac{1}{2} m \omega^2 x^2$ :

$$\begin{aligned} \langle x_b t_b | x_a t_a \rangle &= \sqrt{\frac{m\omega}{2\pi i \sin[\omega(t_b - t_a)]}} \exp\left\{ \frac{i m \omega}{2\hbar \sin[\omega(t_b - t_a)]} [(x_a^2 + x_b^2) \cos[\omega(t_b - t_a)] - 2x_a x_b] \right\} \\ &= \underbrace{\sqrt{\text{determinant of gaussian fluctuation (around classical solution)}}}_{\text{can be calculated exactly for harm. oscillator!}} \cdot \exp\left\{ \frac{i}{\hbar} S_a(\text{harm. osc.}) \right\} \end{aligned} \tag{2.21}$$

can be calculated  
exactly for harm. oscillator!

After these preliminaries, go back to the main problem, changing  $\text{Tre}^{-\beta H}$  to a “path” integral? What paths are there if there is no time? (Paths will be periodic paths in imaginary time!).

We have one particle in 1+1d in some  $V(x)$  (see Fig. 2.7) with the Hamiltonian  $H = H(x, p) = p^2/(2m) + V(x)$ . To evaluate the trace we shall use two complete orthonormal sets of basic states  $|x\rangle$  or  $|p\rangle$ :

$$|p\rangle = \underbrace{\sum_x |x\rangle \langle xp|}_{=1, \text{ completeness}} \equiv \int dx \underbrace{\langle x|p\rangle}_{e^{ipx}} |x\rangle \quad (2.22)$$

To normalize carefully one should use a finite box and let  $L \rightarrow \infty$ . Then simply

$$\text{Tre}^{-\beta H} = \int_{-\infty}^{\infty} dx_1 \langle x_1 | e^{-\beta H} | x_1 \rangle. \quad (2.23)$$

Now comes the trick: write

$$e^{-\beta H} = e^{-\frac{\beta\hbar}{N} \cdot \frac{H}{\hbar}} \cdot e^{-\frac{\beta\hbar}{N} \cdot \frac{H}{\hbar}} \cdot \dots \cdot e^{-\frac{\beta\hbar}{N} \cdot \frac{H}{\hbar}} \quad (N \text{ times}) \quad (2.24)$$

and put

$$\int dx |x\rangle \langle x| = 1 \quad (2.25)$$

to each of the  $N - 1$  intervals, calling the new variables  $x_2, \dots, x_N$  and renaming  $x_1 \rightarrow x_{N+1}$  when it appears for the second time (see Fig. 2.3). One obtains for  $Z$

$$Z = \int_{-\infty}^{\infty} dx_1 dx_2 \dots dx_N \langle x_1 | e^{-\epsilon \frac{H}{\hbar}} | x_2 \rangle \underbrace{\langle x_2 | e^{-\epsilon \frac{H}{\hbar}} | x_3 \rangle}_{\text{new ones}} \dots \langle x_{N-1} | e^{-\epsilon \frac{H}{\hbar}} | x_N \rangle \langle x_N | e^{-\epsilon \frac{H}{\hbar}} | x_{N+1} = x_1 \rangle, \quad (2.26)$$

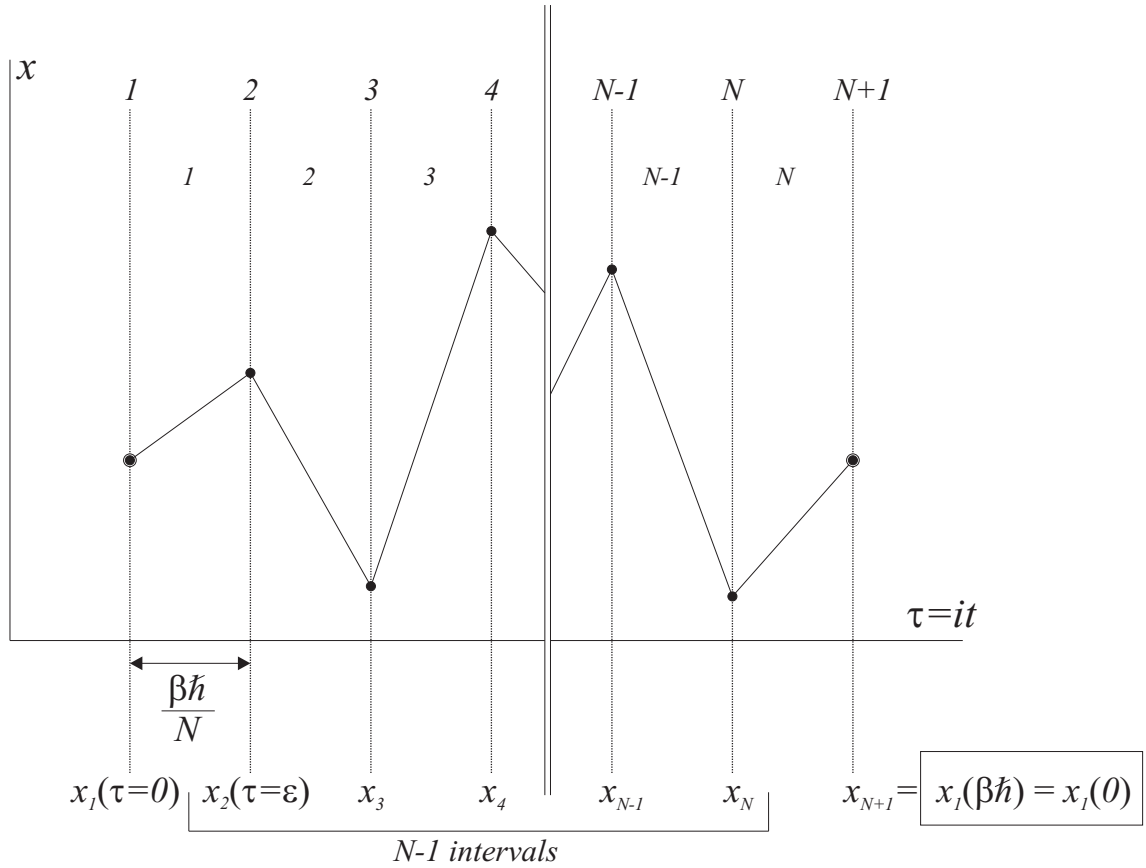
where  $\epsilon = \beta\hbar/N$ . The operator  $e^{-\epsilon H}$  moves the state from  $x_1$  to  $x_2$  in the direction of *imaginary time*  $\tau = it$  ( $U(\tau, 0) = e^{-\tau \frac{H}{\hbar}}$ ). The total motion will be  $N\epsilon = \beta\hbar$ . Since you integrate over all  $x_i$  (keeping  $x_1 = x_{N+1}$ ) you are *summing over all periodic paths* (one such “configuration of  $x(\tau)$ ” is shown in Fig. 2.3) for  $N \rightarrow \infty$ .

The idea now is that for  $N \rightarrow \infty$  the amplitude  $\langle x_{k+1} | e^{-\epsilon H} | x_k \rangle$  in the small interval  $\epsilon \rightarrow 0$  can be reliably estimated by assuming that the potential  $V$  in that interval is essentially a constant:  $\partial_x V \approx 0$  or equivalently  $[p, V] \approx 0$ . For a single step we obtain (put for a while  $\hbar = 1$ ):

$$\langle x_1 | e^{-\epsilon [\frac{p^2}{2m} + V(x)]} | x_2 \rangle = \int dx \langle x_1 | e^{-\epsilon \frac{p^2}{2m}} | x \rangle \langle x | e^{-\epsilon V(x) - \frac{\epsilon^2}{4m} [p^2, V(x)] + \dots} | x_2 \rangle, \quad (2.27)$$

where we used the Baker-Hausdorff expansion  $e^A e^B = e^{A+B + \frac{1}{2}[A, B] + \dots}$ . For sufficiently regular potentials we can write

$$\langle x | e^{-\epsilon V(x) - \frac{\epsilon^2}{4m} [p^2, V(x)] + \dots} | x_2 \rangle = \delta(x - x_2) e^{-\epsilon V(x) + \mathcal{O}(\epsilon^2)}, \quad (2.28)$$


 Figure 2.3: How a periodic path arises,  $x_1 = x_{N+1}$ .

where, to this accuracy, the argument of  $V$  can be  $x_1$ ,  $x_2$  or  $(x_1 + x_2)/2$ . The single-step term becomes

$$\langle x_1 | e^{-\epsilon[\frac{p^2}{2m} + V(x)]} | x_2 \rangle \approx \underbrace{\langle x_1 | e^{-\epsilon\frac{p^2}{2m}} | x_2 \rangle}_{\text{free motion in } \tau} \cdot e^{-\epsilon V(x_1) + \mathcal{O}(\epsilon^2)} \quad (2.29)$$

$$= \int \frac{dp_1}{2\pi} \frac{dp_2}{2\pi} \langle x_1 | p_1 \rangle \underbrace{\langle p_1 | e^{-\epsilon\frac{p^2}{2m}} | p_2 \rangle}_{2\pi e^{-\epsilon\frac{p_1^2}{2m}} \delta(p_1 - p_2)} \overbrace{\langle p_2 | x_2 \rangle}^{e^{ip_2 x_2}} e^{-\epsilon V(x_1)} \quad (2.30)$$

$$= \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ip(x_2 - x_1) - \epsilon\frac{p^2}{2m}} e^{-\epsilon V(x_1)} \quad (2.31)$$

$$= \sqrt{\frac{m}{2\pi\epsilon}} \exp \left\{ -\epsilon \left[ \frac{m}{2} \overbrace{\left( \frac{x_2 - x_1}{\epsilon} \right)^2}^{\Rightarrow \dot{x}(\tau)^2} + V(x_1) \right] \right\}, \quad (2.32)$$

$\Rightarrow$  Euclidean Lagrangian!!

where we have used

$$\int_{-\infty}^{\infty} dx e^{-\alpha x^2 - \beta x} = \sqrt{\frac{\pi}{\alpha}} e^{\frac{\beta^2}{4\alpha}} \quad (2.33)$$

Inserting, for each step, (2.31) to (2.26), we obtain an intermediate form for  $Z$ :

$$Z = \int dx_1 \dots dx_N \frac{dp_1}{2\pi\hbar} \dots \frac{dp_N}{2\pi\hbar} \exp \left\{ \epsilon \left[ ip_1 \frac{x_2 - x_1}{\epsilon} + ip_2 \frac{x_3 - x_2}{\epsilon} + \dots - H(x_1) - \dots - H(x_N) \right] \right\} \quad (2.34)$$

$$\equiv \int \underbrace{\frac{\mathcal{D}x(\tau)\mathcal{D}p(\tau)}{2\pi\hbar}}_{\frac{\Delta x \Delta p}{h}} \exp \left\{ \frac{1}{\hbar} \int_0^{\beta\hbar} d\tau [ip\dot{x} - H(x, p)] \right\}. \quad (2.35)$$

Note that the factor  $ip\dot{x} - H(x, p)$  in the integrand is just the Lagrangian (remembering that  $\tau = it$ ). Note also the basic phase space unit cell volume  $\Delta x \Delta p = h = 2\pi\hbar = 2\pi$ .

Putting everything together, we have an important (Feynman-Hibbs at the end of their book call it “amusing”) result:

$$\begin{aligned} Z &= \text{Tr} e^{-\beta H} = \sum_{\text{states}} e^{-\frac{E_n}{T}}, \quad H = \frac{p^2}{2m} + V(x) \\ &= \int \prod_1^N \frac{dx_i}{\sqrt{\frac{2\pi\hbar\epsilon}{m}}} \exp \left[ -\frac{\epsilon}{\hbar} \left\{ \frac{m}{2} \left[ \left( \frac{x_1 - x_2}{\epsilon} \right)^2 + \dots + \left( \frac{x_N - x_{N-1}}{\epsilon} \right)^2 + \left( \frac{x_1 - x_N}{\epsilon} \right)^2 \right] \right. \right. \\ &\quad \left. \left. + V_1 + V_2 + \dots + V_N \right\} \right] \end{aligned} \quad (2.36)$$

$$\stackrel{N \rightarrow \infty}{\equiv} \int_{x(0)=x(\beta\hbar)} \mathcal{D}x(\tau) \exp \left\{ -\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau \left[ \frac{m}{2} \dot{x}^2(\tau) + V(x(\tau)) \right] \right\} \quad (2.37)$$

$$\equiv \int \mathcal{D}x(\tau) \exp \left( -\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau L(x, \tau) \right) \equiv \int \mathcal{D}x(\tau) \exp \left( -\frac{1}{\hbar} \int_0^{\beta\hbar} d\tau S_E[x] \right), \quad (2.38)$$

where  $S_E$  is the euclidean action. Note that Eq. (2.38) is defined as the  $N \rightarrow \infty$  limit of Eq. (2.37). The partition function also has a similar limit, the thermodynamic limit  $V \rightarrow \infty$ . We have now attained our goal, the partition function has been expressed in terms of the Euclidian Lagrangian of the system ( $L_E(\tau) = -L_M(\tau = it)$ ). For curiosity, note that  $\beta\hbar = 25\text{ps}$  for  $T=300\text{K}$ . This is the amount of imaginary time you have to cover in room temperature!

There are several interesting computations one can do starting from Eq. (2.38). First, it is a very good exercise to work out the integrals in (2.37) for the harmonic oscillator potential and then take the limit  $N \rightarrow \infty$  of the result, to again get the vibrational partition function. Second, one may calculate the same result directly from the gaussian functional integral, using functional methods. Third, one may evaluate the “fluctuation determinant around a classical solution”. We shall return to these after some general remarks about finite  $T$  and imaginary time.

One more good application of the harmonic oscillator is to compute the finite  $T$  expectation value of the time dependent correlator  $\langle x(t)x(0) \rangle$ . Here we really have both real time  $t$  and finite  $T$  in the same quantity, which now can be exactly computed:

$$\langle x(t)x(0) \rangle_T = Z^{-1} \text{Tr} e^{-\beta H} x(t)x(0) \quad (2.39)$$

$$= Z^{-1} \sum_{m,n=0}^{\infty} e^{-\beta\hbar\omega_n + it(\omega_n - \omega_m)} \langle n|x(0)|m\rangle \langle m|x(0)|n\rangle. \quad (2.40)$$

Insert here

$$E_n = \hbar\omega_n = \hbar\omega(n + 1/2) \quad (2.41)$$

$$\langle n|x(0)|m\rangle = \sqrt{\frac{n}{2}}\delta_{m,n-1} + \sqrt{\frac{n+1}{2}}\delta_{m,n+1} \quad (2.42)$$

and obtain

$$\langle x(t)x(0)\rangle_T = \frac{\hbar}{2\omega} \frac{\cosh(\beta\hbar/2 - it)\omega}{\sinh(\beta\hbar\omega/2)} = \frac{\hbar}{\omega} \left[ n_{\text{BE}}(\beta\hbar\omega) \cos(\omega t) + \frac{1}{2}e^{-it\omega} \right]. \quad (2.43)$$

Plot this in imaginary time  $\tau = it!$  It is useful to separate a commutator and anticommutator:

$$\langle x(t)x(0)\rangle_T = \langle \frac{1}{2}\{x(t), x(0)\}\rangle_T + \langle \frac{1}{2}[x(t), x(0)]\rangle_T = \frac{\hbar}{\omega} \left[ n_{\text{BE}}(\beta\hbar\omega) + \frac{1}{2} \right] \cos(\omega t) + \frac{\hbar}{2i\omega} \sin(\omega t) \quad (2.44)$$

Thus the anticommutator is the real part,  $\sim 1 + (\hbar\omega/T)^2/12 + \dots$  and even in  $t$  while the commutator is the imaginary part,  $\mathcal{O}(\hbar)$ , and odd in  $t$ .

How does all this match with classical physics? Harmonic motion with some initial values  $x_c(0), p_c(0)$  is

$$x_c(t) = x_c(0) \cos \omega t + \frac{p_c(0)}{\omega} \sin \omega t. \quad (2.45)$$

Thus

$$\langle x(t)x(0)\rangle_T = \langle x_c^2(0) \cos \omega t + \frac{p_c(0)x_c(0)}{\omega} \sin \omega t\rangle_T = \langle x_c^2(0)\rangle_T \cos \omega t \quad (2.46)$$

since the thermal average of the initial momentum is zero. But here we can insert the fact that the thermal energy per quadratic degree of freedom is  $T/2$ :  $\langle \frac{1}{2}\omega^2 x_c^2(0)\rangle_T = \frac{1}{2}T$  and obtain

$$\langle x(t)x(0)\rangle_T = \frac{T}{\omega^2} \cos \omega t. \quad (2.47)$$

Comparing with the exact quantum mechanics result (2.44) one sees that to order  $\mathcal{O}(\hbar^2)$  the classical result (averaging over initial conditions, taking  $t$  dependence from classical equations of motion) = result from quantum theory. This seems rather trivial but actually forms the groundwork for many numerical attempts to compute field theory correlators  $\langle O(t)O(0)\rangle$ . There is no nonperturbative first-principle method for computing these correlators in gauge field theory and one thus has had to resort to the above approximation, separating

- Equilibrium average over initial conditions,
- Subsequent classical motion.

Applications range from baryon number generation in field theory (the correlator then is that of topological susceptibility,  $FF$ ) to particle production in ultrarelativistic heavy ion collisions.

## 2.2 Finite $T$ means compact imaginary time

We can summarize the properties of the result as follows:

- Thermodynamics is now formulated in terms of the ‘‘Euclidean’’ Lagrangian, which in many cases is much simpler than  $H$ . In particular, in gauge field theories the Lagrangian is Lorentz scalar and a simple singlet under gauge transformations, while defining  $H$  requires gauge fixing.

- The formulation is easy to generalize from one particle in 1d  $\Rightarrow$  N particles in d dimensions  $\Rightarrow$  Field theories in d dimensions = infinite number of particles.
- Very general, applies to any system the dynamics of which is expressed in terms of an action.
- Good starting point for numerics.
- One avoids computing the energy levels  $E_n$ , one gets directly the sum over them! For example, for QCD nobody can compute the full energy spectrum, i.e., the spectrum of hadrons ( $m_\pi$ ,  $m_N$ ,  $m_\delta$ , ...) and it is inconceivable to compute  $Z$  by summing over states. In the path integral formulation this is entirely avoided and, in some sense, computing  $Z(T)$  is as simple (difficult!) as computing a single mass.

We have thus the general result (see Fig. 2.4) that thermal equilibrium means summing over all “periodic configurations”:  $x(0) = x(\beta\hbar)$ . Periodicity reflects the fact that one is computing a trace. For fermions the configurations actually have to be antiperiodic.

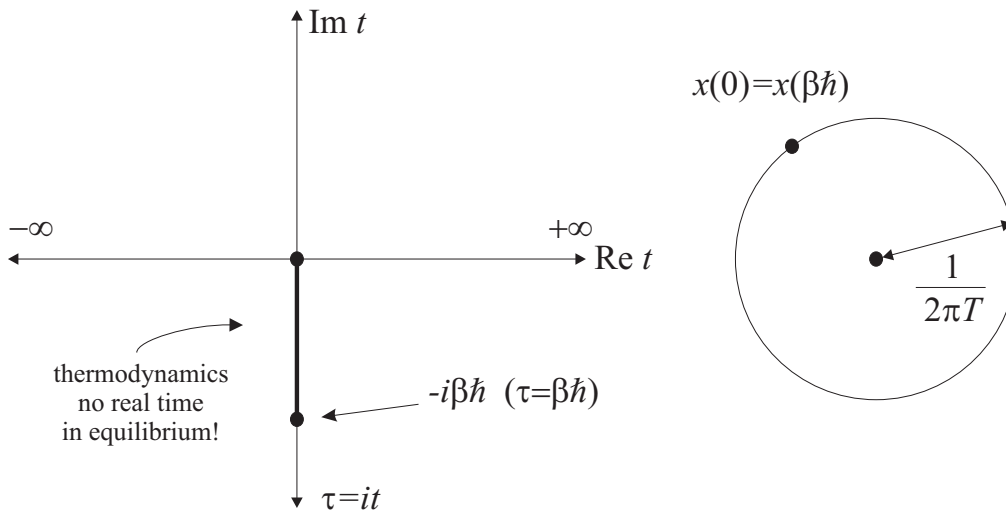


Figure 2.4: Complex time plane

Because of the periodicity the usual continuous energy is replaced by a discrete sum over “Matsubara frequencies”. A physicist frequently wants to analyze time or space dependence in terms of Fourier modes. For usual real time ( $-\infty < t < \infty$ ) one writes:

$$f(t) = \int_{-\infty}^{\infty} \frac{dk_0}{2\pi} e^{-ik_0 t} f(k_0)$$

and we have continuous energy modes. For real  $f(t)$ ,  $f^*(k_0) = f(-k_0)$  and in terms of these, for example,

$$\int_{-\infty}^{\infty} dt [\dot{x}^2(t) + m^2 x^2(t)] = \int_{-\infty}^{\infty} \frac{dk_0}{2\pi} f(k_0) (k_0^2 + m^2) f(-k_0) \quad (2.48)$$

and the whole theory can be formulated in terms of the Fourier components  $f(k_0)$ . Now we want to do Fourier in imaginary time,  $e^{-ik_0 t} = e^{-ik_4 \tau}$  with  $k_0 = ik_4$ ,  $t = -i\tau$ . However,

since  $\tau$  now is varying over a finite interval, we must write a Fourier series to represent  $f(\tau)$ ,  $k_4 \rightarrow \omega_n$ :

$$f(\tau) = T \sum_{n=-\infty}^{\infty} e^{i\omega_n \tau} f(\omega_n) \quad (2.49)$$

and the requirement  $f(0) = f(\beta\hbar)$  specifies  $e^{i\hbar\omega_n\beta} = 1$  or

$$\hbar\omega_n = 2\pi nT, \quad n = 0, \pm 1, \pm 2, \dots \quad (2.50)$$

These are the "Matsubara frequencies", the modes  $f(\omega_n)$  are "Matsubara modes". Going beyond the interval  $0, \beta\hbar$ , the function  $f$  is periodic,  $f(\tau) = f(\tau + \beta\hbar)$ , the  $\tau$  space has become topologically a circle. The factor  $T$  in Eq. (2.49) follows from changing  $k_4$  to  $2\pi Tn$ :

$$\int \frac{dk_4}{2\pi} \Rightarrow T \sum_n. \quad (2.51)$$

On the complex energy plane there will be poles along the imaginary axis  $k_0 = -i2\pi Tn$  (Fig. 2.5).

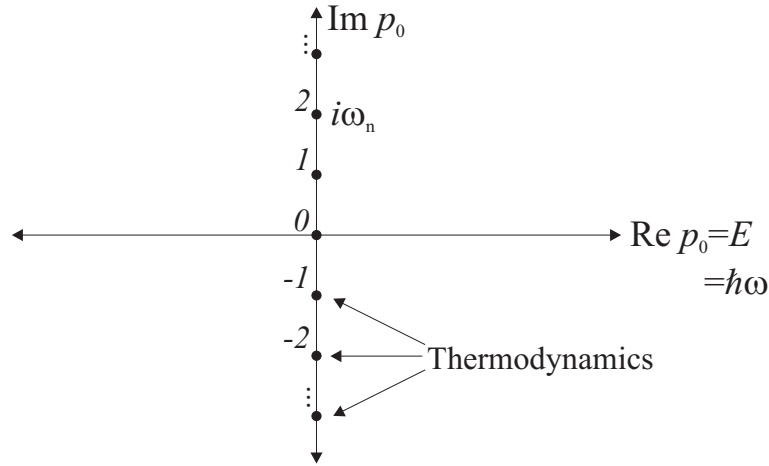


Figure 2.5: Complex energy plane with Matsubara frequencies along the imaginary axis

A parenthesis on Minkowskian  $\leftrightarrow$  Euclidean: How do different quantities behave when  $\tau = it$  or  $x_0 = x^0 = -ix_4$ ? Clearly  $x_\mu x^\mu = x_0^2 - \mathbf{x}^2 = -x_E^2$ . Then  $\partial_0 = i\partial_4$  and one also wants the covariant derivative to behave similarly. Thus  $D_0 = \partial_0 + igA_0$  becomes  $iD_4 = i(\partial_4 + igA_4)$  so that  $A_0 = +iA_4$ ,  $E^i = F_{0i} = iF_{4i} = iE_i^E$  and

$$i \int dt d^3x \frac{1}{2}(\mathbf{E}^2 - \mathbf{B}^2) = - \int d^4x_E \frac{1}{2}(\mathbf{E}_E^2 + \mathbf{B}^2) \quad (2.52)$$

which tells how, for electrodynamics,  $iS_M$  transforms to  $-S_E$ . For fermions the obvious goal  $\{\gamma_\mu^E, \gamma_\nu^E\} = 2\delta_{\mu\nu}$ , replacing  $\{\gamma_\mu, \gamma_\nu\} = 2g_{\mu\nu}$ , is reached by

$$\gamma_0^E = \gamma^0, \quad \gamma_i^E = -i\gamma^i = i\gamma_i. \quad (2.53)$$

$$\Rightarrow \gamma_\mu^{E\dagger} = \gamma_\mu^E, \quad i\gamma^\mu D_\mu = -\gamma_\mu^E D_\mu^E \quad (2.54)$$

so that the fermionic Lagrangian

$$L_M = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi = -\bar{\psi}(\gamma_\mu^E D_\mu^E + m)\psi = -L_E \quad (2.55)$$

where  $\gamma_\mu^E D_\mu^E + m$  is the famous fermion matrix, also a subject of much mathematical research.

## 2.3 Finite $T$ and $T = 0$

Usually the path integral is introduced for 1+1d quantum mechanics in real time. Then there is no  $T$  and no trace to evaluate. Instead of the sum (2.23) over diagonal matrix elements one has a single transition matrix element, for which slight modifications of the previous equations give

$$\langle x_b t_b | x_a t_a \rangle = \langle x_b 0 | \exp \left[ -i \frac{H}{\hbar} (t_b - t_a) \right] | x_a 0 \rangle \quad (2.56)$$

$$= \int \mathcal{D}x \mathcal{D}p \exp \left\{ i \frac{1}{\hbar} \int_{t_a}^{t_b} dt [p\dot{x}(t) - H(x, p)] \right\} \quad (2.57)$$

$$= \int \mathcal{D}x \exp \left\{ i \frac{1}{\hbar} \int_{t_a}^{t_b} dt L(x(t), \dot{x}(t)) \right\}, \quad (2.58)$$

Because of the  $i$  this is mathematically badly behaved; one has to introduce  $i\epsilon$ 's which have a physics reason. Now the paths in real time arise as shown in Fig.2.6.

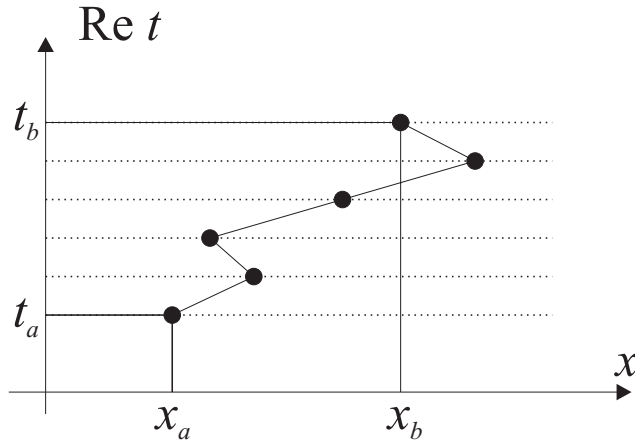


Figure 2.6: Real time paths

One usually also couples the system to an external current  $J(t)$ , some external force affecting the motion. Then the path integral becomes

$$\langle x_b t_b = \infty | x_a t_a = -\infty \rangle_{\mathcal{J}(t)} = \int \mathcal{D}x(t) \exp \left\{ i \frac{1}{\hbar} \int_{-\infty}^{\infty} dt [L(x, \dot{x}) + \mathcal{J}(t)x(t)] \right\} \quad (2.59)$$

$$\equiv Z(\mathcal{J}) \equiv e^{iW(\mathcal{J})} \quad (2.60)$$

Then the functional derivatives  $\delta W / \delta \mathcal{J}(t)$ ,  $\dots$ , give expectation values of products of  $\hat{x}$ -operators. We shall expand on this when discussing extension to field theory.

## 2.4 The path integral of harmonic oscillator using functional methods

Let us now return to the path integral for the 1d harmonic oscillator at finite  $T$ :

$$Z = \int_{x(0)=x(\beta)} \mathcal{D}x \exp \left[ - \int_0^\beta d\tau \left( \frac{1}{2} m \dot{x}^2 + \frac{1}{2} m \omega^2 x^2 \right) \right] \quad (2.61)$$

(here  $\hbar = 1$ ) and complete the circle of arguments by directly showing that this reproduces the almost trivial vibrational partition function,

$$Z_{\text{vib}} = \sum_{n=0}^{\infty} e^{-\beta \hbar \omega (n + \frac{1}{2})} = \frac{1}{2 \sinh \frac{\beta \hbar \omega}{2}}. \quad (2.62)$$

where we started from.

The harmonic oscillator is exactly solvable since the integral (2.61) is Gaussian, quadratic in  $x$ . A complication is the time derivative of  $x$ . The standard way of getting rid of this is by partial integration which casts the expression into the form  $x[\text{operator}]x$ . So use  $d(x\dot{x})/d\tau = \dot{x}^2 + x\ddot{x}$ :

$$\int_0^\beta d\tau \dot{x}^2 = \underbrace{\int_0^\beta x \dot{x}}_{=0: x \text{ periodic}} - \int_0^\beta d\tau x \ddot{x}, \quad (2.63)$$

so that we get the explicitly Gaussian integral,

$$Z = \int_{x(0)=x(\beta)} \mathcal{D}x \exp \left[ - \frac{1}{2} \int_0^\beta d\tau x \left( -m \frac{d^2}{d\tau^2} + m \omega^2 \right) x \right] \quad (2.64)$$

A Gaussian integral can always be carried out using the fundamental formula

$$I = \int_{-\infty}^{\infty} \prod_1^N dx_i \exp \left( - \frac{1}{2} \sum_{ij} x_i A_{ij} x_j + \sum_i b_i x_i \right) = \frac{(2\pi)^{N/2}}{\sqrt{\det A}} \exp \left( \frac{1}{2} \sum_{ij} b_i A_{ij}^{-1} b_j \right), \quad (2.65)$$

which also leads to the Wick formulas for the correlators:

$$\langle x_1 x_2 \rangle \equiv I^{-1} \int \prod_1^N dx_i x_1 x_2 \exp \left[ - \frac{1}{2} x A x \right] = (A^{-1})_{12}, \quad (2.66)$$

$$\langle x_1 x_2 x_3 x_4 \rangle = (A^{-1})_{12} (A^{-1})_{34} + (A^{-1})_{13} (A^{-1})_{24} + (A^{-1})_{14} (A^{-1})_{23}, \quad (2.67)$$

etc. One should understand that the  $\sum_{ij}$  in (2.65) is built in  $\int d\tau$  in the path integral. Thus we can write

$$Z = \underbrace{\text{const}}_{\text{infinite!}} \times (\det K)^{-\frac{1}{2}}, \quad (2.68)$$

where now

$$K = m \left( - \frac{d^2}{d\tau^2} + \omega^2 \right). \quad (2.69)$$

To define and evaluate the determinant of this operator we have to find its eigenvalues  $k_n$ . Then

$$\det K = \prod k_n = e^{\sum \ln k_n} = e^{\text{Tr } \ln K} \quad (2.70)$$

The eigenvalues are obtained by solving the eigenvalue equation

$$K f_n = k_n f_n, \quad (2.71)$$

where  $f_n(\tau) = f_n(\tau + \beta)$  are the periodic eigenfunctions. Clearly, the solutions to

$$\left(-\frac{d^2}{dt^2} + \omega^2\right) f_n = k_n f_n \quad (2.72)$$

are of the form  $f_n = e^{i\alpha\tau}$ , and requiring periodicity  $\tau \rightarrow \tau + \beta$  we find  $f_n = e^{2\pi i n \tau / \beta}$  so that the eigenvalues are

$$k_n = \omega^2 + (2\pi n T)^2 \equiv \omega^2 + \omega_n^2; \quad (2.73)$$

the Matsubara frequencies have reappeared and

$$Z(\omega) = \frac{\text{const}}{\sqrt{\prod_{-\infty}^{\infty} (\omega^2 + \omega_n^2)}} = \frac{\text{const}}{\omega \prod_1^{\infty} (\omega^2 + \omega_n^2)}. \quad (2.74)$$

The determinant is obviously infinite, but this need not worry us: in any case, we have to normalize to determine the constant. It is natural to normalise by the path integral of a free theory with  $\omega = 0$ . However, the  $n = 0$  zero mode term in Eq. (2.74) diverges in this limit. The physical reason is that if  $V = 0$  the particle is free to move anywhere in space which leads to this "infrared divergence". Mathematically, the problem is that the operator  $d^2/d\tau^2$  has a zero eigenvalue, which clearly must be removed from the definition  $\det K = \prod k_n$  for this to make sense. This situation is very common when evaluating functional determinants. Other arguments must be used to evaluate their contribution. Here we simply say that to keep  $Z_0$  dimensionless, we must include a factor of dimension  $\omega$  and there is just  $T$ . So we write

$$Z(\omega = 0) \equiv Z_0 = \det \left(-m \frac{d^2}{d\tau^2}\right)^{-\frac{1}{2}} \times \text{const} = \frac{\text{const}}{T \prod_1^{\infty} \omega_n^2} \quad (2.75)$$

The properly normalized harmonic oscillator partition function  $Z_{\text{HO}}$  is thus

$$Z_{\text{HO}} \equiv \frac{Z(\omega)}{Z(0)} = \frac{1}{\beta \omega \prod_{n=1}^{\infty} \left(1 + \frac{\omega^2 \beta^2}{4\pi^2 n^2}\right)} = \frac{1}{2 \sinh \frac{\beta \omega}{2}}, \quad (2.76)$$

where in the last step  $\sinh x = x \prod_1^{\infty} (1 + x^2/(\pi n)^2)$  (Gradshteyn-Ryzhik 1.431) was used. So we are back to Eq. (2.62) where we started from.

## 2.5 Generating functionals

By computing  $Z$  one obtains the thermodynamic potential of the system. In practise, for interacting systems, this is unfortunately a calculation we do not know how to do analytically

(recall that physicists can, with some exceptions, do only gaussian integrals!). Therefore one has to resort to perturbation theory (i.e. assume that the interaction is weak) or numerics.

We need a path integral which generates correlators (=Green's functions). The task is then to evaluate the correlators in perturbation theory. To this end, let us define the *generating functional* which in 1+1 dimensions can be written as

$$Z[J] = N \int \mathcal{D}x e^{-[S + \int_0^\beta d\tau J(\tau)x(\tau)]}, \quad (2.77)$$

where  $J(\tau) = J(\tau + \beta)$  is an arbitrary (periodic) source function so that formally

$$\begin{aligned} \left. \frac{\delta Z}{\delta J(\tau_1) \dots \delta J(\tau_n)} \right|_{J=0} &= N \int \mathcal{D}x x(\tau_1) \dots x(\tau_n) e^{-S} (-1)^n \\ &\equiv \langle x(\tau_1) \dots x(\tau_n) \rangle (-1)^n \end{aligned} \quad (2.78)$$

with  $N = Z[0]^{-1}$ . For the harmonic oscillator we immediately obtain, using Eq.(2.65),

$$\begin{aligned} Z[J] &= N \int \mathcal{D}x \exp \left[ - \int d\tau \left( \frac{1}{2} m \dot{x}^2 + \frac{1}{2} m \omega^2 x^2 \right) - \int d\tau J(\tau)x \right] \\ &\propto \left[ \det \left( - \frac{d^2}{d\tau^2} + \omega^2 \right) \right]^{-\frac{1}{2}} \exp \left[ - \frac{1}{2m} \int_0^\beta d\tau d\tau' J(\tau') \left( - \frac{d^2}{d\tau^2} + \omega^2 \right)^{-1} J(\tau) \right]. \end{aligned} \quad (2.79)$$

## 2.6 Perturbation theory

The harmonic oscillator,  $V(x) \sim x^2$ , can be done exactly, as a Gaussian integral. For more complicated interactions various approximation methods have to be applied. We will outline two main methods. Both boil down to doing a Gaussian integral as a leading term and then computing corrections. Firstly, one may assume all the non-Gaussianity is a small effect and can be regarded as a perturbation. Secondly, one may attempt a semiclassical  $\hbar \rightarrow 0$  saddle point computation.

The substance of perturbation theory is easy to formulate. Suppose we have a theory with action  $S[\Phi] = S_0[\Phi] + S_1[\Phi]$ , where  $\Phi$  is a set of degrees of freedom, and  $S_0$  contains all the quadratic terms. In the 1d case  $S_0 = \int dt (\frac{1}{2} m \dot{x}^2 + \frac{1}{2} m \omega^2 x^2)$ . All the physics is in expectation values of operators  $O(\Phi)$  and to compute them we expand in  $S_1$ :

$$\begin{aligned} \langle O \rangle &= \frac{\int \mathcal{D}\Phi O \exp[-S_0 - S_1]}{\int \mathcal{D}\Phi \exp[-S_0 - S_1]} \\ &= \frac{\int \mathcal{D}\Phi O \exp[-S_0] \sum_0^\infty \frac{(-)^n}{n!} S_1^n}{\int \mathcal{D}\Phi \exp[-S_0] \sum_0^\infty \frac{(-)^n}{n!} S_1^n} \\ &\equiv \frac{\sum_0^\infty \frac{(-)^n}{n!} \langle O S_1^n \rangle}{\sum_0^\infty \frac{(-)^n}{n!} \langle S_1^n \rangle} \\ &= \frac{\langle O - O S_1 + \frac{1}{2} O S_1^2 - \dots \rangle}{\langle 1 - S_1 + \frac{1}{2} S_1^2 - \dots \rangle} \end{aligned} \quad (2.80)$$

Thus perturbation theory boils down to computing Gaussian expectation values of powers of the interaction term and of the operator  $O$  multiplied by powers of  $S_1$ . Effectively, this is an application of the Gaussian master formula (2.65) with the correlator formulas (2.66), (2.67) and their generalisations.

**Example: 1+1d interacting harmonic oscillator.** Consider a theory defined by the Lagrangian

$$L(x) = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2 x^2 + \frac{1}{4}\lambda m\omega_0^4 x^4, \quad \lambda \ll 1. \quad (2.81)$$

Here  $\omega$ ,  $\omega_0$ ,  $\lambda$  are some constants. The constants are chosen such that in the units  $\hbar = c = 1$ ,  $\lambda$  is a pure number and can be used as an expansion parameter. For general  $\hbar, c$  one could write the interaction, e.g., in the form  $+\lambda m^2 \omega_0^4 / \hbar x^4$ , where  $\omega_0$  is a frequency. We may write down the path integral and, assuming a weak interaction, make an expansion in the small coupling constant  $\lambda$ :

$$\begin{aligned} Z_\lambda &= \int \mathcal{D}x e^{-S_{\text{HO}} - \frac{1}{4} \int_0^\beta d\tau \lambda m\omega_0^4 x^4} \\ &= \int \mathcal{D}x \exp \left\{ -S_{\text{HO}} \left[ 1 - \frac{\lambda}{4} \int_0^\beta d\tau m\omega_0^4 x^4 + \mathcal{O}(\lambda^2) \right] \right\} \\ &= Z_{\text{HO}} - \frac{\lambda}{4} m\omega_0^4 \int_0^\beta d\tau \int \mathcal{D}x e^{-S_{\text{HO}}} x^4 \\ &= Z_{\text{HO}} - \frac{\lambda}{4} m\omega_0^4 \int_0^\beta d\tau \underbrace{\frac{\delta^4 Z_{\text{HO}}[J]}{\delta J(t) \dots \delta J(t)} \Big|_{J=0}}_{\text{this can be computed}} + \mathcal{O}(\lambda^2). \end{aligned} \quad (2.82)$$

(2.83)

Thus we may write

$$\frac{Z_\lambda}{Z_{\lambda=0}} = 1 - \frac{\lambda}{4} m\omega_0^4 Z_{\text{HO}}^{-1} \int_0^\beta d\tau \frac{\delta^4 Z_{\text{HO}}}{\delta J^4} \Big|_{J=0}, \quad (2.84)$$

where the second term represents the first-order correction to the path integral of the ordinary harmonic oscillator.

**Exercise:** evaluate  $Z_\lambda$ .

## 2.7 Semiclassical approximation, Gaussian fluctuation determinant

Instead of expanding the potential with respect to some small dimensionless parameter, we may also use another, different method called the semiclassical approximation or the loop expansion, which does not require weak interactions. The following is equivalent to the saddle point evaluation of the integral  $\int dx \exp[-S(x)/\hbar]$  in the first chapter, in the limit  $\hbar \rightarrow 0$ . Here  $\hbar$  may be the Planck constant, but it can also be some formal parameter counting how many corrections are included. We discuss only the leading classical term and the first correction, the Gaussian fluctuation determinant.

Let us consider a general 1+1d Euclidean action

$$S = \int_0^\beta d\tau \left[ \frac{1}{2} m \dot{x}^2 + V(x) \right] = \int_0^\beta d\tau \left[ \frac{1}{2} m x (-\partial_\tau^2) x + V(x) \right]. \quad (2.85)$$

Here  $V(x)$  is some arbitrary potential. In general, the configurations that contribute most to  $Z$  are those for which  $S$  is at its minimum. These are the saddle points  $\delta S/\delta x = 0$  which correspond to the classical trajectories  $x_{cl}(t)$  given by the equation of motion  $V'(x) - m\ddot{x} = 0$ . Therefore, it makes sense in the path integral to expand about the classical solution  $x(t) = x_{cl}(t)$ :

$$\begin{aligned} S[x] &= S[x_{cl}] + \int \underbrace{\frac{\delta S}{\delta x(\tau_1)} \Big|_{x=x_{cl}}}_{=0, \text{ eq. of motion}} (x(\tau_1) - x_{cl}) d\tau_1 \\ &+ \frac{1}{2} \int \frac{\delta^2 S}{\delta x(\tau_1) \delta x(\tau_2)} \Big|_{x=x_{cl}} (x(\tau_1) - x_{cl})(x(\tau_2) - x_{cl}) d\tau_1 d\tau_2 + \dots \end{aligned} \quad (2.86)$$

Note that  $-\partial_\tau^2$  is a linear operator so that we may write

$$\begin{aligned} \frac{\delta S}{\delta x(\tau_1)} &= \frac{\delta}{\delta x(\tau_1)} \int d\tau \left( \frac{1}{2} m x (-\partial_\tau^2) x + V(x) \right) \\ &= \int d\tau \frac{\delta V(x)}{\delta x(\tau)} \underbrace{\frac{\delta x(\tau)}{\delta x(\tau_1)}}_{\delta(\tau-\tau_1)} - \frac{1}{2} m \int d\tau d\tau' x(\tau) \underbrace{K(\tau, \tau')}_{\text{symmetric kernel}} x(\tau') \\ &= V'(x(\tau_1)) - \frac{1}{2} m \int d\tau d\tau' [\delta(\tau - \tau_1) K(\tau, \tau') x(\tau') + \delta(\tau_1 - \tau') K(\tau, \tau') x(\tau)] \\ &= V'(x(\tau_1)) - m \int d\tau K(\tau_1, \tau) x(\tau) \\ &= V'(x) - m \partial_\tau^2 x . \end{aligned} \quad (2.87)$$

Then

$$\frac{\delta^2 S}{\delta x(\tau_1) \delta x(\tau_2)} = V'' \delta(\tau_1 - \tau_2) - m K(\tau_1, \tau_2) \quad (2.88)$$

so that, defining  $x - x_{cl} \equiv x_q$  (where "q" stands for quantum fluctuation), we find that

$$\begin{aligned} S[x] &= S[x_{cl}] + \frac{1}{2} \int d\tau_1 d\tau_2 [V''(x_{cl}) \delta(\tau_1 - \tau_2) - m K(\tau_1, \tau_2)] x_q(\tau_1) x_q(\tau_2) + \mathcal{O}(x_q^3) \\ &= S[x_{cl}] + \frac{1}{2} \int d\tau_1 [x_q(\tau_1) (-m \partial_\tau^2 + V''(x_{cl})) x_q(\tau_1)] + \mathcal{O}(x_q^3) . \end{aligned} \quad (2.89)$$

If we neglect the terms of order  $\mathcal{O}(x_q^3)$  and note that in the path integral measure we may perform the shift  $\mathcal{D}x \rightarrow \mathcal{D}(x - x_{cl}) = \mathcal{D}x_q$  because  $x_{cl}$  is just a point in the space of all configurations, we again have a Gaussian integral. Hence in the Gaussian approximation  $Z$  is obtained by an integration over small fluctuations:

$$Z = \int \mathcal{D}x e^{-S[x]} \simeq e^{-S[x_{cl}]} \int \mathcal{D}x_q e^{-\frac{1}{2} \int d\tau x_q K x_q} \propto e^{-S[x_{cl}]} [\det K]^{-\frac{1}{2}} . \quad (2.90)$$

So we again end up evaluating a functional determinant, now the determinant of the operator  $K = -m \partial_\tau^2 + V''(x_{cl})$ . Evaluating  $\det K$  is often tricky because unless  $x_{cl}$  is the trivial constant vacuum configuration (e.g.  $x_{cl} = 0$ ), the determinant requires the solution of a complicated eigenvalue problem.

**Example:** Assume the potential is of the double-well form  $V(x) = \frac{1}{4}\lambda(x^2 - v^2)^2$  with minima at  $x = \pm v$ . Then the classical EOM has a "kink" solution, a solution of  $\ddot{x} = V'(x)$ , taking us from one minimum to the other:

$$x_{\text{cl}}(\tau) = v \tanh \sqrt{\lambda/2}v(\tau - \tau_0) \quad (2.91)$$

with the classical action

$$S[x_{\text{cl}}] = \frac{4}{3}\sqrt{\frac{\lambda}{2}}v^3 = \frac{m_H^3}{3\lambda}, \quad m_H^2 = V''(\pm v) = 2\lambda v^2 \quad (2.92)$$

and with

$$V''(x_{\text{cl}}(\tau)) = \lambda v^2[(3 \tanh^2(\tau/\tau_1) - 1), \quad \tau_1^2 \lambda v^2 = 2; \quad \tau_0 = 0. \quad (2.93)$$

In (2.91)  $\tau_0$  is the "position of the kink" and we assume that  $\beta\hbar$  and the parameters are such that the kink fits in the interval  $0, \beta\hbar$ , i.e., we can take  $\tau \rightarrow \pm\infty$  in (2.91). A periodic configuration then is one in which one jumps from one minimum to the other and then returns, a kink + antikink. The nontrivial zero mode is easy to identify: by construction  $x_{\text{cl}}$  satisfies  $\ddot{x}_{\text{cl}} - V'(x_{\text{cl}}) = 0$ , take the derivative of this with respect to  $\tau$  and find

$$[-\partial_\tau^2 + V''(x_{\text{cl}})]\frac{dx_{\text{cl}}}{d\tau} = 0 \quad (2.94)$$

so that the normalised zero mode is

$$x_0(\tau) = \sqrt{\frac{3}{4\tau_1}} \frac{1}{\cosh^2(\tau/\tau_1)}. \quad (2.95)$$

Finding the eigenvalues  $a_n$  of the operator  $K = -m\partial_\tau^2 + V''(x_{\text{cl}})$  we must, scaling variables suitably, solve

$$-\frac{1}{2}\ddot{x} + (3 \tanh^2 \tau - 1)x = \tau_1 a_n x \quad (2.96)$$

Astonishingly, these can be obtained analytically - not so many cases where analytic solutions of the eigenvalue equation can be given. There are two discrete eigenvalues and -functions:

$$\begin{aligned} a_0 &= 0 & x_0 &= \frac{1}{\cosh^2 \tau} \\ a_1 &= \frac{3}{2\tau_1^2} & x_1 &= \frac{\sinh \tau}{\cosh^2 \tau} \end{aligned} \quad (2.97)$$

and a continuum

$$\tau_1^2 a_p = 2 + \frac{1}{2}p^2, \quad x_p = e^{ip\tau} (3 \tanh^2 \tau - 1 - p^2 - 3ip \tanh \tau). \quad (2.98)$$

These may seem like very formal developments, but the applications are very practical: physics of the  $\text{NH}_3$  molecule, symmetric and antisymmetric ground states and the tunneling between the two minima of the potential.

## 2.8 Effective actions\*

An effective action is the fluctuation corrected action. The basic definition of the effective action for a fixed background  $x_b$  is

$$\Gamma(x_b) = W(J) - \int d\tau J(\tau)x_b(\tau). \quad (2.99)$$

One may then trivially divide the effective action into kinetic and potential parts:

$$\Gamma(x_b) = \int_0^\beta d\tau \left[ E_{\text{kin}}(x_b) + V_{\text{eff}}(x_b) \right] \quad (2.100)$$

so that for  $x_b = \text{const} \equiv x_0$

$$\Gamma(x_0) = \frac{V_{\text{eff}}(x_0)}{T}. \quad (2.101)$$

The question one should then pose is: What is the value of the fixed background at which the effective action is minimized, i.e. what is the ground state of temperature-corrected system.

Here are a number of general equations on the effective potential in a compact notation. They may look very formal and boring but are actually very important for any computations in theories defined by path integrals. The basic definition is

$$\begin{aligned} Z(J) &= \int \mathcal{D}x e^{-S(\phi) - \int d\tau Jx} = \\ &= e^{-W(J)} = e^{-\Gamma(\bar{x}) - \int d\tau J\bar{x}} \end{aligned}$$

( $e^{\dots + \int d\tau J\bar{x}}$  is perhaps nicer: then  $J > 0 \rightarrow \bar{x} > 0$ ) where the *mean field* or the *expectation value*  $\bar{x}$  is defined as

$$\bar{x}_J = \langle x \rangle_J = Z^{-1}(J) \int \mathcal{D}x e^{-S - \int d\tau Jx} x = -\frac{1}{Z(J)} \frac{\delta Z(J)}{\delta J} = W'(J), \quad (2.102)$$

where the subscript  $J$  reminds us that the expectation value depends on the fixed source. From (2.102)

$$\frac{\delta \bar{x}_{J_1}}{\delta J_2} = \frac{1}{Z(J)^2} \frac{\delta Z}{\delta J_1} \frac{\delta Z}{\delta J_2} - \frac{1}{Z(J)} \frac{\delta^2 Z}{\delta J_1 \delta J_2} = \bar{x}^2 - \langle x(\tau_1)x(\tau_2) \rangle. \quad (2.103)$$

Noting that  $\langle (\bar{x} - x(\tau_1))(\bar{x} - x(\tau_2)) \rangle = -\bar{x}^2 - \langle x(\tau_1)x(\tau_2) \rangle$  we may also write

$$\frac{\delta \bar{x}_J}{\delta J} = W''(J) = \langle (\bar{x} - x)^2 \rangle \quad (2.104)$$

so that  $W''$  is the fluctuation width.

Now perform a Legendre transformation and take  $\bar{x}$  as a variable, instead of  $J$ :

$$\Gamma(\bar{x}) = W(J) - \int d\tau J\bar{x}. \quad (2.105)$$

Then

$$\Gamma'(\bar{x}) = \frac{\delta W}{\delta \bar{x}} - \frac{\delta}{\delta \bar{x}} \int d\tau J\bar{x} = \int \frac{\delta W}{\delta J} \frac{\delta J}{\delta \bar{x}} d\tau - J - \int \frac{\delta J}{\delta \bar{x}} \bar{x} d\tau = -J \quad (2.106)$$

and thus  $\Gamma'(\bar{x}) = 0$  gives the true ground state ( $J=0$ ). Further derivatives are

$$\Gamma''(\bar{\phi}) = -\frac{dJ}{d\bar{\phi}} = -\frac{1}{W''(J)}, \quad \Gamma'''(\bar{\phi}) = W'''/(W'')^3,$$

$$\Gamma^{(4)}(\bar{\phi}) = W^{(4)}/(W'')^4 - 3(W''')^2/(W'')^5, \dots$$

The physics behind this is that an external current  $J$  is used to tune  $\langle \phi \rangle$  to the value  $\bar{\phi}$ ; otherwise it relaxes to the value of  $\bar{\phi}$  in the ground state.

Since  $\Gamma$  determines the ground state, it is very important to find methods to compute it. This can be done in the loop expansion (Jackiw74). Very schematically, taking  $J(\tau) \equiv J$  and  $x(\tau) \equiv \phi$  to be constants instead of functions so that we may perform the imaginary time integrals trivially, the following steps are needed:

1. Compute  $W(J)$  expanding about the classical saddle point  $\phi_c$ :

$$\begin{aligned} S(\phi) + J\phi &= S(\phi_c) + J\phi_c + [S'(\phi_c) + J](\phi - \phi_c) + \frac{1}{2!}S_c''(\phi - \phi_c)^2 + \\ &\quad + \frac{1}{3!}S_c'''(\phi - \phi_c)^3 + \frac{1}{4!}S_c^{(4)}(\phi - \phi_c)^4 + \dots \end{aligned}$$

where the saddle point is chosen by

$$S'(\phi_c) + J = 0.$$

Then  $W(J)$  is given by the Gaussian integral

$$\begin{aligned} e^{-W(J)} &= e^{-(S_c + J\phi_c)} \int \mathcal{D}\phi e^{-\frac{1}{2!}S_c''(\phi - \phi_c)^2 - \dots} \\ &= e^{-(S_c + J\phi_c)} \int \mathcal{D}\chi e^{-\frac{1}{2!}S_c''\chi^2} \left[ 1 - \frac{1}{3!}S_c'''\chi^3 - \frac{1}{4!}S_c^{(4)}\chi^4 + \frac{1}{2(3!)^2}(S_c''')^2\chi^6 + \dots \right] \\ &= e^{-(S_c + J\phi_c)} \sqrt{\frac{2\pi}{S_c''}} \left[ 1 - \frac{S_c^{(4)}}{8(S_c'')^2} + \frac{5(S_c''')^2}{24(S_c'')^3} + \dots \right] \end{aligned}$$

leading to

$$\begin{aligned} W(J) &= S(\phi_c) + J\phi_c + \frac{\hbar}{2} \log S''(\phi_c) + \frac{\hbar^2 S_c^{(4)}}{8(S_c'')^2} - \frac{5\hbar^2 (S_c''')^2}{24 (S_c'')^3} + \dots \\ &\equiv S(\phi_c) + J\phi_c + \Gamma_1(\phi_c). \end{aligned}$$

Here we have scaled  $\phi - \phi_c = \sqrt{\hbar}\chi$  to demonstrate that we are dealing with an expansion in  $\hbar$ , the loop expansion ( $\hbar$  is brought back into the equations by the scaling  $S \rightarrow S/\hbar$ ). Thus  $\Gamma/\hbar = S/\hbar + \frac{1}{2}\log S'' + \mathcal{O}(\hbar)$  and the gaussian contribution  $\propto \log S''$  is thus of the order  $\mathcal{O}(\hbar^0)$ .

2. Compute  $\Gamma(\bar{\phi})$ , the effective action of the mean field ( $\neq$  the saddle point  $\phi_c$  if we go beyond the lowest order). From  $\bar{\phi} = W'(J)$  and the above result for  $W(J)$  one finds that

$$\bar{\phi} = \phi_c - \frac{S_c'''}{2(S_c'')^2} \equiv \phi_c - \phi_1.$$

Then write  $W(J) - \bar{\phi}J$  in terms of  $\bar{\phi} + \phi_1$ , expand in  $\phi_1$  and find that

$$\begin{aligned} \Gamma(\bar{\phi}) &= S(\bar{\phi}) + \Gamma_1(\bar{\phi}) + \text{terms combining to 1 - particle reducible diagrams} \\ &= S(\bar{\phi}) + \Gamma_1(\bar{\phi})|_{\text{1-part.irred.diags}} \\ &= S(\bar{\phi}) + \frac{1}{2}\log S''(\bar{\phi}) + \frac{S^{(4)}}{8(S'')^2} - \frac{(S''')^2}{12(S'')^3} \end{aligned}$$

Actually in  $W(J)$

$$\frac{5}{24} = \frac{1}{8} + \frac{1}{12} = \text{spectacle} + \text{sunset}$$

and the  $1/8$  is cancelled by 1PI. **Some figure needed here!**

Compact form of the result:

$$V_{\text{eff}}(\phi) = V_0(\phi) - \frac{1}{V_3} \ln \int \mathcal{D}\phi e^{-S_0} - \frac{1}{V_3} \langle e^{-S_1} \rangle_{1\text{PI}}$$

where one has shifted one of the components  $\phi_i$  by  $\phi$ , neglected linear terms and grouped the quadratic terms in  $S_0$  and the rest + counter terms in  $S_1$ .

**Example: Inverted oscillator.** Let us return to quantum mechanics and consider the 1+1 dimensional inverted oscillator with the Lagrangian

$$L = \frac{1}{2}m\dot{x}^2 + V(x), \quad V(x) = -\frac{1}{2}m\omega^2x^2 + \underbrace{\frac{1}{4}\lambda m\omega_0^4x^4}_{\text{needed for stabilizing } V}. \quad (2.107)$$

Here we have chosen the coefficient of the  $x^4$  such that  $\lambda$  is dimensionless.

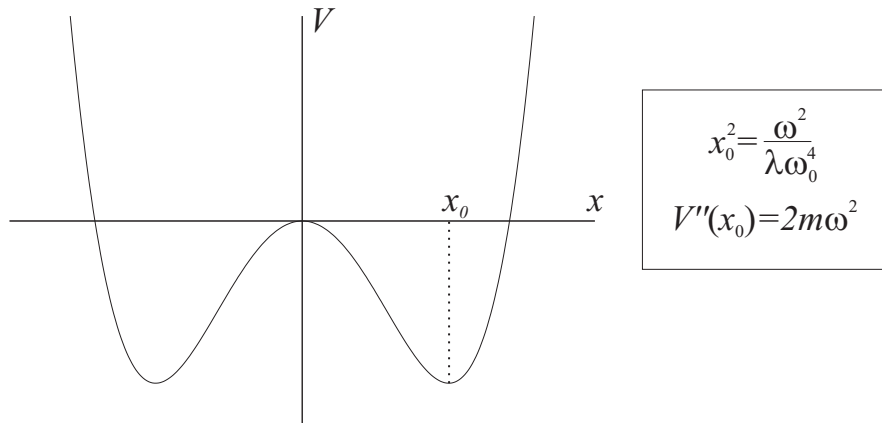


Figure 2.7: Potential of inverted oscillator

Let us take a constant background  $x_c = \text{const.}$ ; then  $V''(x_c) = -m\omega^2 + 3\lambda m\omega_0^4x_c^2$ . From pages [49 prujussa] and [76] we find that the gaussian integration yields

$$\text{“det } K \text{”} = \text{const.} \cdot e^{\sum_n \ln(3\lambda\omega_0^4x_c^2 + 4\pi^2n^2T^2)} \quad (2.108)$$

so that for a constant background we may immediately write

$$\Gamma(x_c) = \frac{V_{\text{eff}}(x_c)}{T} = \frac{V(x_c)}{T} + \underbrace{\frac{1}{2} \sum_n \ln(3\lambda\omega_0^4x_c^2 - \omega^2 + 4\pi^2n^2T^2)}_{\text{diverges} \rightarrow \text{must renormalize}}. \quad (2.109)$$

The divergence is here due to the zero point quantum fluctuations, which are present already at  $T = 0$ . It is a theorem that no new divergences appear at finite  $T$  so that the infinities can be absorbed by the redefinition

of the parameters of the  $T = 0$  theory; this is just the usual renormalization procedure. Thus at large  $T$  we may write the effective potential as

$$V_{\text{eff}}(x_c) \simeq \frac{1}{2}T \sum_n \ln(3\lambda\omega_0^2 x_c^2 - \omega^2 + 4\pi^2 n^2 T^2) + \underbrace{\text{terms independent of } T}_{\text{these cancel the infinities}}. \quad (2.110)$$

Strictly speaking, the expression is well defined only when

$$U \equiv 3\lambda\omega_0^4 x_c^2 - \omega^2 \geq 0. \quad (2.111)$$

We may sidestep the issue of infinities by taking a derivative with respect to  $U$  (recall that  $x_c$  is just some fixed constant). Then

$$\begin{aligned} \frac{\partial V_{\text{eff}}}{\partial U} &= \frac{1}{2}T \sum_n \left[ \frac{1}{U + 4\pi^2 n^2 T^2} \right] \\ &= \frac{1}{2} \frac{1}{\sqrt{U}} \sum_n \frac{T\sqrt{U}}{U + 4\pi^2 n^2 T^2} \\ &= \frac{1}{2} \frac{1}{\sqrt{U}} \left[ \frac{1}{2} + \frac{1}{e^{\beta\sqrt{U}} - 1} \right]. \end{aligned} \quad (2.112)$$

Thus the  $T$ -dependent part of the effective potential close to the origin  $x_c \approx 0$  is found from

$$\begin{aligned} \frac{\partial V_{\text{eff}}}{\partial x^2} &= \frac{\partial U}{\partial x_c^2} \frac{\partial V_{\text{eff}}}{\partial U} = \frac{3}{2} \lambda \omega_0^4 \frac{1}{\sqrt{U}} \frac{1}{e^{\beta\sqrt{U}} - 1} \\ &\simeq \frac{3}{2} \lambda \omega_0^4 \frac{T}{U} \end{aligned} \quad (2.113)$$

i.e.  $V_{\text{eff}} \propto x_c^2 T$  as  $T \rightarrow \infty$ . Thus, at very high temperatures, the term proportional to  $x_c$  would dominate over the zero temperature potential (at least close to  $x_c \sim 0$ ). As a consequence, the high temperature ground state is  $x_c = 0$ . When the temperature decreases, eventually the vacuum term  $-m\omega^2 x_c^2$  takes over and  $x_c = 0$  becomes unstable, triggering a phase transition from  $x_c = 0$  to  $x_c \neq 0$ .

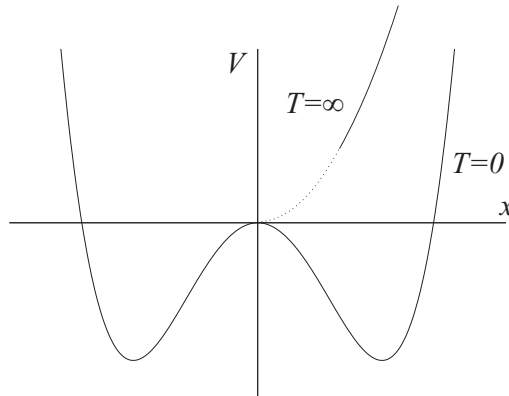


Figure 2.8: Phase transition

## 2.9 Effective theories in general\*

Note that the notion of an effective action is not unique; there are an infinite number of effective actions. Starting with the path integral

$$Z = \int \mathcal{D}\phi e^{-S_E[\phi]} \quad (2.114)$$

we may organize the degrees of freedom into different sets, for example

$$Z = \int \Pi \mathcal{D}\phi_L \mathcal{D}\phi_S e^{-S_E[\phi_L, \phi_S]} \quad (2.115)$$

where  $\phi_L$  stands for long wavelengths and  $\phi_S$  for shortwavelengths; integrating the latter out we find

$$Z = \int \mathcal{D}\phi_L e^{-S_E^{\text{eff}}[\phi_L]} \quad (2.116)$$

which is an effective action for the long wavelength degrees of freedom. How the division is actually done is of course dictated by the physical problem at hand. Nevertheless, this demonstrates a general principle of *coarse graining*: irrelevant degrees of freedom have been *averaged out*. An example is chemistry, which can be viewed as coarse grained QED with an integration over short wavelength modes.

Note that, because of nonlinearities, coarse graining gives rise to qualitatively new "laws" as the fundamental degrees of freedom  $q$  are replaced by the effective degrees of freedom  $\langle q \rangle_{\text{time, space, ...}}$ . This means that the equations of motion, which typically are of the form  $\mathcal{D}q = \lambda q^2 + \gamma q^3 + \dots$  where  $\mathcal{D}$  is some differential operator, gets replaced by

$$\mathcal{D}\langle q \rangle = \lambda \langle q^2 \rangle + \gamma \langle q^3 \rangle + \dots \neq \lambda \langle q \rangle^2 + \gamma \langle q \rangle^3 . \quad (2.117)$$

As a consequence, even simple fundamental laws may give rise to complicated laws for the coarse grained quantities.

**Example. Effective theories in quantum mechanics.** Consider a quantum mechanical system (such as a two-particle spin system) in an entangled state:

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|+\rangle|-\rangle + |-\rangle|+\rangle) . \quad (2.118)$$

The density matrix reads

$$\rho = |\psi\rangle\langle\psi| = \underbrace{\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}_{\substack{++ \quad + - \quad - + \quad --}} \quad (2.119)$$

and we are obviously dealing with a pure state:  $\rho^2 = \rho$ . An effective theory, describing only a reduced number of degrees of freedom (here = 1), is obtained by integrating out (= taking a trace over) the superfluous degrees of freedom. The effective density matrix reads

$$\begin{aligned} \rho_{\text{eff}} &= \underbrace{\text{Tr} \rho}_{\text{over states 2}} = \langle +|\rho|+\rangle + \langle -|\rho|-\rangle \\ &= \frac{1}{2} (|+\rangle\langle +| + |+\rangle\langle -|) \end{aligned} \quad (2.120)$$

which describes now a mixed state:  $\rho_{\text{eff}}^2 = \rho_{\text{eff}}$ .

The very interesting question is: given that at the fundamental level the world is quantum mechanical with  $Z = \int \mathcal{D}x e^{iS}$ , how come for large ensembles we nevertheless write  $Z = \int \mathcal{D}x e^{-SE}$ ?

The answer appears to be decoherence. Consider a quantum system that consist of a small subsystem  $|a\rangle$ , with possible states labeled by  $|n\rangle$  so that  $|a\rangle = \sum_n c_n |n\rangle$ , and the environment  $|\phi_0\rangle$ . The total density matrix is  $\rho_{\text{tot}} = |\phi_0\rangle|a\rangle\langle a|\langle\phi_0|$ . The density matrix of the subsystem  $\rho = \text{Tr}_{\text{env}}\rho_{\text{tot}} = |a\rangle\langle a|$  is subject to evolution, which has two sources, internal and interaction with the environment:

$$i\frac{\partial\rho}{\partial t} = [H_{\text{int}}, \rho] + i\frac{\partial\rho}{\partial t}\Big|_{\text{scatt}}. \quad (2.121)$$

Let us assume slow internal dynamics. Then, with a single scattering event, the initial state  $|a\rangle|\phi_0\rangle \rightarrow S|a\rangle|\phi_0\rangle$ , where  $S$  is the S-matrix. Assuming no recoil the subsystem remains the same even after the scattering. Thus

$$S|a\rangle|\phi_0\rangle = \sum_n c_n |n\rangle|\phi_n\rangle, \quad (2.122)$$

where  $|\phi_n\rangle$  is the environment state corresponding to the subsystem state  $|n\rangle$  (the environment could be considered as a measuring device with  $n$  pointer position; after scattering, the device would be in a superposition of the pointer positions). Thus, after scattering, the reduced density matrix of the subsystem

$$\rho = \sum c_m^* c_n |n\rangle\langle m| \rightarrow \sum c_m^* c_n \langle\phi_n|\phi_m\rangle |n\rangle\langle m| \quad (2.123)$$

or

$$\rho_{nm} \rightarrow \rho_{nm} \langle\phi_m|\phi_n\rangle = \rho_{nm} \langle\phi_0|S_n^\dagger S_m|\phi_0\rangle. \quad (2.124)$$

We now assume that a single scattering is not enough to resolve the different system states; the system remains in "almost unmeasured" state and  $S_n^\dagger S_m \approx 1 - \epsilon$ . The scattering rate  $\Gamma = \sigma v n$  depends on the dynamics, but in general we may now write

$$\rho_{nm} \rightarrow \rho_{nm} (1 - \epsilon)^{\Gamma t} \approx \rho_{nm} e^{-\epsilon\Gamma t} \quad (2.125)$$

so that the non-diagonal elements of the density matrix vanish exponentially fast. Because of quantum entanglement, the subsystem is thus seen to become a statistical ensemble.

Here we may echo the sentiments of the French mathematician Emile Borel, who in 1914 wrote: "Statistical mechanics is not mechanics of large complicated systems, rather it is the mechanics of limited, not completely isolated systems".

## 2.10 Tunneling\*

Let us now apply path integral methods to tunneling, which relates directly to first order phase transitions (phase transitions will be discussed in detail in Ch. X). From quantum

mechanics we recall that in the WKB-approximation the tunneling rate  $\Gamma$  is given by

$$\Gamma = \frac{1}{\tau} \approx \frac{\omega}{2\pi} e^{-2 \int_{x_1}^{x_2} dx K(x)}, \quad K(x) = \frac{2m}{\hbar^2} (V_{\text{eff}} - E) \quad (2.126)$$

where  $V_{\text{eff}}$  is the effective potential. For example, for a 3-d problem with spherical symmetry  $V_{\text{eff}} = V(r) + \hbar^2 l(l+1)/(2mr^2)$ . Quantum mechanics gives directly the barrier penetration probability  $e^{-2 \int dx K}$ ; the prefactor  $\omega$  is in general more difficult to compute. Quantum indeterminacy allows the system to go over (or rather, through) the barrier  $V(x_0)$  even though the energy is less than the barrier height. **KUVA PUUTTUU**

For a thermal system the situation is analogous. However, since the probability for a thermal fluctuation is given by the Boltzmann factor  $e^{-\beta E}$ , the tail of the distribution may escape from the potential well simply by going classically over the wall. Let us consider the situation where at  $x \approx 0$  the potential is given by  $V \approx \frac{1}{2} m \omega_0^2 x^2$  while at the barrier  $V \approx V(x_0) - \frac{1}{2} m \omega^2 (x - x_0)^2$ . We assume that  $T \ll V(x_0)$ . Then classically the differential probability for going over the wall is

$$\frac{d\Gamma}{dx dp} = \underbrace{P(E \geq V(x_0))}_{\propto e^{-\beta E} \approx e^{-\beta V(x_0)}} \underbrace{v \theta(v) \delta(x - x_0)}_{\text{rightmoving flux}}. \quad (2.127)$$

Then, assuming that most contribution to the path integral is obtained from  $x \approx 0$ , we may write

$$\Gamma = \frac{e^{-V(x_0)} \int dp \frac{p}{m} \theta(p) e^{-\beta p^2/2m}}{\int dp e^{-\beta p^2/2m} \underbrace{\int dx e^{-\frac{1}{2} m \omega_0^2 x^2 + \dots}}_{\sqrt{\frac{2\pi}{\beta m \omega_0^2}}}} \approx \frac{\omega_0}{2\pi} e^{-\beta V(x_0)}. \quad (2.128)$$

Note that here we closed our eyes to the fact that at  $x \approx x_0$

$$e^{-V(x)} \approx e^{-V(x_0)} e^{+\frac{1}{2} m \omega^2 (x - x_0)^2} \quad (2.129)$$

where the second factor is formally divergent but when analytically continued, gives rise to an imaginary contribution. In a proper treatment, it is really this imaginary part which is the source of non-zero tunneling rate. You should recall from quantum mechanics that the probability distribution decays if there is an imaginary component in energy:

$$|\psi(t)|^2 = |e^{-iHt} \psi(0)|^2 = |e^{-i\text{Re}Et + \text{Im}Et} \psi(0)|^2 = e^{2\text{Im}Et} |\psi(0)|^2 \quad (2.130)$$

so that  $\Gamma = -2\text{Im}E$ .

In a thermal system the instability of the (ground) state is signalled by a non-zero imaginary part of the free energy. Indeed, classically

$$\begin{aligned} \text{Im}F &= -T \frac{\text{Im}Z}{Z} = -T \frac{\text{Im} \int dx dp e^{-\beta p^2/2m} e^{-\beta[V(x_0) - \frac{1}{2} m \omega^2 (x - x_0)^2]}}{\int dx dp e^{-\beta p^2/2m} e^{-\frac{1}{2} m \omega_0^2 x^2}} \\ &= -T \frac{\text{Im} e^{-\beta V(x_0)} \sqrt{\frac{2\pi T}{-\omega^2}}}{\sqrt{\frac{2\pi T}{\omega_0^2}}} \\ &= T \frac{\omega_0}{2\omega} e^{-\beta V(x_0)}, \end{aligned} \quad (2.131)$$

where we now have continued analytically the gaussian integral in the numerator. Thus we find

$$\Gamma = T \frac{\omega_0}{\omega} e^{-\beta V(x_0)} \quad (2.132)$$

which agrees with (2.128) if we choose  $T = \hbar\omega/(2\pi)$  (see Affleck, Phys. Rev. Lett. 46 (1981) 388.)

In the quantum case we should again look for the imaginary part of  $F$  (or  $Z$ ). Let us consider the potential shown in Figure XXXXX. We already know that integration about the trivial saddle point  $x = x_0$  yields the usual result (2.76) for the harmonic oscillator. But what about other saddle points? These are given by the euclidean equation of motion

$$\frac{1}{2}m\ddot{x} - V'(x) = 0 \rightarrow \frac{1}{2}m\dot{x}^2 - V(x) = -E = \text{const.} \quad (2.133)$$

The question is: are there non-trivial solutions such that  $x(0) = x(\beta)$ ? As can be seen from (2.133), these can be viewed as non-euclidean solutions for motion in an inverted potential starting from  $x_1$  and coming to rest at  $x_2$  (see Fig. XXXXX). At  $x \approx x_0$  the potential is approximately harmonic with frequency  $\omega$ , and  $x_+ > x_2$  is defined by  $V(x_+) = 0$ . The period  $P$  of such a motion is given by

$$\begin{aligned} P(E) &= 2 \int_{\tau_1}^{\tau_2} d\tau = 2 \int_{x_1}^{x_2} dx \left[ \frac{2}{m} (V(x) - E) \right]^{-1/2} \\ &\geq \int_{x_+ - x_0}^{x_+} dx \underbrace{\sqrt{\frac{2}{m} \left( V(x_0) - E - \frac{1}{2}m\omega^2(x - x_0)^2 \right)}}_{\text{harmonic oscillator}}^{-1/2} = \frac{2\pi}{\omega}. \end{aligned} \quad (2.134)$$

Thus we conclude that the motion is periodic, i.e.  $P(E) = \beta$ , whenever  $\beta \geq 2\pi/\omega$ . In that case there always exists an orbit  $\bar{x}$  such that  $\bar{x}(0) = \bar{x}(\beta)$  which is also a saddle point (if  $T \geq \omega/(2\pi)$  the only solution is the classical  $x = x_0$ ). We may call the solution  $\bar{x}$  an *instanton*.

Expanding about the instanton we find

$$Z = N \left[ \det \left( -\frac{d^2}{d\tau^2} + V''(\bar{x}(\tau)) \right) \right]^{-1/2} e^{-S_E[\bar{x}]} . \quad (2.135)$$

The aim is then to show that the determinant has one negative eigenvalue, giving rise to an imaginary part of  $Z$ ; this is a non-trivial task but can be done (see. Phys. Rev. D25 (1982) 330).

## 2.11 Tunneling in field theory\*

Tunneling in field theory is analogous to the quantum mechanical case considered in the previous Section. At high  $T$  we may simplify things by noting that as  $\beta \rightarrow 0$ , only the static

modes with  $\dot{\phi} = 0$  contribute to the action so that

$$S = \int_0^\beta d\tau d^3x \left[ \frac{1}{2} \dot{\phi}^2 + \frac{1}{2} (\nabla\phi)^2 + V(\phi, T) \right] \approx \frac{1}{T} \int d^3x \left[ \frac{1}{2} (\nabla\phi)^2 + V(\phi, T) \right] \equiv \frac{1}{T} S_3[T]. \quad (2.136)$$

The tunneling rate is then given by

$$\Gamma = A e^{-S[\phi_*]/T} \quad (2.137)$$

where  $A$  is the fluctuation determinant (from a gaussian integration) and  $\phi_*$  is the *critical field* configuration, which is the solution to the euclidean equation of motion that connects the two vacua.

In general there is an infinity of configurations connecting any two vacua. The issue then is, which of these has the lowest action and thus corresponds to the fastest tunneling rate? Usually the answer is: the most symmetric one. Let us therefore assume that the critical field configuration is spherically symmetric. The euclidean equation of motion reads then

$$\frac{d^2\phi_*}{dr^2} + \frac{2}{r} \frac{d\phi_*}{dr} = V'(\phi_*, T). \quad (2.138)$$

The solution  $\phi_* = \phi_*(r)$  is called the critical bubble.

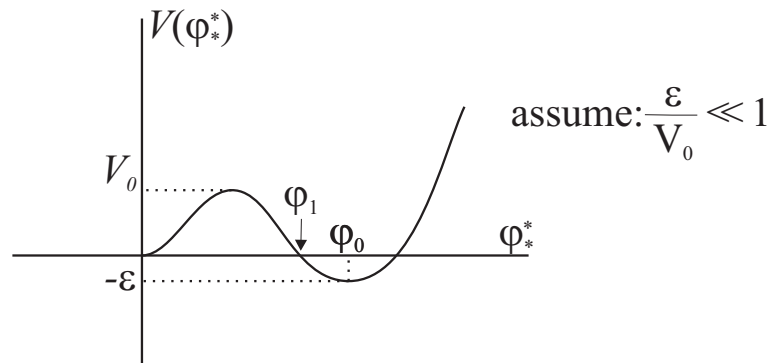


Figure 2.9: The potential appropriate for the thin wall approximation.

**Thin wall approximation.** The critical bubble can be found analytically in the thin wall approximation<sup>1</sup> which is appropriate for the potential of the type depicted in Fig. 2.9. There one assumes that the energy difference  $\epsilon$  between the two vacua is small compared with the height of the potential wall  $V_0$  that separates them. In that case we may seek for a solution where  $\phi_* \approx \phi_0 = \text{const}$  when  $r < R$ , the size of the bubble, and  $d\phi_*/dr \neq 0$  only in a narrow region  $\ll R$ , while outside the bubble we have  $\phi_* \approx 0$  (see Fig. 2.10). Close to the thin wall  $r$  is large so that we may write

$$\frac{d^2\phi_*}{dr^2} \approx V'(\phi_*, T) = \frac{dV}{d\phi_*} \frac{dr}{dr} \quad (2.139)$$

so that  $\phi_*'^2 \approx V(r)$  and

$$r \approx \int_\phi^{\phi_0} \frac{\phi_*}{\sqrt{V}}. \quad (2.140)$$

<sup>1</sup>S. Coleman, Phys. Rev. D15, 2929 (1977).

We then find that

$$\begin{aligned} S_3 &= 4\pi \int_0^\infty dr r^2 \left[ \frac{1}{2} \frac{d^2 \phi_*}{dr^2} + V(\phi_*, T) \right] \\ &= -\frac{4}{3} \pi R^3 \epsilon + 4\pi R^2 S_1(T), \end{aligned} \quad (2.141)$$

where  $S_1$  is the surface tension, which is the integral over the region where  $\phi_*$  changes rapidly; it can be calculated explicitly once  $V(\phi_*, T)$  is specified.

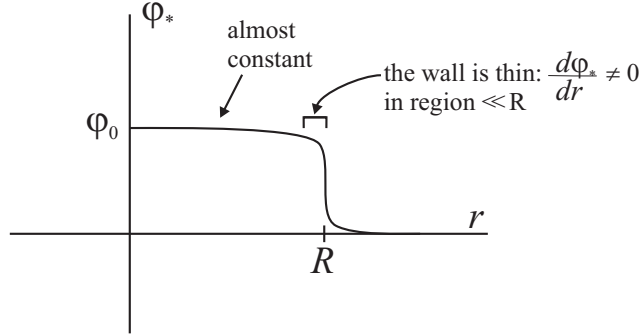


Figure 2.10: The critical field in the thin wall approximation.

The remaining task is now to minimize the action as a function of the free parameter  $R$ , the size of the critical bubble:

$$\frac{dS_3}{dR} = 0 \rightarrow R = \frac{2S_1}{\epsilon}. \quad (2.142)$$

Since  $\epsilon$  is assumed to be small, the bubble is large, as it should for the thin wall approximation to be valid. We can also find the action, which reads

$$S_3 = \frac{16\pi S_1^3}{3\epsilon^2}. \quad (2.143)$$

Hence in the thin wall approximation the tunneling rate  $\Gamma \sim e^{S_3/T}$  is small and the transition could be called slow boiling.

Finding the fluctuation determinant is again much more complicated. A good guess is always that  $A \sim T^4$  since  $T$  is often the only relevant mass scale in the problem.



# Chapter 3

## Path integrals in finite $T$ field theory

Previously we had one degree of freedom,  $x(t)$ , which we could as well call  $\phi(t)$ . Let us now assume that we have one degree of freedom in each point  $\mathbf{x}$  of space. Then we come to field theory for a real scalar field  $\phi(t, \mathbf{x})$ . The baseline case is again that of a harmonic oscillator potential, the frequency of which is now conventionally called the mass  $m$  of the field. If the field degrees of freedom are taken to be the spatial Fourier components  $\phi(t, \mathbf{k})$ , the effective binding frequency becomes  $\omega_{\mathbf{k}} = \sqrt{m^2 + \mathbf{k}^2}$ . This collection of harmonic oscillators is called free field theory.

Using a relativistic notation  $k^\mu = (k^0, k^i)$ ,  $k^2 = k^\mu k_\mu = k_0^2 - \mathbf{k}^2$ ,  $\partial_\mu = \partial/\partial x^\mu$ , a natural generalisation of the harmonic oscillator action with an interaction term is

$$S = \int dt d^3x \left[ \frac{1}{2} \partial_\mu \phi \partial^\mu \phi - \frac{1}{2} m^2 \phi^2 - \frac{1}{4} \lambda \phi^4 \right] = \int d^4x \mathcal{L}(\phi, \partial_\mu \phi) \quad (3.1)$$

The classical equation of motion extremising this action is

$$(\square + m^2 + \lambda \phi^2) \phi = 0, \quad (3.2)$$

where  $\square = \partial_\mu \partial^\mu = \partial_t^2 - \partial_{\mathbf{x}}^2$ . The plane wave solutions of the Klein-Gordon equation ( $\lambda = 0$ ) are  $\phi = e^{ik \cdot x}$  with a dispersion relation  $k^2 - m^2 = 0$ ,  $k_0 = \pm \sqrt{\mathbf{k}^2 + m^2}$ .

**Non-relativistic limit.** To find the non-relativistic limit,  $\sqrt{\mathbf{k}^2 + m^2} = m + \mathbf{k}^2/(2m) + \dots$  of the scalar field equation, one has to separate the positive and negative frequency modes. This can be done by writing, identically,

$$-\frac{1}{2m} (\square + m^2) \phi = \left[ i\partial_t - m + \frac{1}{2m} (i\partial_t - m)^2 + \frac{1}{2m} \nabla^2 \right] \phi. \quad (3.3)$$

For large  $m$  the term with  $(i\partial_t - m)^2$  is negligible and the usual Schrödinger equation is obtained, measuring energies starting from  $m$ .

We shall now compute the partition function of the free scalar field using field theory methods. As discussed previously, at  $T \neq 0$ , we take the euclidean action and periodic fields so that

$$Z = N \int \mathcal{D}\phi \exp \left[ - \int_0^\beta d\tau \int d^3x \left[ \frac{1}{2} (\partial_\tau \phi)^2 + \frac{1}{2} (\partial_i \phi)^2 + \frac{1}{2} m^2 \phi^2 \right] \right], \quad (3.4)$$

where  $\phi(\tau + \beta, \mathbf{x}) = \phi(\tau, \mathbf{x})$  and  $N$  is an irrelevant constant. Let us first note that

$$\begin{aligned} \int d^3x d\tau \frac{1}{2} \partial_\mu \phi \partial_\mu \phi &= \int d^4x \left[ \frac{1}{2} \partial_\mu (\phi \partial^\mu \phi) - \frac{1}{2} \phi \square \phi \right] \\ &= \underbrace{\frac{1}{2} \oint dS_\mu \phi \partial_\mu \phi}_{= 0 \text{ for } \phi(\mathbf{x}) \rightarrow 0 \text{ as } \mathbf{x} \rightarrow \infty} - \frac{1}{2} \int d^4x \phi \square \phi. \end{aligned} \quad (3.5)$$

The surface term thus vanishes because there is no field at infinity. We can evaluate this, again using the fundamental Gaussian integral (2.65),

$$Z = N \int \mathcal{D}\phi \exp \left( - \int d\tau d^3x \frac{1}{2} \phi K \phi \right) \propto (\det K)^{-\frac{1}{2}} \quad (3.6)$$

where now

$$K = -\partial_\tau^2 - \nabla^2 + m^2. \quad (3.7)$$

The periodic eigenfunctions of the operator  $K$  are now  $e^{i\omega_n \tau - i\mathbf{k} \cdot \mathbf{x}}$  with the eigenvalues  $\omega_n^2 + \mathbf{k}^2 + m^2$  and we can immediately write  $\det K$  as a product of eigenvalues or  $\log \det K = \text{Tr} \log K$  as a sum of logs of eigenvalues:

$$F = \frac{1}{2} T \log \det K = \frac{1}{2} T \text{Tr} \ln K = V \frac{1}{2} T \sum_{n=-\infty}^{\infty} \int \frac{d^3k}{(2\pi)^3} \ln \left( (2\pi n T)^2 + \mathbf{k}^2 + m^2 \right). \quad (3.8)$$

To proceed further, we note that the integral is divergent, but the divergence is there already for  $T = 0$ , i.e., is  $T$ -independent. One can get rid of constants by taking derivatives, so let us improve the convergence by taking a derivative with respect to  $m^2$ :

$$I(m) \equiv T \sum_{n=-\infty}^{\infty} \int \frac{d^3k}{(2\pi)^3} \frac{1}{(2\pi n T)^2 + \mathbf{k}^2 + m^2}. \quad (3.9)$$

Then apply a magic formula from 19th-century mathematics

$$\sum_{n=-\infty}^{\infty} \frac{x}{(2\pi n)^2 + x^2} = \frac{1}{x} + 2 \sum_1^{\infty} \frac{x}{(2\pi n)^2 + x^2} = \frac{1}{2} + \frac{1}{e^x - 1}. \quad (3.10)$$

and derive

$$I(m) = \int \frac{d^3k}{(2\pi)^3} \left[ \frac{1}{2E_k} + \frac{1}{E_k} \frac{1}{e^{\beta E_k} - 1} \right]. \quad (3.11)$$

Further, by integrating over  $m^2$  with  $dm^2 = 2E dE$  and noting that the lower limit gives an additive constant:

$$\begin{aligned} F(T)/V = -p(T) &= \frac{1}{2} \int_0^{m^2} dm^2 I(m) = \int \frac{d^3k}{(2\pi)^3} \int^{E_k} dE \left( \frac{1}{2} + \frac{1}{e^{\beta E} - 1} \right) \\ &= \int \frac{d^3k}{(2\pi)^3} \left\{ \frac{1}{2} E_k + T \log[1 - e^{-\beta E_k}] \right\}. \end{aligned} \quad (3.12)$$

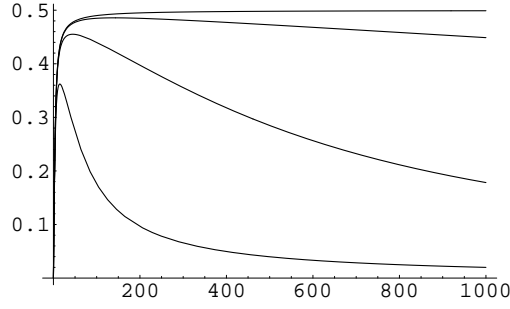


Figure 3.1: How the summation formula (3.10) works; the top curve shows the RHS  $-1/x$  as a function of  $x$ ; the lower ones show respectively sums up to 1000, 100, and 10 terms.

Here all the divergences are dumped in the first term, which obviously sums over all the zero point energies. It is  $T$ -independent, as promised, and if we only are interested in  $T$ -dependence, we can forget it. And the second term is precisely Eq. (3.12) with  $\mu = 0$ .

However, if one really wants to find out the correct way of handling divergences, it is important to keep even the first term. Also, often  $m$  has an important dynamic significance (in symmetry breaking, for example) and cannot be forgotten. Then the simplest way of handling the divergence of the first term in Eq. (3.11) is to keep  $d$  arbitrary. As we want to be close to  $3d$  we write  $d = 3 - 2\epsilon$ ; then for small  $\epsilon$  the integral is simply given by the expansion

$$\int \frac{d^d k}{(2\pi)^d} \frac{1}{2(\mathbf{k}^2 + m^2)^{1/2}} = -\frac{m^2}{8\pi^2} \left( \frac{1}{\epsilon} + 1 - \gamma_{\text{Euler}} + \mathcal{O}(\epsilon) \right) \quad (3.13)$$

so that the divergence is isolated in the  $\frac{1}{\epsilon}$  singularity; this is an example of *dimensional regularisation*. We shall return to this in a moment when discussing the  $T \gg m$ -expansion of (3.12).

Why all this trouble with sums over  $n$ ? The reason is that to include the effects of interactions perturbatively, you cannot avoid doing sums.

**Note: the Hardy-Ramanujan formula.** Define  $p^s(n)$  as the number of ways an integer can be expressed as a sum of  $s$ th powers of integers. For example,  $p^1(5) = 7$  since the ways are 5, 4+1, 3+2, 3+1+1, 2+2+1, 2+1+1+1, 1+1+1+1+1. Similarly,  $p^2(5) = 2$  since  $5 = 2^2 + 1^2 = 1^2 + 1^2 + 1^2 + 1^2 + 1^2$ . Assume now that the energy spectrum is  $E_n = n^s$ ,  $n \geq 1$ ,  $s > 0$ . If  $x \equiv e^{-\beta}$ , the bosonic partition function (1.55) with  $\mu = 0$  is nothing but the generating function of  $p^s(n)$ :

$$Z(x = e^{-\beta}) = \prod_{n=1}^{\infty} \frac{1}{1 - x^{n^s}} = \sum_{n=1}^{\infty} p^s(n) x^n \approx \int_1^{\infty} dn p^s(n) e^{-\beta n}. \quad (3.14)$$

One can now invert this by saddle point methods to obtain the famous Hardy-Ramanujan formula (1918) for  $p^s(n)$ . For example, for the harmonic spectrum  $s = 1$ ,

$$p(n) = \frac{1}{4\sqrt{3}N} e^{\pi\sqrt{2N/3}}. \quad (3.15)$$

In string theory, the spectrum of string excitations goes like  $M^2 \sim 4N/\alpha'$  so that the number of states grows exponentially with mass.

**Note: Field theory in curved space.** Einstein's general theory of relativity replaces the metric  $\eta_{\mu\nu} = \text{diag}(1, -1, -1, -1)$  by a general 10-component tensor  $g_{\mu\nu}(x)$ , given as a solution of Einstein's gravity equations. Then the quadratic terms of the action of scalar field theory are written in the form

$$S[\phi] = \int d^4x \sqrt{-g(x)} \left[ \frac{1}{2} g^{\mu\nu}(x) \partial_\mu \phi(x) \partial_\nu \phi(x) - \frac{1}{2} m^2 \phi^2(x) \right], \quad (3.16)$$

where  $g(x) = \det g_{\mu\nu}(x)$ . This form is specified by the requirement of reparametrisation invariance, the action should be invariant under any coordinate transformation  $x^\mu \rightarrow x'^\mu(x)$ . To do thermodynamics one proceeds exactly as above: goes to imaginary time, does the gaussian integral with the result  $Z^{-\frac{1}{2}} \sim \det(\square + m^2)$ , where now in curved space  $\square = \sqrt{-g}^{-1} \partial_\mu \sqrt{-g} g^{\mu\nu} \partial_\nu$ . The problem thus boils down to a computation of this functional determinant, for example, by finding out the mode functions and eigenvalues. Many interesting new effects appear <sup>1</sup>, but basic ideas of thermodynamics are the same.

### 3.1 Photon gas

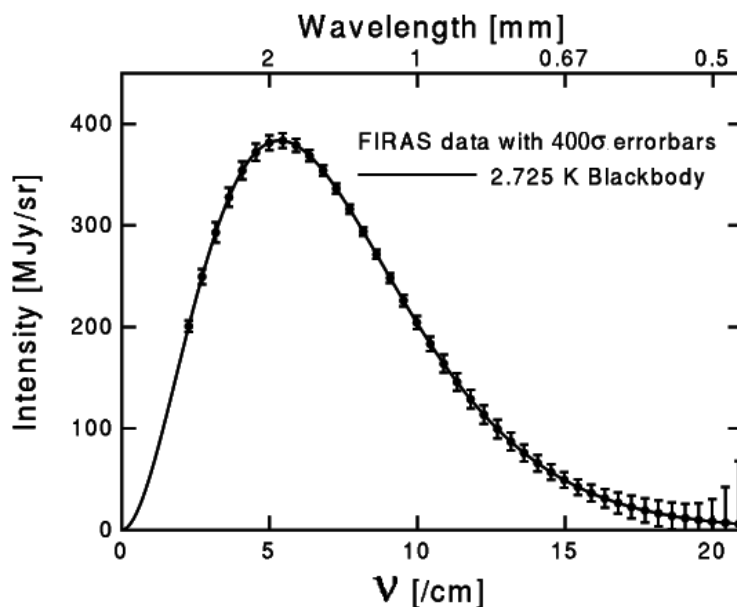


Figure 3.2: Spectrum of cosmic background radiation: perfect massless Bose-Einstein. Note that the error bars in the Figure are multiplied by 400.

As a first application, consider the photon gas. Photons propagate with the velocity of light, but when a collection of photons has, due to physical thermalisation effects like boundaries, momenta that are isotropic and thermally distributed, the system is thermal gas. An example of photon gas which plays an important role in contemporary physics is the cosmic microwave background.

For the purposes of statistical physics, photons are bosons with  $m = 0$  and their degeneracy factor is 2 for the two helicities of massless vector bosons. In general, in the presence

<sup>1</sup>see N.D.Birrel and P.C.W.Davies, Quantum fields in curved space, Cambridge University Press 1999

of interactions the number of photons is not conserved so that  $\mu = 0$ . Remembering that

$$\int_0^\infty dx \frac{x^{\alpha-1}}{e^x \mp 1} = \begin{cases} \zeta(\alpha)\Gamma(\alpha) & \text{BE} \\ (1 - \frac{1}{2^{\alpha-1}})\zeta(\alpha)\Gamma(\alpha) & \text{FD} \end{cases} \quad (3.17)$$

we find the following expressions:

$$n_\gamma = \frac{N}{V} = 2 \cdot \frac{1}{(2\pi)^3} \int d^3k \frac{1}{e^{\frac{k}{T}} - 1} = \frac{T^3}{\pi^2} \int_0^\infty dx \frac{x^2}{e^x - 1} = \frac{2\zeta(3)}{\pi^2} T^3 \quad (3.18)$$

$$\epsilon_\gamma = \frac{E}{V} = 2 \cdot \frac{1}{(2\pi)^3} \int d^3k \frac{k}{e^{\frac{k}{T}} - 1} = \frac{T^4}{\pi^2} \int_0^\infty dx \frac{x^3}{e^x - 1} = \frac{\pi^2}{15} T^4 \equiv \frac{\pi^2}{15c^3 \hbar^3} T^4 = 3p \quad (3.19)$$

$$s_\gamma = p'(T) = \frac{4}{3} \frac{\pi^2}{15} T^3 = \frac{2\pi^4}{45\zeta(3)} n \quad (3.20)$$

From here one can derive various differential forms for  $d\epsilon/d\omega$ ,  $d\epsilon/d\lambda$ , etc, using

$$E = \hbar\omega = h\nu = pc = \hbar ck \quad (3.21)$$

$$p = \hbar k = \frac{h}{\lambda} \quad (\text{here } p \text{ is momentum!}). \quad (3.22)$$

For example, the energy density per unit frequency  $\nu$  becomes

$$\frac{d\epsilon}{d\nu} = \frac{8\pi h}{c^3} \frac{\nu^3}{e^{h\nu/T} - 1}. \quad (3.23)$$

This is the celebrated black body spectrum; it is called "black" for historical reasons. The most perfect black body observed in Nature is the cosmic microwave background (see Fig. 3.2). Note also that "radiation emittance" = energy emitted by a black body per unit time per unit area =  $c/4 \times$  energy density.

In  $d$  spatial dimensions one finds

$$p(T) = \frac{1}{d} \epsilon(T) = \frac{2\Gamma(d+1)\zeta(d+1)}{d\Gamma(d/2)(4\pi)^{d/2}} T^{d+1}. \quad (3.24)$$

**Massless BE and FD gases; basic equations in early cosmology.** Here we summarize the relevant ultrarelativistic expressions for Bose-Einstein and Fermi-Dirac gases emphasising unit choices. Both are very much needed in cosmology (units K, m), also in relativistic heavy ion collisions (units GeV, fm). The appropriate conversion relations, given in the Appendix, are

$$\begin{aligned} 1 \text{ eV} &= 1.602 \times 10^{-19} \text{ J}; \\ \hbar &= 1 = 6.58 \times 10^{-22} \text{ MeVs} = 7.64 \times 10^{-12} \text{ Ks}; \\ \hbar c &= 1 = 0.19733 \text{ GeVfm} = 0.2290 \text{ Kcm}; \\ 1 \text{ K} &= 0.1532 \times 10^{-36} \text{ gc}^2. \end{aligned}$$

Then  $\epsilon = 3p$  with

$$\begin{aligned} \epsilon &= \frac{g}{2} \cdot \left(\frac{7}{8}\right) \cdot \frac{\pi^2}{15} T^4 = \frac{g}{2} \cdot \left(\frac{7}{8}\right) 85.633 \left(\frac{T}{\text{GeV}}\right)^4 \frac{\text{GeV}}{\text{fm}^3} = \frac{g}{2} \cdot \left(\frac{7}{8}\right) \cdot 0.841 \cdot 10^{-36} \left(\frac{T}{\text{K}}\right)^4 \frac{g}{\text{cm}^3}; \\ n &= \frac{g}{2} \cdot \left(\frac{3}{4}\right) \cdot \frac{2\zeta(3)}{\pi^2} T^3 = \frac{g}{2} \cdot \left(\frac{3}{4}\right) 31.700 \left(\frac{T}{\text{GeV}}\right)^3 \frac{1}{\text{fm}^3} = \frac{g}{2} \cdot \left(\frac{3}{4}\right) \cdot 20.288 \left(\frac{T}{\text{K}}\right)^3 \frac{1}{\text{cm}^3}; \\ s &= \frac{g}{2} \cdot \left(\frac{7}{8}\right) \cdot \frac{4\pi^2}{45} T^3 = \left(\frac{7}{6}\right) \frac{2\pi^4}{45\zeta(3)} n. \end{aligned} \quad (3.25)$$

For BE remove the bracketed fractions  $(\frac{7}{8}), (\frac{3}{4}), (\frac{7}{6})$ . Some further numerical relations are

$$\begin{aligned} T_\gamma &= 2.725K \Rightarrow n_\gamma = 410 \frac{1}{\text{cm}^3}; \\ T_\nu &= \left(\frac{4}{11}\right)^{\frac{1}{3}} 2.7K = 1.9K \Rightarrow n_\nu = 54 \frac{1}{\text{cm}^3} \text{ for } g_\nu = 1; \\ s_0 &= \frac{4\pi^2}{45} \left[1 + \frac{2 \cdot 3}{2} \cdot \frac{7}{8} \cdot \frac{4}{11}\right] T_{0\gamma}^3 = 2810 \frac{1}{\text{cm}^3} \left(\frac{T_{0\gamma}}{2.7K}\right)^3 = 7.03 n_{0\gamma}. \end{aligned}$$

## 3.2 Large $T$ expansion

For  $\mu = 0$  we may write for bosons from Eq. (3.12)

$$-p(T, m) = \frac{T^4}{2\pi^2} \int_0^\infty dx x^2 \log[1 - e^{-\sqrt{x^2+y^2}}] \Big|_{y=m/T}. \quad (3.26)$$

The integral in Eq. (3.26) has the following expansions:

$$-\frac{p_{\text{BE}}(T, m)}{T^4} = -\left(\frac{y}{2\pi}\right)^{3/2} e^{-y} \quad (y \gg 1) \quad (3.27)$$

$$= -\frac{\pi^2}{90} + \frac{y^2}{24} - \frac{y^3}{12\pi} - \frac{y^4}{32\pi^2} [\log y + \gamma_E - \log 4\pi - \frac{3}{4}] + \frac{\zeta(3)y^6}{768\pi^4} + \dots \quad (3.28)$$

Similarly, for the FD free energy (1.63) one has the expansion

$$-\frac{p_{\text{FD}}(T, m)}{T^4} = -\frac{7\pi^2}{720} + \frac{y^2}{48} + \frac{y^4}{32\pi^2} [\log y + \gamma_E - \log \pi - \frac{3}{4}] + \frac{7\zeta(3)y^6}{4 \cdot 768\pi^4} + \dots \quad (3.29)$$

Finding the small- $y$  expansion is an interesting mathematical problem. Note that the integral seems to depend on  $y^2$  but the expansion (3.28) contains the term  $y^3$ . There is no such in (3.29). The reason is that expanding the integrand for small  $y$  leads to a divergent integral for bosons. The physics reason is that the BE distribution function  $1/(e^x - 1)$  diverges at  $x \rightarrow 0$ , the FD distribution is finite. There are lots of infrared bosons at finite  $T$ !

To derive the  $T \gg m$  expansion return to the  $m^2$ -derivative of  $I(m)$  in Eq. (3.9) and replace there  $3 \rightarrow d = 3 - 2\epsilon$ . One sees that all the terms with  $n \neq 0$  can be expanded for small  $m/T$ , the zero mode  $n = 0$  is the dangerous one. So separate it:

$$\begin{aligned} I(T, m) &= I^{(n=0)}(T, m) + I^{n \neq 0}(T, m) \\ &= T \int \frac{d^d k}{(2\pi)^d} \frac{1}{\mathbf{k}^2 + m^2} + 2T \sum_{n=1}^{\infty} \int \frac{d^d k}{(2\pi)^d} \frac{1}{(2\pi n T)^2 + \mathbf{k}^2 + m^2}. \end{aligned} \quad (3.30)$$

The zero mode term is seemingly a function of  $m^2$  but actually is divergent for  $d = 3$  so a consistent regularisation is needed. Try

$$\int \frac{d^3 k}{(2\pi)^3} \frac{1}{\mathbf{k}^2 + m^2} = \int_0^\infty \frac{dk}{2\pi^2} \frac{k^2 + m^2 - m^2}{k^2 + m^2} = \int_0^\infty \frac{dk}{2\pi^2} - \frac{m^2}{2\pi^2} \int_0^\infty \frac{dk}{k^2 + m^2}. \quad (3.31)$$

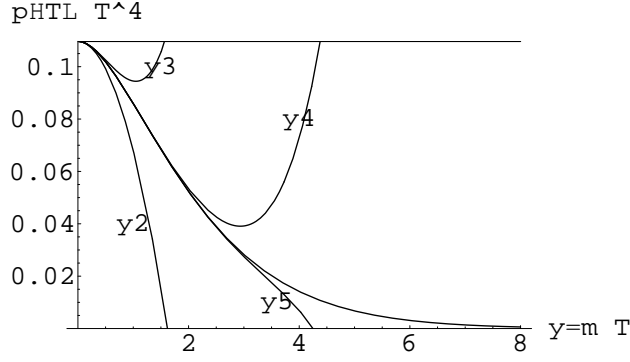


Figure 3.3: The exact result for  $p(T)/T^4$  from (3.26) and the various terms of the large- $T$  or small- $y$  expansion in (3.28).

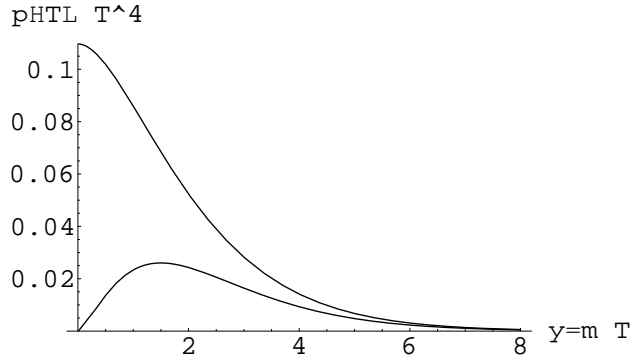


Figure 3.4: The exact result from (3.26) compared with the low- $T$  approximation in (3.28).

Thus

$$\int \frac{d^3 k}{(2\pi)^3} \frac{1}{\mathbf{k}^2 + m^2} = +\infty - \frac{Tm}{4\pi} \quad (3.32)$$

and an obviously positive function of  $m^2$  has become a negative function of  $m$  – provided that the positive infinity can be disposed of. The second term in Eq. (3.30) can now be expanded for  $T \gg m$ :

$$\frac{1}{(2\pi n T)^2 + \mathbf{k}^2 + m^2} = \sum_{l=0}^{\infty} \frac{(-)^l (m^2)^l}{[(2\pi n T)^2 + \mathbf{k}^2]^{l+1}} \quad (3.33)$$

and then integrated term by term over  $\mathbf{k}$  using

$$d^d k = \frac{\pi^{d/2}}{\Gamma(d/2)} (\mathbf{k}^2)^{d/2-1} dk^2 \quad (3.34)$$

together with the definition of the gamma function:

$$\int \frac{d^d k}{(2\pi)^d} \frac{1}{(\mathbf{k}^2 + m^2)^A} = \frac{1}{(4\pi)^{d/2}} \frac{\Gamma(A - d/2)}{\Gamma(A)} \frac{1}{(m^2)^{A-d/2}}. \quad (3.35)$$

After the integration the sum over  $n$  can be written as a zeta function and the final answer reads

$$I^{n \neq 0}(T, m) = \frac{2T}{(4\pi)^{d/2}} \frac{1}{(2\pi T)^{2-d}} \sum_{l=0}^{\infty} \left( \frac{-m^2}{4\pi^2 T^2} \right)^l \frac{\Gamma(l+1-d/2)}{\Gamma(l+1)} \zeta(2l+2-d). \quad (3.36)$$

Expanding for small  $\epsilon$ , including terms up to  $l = 2$ , using the values of the zeta function,  $\zeta(-1)$ ,  $\zeta(1+2\epsilon)$ ,  $\zeta(3)$  given below in Sect. 3.3 and adding the  $n = 0$  term ( $\gamma_E$  is the Euler constant) leads to

$$I(T, m) = \frac{T^2}{12} - \frac{Tm}{4\pi} - \frac{m^2}{16\pi^2} \left( \frac{1}{\epsilon} + \log \frac{4\pi}{T^2} - 2 \log(2\pi) + 2\gamma_E + \mathcal{O}(\epsilon) \right) + \frac{m^4 \zeta(3)}{128\pi^4 T^2} + \mathcal{O}(m^6/T^4), \quad (3.37)$$

which ( $\times 1/2$ ) still has to be integrated over  $m^2$  to give (3.28).

The extremely accurate computations of the Standard Model in particle physics express their results in terms of the numbers  $\log \pi$ ,  $\gamma_E$ ,  $\zeta(N)$  appearing here (plus further related ones). Why does Nature choose them?

### 3.3 Chemical potential, charged scalar field

To introduce chemical potential we need a conserved quantum number. The simplest way to do this is to consider a charged scalar field with the Lagrangian density

$$\mathcal{L}[\phi, \partial_\mu \phi, \phi^*, \partial_\mu \phi^*] = \partial_\mu \phi^* \partial^\mu \phi - m^2 \phi^* \phi - \lambda(\phi^* \phi)^2, \quad (3.38)$$

$$\phi = \frac{1}{\sqrt{2}} (\phi_1 + i\phi_2). \quad (3.39)$$

The Lagrangian is invariant under  $\phi \rightarrow e^{i\alpha} \phi \approx \phi + i\alpha \phi$ ,  $\phi^* \rightarrow e^{-i\alpha} \phi^* \approx \phi^* - i\alpha \phi^*$ . Under this transformation

$$\begin{aligned} 0 = \delta L &= \frac{\partial L}{\partial \phi} \delta \phi + \frac{\partial L}{\partial \partial_\mu \phi} \partial_\mu \delta \phi + (\phi \rightarrow \phi^*) \\ &= \left( \frac{\partial L}{\partial \phi} - \partial_\mu \frac{\partial L}{\partial \partial_\mu \phi} \right) \delta \phi + \partial_\mu \left( \frac{\partial L}{\partial \partial_\mu \phi} \cdot \delta \phi \right) + (\phi \rightarrow \phi^*). \end{aligned} \quad (3.40)$$

Inserting here  $\delta \phi = i\phi$ ,  $\delta \phi^* = -i\phi^*$  (canceling the small parameter  $\alpha$ ) and evaluating the partial derivatives, one obtains, for the field configurations satisfying the equation of motion, the conserved current

$$\partial_\mu J^\mu = 0, \quad J_\mu = i(\partial_\mu \phi^* \cdot \phi - \partial_\mu \phi \cdot \phi^*) = 2\text{Im}(\phi^* \partial_\mu \phi), \quad (3.41)$$

with the conserved total charge

$$Q = \int d^3x J^0 = \int d^3x i(\partial_t \phi^* \cdot \phi - \partial_t \phi \cdot \phi^*) = \int d^3x (\phi^* \partial_\tau \phi - \phi \partial_\tau \phi^*). \quad (3.42)$$

We can now understand the path integral result for the grand partition function

$$\begin{aligned} \mathcal{Z}(T, V, \mu) &= \text{Tre}^{-\beta(H-\mu Q)} = \\ &N \int \mathcal{D}\phi \mathcal{D}\phi^* \exp \left\{ - \int_0^\beta d\tau \int d^3x [((\partial_\tau + \mu)\phi^*) \cdot ((\partial_\tau - \mu)\phi) + \partial_i \phi^* \partial_i \phi + m^2 \phi^* \phi + \lambda(\phi^* \phi)^2] \right\}. \end{aligned} \quad (3.43)$$

The cross terms in (3.44) involving  $\partial_\tau$  just produce the needed term  $\mu Q$ , there further is the term  $\mu^2 \phi^* \phi$ . This has one very important consequence, the integrand does not contain the

term  $|(\partial_\tau + \mu)\phi|^2$ , for real chemical potential it is complex. In fact, using the real components (3.39)

$$\mathcal{Z}(T, V, \mu) = N \int \mathcal{D}\phi_1 \mathcal{D}\phi_2 \cos \left[ \mu \int d\tau d^3x (\phi_1 \partial_\tau \phi_2 - \phi_2 \partial_\tau \phi_1) \right] e^{-S_R}, \quad (3.44)$$

where the real action is

$$S_R = \int d\tau d^3x [|\partial_\tau \phi|^2 + (m^2 - \mu^2)\phi^* \phi + \lambda(\phi^* \phi)^2]. \quad (3.45)$$

Because of the oscillating factor it is, in practise, impossible to use numerical methods to evaluate the path integral for finite real  $\mu$ .

To evaluate the path integral it is convenient to go to the real components (3.39). The term  $\frac{1}{2}\phi(-\partial_\tau^2)\phi$  in the single-component case is then replaced by

$$\frac{1}{2}(\phi_1, \phi_2) \begin{pmatrix} -\partial_\tau^2 - \mu^2 + E_k^2 & 2i\mu\partial_\tau \\ -2i\mu\partial_\tau & -\partial_\tau^2 - \mu^2 + E_k^2 \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}, \quad (3.46)$$

where  $E_k = \sqrt{k^2 + m^2}$ . Replacing here  $\partial_\tau \rightarrow i\omega_n$ , evaluating the determinant and using the identity  $(\omega_n^2 + E_k^2 - \mu^2)^2 + 4\mu^2 E_k^2 = [\omega_n^2 + (E_k - \mu)^2][\omega_n^2 + (E_k + \mu)^2]$  one sees that the result is the sum of two terms of the form (3.8) in which  $E_k \rightarrow E_k \pm \mu$ . Thus finally, generalising Eq. (3.12),

$$\Omega(T, \mu)/V = -p(T, \mu) = \int \frac{d^3k}{(2\pi)^3} \left\{ E_k + T \log \left[ 1 - e^{-\beta(E_k - \mu)} \right] + T \log \left[ 1 - e^{-\beta(E_k + \mu)} \right] \right\}. \quad (3.47)$$

Note 1: In connection with chemical potential the following generalisations of the beautiful formula (3.10) are often useful

$$T \sum_{n=-\infty}^{\infty} \frac{1}{(2\pi nT + C)^2 + E^2} = \frac{1}{2E} \left( 1 + \frac{1}{e^{\beta(E+iC)} - 1} + \frac{1}{e^{\beta(E-iC)} - 1} \right), \quad (3.48)$$

$$T \sum_{n=-\infty}^{\infty} \frac{1}{((2n+1)\pi T + C)^2 + E^2} = \frac{1}{2E} \left( 1 - \frac{1}{e^{\beta(E+iC)} + 1} - \frac{1}{e^{\beta(E-iC)} + 1} \right). \quad (3.49)$$

The terms in the RHS here are distribution functions with chemical potential  $= \pm iC$ .

### 3.4 Fermion-antifermion mixtures at large $T$

In relativistic plasmas one must include also the antiparticles. Since the two can annihilate to vacuum, the chemical potential of an antiparticle is  $-\mu$ . For a FD system one then has, in analogy with Eq. (3.47),

$$p(T, \mu) = 2 \int \frac{d^d k}{(2\pi)^d} \left\{ E_k + T \left[ \log(1 + e^{-\beta(E_k - \mu)}) + \log(1 + e^{-\beta(E_k + \mu)}) \right] \right\}, \quad (3.50)$$

where  $E_k = \sqrt{k^2 + m^2}$ , 2 counts the number of spin states and, for the first vacuum energy term,  $d = 3 - 2\epsilon$ .

As for  $\mu = 0$ , for the massless case the above result can be written in a very simple form. Dropping the vacuum term

$$\begin{aligned}
p(T, \mu; m = 0) &= \frac{T^4}{\pi^2} \int_0^\infty dx x^2 [\log(1 + e^{y-x}) + \log(1 + e^{-y-x})] \Big|_{y=\beta\mu} \\
&= \frac{T^4}{\pi^2} \left( \frac{7\pi^4}{180} + \frac{\pi^2}{6} y^2 + \frac{1}{12} y^4 \right) \\
&= \frac{7\pi^2}{180} T^4 + \frac{1}{6} T^2 \mu^2 + \frac{1}{12\pi^2} \mu^4.
\end{aligned} \tag{3.51}$$

Here the coefficient of the  $T^4$  term is  $2 \cdot 2 \cdot \frac{7}{8} \cdot \frac{\pi^2}{90}$  with obvious interpretations (2 for spin, 2 for particle+antiparticle at  $\mu = 0$ ,  $7/8$  for relating fermions and bosons and  $\pi^2/90$  the factor for one bosonic degree of freedom. For a quark-antiquark gas one would further have 3 for color and  $N_F$  for number of flavours). What is surprising here is that the sum of the two terms (which has to be even in  $y$ ) is so simple while the log-terms separately just define some functions of  $y$ . Further analogous relations are

$$\int_0^\infty dx x \left( \frac{1}{e^{x-y} + 1} + \frac{1}{e^{x+y} + 1} \right) = \frac{\pi^2}{6} + \frac{1}{2} y^2 \tag{3.52}$$

$$\int_0^\infty dx x^2 \left( \frac{1}{e^{x-y} + 1} - \frac{1}{e^{x+y} + 1} \right) = \frac{\pi^2}{3} y + \frac{1}{3} y^3 \tag{3.53}$$

$$\int_0^\infty dx x^3 \left( \frac{1}{e^{x-y} + 1} + \frac{1}{e^{x+y} + 1} \right) = \frac{7\pi^4}{60} + \frac{\pi^2}{2} y^2 + \frac{1}{4} y^4 \tag{3.54}$$

Here the last is basically the same as (3.51), as shown earlier by partial integration. Note the minus sign in the middle equation, what is simple is the **net** fermion number,  $n - \bar{n}$ .

There are many ways of deriving the above integrals. Actually all the terms are polylogarithms  $L_s(z)$ :

$$L_s(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^s} = \frac{1}{\Gamma(s)} \int_0^\infty dx \frac{x^{s-1}}{z^{-1}e^x - 1}, \quad L_s(1) = \zeta(s), \tag{3.55}$$

where  $z$  is a complex number and where the analytic continuation to the complex plane is quite non-trivial. Note, e.g., that the sum defines the function only for  $|z| < 1$ . The general result for an integral with arbitrary integer power of  $x$  is given later in (3.71). An elegant way of evaluating the integrals is Taylor expanding around  $y = 0$ . To calculate the derivatives with respect to  $y$  one should not work out  $dn(x, y)/dy$  explicitly but note that this is equal to  $\pm dn(x, y)dx$  and get rid of  $d/dx$  by partial integration, which simultaneously decreases the power of  $x$ . With proper sign between the terms one ultimately comes to constant derivative so that the expansion terminates.

Somewhat more laborious is to get the result by expanding the FD distributions using  $1/(1-x) = \sum_0^\infty x^n$ . Now  $e^{x+y} \geq 1$  always, but  $e^{x-y} \geq 1$  for  $x \geq y$  so we have to expand differently for  $0 < x < y$  and  $y < x < \infty$ .

For the middle one we have

$$\begin{aligned}
&= \int_0^\infty dx x^2 \left\{ -\Theta(x-y) \sum_1^\infty (-e^{-x+y})^n + \Theta(y-x) \left[ 1 + \sum_1^\infty (-e^{x-y})^n \right] + \sum_1^\infty (-e^{-x-y})^n \right\} \\
&= \int_0^y dx x^2 + \sum_1^\infty (-)^n \left\{ -\int_y^\infty dx x^2 e^{-nx} e^{ny} + \int_0^y dx x^2 e^{nx} e^{-ny} + \int_0^\infty dx x^2 e^{-nx} e^{-ny} \right\} \\
&= \frac{1}{3} y^3 + \sum_1^\infty (-)^n \left\{ \int_0^\infty dx x^2 e^{-nx} (e^{-ny} - e^{ny}) + \int_0^y dx x^2 (e^{-nx} e^{ny} + e^{nx} e^{-ny}) \right\} \\
&= \frac{1}{3} y^3 + \sum_1^\infty (-)^n \left( -\frac{4y}{n^2} \right) = \frac{1}{3} y^3 + \frac{\pi^2}{3} y. \tag{3.56}
\end{aligned}$$

To get from the second to the third line we have added to the integrand of the last term  $0 = e^{-nx} e^{ny} - e^{-nx} e^{ny}$ . To get from the third to the last line, simple integrals were carried out explicitly, lots of terms then cancel.

### 3.5 Mathematical interlude: Properties of the $\zeta$ function

The  $\zeta$  function appears frequently. It is defined by

$$\begin{aligned}
\zeta(s) &= \sum_{n=1}^\infty \frac{1}{n^s} = \frac{1}{\Gamma(s)} \int_0^\infty dx \frac{x^{s-1}}{e^x - 1} \quad \text{Res} > 1 \\
&= \frac{1}{1 - 2^{1-s}} \sum_{n=1}^\infty \frac{(-1)^{n+1}}{n^s} = \frac{1}{(1 - 2^{1-s})\Gamma(s)} \int_0^\infty dx \frac{x^{s-1}}{e^x + 1} \quad \text{Res} > 0 \\
&= 2(2\pi)^{s-1} \sin \frac{\pi s}{2} \Gamma(1-s) \zeta(1-s) = \prod_{p=\text{prime}} \frac{1}{1 - \frac{1}{p^s}}. \tag{3.57}
\end{aligned}$$

The middle line follows from the identity

$$\frac{1}{e^x + 1} = \frac{1}{e^x - 1} - \frac{2}{e^{2x} - 1}. \tag{3.58}$$

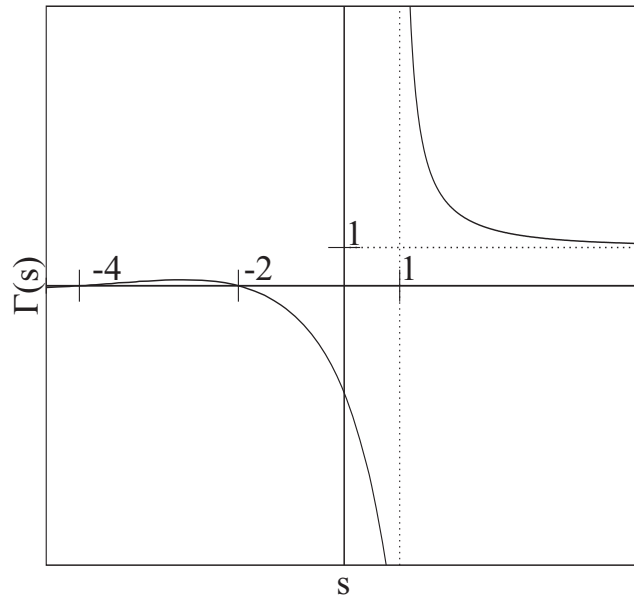
From this analytic continuation we have a beautiful result of the sum of all positive integers:

$$\zeta(-1) = 1 + 2 + 3 + 4 + \dots = \frac{2}{4\pi^2} \sin\left(-\frac{\pi}{2}\right) \Gamma(2) \zeta(2) = -\frac{1}{12}. \tag{3.59}$$

This may look like something completely unphysical, but the contrary is the case. For example, when you hear that bosonic string theories are consistent only in a world of 26 dimensions, this number 26 is the solution of  $1 + 2 + 3 + 4 + \dots = 2/(2-d)$ .

What then is the product  $1 \cdot 2 \cdot 3 \cdot 4 \dots$  of all the integers? Now use

$$\zeta'(s) = \sum_{n=1}^\infty -\frac{\log n}{n^s} \Rightarrow \zeta'(0) = -\sum_1^\infty \log n = -\log \prod_1^\infty n$$

Figure 3.5: Plot of  $\zeta(s)$ .

so that

$$\prod_1^{\infty} n = 1 \cdot 2 \cdot 3 \cdot 4 \cdots = e^{-\zeta'(0)} = \sqrt{2\pi}, \text{ since } \zeta'(0) = -\frac{1}{2} \log 2\pi.$$

A very important generalisation of this is the widely used “zeta function regularisation of functional determinants. Assume  $A$  is an operator with  $Au_n = a_n u_n$ , where  $a_n$  are its eigenvalues and  $u_n$  its eigenfunctions,  $n = 1, 2, \dots$ . For any operator its determinant is an important quantity. In terms of the eigenvalues it is  $\det A = a_1 \cdot a_2 \cdot a_3 \cdots$ , but for infinite dimensional functional operators this product is most likely infinite. How do you regulate it? If one defines:

$$\zeta_A(s) = \sum_{n=1}^{\infty} \frac{1}{a_n^s} \quad (3.60)$$

one has

$$\det A = a_1 \cdot a_2 \cdot a_3 \cdots = e^{-\zeta'_A(0)} \quad (3.61)$$

and these equations define an analytic continuation of the product of eigenvalues from the region of large  $\text{Re } s$ , where the product converges, to a region where one needs the value of the product. Since the eigenvalues of the harmonic oscillator are equally spaced, one notices that  $\zeta(s)$  is essentially just the  $\zeta_A(s)$  for  $A =$  harmonic oscillator!

Some special values of  $\zeta(s)$  are

$$\zeta(-2n, n \geq 1) = 0, \quad \zeta(-3) = \frac{1}{120}, \quad \zeta(-1) = -\frac{1}{12}, \quad \zeta(0) = -\frac{1}{2}, \quad (3.62)$$

$$\zeta(2) = \frac{\pi^2}{6}, \quad \zeta(3) = 1.20206, \quad \zeta(4) = \frac{\pi^4}{90}, \quad (3.63)$$

$$\zeta(1 + \epsilon) = \frac{1}{\epsilon} + \gamma_{\text{Euler}} + \mathcal{O}(\epsilon) \quad \text{the only singularity!} \quad (3.64)$$

Riemann's hypothesis is that all the nontrivial zeroes of  $\zeta(s)$  have  $\text{Re } s = \frac{1}{2}$ . Numerical verification has been extended up to  $10^{12}$  zeroes, all of type  $\frac{1}{2} + it$ . Note that up to some value of  $t$ , there will be  $t \cdot [\log(t/(2\pi e))/(2\pi) + \mathcal{O}(\log t/t)]$  zeroes, for example, the  $10^{20}$ th zero is at  $\frac{1}{2} + i1.52024\dots 10^{19}$ .

A function closely related to the  $\zeta$  function is the polylogarithm

$$L_s(z) = \sum_{n=1}^{\infty} \frac{z^n}{n^s} = \frac{1}{\Gamma(s)} \int_0^{\infty} dx \frac{x^{s-1}}{z^{-1}e^x - 1}, \quad L_s(1) = \zeta(s), \quad (3.65)$$

$$L_0(z) = \frac{z}{1-z}, \quad L_1(z) = \log \frac{1}{1-z}, \quad L_2(z) = - \int_0^z dt \frac{\log(1-t)}{t}, \dots \quad (3.66)$$

If we define the integral

$$I(s) = \int_0^{\infty} dx x^{s-1} \left( \frac{1}{e^{x-y} + 1} + (-)^s \frac{1}{e^{x+y} + 1} \right) \quad (3.67)$$

then from (3.65)

$$I(s) = -\Gamma(s)[L_s(-e^y) + (-)^s L_s(-e^{-y})]. \quad (3.68)$$

The polylog satisfies the functional relation

$$L_s(z) = (-)^{s-1} L_s(1/z) - \frac{(2\pi i)^s}{s!} B_s \left( \frac{\log(-z)}{2\pi i} + \frac{1}{2} \right), \quad (3.69)$$

where  $B_s(x)$  is a Bernoulli polynomial,

$$\begin{aligned} B_1(x) &= \frac{1}{2} + x, \\ B_2(x) &= \frac{1}{6} - x + x^2, \\ B_3(x) &= x \left( \frac{1}{2} - x \right) (1 - x), \\ B_4(x) &= -\frac{1}{30} + x^2 (1 - x)^2, \end{aligned} \quad (3.70)$$

etc. Using this one finds

$$I(s) = \frac{1}{s} (2\pi i)^s B_s \left( \frac{1}{2} + \frac{y}{2\pi i} \right), \quad (3.71)$$

which together with the explicit forms Eq. (3.70) reproduces the integrals Eq. (3.54).

Finally, are you interested in the 10 000 000th (hexadecimal) digit of  $\zeta(3)$  (and who wouldn't)? From D. J. Broadhurst, math.CA/9803067 you find that  $\zeta(3)$  goes like 1.202056903159594.....CDA018F4E....., where the C is the 10Mth hexadecimal digit.

## 3.6 Casimir effect

As discussed in Ch. 2, at finite  $T$  the time direction is imaginary and of finite length,  $0 < \tau < \beta$ , while the spatial directions satisfy  $0 < x < L \rightarrow \infty$ . Let us now make one

spatial direction of finite length,  $0 < z < a$ , while keeping the other two spatial directions and imaginary time infinite,  $0 < x, y, \tau < L \rightarrow \infty$ . From the symmetry of the problem it should be obvious that there is a physical quantity  $\mathcal{E}(a)$  obtainable from  $p(T)$  by  $1/T \leftrightarrow 2a$  (for the factor 2, see below):

$$p(T)/T = -\mathcal{E}(a = \frac{1}{2T}), \quad \mathcal{E}(a) = -\frac{\pi^2 \hbar c}{720 a^3}. \quad (3.72)$$

Take a look at Eq. (3.4): as it stands it would yield  $Z = \exp(-F/T) = \exp(pL^3/T)$ , and replacing  $1/T \rightarrow 2a$  we have  $Z = \exp(L \cdot L^2 \mathcal{E})$ . The quantity  $\mathcal{E}(a)$  is the *Casimir energy*<sup>2</sup>, the energy per area between two infinite plates arising just from the fact that one has cut away a finite region from an infinite space. It is thus a macroscopic manifestation of the quantum mechanical zero point energy for field fluctuations, a "cosmological constant". Changing the shape of the region changes the constant, but as long as there is no other quantity with dimensions of mass (now  $m_e = \infty!$ ),  $\mathcal{E}(a)$  must behave as  $\sim 1/a^3$ . Since  $\mathcal{E}(a) \sim -1/a^3$ , the associated force  $\mathcal{E}'(a)$  (which corresponds to entropy density at finite  $T$ ) is attractive. That is,  $\mathcal{E}(a)$  wants to be smaller and, since

$$\frac{\hbar c}{a^4} \approx 10^{-14} \frac{\text{N}}{\text{m}^2} \left( \frac{\text{mm}}{a^4} \right),$$

the force is small indeed, but nevertheless measurable.

Let us derive the above result doing the mode sum explicitly using dimensional regularisation:

$$\begin{aligned} E &= \sum \frac{1}{2} \hbar \omega = \frac{1}{2} \hbar c \sum \sqrt{k_x^2 + k_y^2 + k_z^2} \\ &= \frac{1}{2} \hbar c \sum_{n=0, \pm 1, \dots} \int \frac{L^2}{(2\pi)^2} d^2 k \sqrt{\mathbf{k}_T^2 + \left(\frac{\pi n}{a}\right)^2}, \\ &= \frac{1}{2} \hbar c \sum_{n=0, \pm 1, \dots} \left(-\frac{L^2}{6\pi}\right) \left(\frac{\pi}{a} |n|\right)^3 \\ &= \frac{1}{2} \hbar c \left(-\frac{\pi^2}{6a^3}\right) L^2 \sum_{n=0, \pm 1, \dots} |n|^3 \\ &= -\frac{\pi^2 \hbar c}{720 a^3} L^2, \end{aligned} \quad (3.73)$$

where the momentum integral was done by setting  $s = 0$  in

$$\int \frac{d^2 k}{(2\pi)^2} (\mathbf{k}_T^2 + m^2)^{1/2-s} = \frac{m^{3-2s}}{4\pi} \frac{1}{s-3/2}$$

and where  $\zeta(-3) = 1/120$  was used. Remarkably, the analytic continuation of a divergent integral (this even fixes the sign!) and the sum of a divergent series, properly done, gives a physical measurable result. Note that above the mode functions are those for a finite box,  $\exp(ik_n z)$ ,  $k_n = \pi/a n$ , (both periodic and antiperiodic) while for finite  $T$  bosons one has to include only the periodic ones,  $\omega_n = 2\pi/\beta n$ , since the space is topologically a circle<sup>3</sup>.

<sup>2</sup>For a review, see V. M. Mostepanenko, arXiv:quant-ph/0702061

<sup>3</sup>Actually, there is much discussion in the literature on the correct choice of modes.