Advanced Statistical Physics: 3. Quantum Statistical Physics

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3.1 The quantum - classical connection

Many quantum mechanical problems in d spatial dimensions evolving in real time can be transformed into classical statistical physics ones in $d+1$ spatial dimensions. The relation can be interpreted in reverse sense as well. This can be seen in lattice models in which the spatial coordinates are discrete and also in the continuum limit in which the statistical field theory is related to a quantum field theory. We now discuss different ways of proving this relation.

We note that the classical partition function generated by a legitimate quantum problem (with a Hermitian Hamiltonian) could be non-physical in the sense of having negative or even complex Boltzmann weights. When this happens the interpretation of the classical problem and its numerical simulation of the classical model, with for example Monte Carlo Methods, become more than tricky.

3.1.1 From classical to quantum

The transfer matrix

For the sake of simplicity, take a classical model defined on a chain with N sites, $i = 1, \ldots, N$, and periodic boundary conditions ($s_{N+1} = s_1$ and $s_0 = s_N$). The partition function takes the familiar form

$$\mathcal{Z} = \sum_{\{s_i\}} e^{-\beta H(\{s_i\})} \qquad \text{with} \qquad H(\{s_i\}) = \sum_{i=1}^{N} U(s_i) + \sum_{i=1}^{N} V(s_i, s_{i+1}) \; . \tag{3.1}$$

Although we use the s_i notation, the variables s_i are completely general. U is a local energy. For example, $U(s_i) = -h_i s_i$ with h_i a local magnetic field, or $U(s_i) = a(s_i^2 - 1)^2$ which is a non trivial function if the s_i's are not Ising variables. V is the contribution of the nearest neighbour interactions on which we focus here. The classical Hamiltonian can be rewritten as

$$H(\{s_i\}) = \sum_{i=1}^{N} W(s_i, s_{i+1}) \; , \tag{3.2}$$

$$W(s_i, s_{i+1}) = \frac{U(s_i) + U(s_{i+1})}{2} + V(s_i, s_{i+1}) \; , \tag{3.3}$$

with the two terms involving two nearest neighbour variables. The partition sum now

becomes

$$\begin{aligned}\mathcal{Z} &= \sum_{\{s_i\}} e^{-\beta \sum_{i=1}^{N} W(s_i,s_{i+1})} = \sum_{\{s_i\}} \prod_{i=1}^{N} e^{-\beta W(s_i,s_{i+1})} \\ &= \sum_{\{s_1=s_{N+1}\}} \sum_{\{s_N\}} e^{-\beta W(s_N,s_1=s_{N+1})} \sum_{\{s_{N-1}\}} e^{-\beta W(s_{N-1},s_N)} \quad \dots \quad \sum_{\{s_2\}} e^{-\beta W(s_1,s_2)} \,. \end{aligned} \tag{3.4}$$

In this way it is clear that each factor

$$\exp[-\beta W(s_i, s_{i+1})] = \exp\left[-\beta\left(\frac{U(s_i)+U(s_{i+1})}{2} + V(s_i, s_{i+1})\right)\right] \tag{3.5}$$

is the weight of the link joining the site i and the subsequent site $i+1$ on the chain. This way of writing the factors is not unique but it has the advantage of being symmetric $W(s_i, s_{i+1}) = W(s_{i+1}, s_i)$.

If the variables s_i took n values, say, $s_i = x^1, x^2, \dots x^n$, the Boltzmann factors $e^{-\beta W(s_{i-1},s_i)}$ can take $n \times n$ values which can be arranged in an $n \times n$ matrix, in which the evaluation of s_{i-1} spans the rows and the one of s_i the columns. Explicitly,

$$\begin{pmatrix} e^{-\beta W(s_{i-1}=x^1,\, s_i=x^1)} & e^{-\beta W(s_{i-1}=x^1,\, s_i=x^2)} & \cdots & e^{-\beta W(s_{i-1}=x^1,\, s_i=x^n)} \\ e^{-\beta W(s_{i-1}=x^2,\ s_i=x^1)} & e^{-\beta W(s_{i-1}=x^2,\, s_i=x^2)} & \cdots & e^{-\beta W(s_{i-1}=x^2,\, s_i=x^n)} \\ \cdots & \cdots & \cdots & \cdots \\ e^{-\beta W(s_{i-1}=x^n,\, s_i=x^1)} & e^{-\beta W(s_{i-1}=x^n,\, s_i=x^2)} & \cdots & e^{-\beta W(s_{i-1}=x^n,\, s_i=x^n)} \end{pmatrix}$$

The partition sum over the intermediate spin s_i, situated between s_{i-1} and s_{i+1}, is the sum over all its possible values:

$$\sum_{s_i=x^1,\dots,x^n} e^{-\beta W(s_{i-1},s_i)} e^{-\beta W(s_i,\, s_{i+1})} \,. \tag{3.6}$$

In the matricial notation just introduced, it corresponds to the the s_{i-1}, s_{i+1} element of the product of two such matrices. For example, if $s_{i-1} = x^2$ and $s_{i+1} = x^1$, this is:

$$\begin{pmatrix} & \cdots & \\ e^{-\beta W(x^2,\ x^1)} & \cdots & e^{-\beta W(x^2,x^n)} \\ \cdots & \cdots & \cdots \\ & \cdots & \end{pmatrix} \begin{pmatrix} e^{-\beta W(x^1,\, x^1)} & \cdots & \\ e^{-\beta W(x^2,\ x^1)} & \cdots & \\ \cdots & \cdots & \cdots \\ e^{-\beta W(x^n,\, x^1)} & \cdots & \end{pmatrix} = \begin{pmatrix} & \cdots & \\ A_{21} & \cdots & \\ \cdots & \cdots & \cdots \\ & \cdots & \end{pmatrix}$$

with $A_{21} = e^{-\beta W(x^2,x^1)} e^{-\beta W(x^1,x^1)} + e^{-\beta W(x^2,x^2)} e^{-\beta W(x^2,x^1)} + \dots + e^{-\beta W(x^2,x^n)} e^{-\beta W(x^n,x^1)}$. This product gives the 21 element of the resulting matrix. Since one also has to sum over all the configurations of the other spins, s_{i-1} and s_{i+1}, it is not hard to see that an N matricial product is generated.

In conclusion, $\mathcal{Z}$ can then be arranged as the trace of the product of the

$$n \times n \text{ symmetric } \textit{transfer matrix } \mathbb{T} \tag{3.7}$$

with elements

$$T_{ab} = T_{ba} \qquad a, b = 1, \ldots, n \ , \tag{3.8}$$

introduced by Kramers & Wannier [1] (formally, n can also be continuous). In "normal" statistical physics models, the elements $T_{ab} \in \mathbb{R}^+$. The partition function is then a trace over a matrix product, with one matrix for each site on the chain:

$$\mathcal{Z} = \mathrm{Tr}\, \mathbb{T}_N \mathbb{T}_{N-1} \ldots \mathbb{T}_1 \ . \tag{3.9}$$

We note that the parameters in the link energy and local energy, which could be the exchange and magnetic field in a classical spin chain, for example, could depend on the site indices (disorder). We will not consider these heterogeneous cases here and then $\mathbb{T}_1 = \cdots = \mathbb{T}_N$. The partition function for homogeneous models is simply

$$\mathcal{Z} = \mathrm{Tr}\, \mathbb{T}^N \ . \tag{3.10}$$

The trace of a matrix is equal to the sum of its diagonal elements, $\mathrm{Tr}\, \mathbb{M} = \sum_a M_{aa}$. If the matrix is diagonalizable, and this is the case of $\mathbb{T}$ (it is real symmetric), it is also equal to the sum of its eigenvalues. The eigenvalues of the matrix $\mathbb{T}^N$ are the eigenvalues of $\mathbb{T}$ to the power N. Then,

$$\mathcal{Z} = \sum_{a=1}^{n} \lambda_a^N \ , \tag{3.11}$$

with λ_a the n eigenvalues of $\mathbb{T}$. Assuming the ordering $|\lambda_1| > |\lambda_2| \geq \cdots \geq |\lambda_n|$ (and thanks to the Perron-Frobenius theorem, which states that "a square matrix with positive non-zero real entries will have a non-degenerate largest positive eigenvalue and a corresponding eigenvector with strictly positive components", the non-degeneracy of the largest eigenvalue is justified), after taking ln and dividing by N,

$$\begin{aligned} \frac{1}{N} \ln \mathcal{Z} &= \ln \lambda_1 + \frac{1}{N} \ln \left[1 + \left(\frac{\lambda_2}{\lambda_1} \right)^N + \ldots \right] \\ &\sim \ln \lambda_1 \end{aligned} \tag{3.12}$$

since $\lambda_2 < \lambda_1$, etc. The corrections are expected to be negligible in the $N \to \infty$ limit. Thus, finding the free energy density, $-\beta f = N^{-1} \ln \mathcal{Z}$, reduces to determining the largest eigenvalue of the transfer matrix.

The transfer operator

One then associates the elements of the transfer matrix with the outcome of the *quantum computation*

$$\langle s_{i+1}|\hat{T}|s_i\rangle \tag{3.13}$$

where $\hat{T}$ is the *transfer operator*, and the $|s\rangle$ are a complete set of states (bra and ket Dirac notation), at sites i and $i+1$, and rewrites $\mathcal{Z}$ as

$$\mathcal{Z} = \mathrm{Tr}_{s_1}\mathrm{Tr}_{s_N}\langle s_1|\hat{T}|s_N\rangle\mathrm{Tr}_{s_{N-1}}\langle s_N|\hat{T}|s_{N-1}\rangle\ldots\mathrm{Tr}_{s_2}\langle s_3|\hat{T}|s_2\rangle\langle s_2|\hat{T}|s_1\rangle \tag{3.14}$$

where the symbols Tr represent here the sum over all possible states. At each stage one sums over all states at a new site. This form can be interpreted as a successive matrix multiplication, with the numbers $\langle s_{i+1}|\hat{T}|s_i\rangle$ being the elements of the transfer matrix $\mathbb{T}$, and a final trace operation, just as what we claimed above, in the classical formulation. Using now $\mathrm{Tr}_{s_k}|s_k\rangle\langle s_k| = 1$ for all $k = 1,\ldots,N$, and for cases in which the parameters in U and V are homogeneous and do not depend on the site indices themselves, this expression simplifies considerably and

$$\mathcal{Z} = \mathrm{Tr}_{s_1}\langle s_1|\hat{T}^N|s_1\rangle = \mathrm{Tr}\,\hat{T}^N \tag{3.15}$$

which is equivalent to (3.10).

In cases in which the transfer operator $\hat{T}$ has $a = 1,\ldots,n$ positive eigenvalues, one proposes

$$\hat{T} = e^{-\epsilon\hat{\mathcal{H}}} \qquad \text{and} \qquad \mathcal{Z} = \mathrm{Tr}\,e^{-N\epsilon\hat{\mathcal{H}}} = \sum_a e^{-N\epsilon e_a} \tag{3.16}$$

with a quantum (Hermitian) Hamiltonian $\hat{\mathcal{H}}$, e_a its energy levels, and ϵ a parameter that is there to make the object in the exponential adimensional (like an inverse temperature). Thus,

> the partition function of a classical chain model ($d = 1$) with Hamiltonian H is identical to the one of a quantum "particle" (no space, $d = 0$) with Hamiltonian $\hat{\mathcal{H}}$.

The length of the chain N times the parameter ϵ should then be the inverse temperature β_q of the quantum particle (which is not the same as the inverse temperature of the original classical model):

$$\beta_q = N\epsilon\,. \tag{3.17}$$

We will examine this relation in some concrete examples below. The parameters of the classical model (its inverse temperature β and coupling constants) are related to the parameters in the quantum models in ways that have to be determined on a case by case basis.

Exercise 3.1 Show that the statistical average of an observable of the classical system in its thermodynamic limit can be obtained as the expectation value of the operator which represents the observable in question in the ground state of the quantum system.

In the limit $N \to \infty$, the sum over a is dominated by the contribution of the *ground state* of $\hat{\mathcal{H}}$

$$\lim_{N\to\infty} \mathcal{Z} = e^{-N\epsilon e_0} \tag{3.18}$$

(exploiting again the non-degeneracy of energy levels). The first correction leads to $\ln[e^{-N\epsilon e_0} + e^{-N\epsilon e_1} + \dots] \sim \ln\{e^{-N\epsilon e_0}[1 + e^{-N\epsilon(e_1-e_0)}]\}$, and for large N

$$\frac{1}{N}\ln \mathcal{Z} \sim -\epsilon e_0 + \frac{1}{N}\ln[1 + e^{-N\epsilon(e_1-e_0)}] \sim -\epsilon e_0 + \frac{1}{N}e^{-N\epsilon(e_1-e_0)} \ . \tag{3.19}$$

Exercise 3.2 For details on how to calculate space correlation functions and the correlation length with the transfer matrix, see [3, 4] and TD6.

Imaginary time

The transfer matrix lets the calculation of the partition function of the classical problem advance progressively on the chain from site to site. Once written as the exponential of a quantum Hamiltonian, the latter plays the role of a *time translation operator*. However, time-translations in real time are generated by $\exp(-\mathrm{i}\hat{\mathcal{H}}t/\hbar)$ (with an i) while here we have $\exp(-N\epsilon\hat{\mathcal{H}})$ with no i and a minus sign. It is as if,

$$\exp(-\mathrm{i}\hat{\mathcal{H}}t/\hbar) \ \mapsto \ \exp(-N\epsilon\hat{\mathcal{H}}) \tag{3.20}$$

$$t \ \mapsto \ -\mathrm{i}N\epsilon\hbar = -\mathrm{i}\beta_q\hbar \equiv \tau \ , \tag{3.21}$$

and the transfer operator corresponds to a quantum evolution in *imaginary time* over a time span $\beta_q\hbar$ with periodic boundary conditions, because of the trace present in the calculation of the partition sum.

Another way of making the same statement is the following. If we imagine that the spatial axis of the lattice on which the classical model is defined is a discrete time axis of quantum mechanics, then $\hat{T}$ carries information from one time step t to the next one $t+\delta t$. The transfer operator is then identified as the *time evolution operator* for a quantum system of a single "particle", evolving in *imaginary time*. The reason for "imaginary" is that there is no i in the exponential in (3.16) and the infinitesimal time step would be $\delta t = -\mathrm{i}\epsilon\hbar$. The periodicity in the spatial dimension is translated in a periodicity in the imaginary time one. This interpretation will be further developed when we describe the evolution operator.

We discuss below the one dimensional Ising chain as a particularly simple example exhibiting this connection. The generalisation to higher dimensional cases, in which the transfer matrix acts along one out of the $d+1$ coordinates of the classical model is straightforward. For example, the anisotropic classical bidimensional classical Ising model maps on a quantum Ising chain.

In general we have an equivalence between a d dimensional quantum problem and a $d+1$ dimensional classical one, both in canonical equilibrium at inverse temperatures $\beta_q = N\epsilon$ and β, respectively.

The one dimensional Ising chain

Take a classical Ising chain with ferromagnetic coupling, under an external field, and in contact with a thermal bath at inverse temperature β. The matrix elements should be evaluated from

$$e^{-\beta W(s_i,s_{i+1})} = e^{\beta J s_i s_{i+1} + \beta \frac{h}{2}(s_i+s_{i+1})} = \langle s_{i+1}|\hat{T}|s_i\rangle \ . \tag{3.22}$$

The spins s_i and s_{i+1} take two possible values each, $s_i = +1$ and $s_i = -1$, and the transfer matrix is therefore 2×2:

$$\mathbb{T} = \begin{pmatrix} ++ & +- \\ -+ & -- \end{pmatrix} = \begin{pmatrix} e^{K+H} & e^{-K} \\ e^{-K} & e^{K-H} \end{pmatrix} \tag{3.23}$$

with the notation $K = \beta J$ and $H = \beta h$, $a, b = 1, 2$ and $n = 2$. (This adimensional magnetic field should not be confused with the classical Hamiltonian also denoted H, of course.) We have to keep in mind that the temperature influence in the classical problem is encoded in these two parameters.

Exercise 3.3 Find the eigenvalues of the matrix $\mathbb{T}$ in Eq. (3.23). Use them to write the parameter dependence of the partition function and the free-energy density in the infinite size limit, and to show that the latter is analytic for all values of K and H. Derive the magnetisation density as a function of the parameters and find that it vanishes for $H \to 0$ and saturates for $H \to \infty$.
Solution: The characteristic polynomial is $(e^{K+H} - \lambda)(e^{K-H} - \lambda) - e^{-2K} = 0$ with roots $2\lambda_{1,2} = (e^{K+H} + e^{K-H}) \pm [(e^{K+H} + e^{K-H})^2 + 4(e^{2K} - e^{-2K})]^{1/2} = 2e^K \cosh H \pm 2e^K [\sinh^2 H + e^{-4K}]^{1/2}$. The partition function is $\mathcal{Z} = \lambda_1^N$ and the free-energy density $-\beta f = \ln \lambda_1$. One notes that for $K > 0$ the square root acts on a positive definite quantity and f is analytic with respect to the parameters: there is no phase transition. For $K \to \infty$ the exponential term vanishes and $f = -J - k_B T \ln(\cosh H \pm |\sinh H|)]$. With $m = N^{-1} \partial \ln \mathcal{Z}/\partial H = -\partial f/\partial h$ we get $m = e^K \sinh H / [e^{2K} \sinh^2 H + e^{-2K}]^{1/2}$ which vanishes for $H \to 0$ and tends to one for $H \to \infty$. Moreover, at $T \to 0$ one sees that $m = 1$ for $H > 0$ and $m = -1$ for $H < 0$.

In TD6 we will show that the correlation length can be expressed in terms of λ_1 and λ_2 as

$$\xi = \left[\ln \left(\frac{\lambda_1}{\lambda_2} \right) \right]^{-1} \ . \tag{3.24}$$

(A very detailed analysis of this problem can be found in [2, 4, 5].)

With a little bit of thinking, the elements of $\mathbb{T}$ in Eq. (3.23) can be recovered from a linear combination of the Pauli matrices, $\sigma_{x,y,z}$, see App. 3.A for their definition and

properties,

$$\mathbb{T} = e^K \cosh H \, \mathbb{I} + e^{-K}\sigma_x + e^K \sinh H \, \sigma_z \, , \tag{3.25}$$

where we exploited the fact that any Hermitian matrix can be written in the form $a_0\mathbb{I} + a_x\sigma_x + a_y\sigma_y + a_z\sigma_z$.

Similarly, considering $\hat{T}$ as an operator acting in a two-dimensional *Hilbert space* with the basis $|\pm\rangle$ (bra and ket Dirac notation) and the association

$$|+\rangle \mapsto \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |-\rangle \mapsto \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{3.26}$$

we can write

$$\hat{T} = e^K \cosh H \, \mathbb{I} + e^{-K} \, \hat{\sigma}_x + e^K \sinh H \, \hat{\sigma}_z \, . \tag{3.27}$$

The terms proportional to σ_z in (3.25) or $\hat{\sigma}_z$ in (3.27) are present only if $H \neq 0$.

Exercise 3.4 Prove eq. (3.25).

The idea now is to compare the classical partition function of the Ising chain to the one of a single quantum spin 1/2 at inverse temperature β_q. The latter is

$$\mathcal{Z}_q = \mathrm{Tr}\, e^{-\beta_q \hat{\mathcal{H}}} = \sum_s \langle s | e^{-\beta_q \hat{\mathcal{H}}} | s \rangle \, . \tag{3.28}$$

The exponential is also the product of N identical factors $e^{-\beta_q \hat{\mathcal{H}}} = e^{-\epsilon \hat{\mathcal{H}}} e^{-\epsilon \hat{\mathcal{H}}} \dots e^{-\epsilon \hat{\mathcal{H}}}$ with

$$\epsilon N = \beta_q \, . \tag{3.29}$$

Then

$$\begin{aligned} \mathcal{Z}_q &= \sum_s \langle s | e^{-\beta_q \hat{\mathcal{H}}} | s \rangle \\ &= \sum_{\{s_j\}} \langle s_1 | e^{-\epsilon \hat{\mathcal{H}}} | s_N \rangle \langle s_N | e^{-\epsilon \hat{\mathcal{H}}} | s_{N-1} \rangle \dots \langle s_2 | e^{-\epsilon \hat{\mathcal{H}}} | s_1 \rangle \, , \end{aligned} \tag{3.30}$$

where we introduced $N-1$ identities, and we renamed $|s\rangle$, $|s_1\rangle$. This partition function has the same form as the classical partition function of the Ising chain. One identifies $\hat{T}$ and $e^{-\epsilon \hat{\mathcal{H}}}$ with ϵ a parameter with dimension of inverse temperature and takes $\hat{\mathcal{H}}$ to be a local Hermitian operator, like a Hamiltonian operator. For the latter one proposes

$$-\epsilon \hat{\mathcal{H}} = \epsilon b_0 \, \mathbb{I} + \epsilon b_1 \hat{\sigma}_x + \epsilon b_3 \hat{\sigma}_z \tag{3.31}$$

($\hat{\sigma}_y$ does not enter since there are no complex numbers in the classical problem and we can simply set $b_2 = 0$), expands the exponential in Taylor series, and collects all terms of the same kind, to find

$$\hat{T} = e^{-\epsilon \hat{\mathcal{H}}} = e^{\epsilon b_0} \cosh(\epsilon b) \, \mathbb{I} + e^{\epsilon b_0} \sinh(\epsilon b) \frac{b_1}{b} \hat{\sigma}_x + e^{\epsilon b_0} \sinh(\epsilon b) \frac{b_3}{b} \hat{\sigma}_z \, , \tag{3.32}$$

where $b = (b_1^2 + b_3^2)^{1/2}$. Identifying coefficient by coefficient

$$e^{\epsilon b_0} \cosh(\epsilon b) = e^K \cosh H \ , \tag{3.33}$$

$$e^{\epsilon b_0} \sinh(\epsilon b) \frac{b_1}{b} = e^{-K} \ , \tag{3.34}$$

$$e^{\epsilon b_0} \sinh(\epsilon b) \frac{b_3}{b} = e^K \sinh H \ . \tag{3.35}$$

Exercise 3.5 Prove eqs. (3.33)-(3.35) and their $H = 0$ limit. Trick: use the identity $(b_1\hat{\sigma}_x + b_3\hat{\sigma}_z)^2 = b^2\mathbb{I}$ where $b = (b_1^2 + b_3^2)^{1/2}$ to show that the even terms in the Taylor expansion of the exponential are proportional to $\mathbb{I}$ and the odd ones to $b_1\hat{\sigma}_x + b_3\hat{\sigma}_z$ itself.

Rearranging a bit

$$\epsilon b_0 = \frac{1}{2} \ln[2 \sinh(2K)] \ , \tag{3.36}$$

$$\epsilon b_1 = -\frac{1}{2} \frac{1}{\sqrt{1 + e^{4K} \sinh^2 H}} \ln \left[\frac{1 - e^{-2K} \cosh H \sqrt{1 + e^{4K} \sinh^2 H}}{1 + e^{-2K} \cosh H \sqrt{1 + e^{4K} \sinh^2 H}} \right] \ , \tag{3.37}$$

$$\epsilon b_3 = e^{2K} \sinh H \ \epsilon b_1 \ . \tag{3.38}$$

(The relation between b_1 and b_3 comes from dividing Eq. (3.35) by Eq. (3.34). b_0 is found taking b/b_1 to the right-hand-side of (3.34), squaring Eq. (3.33) and the new resulting Eq. (3.34) and subtracting them; in b/b_1 one uses the relation between b_1 and b_3 to get rid of the two.)

We focus now on the $H = 0$ case to keep the expressions more manageable. They simplify and yield

$$\epsilon b_0 = \frac{1}{2} \ln[2 \sinh(2K)] \ , \tag{3.39}$$

$$\epsilon b_1 = -\frac{1}{2} \ln[\tanh K] \ , \tag{3.40}$$

$$b_3 = 0 \ , \tag{3.41}$$

$b = |b_1|$, and replacing in Eq. (3.31) one simply has

$$-\epsilon \hat{\mathcal{H}} = \frac{1}{2} \ln[2 \sinh(2K)] \, \mathbb{I} - \frac{1}{2} \ln[\tanh K] \, \hat{\sigma}_x \ . \tag{3.42}$$

The first term is proportional to the identity and it only contributes to the normalisation of the operator $e^{-\epsilon \hat{\mathcal{H}}}$. The interesting term is the second one and tells us that the classical Ising chain with length N is represented by a single quantum spin 1/2 model, in equilibrium at inverse temperature $\beta_q = \epsilon N$, with Hamiltonian

$$\begin{aligned} -\epsilon \hat{\mathcal{H}} &= -\frac{\delta}{2} \hat{\sigma}_x \quad \text{with} \quad \delta = \ln[\tanh K] \quad \text{and} \\ -\beta_q \hat{\mathcal{H}} &= -\frac{\Delta}{2} \hat{\sigma}_x \quad \text{with} \quad \beta_q = \epsilon N \ \text{ and } \ \Delta = N\delta = N \ln[\tanh K] \ . \end{aligned} \tag{3.43}$$

Note that the inverse temperature of the classical system is in $K = \beta J$, it then fixes Δ, together with N. Moreover, it is important to notice that $\beta_q \neq \beta$. Had we kept $H \neq 0$, we would have obtained a quantum Hamiltonian $-\epsilon\hat{\mathcal{H}} = -\delta/2\ \hat{\sigma}_x - H_q/2\ \hat{\sigma}_z$, that is, with two fields, both with dependencies on K and H.

If we fix the parameters in the classical model, K, Δ and H if present, we still have some freedom to choose the ϵ and b_1, b_3 that correspond to them. Indeed, in the limit $\epsilon \to 0$ Eqs. (3.33)-(3.35) impose

$$\epsilon b_1 \sim e^{-K} \qquad \text{and} \qquad \epsilon b_3 \sim e^{K} \sinh H \ . \tag{3.44}$$

Say that we fix b_1. The first equation yields $\epsilon = e^{-K}/b_1$ which, once inserted in the second one, yields $b_3 = e^{2K} \sinh H\, b_1$. In short, K and H determine ϵ, the step between imaginary time-slices, and the parameter b_3 in units set by b_1.

The classical system size in the additional direction is proportional to the quantum inverse temperature β_q. This means that if we are interested in studying a quantum problem at finite temperature, we have to work with a classical system with finite size in this direction. Instead, to reach the zero temperature limit of the quantum model, which is particularly important in the analysis of quantum phase transitions, not surprisingly, we have to take the thermodynamic limit of the classical model in this direction as well.

One can also show, see TD 6, that the quantum energy gap, $e_1 - e_0$, and the classical correlation length, ξ, are inversely related.

A full field of research

The relation between quantum spin chains and two dimensional classical models based on the transfer matrix solution of the latter has opened a full field of research in theoretical physics [5]. Indeed, the transfer matrix of many equilibrium classical statistical mechanics problems can be chosen to be Hermitian. This follows partially because the Boltzmann weights are positive real numbers and more generally because of reflection positivity.

In TD6 we will study the mapping between the classical two dimensional Ising model and the quantum transverse field Ising chain, which is the simplest quantum model exhibiting a zero temperature quantum phase transition. The need for a zero temperature limit (of the quantum problem) to have a phase transition should not be surprising at this stage, since the temperature of the quantum model maps on the length of the classical system in the singled out spatial direction.

For quantum spin chains and two dimensional classical spin models it is relatively easy to find the relation between the two formulations. In generic cases, the Boltzmann weight of the quantum model is a product of exponentials of non-commuting operators, and the explicit connection may be hard or impossible to work out. Still, the asymptotic behaviour in the $N \to \infty$ limit is dominated by the largest eigenvalue of $\hat{T}$ or the ground state of $\hat{\mathcal{H}}$.

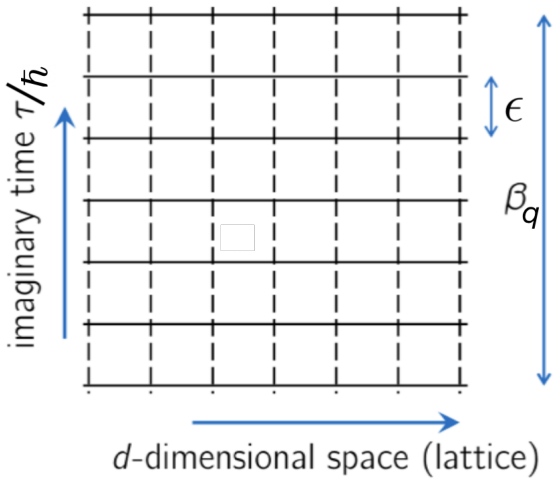

Figure 3.1: The $d+1$ dimensional lattice with, in the vertical direction, the imaginary time running from 0 to $\beta_q\hbar = \epsilon\hbar N_\tau$. The original classical spins sit on the vertices of the horizontal lattice. Note that the number of lattice sites in the spatial and imaginary time directions need not be the same, that is the reason why one calls N_τ the number in the imaginary time direction. ϵ is the lattice spacing in the imaginary time direction which can also be different from the one in the spatial ones.

3.1.2 From quantum to classical

One can follow an inverse path. Say that one is interested in understanding a quantum model in d dimensions and, to do it, one maps it to a classical one in $d+1$ dimensions, exploiting the Trotter relation. This is the route followed by Suzuki [6] in a series of very influential papers. It is what is done to set up the so-called *quantum Monte Carlo* (QMC) methods to study the equilibrium properties of a quantum model (with positive matrix elements of $e^{-\epsilon\hat{\mathcal{H}}}$, otherwise *sign problems* inhibit the good functioning of the QMC).

Let us present the connection in generic form. The quantum spins are noted $\vec{s}$. The vector refers to the three components s^x, s^y, s^z and, on top of this, they can encode a site index which determines the identity of the spin, as given for example by its position in a d dimensional lattice. The Hamiltonian is $\hat{\mathcal{H}}$ and the inverse temperature β_q. The quantum partition function reads

$$\mathcal{Z}_q = \mathrm{Tr} e^{-\beta_q\hat{\mathcal{H}}} = \sum_{\vec{s}_1} \langle \vec{s}_1 | e^{-\beta_q\hat{\mathcal{H}}} | \vec{s}_1 \rangle \tag{3.45}$$

with $|\vec{s}_1\rangle$ an orthonormal basis of the Hilbert space. Split the Boltzmann operator in N_τ identical factors, with $\beta_q = N_\tau\epsilon$. Eventually, one could take $\epsilon \to 0$, $N_\tau \to \infty$ with $N_\tau\epsilon$

Quantum	**Classical**
imaginary time τ	extra space dimension τ
inverse temperature β_q	system size in new direction $L_\tau = \epsilon N_\tau$
imaginary time-evolution $e^{-\tau\hat{\mathcal{H}}}$	Boltzmann weight $e^{-\beta\mathcal{E}(\vec{s}_\ell,\vec{s}_{\ell+1})}$
$\tau = -\mathrm{i}\beta_q\hbar$	
path integral	sum over configurations

fixed. Insert identities $1 = \sum_{\vec{s}} |\vec{s}\rangle\langle\vec{s}|$ in between each of these factors

$$\mathcal{Z}_q = \sum_{\vec{s}_1}\sum_{\vec{s}_{N_\tau}}\cdots\sum_{\vec{s}_2} \langle\vec{s}_1|e^{-\epsilon\hat{\mathcal{H}}}|\vec{s}_{N_\tau}\rangle \quad \ldots \quad \langle\vec{s}_2|e^{-\epsilon\hat{\mathcal{H}}}|\vec{s}_1\rangle \ . \tag{3.46}$$

Each of the operators $e^{-\epsilon\hat{\mathcal{H}}}$ can be interpreted as the evolution operator $e^{-\mathrm{i}\hat{\mathcal{H}}t/\hbar}$ on an infinitesimal time step $\delta t = -\mathrm{i}\delta\tau$ with $\delta\tau = \epsilon\hbar$. The sum over all states $\vec{s}_\ell$, for each $\ell = 1, \ldots, N_\tau$, can be interpreted as a *path integral*. Define now

$$\beta\mathcal{E}(\vec{s},\vec{s}\,') = -\ln\langle\vec{s}|e^{-\epsilon\hat{\mathcal{H}}}|\vec{s}\,'\rangle \tag{3.47}$$

(which is adimensional by definition, and we introduced a β to make the connection with the classical equilibrium writing clearer) and rewrite the partition sum as

$$\mathcal{Z}_q = \sum_{\{\vec{s}_\ell\}} e^{-\beta\sum_{\ell=1}^{N_\tau}\mathcal{E}(\vec{s}_\ell,\vec{s}_{\ell+1})} \ . \tag{3.48}$$

and $\vec{s}_{N_\tau+1} = \vec{s}_1$. If $\mathcal{E}(\vec{s}_\ell, \vec{s}_{\ell+1})$ is real, the last expression can be interpreted as the classical partition sum of a system in $d+1$ dimensions. The local energy contributions, $\mathcal{E}(\vec{s}_\ell, \vec{s}_{\ell+1})$, will have "intra"-layer (on real space) and "inter"-layer (on the imaginary time direction) contributions (one goes from one layer to the next by following the τ direction). They are the elements of the transfer matrix in the selected τ direction.

At zero temperature, $\beta_q \to \infty$, the quantum system maps to a classical system with a diverging size in the τ direction. If the transverse size also diverges the quantum system can undergo a *zero temperature phase transition* at special values of the remaining parameters, which correspond to the critical point of the classical counter-part. We will address this problem in the next chapter.

As our recurrent example, take a quantum spin model defined on a d dimensional cubic lattice. The coordinates are labelled with $k = 1, \ldots, d$ and the sites on each direction with $i_k = 1, \ldots, L/a$, with L the linear length and a the lattice spacing. There are $N = (L/a)^d$ sites in the system. We consider two-body couplings J, a *longitudinal field* (coupled to the spin component which also appears in the two-body interacting term) and a *transverse field* (coupled to another component, $\hat{\sigma}^x$ in this case). These parameters, multiplied by

the inverse temperature of the quantum system β_q are $\{K_q, H_q, \Delta\}$. For example, the quantum Ising model in a longitudinal (H_q) and a transverse (Δ) field is

$$-\beta_q \hat{\mathcal{H}} = \sum_{k=1}^{d} \sum_{\langle i_k, j_k \rangle}^{L/a} K_q \, \hat{\sigma}_{i_k}^z \hat{\sigma}_{j_k}^z + H_q \sum_{k=1}^{d} \sum_{i_k=1}^{L/a} \hat{\sigma}_{i_k}^z + \Delta \sum_{k=1}^{d} \sum_{i_k=1}^{L/a} \hat{\sigma}_{i_k}^x \; . \tag{3.49}$$

The notation is a bit unusual. The $\langle i_k, j_k \rangle$ denote nearest neighbour on the kth plane. The upper limit L/a indicates that one of these indices runs over all sites in a row, say, and the other one over the first neighbours on the transverse direction. Its quantum partition function $\mathcal{Z}_q = \mathrm{Tr}\, e^{-\beta_q \hat{\mathcal{H}}}$, at an inverse temperature β_q, is related to the one of a classical Ising spin model defined on a $d+1$ anisotropic space with the parameters grouped in the set $\{K_q/N_\tau, H_q/N_\tau, 1/2 \, \ln \coth(\Delta/N_\tau)\}$, where K_q/N_τ are the exchanges in the "original" d dimensions, H_q/N_τ is an applied field acting on all classical spins, and $1/2 \, \ln \coth(\Delta/N_\tau)$ is the exchange in the singled out direction. The relation is

$$\mathcal{Z}_q = \lim_{N_\tau \to \infty} \left(\frac{1}{2} \sinh \frac{2\Delta}{N_\tau} \right)^{N N_\tau / 2} \mathcal{Z} \; . \tag{3.50}$$

In the classical model the Ising spins $s_{i_k,\ell}$ are labeled by two indices i_k, ℓ, with the first one being the same as for the quantum model and referring to the original d dimensional space, and the second one running along the additional direction, from 1 to N_τ. The classical partition function is

$$\mathcal{Z} = \sum_{\{s_{i_k,\ell}\}=\pm 1} e^{-\beta H} \tag{3.51}$$

$$\begin{aligned} -\beta H = & \sum_{\ell=1}^{N_\tau} \sum_{k=1}^{d} \sum_{\langle i_k, j_k \rangle}^{L/a} \frac{K_q}{N_\tau} s_{i_k,\ell} s_{j_k,\ell} + \frac{1}{2} \, \ln \coth \left(\frac{\Delta}{N_\tau} \right) \sum_{\ell=1}^{N_\tau} \sum_{k=1}^{d} \sum_{i_k=1}^{L/a} s_{i_k,\ell} s_{i_k,\ell+1} \\ & + \frac{H_q}{N_\tau} \sum_{\ell=1}^{N_\tau} \sum_{k=1}^{d} \sum_{i_k=1}^{L/a} s_{i_k,\ell} \end{aligned} \tag{3.52}$$

The proof of the equation above goes as follows. To avoid carrying many indices, let us focus once again on the single quantum spin ($d = 0$) which is related to the classical Ising chain (0+1 dimensional). We start from the quantum partition function

$$\mathcal{Z}_q = \mathrm{Tr}\, e^{-\beta_q \hat{\mathcal{H}}} = \sum_{s=\pm 1} \langle s | e^{-\beta_q \hat{\mathcal{H}}} | s \rangle \qquad \text{with} \qquad \hat{\mathcal{H}} = -\delta \hat{\sigma}_x - h_q \hat{\sigma}_z \tag{3.53}$$

where the sum runs over all eigenvalues of $\hat{\sigma}_z$, $\hat{\sigma}_z|s\rangle = \sigma_z|s\rangle$, $\sigma_z = \pm 1$. We rewrite[1]

$$\mathcal{Z}_q = \sum_{s=\pm 1} \langle s|(e^{-\epsilon\hat{\mathcal{H}}})^{N_\tau}|s\rangle = \sum_{s_1=\pm 1} \sum_{s_{N_\tau}=\pm 1} \cdots \sum_{s_2=\pm 1} \langle s_{N_\tau+1}|e^{-\epsilon\hat{\mathcal{H}}}|s_{N_\tau}\rangle \ldots \langle s_2|e^{-\epsilon\hat{\mathcal{H}}}|s_1\rangle \quad (3.55)$$

keeping in mind that $\langle s_{N_\tau+1}| = \langle s_1|$ because of the periodic boundary conditions. We can now calculate, in the $\epsilon = \beta_q/N_\tau \to 0$ limit, the matrix elements:

$$\begin{aligned}
\langle s_{j+1}|e^{-\epsilon\hat{\mathcal{H}}}|s_j\rangle &= \langle s_{j+1}|e^{\epsilon\delta\hat{\sigma}_x+\epsilon h_q\hat{\sigma}_z}|s_j\rangle \\
&= \langle s_{j+1}|e^{\epsilon\delta\hat{\sigma}_x}e^{\epsilon h_q\hat{\sigma}_z} + \mathcal{O}(\epsilon^2)|s_j\rangle \\
&\sim e^{\epsilon h_q s_j}\langle s_{j+1}|e^{\epsilon\delta\hat{\sigma}_x}|s_j\rangle \\
&= e^{\epsilon h_q s_j}\langle s_{j+1}|\left[\cosh(\epsilon\delta) + \sinh(\epsilon\delta)\hat{\sigma}_x\right]|s_j\rangle \\
&= e^{\epsilon h_q s_j}\left[\cosh(\epsilon\delta)\delta_{s_j,s_{j+1}} + \sinh(\epsilon\delta)\delta_{-s_j,s_{j+1}}\right] . \qquad (3.56)
\end{aligned}$$

At this point we can compare these elements to the Boltzmann weights of the classical Ising chain under a field

$$s_j = s_{j+1} = \pm 1 \qquad \Longrightarrow \qquad A\, e^{K\pm H} \qquad (3.57)$$

$$s_j = -s_{j+1} = \pm 1 \qquad \Longrightarrow \qquad A\, e^{-K\pm H} \qquad (3.58)$$

The first line implies $H \equiv \beta h = \epsilon h_q = \beta_q h_q/N_\tau$. The ratio between the second and first lines then yields $K \equiv \beta J = -(1/2)\ln\tanh(\epsilon\delta)$. h is the classical magnetic field and J the magnetic exchange. β is, here, the inverse temperature of the classical model and appears in $K = \beta J$ and $H = \beta h$. We note that, if h_q and δ are finite

$H \propto \epsilon$ is infinitesimal and K diverges as $-\ln\epsilon$.

The length of the new spatial dimension is $N_\tau\epsilon = \beta_q$. It has N_τ steps, with lattice spacing ϵ in such a way that their product is the inverse temperature of the quantum system.

From the point of view of the classical Ising model, it is for these infinitesimal parameters that the mapping to the quantum model applies. In these cases, we map it to the eigenvalue problem of the quantum $\hat{\mathcal{H}}$ above, which is a lot easier than the eigenvalue problem of the full transfer matrix.

[1] Recall *Trotter's formula*

$$\exp(A+B) = \lim_{N\to\infty}[\exp(A/N)\ \exp(B/N)]^N \qquad (3.54)$$

for the product of the exponential of two operators or matrices A and B which do not necessarily commute.

Strictly speaking, the identity holds for $N_\tau \to \infty$, $\epsilon \to 0$ and $\beta_q = N_\tau \epsilon$ fixed (we used Trotter's) which could diverge to capture zero temperature quantum behaviour.

Quantum Monte Carlo

The usual way of implementing the quantum Monte Carlo method is to map the quantum problem to a classical one and simply use the standard Monte Carlo technique to simulate the equilibrium properties of the latter. When $\mathcal{E}$ is real, and for the translation of the parameters relevant to the problem of interest, the Monte Carlo technique should converge to the equilibrium searched. In cases in which $e^{-\mathcal{E}}$ is not positive definite, sign problems may inhibit the good functioning of the method.

Mapping via the evolution operator

Take the *time-dependent Schrödinger equation*

$$\mathrm{i}\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{\mathcal{H}} |\psi\rangle \tag{3.59}$$

and formally solve it

$$|\psi(t)\rangle = \hat{U}(t,t')|\psi(t')\rangle \qquad \text{with} \qquad \hat{U}(t,t') = e^{-\mathrm{i}\hat{\mathcal{H}}(t-t')/\hbar} \tag{3.60}$$

the *evolution operator*. Since the Hamiltonian is a time-independent Hermitian operator, $\hat{\mathcal{H}} = \hat{\mathcal{H}}^\dagger$, the operator $\hat{U}$ is unitary and satisfies $\hat{U} = \hat{U}^\dagger = \mathbb{I}$; therefore, the norm is preserved $\langle\psi(t)|\psi(t)\rangle = \langle\psi(t')|\hat{U}^\dagger(t,t')U(t,t')|\psi(t')\rangle = \langle\psi(t')|\psi(t')\rangle$.

Multiplying on the left by $\langle x|$, an eigenstate of the (time-independent in the Schrödinger picture) position operator $\hat{x}$, we introduce the wave function in the position representation

$$\begin{aligned} \psi(x,t) &\equiv \langle x|\psi(t)\rangle = \langle x|\hat{U}(t,t')|\psi(t')\rangle = \int dx' \, \langle x|\hat{U}(t,t')|x'\rangle \, \langle x'|\psi(t)\rangle \\ &\equiv \int dx' \, U(x,t;x',t') \, \psi(x',t) \, . \end{aligned} \tag{3.61}$$

(For simplicity we focus on a one space dimensional problem.) $U(x,t;x',t')$ is the x, x' component of the evolution operator between times t' and t.

The partition function is

$$\mathcal{Z}_q = \mathrm{Tr}\; e^{-\beta_q \hat{\mathcal{H}}} = \int dx \, \langle x|e^{-\beta_q \hat{\mathcal{H}}}|x\rangle = \int dx \, U(x, t = -\mathrm{i}\beta_q\hbar; x, t' = 0) \, . \tag{3.62}$$

Once again we see that in quantum statistical physics the inverse temperature β_q multiplied by $\hbar$ behaves as an imaginary time with periodic boundary conditions, because of the trace.

Back to the classical Ising chain - the evolution operator

We saw in the analysis of the classical Ising chain that the elements of the transfer matrix $\mathbb{T}$ can be interpreted as the ones of a quantum operator $\exp(-\epsilon\hat{\mathcal{H}})$, with $\hat{\mathcal{H}}$ a quantum Hamiltonian and ϵ a parameter inserted in the exponential to arrange the units. But not only that, ϵ can also be interpreted as an *infinitesimal imaginary time-step* (divided by $\hbar$) in a quantum evolution operator.

To make the connection more explicit, one can look at Eqs. (3.33)-(3.35) in the limit $\epsilon \to 0$ and derive an approximation for b_1 and b_3,

$$\epsilon b_1 \sim e^{-K} \qquad \text{and} \qquad \epsilon b_3 \sim e^{K} \sinh H \tag{3.63}$$

which indicates that $\epsilon \to 0$ implies $H \to 0$ first and $K \to \infty$ next if one wanted to keep both b_1 and b_3 finite:

$$H \to 0 \ \text{ and } \ K \to \infty \ . \tag{3.64}$$

Therefore, for these parameters of the classical Ising model, the quantum representation trully corresponds to the infinitesimal time-evolution

$$\hat{U}(\tau_k + \epsilon\hbar, \tau_k) = e^{-\epsilon\hat{\mathcal{H}}} \sim 1 - \epsilon\hat{\mathcal{H}} + \mathcal{O}(\epsilon^2) \tag{3.65}$$

with

$$-\epsilon\hat{\mathcal{H}} = \epsilon b_1(K,H)\hat{\sigma}^x + \epsilon b_3(K,H)\hat{\sigma}^z \ . \tag{3.66}$$

> Classical one dimensional Ising models for these parameters (small H and large K) are "identical" to the eigenvalue problem of the quantum $\hat{\mathcal{H}}$ above.

Discussion

Let us discuss the meaning of the various limits obtained by taking the parameters to vanish or diverge, with different choices of what is held constant.

- Consider the classical Ising model with parameters K and H and system size N. In the thermodynamic $N \to \infty$ limit, holding K and H *fixed*, the statistical properties are dominated by the largest eigenvalue of the transfer matrix, and it corresponds to the ground state of the corresponding quantum Hamiltonian $\hat{\mathcal{H}}$ (since $\beta_q = \epsilon N_\tau \to \infty$).

- When we map a quantum partition function to a classical one, there are two different temperatures. On the one hand, we have β_q, the quantum temperature, which controls the length $\beta_q\hbar$ of the classical system system in this additional τ direction. On the other hand, we have the temperature of the classical model (hidden inside, say, $K = \beta J$ and $H = \beta h$ in the Ising model example), which varies with the parameters of the quantum problem (such as b_1 and b_3 in the Ising classical chain example) as well as the value of $\epsilon = \hbar\beta_q/N_\tau$.

– At zero temperature, $\beta_q \to \infty$, $\tau = \beta_q \hbar \to \infty$. This is when the ground state of the quantum system dominates. If $\epsilon \to 0$, the number of points in any fixed τ interval diverges. Moreover, the length of the overall imaginary time interval $\beta_q \hbar$ diverges as well. This poses a double problem for numerical (Monte Carlo) work since the number of variables the computer has to keep track of diverges in this double sense. One then has to extrapolate the numerical results obtained from a large but necessarily finite value of N_τ to the continuum and zero-temperature ($\beta_q \to \infty$) limits.

3.2 Path integrals

Concise presentations of the path integral formalism can be found in the lecture notes by B. Simons [7] and D. J. Amit's book [8]. The method was suggested by Dirac in the 30s and then developed by Feynman in the 40s.

The path integral method provides a way to write the matrix element of the evolution operator, or *amplitude* to find the particle at x at time t knowing that it was at x' at time t',

$$\langle x, t | x', t' \rangle = \langle x | \hat{U}(t, t') | x' \rangle = U(x, t; x', t') \; , \tag{3.67}$$

as an *integral over classical paths*. (Extensions to spins, fields or other kinds of variables also exist.) Before presenting its construction we take a few paragraphs to explain how functional integration methods were introduced in the context of stochastic processes

3.2.1 The Wiener construction for Langevin equations

We open a parenthesis and comment on a classical analogy of what Feynman did quantum mechanically. It concerns the description of stochastic processes developed by Wiener in the 20s. Consider a time-dependent random process as described, for example, by the over-damped Langevin equation

$$\frac{dx(t)}{dt} = \xi(t) \; . \tag{3.68}$$

The right-hand-side is a random function, and its statistical properties have to be specified. A usual choice is Gaussian, as a zero mean white noise, that is, $\langle \xi(t'') \rangle = 0$ and $\langle \xi(t'') x(t''') \rangle = 2 k_B T \delta(t'' - t''')$ for all t'' and t'''. The angular brackets represent here the average over the Gaussian probability distribution of the noise. This noise has *no memory* or, in other terms, the process is *Markovian*. We will come back to what this means below. The friction coefficient has been absorbed in a time redefinition and T is the temperature of the bath. The particle has fixed initial condition $x(t') = x'$ and it evolves according to (3.68). Observables are noise averages of the particle's position and can be readily calculated from the solution of the above equation, $x(t) = x(t') + \int_{t'}^{t} dt'' \, \xi(t'')$. For example, $\langle x(t) \rangle = x'$ and $\langle (x(t) - x(t'))^2 \rangle = 2D(t - t')$ with diffusion coefficient $D = k_B T$.

Time is now discretized in infinitesimal steps of length $\delta t = (t-t')/N$ with $t_k = t' + k\,\delta t$ and $k = 0, \ldots, N$; then $t_0 = t'$ and $t_N = t$. The evaluation of the position at the discrete time will be denoted $x_k = x(t_k)$. Equation (3.68) then reads

$$\delta x_k \equiv x_{k+1} - x_k = \delta t\ \xi_k\ . \tag{3.69}$$

(We adopt here what is called Ito's discretization scheme in which the noise is evaluated in the pre-point.) The Gaussian white noise has joint probability distribution

$$P(\xi) \equiv P(\{\xi_k\}) = \prod_k \frac{1}{(2\pi\ 2k_BT/\delta t)^{1/2}}\ e^{-\frac{1}{2}\frac{\delta t}{2k_BT}\,\xi_k^2}\ . \tag{3.70}$$

This ensures that

$$\langle \xi_k \rangle = 0\ , \qquad\qquad \langle \xi_k \xi_{k'} \rangle = 2k_BT\ \frac{1}{\delta t}\ \delta_{kk'} \tag{3.71}$$

giving the scalings $\xi_k = \mathcal{O}(\delta t^{-1/2})$ and $x_{k+1} - x_k = \mathcal{O}(\delta t^{1/2})$ typical of over-damped (no second time derivative) white noise processes. The weird normalization of the Kronecker delta in the second relation ensures that it approaches the Dirac delta in the continuous time limit. The noise average of a generic function O of the variable x is then,

$$\langle O \rangle = \int \mathcal{D}\xi\ O(x^{(\xi)})\ P(\xi) \tag{3.72}$$

where $O(x^{(\xi)})$ indicates that x has to be expressed as a solution of the Langevin equation, in terms of the noise, the measure $\mathcal{D}\xi$ is just $\prod_k d\xi_k$ and all integrals over the noise run from $-\infty$ to ∞.

Thanks to the Markov property of the process, the probability to find the particle at a position $x = x_N$ at time $t = t_N$ knowing that it departed from $x' = x_0$ at time $t' = t_0$ is

$$\begin{aligned} &p(x,t|x',t') \\ &\quad = \int_{-\infty}^{\infty} dx_{N-1} \cdots \int_{-\infty}^{\infty} dx_1\ p(x_N = x, t_N = t | x_{N-1}, t_{N-1}) \ldots p(x_1, t_1 | x' = x_0, t_0 = t')\ . \end{aligned} \tag{3.73}$$

The evolution over an infinitesimal time step is ruled by Eq. (3.69). Take the first time-step $x_1 = x_0 + \delta t\,\xi_0$. x_0 is fixed to x', and x_1 is just a linear function of ξ_0. One has

$$\begin{aligned} p(x_1,t_1|x_0,t_0) &= \int d\xi_0\ \delta(x_1 - (x_0 + \delta t\,\xi_0))\ \frac{1}{(2\pi\ 2k_BT/\delta t)^{1/2}}\ e^{-\frac{1}{2}\frac{\delta t}{2k_BT}\,\xi_0^2} \\ &= \frac{1}{(2\pi\ 2k_BT/\delta t)^{1/2}} \int d\xi_0\ \delta(x_1 - x_0 - \delta t\,\xi_0))\ e^{-\frac{1}{2}\frac{\delta t}{2k_BT}\,\xi_0^2} \\ &= \frac{1}{(2\pi\ 2k_BT/\delta t)^{1/2}}\ \frac{1}{\delta t} \int d\overline{\xi}_0\ \delta(\overline{\xi}_0 - (x_1 - x_0))\ e^{-\frac{1}{2}\frac{\delta t}{2k_BT}\left(\frac{\overline{\xi}_0}{\delta t}\right)^2} \\ &= \frac{1}{(2\pi\ 2k_BT\delta t)^{1/2}}\ e^{-\frac{1}{2}\frac{\delta t}{2k_BT}\left(\frac{x_1 - x_0}{\delta t}\right)^2}\ . \end{aligned} \tag{3.74}$$

Replacing now in (3.73)

$$p(x,t|x',t') = \frac{1}{(2\pi\ 2k_BT\ \delta t)^{(N-1)/2}} \int_{-\infty}^{\infty} dx_{N-1} \cdots \int_{-\infty}^{\infty} dx_1\ e^{-\frac{1}{2}\frac{1}{2k_BT}\ \delta t\ \sum_k \left(\frac{x_{k+1}-x_k}{\delta t}\right)^2}$$
$$= \int \mathcal{D}x\ e^{-\frac{1}{2}\frac{1}{2k_BT}\int_{t'}^{t} dt'' \left(\frac{dx(t'')}{dt''}\right)^2} . \tag{3.75}$$

The compact notation $\int \mathcal{D}x$ represents

$$\int \mathcal{D}x\ \ldots = \frac{1}{(2\pi\ 2k_BT\ \delta t)^{(N-1)/2}} \int_{-\infty}^{\infty} dx_{N-1} \cdots \int_{-\infty}^{\infty} dx_1\ \ldots \tag{3.76}$$

We have expressed the transition probability as a sum over all paths linking the initial value to the final one.

For the generalization of this construction to stochastic Langevin equations with deterministic forces and also multiplicative noise, see [10, 11].

3.2.2 The Feynman path integral construction

Going back to the quantum problem, the propagator is

$$\langle x|\hat{U}(t,t')|x'\rangle = U(x,t;x',t') \qquad \hat{U}(t,t') = e^{-\mathrm{i}\hat{\mathcal{H}}(t-t')/\hbar} . \tag{3.77}$$

The idea is to discretise the real time interval $[t',t]$, with the definitions

$$t_k = t' + k\,\delta t \qquad k = 0,\ldots,N \quad \text{and} \quad \delta t = (t-t')/N \tag{3.78}$$

in such a way that $t' = t_0$ and $t = t_N$. Eventually one takes $\delta t \to 0$ and $N \to \infty$ with $t - t'$ fixed.

We first factorize the evolution operator

$$e^{-\mathrm{i}\hat{\mathcal{H}}(t-t')/\hbar} = e^{-\mathrm{i}\hat{\mathcal{H}}\delta t/\hbar}\ \ldots\ e^{-\mathrm{i}\hat{\mathcal{H}}\delta t/\hbar} \tag{3.79}$$

in N factors such that $N\delta t = t - t'$. Then we introduce resolutions of the identity in position space

$$\mathbb{I} = \int dx_k\ |x_k\rangle\langle x_k| \tag{3.80}$$

and we derive

$$e^{-\mathrm{i}\hat{\mathcal{H}}(t-t')/\hbar} = \int dx_{N-1}|x_{N-1}\rangle\langle x_{N-1}|e^{-\mathrm{i}\hat{\mathcal{H}}\delta t/\hbar} \int dx_{N-2}|x_{N-2}\rangle\langle x_{N-2}|e^{-\mathrm{i}\hat{\mathcal{H}}\delta t/\hbar}\ \ldots$$
$$\ldots \int dx_1|x_1\rangle\langle x_1|e^{-\mathrm{i}\hat{\mathcal{H}}\delta t/\hbar} \tag{3.81}$$

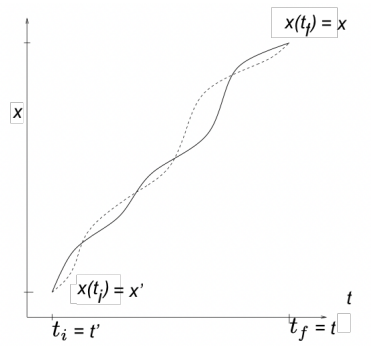

Figure 3.2: Two paths out of many contributing to the path integral that represents the bracket of the evolution operator between an initial and a final state at times t_i and t_f respectively.

Sandwiched between $\langle x|$ and $|x'\rangle$, this expression can also be written as

$$\begin{aligned}\langle x,t|x',t'\rangle &= \int dx_{N-1}\ \ldots \int dx_2 \int dx_1\ \langle x,t|x_{N-1},t_{N-1}\rangle \\ &\qquad \langle x_{N-1},t_{N-1}|x_{N-2},t_{N-2}\rangle \ldots \langle x_2,t_2|x_1,t_1\rangle\langle x_1,t_1|x',t'\rangle\ . \end{aligned} \tag{3.82}$$

Each factor in the product is

$$\langle x_k,t_k|x_{k-1},t_{k-1}\rangle = \langle x_k|\hat{U}(t_k,t_{k-1})|x_{k-1}\rangle = U(x_k,t_k;x_{k-1},t_{k-1})\ . \tag{3.83}$$

Inserting now identities in momentum space $\mathbb{I} = \int dp_k\ |p_k\rangle\langle p_k|$

$$\begin{aligned} U(x_k,t_k;x_{k-1},t_{k-1}) &= \langle x_k|e^{-\mathrm{i}\hat{\mathcal{H}}\delta t/\hbar}|x_{k-1}\rangle = \int \frac{dp_k}{2\pi\hbar}\ \langle x_k|p_k\rangle\ \langle p_k|e^{-\mathrm{i}\hat{\mathcal{H}}\delta t/\hbar}|x_{k-1}\rangle \\ &= \int \frac{dp_k}{2\pi\hbar}\ \exp\left[\frac{\mathrm{i}}{\hbar}\left(p_k\dot{x}_k - \mathcal{H}(p_k,x_k)\right)\delta t\right] \end{aligned} \tag{3.84}$$

where we have dropped any $\mathcal{O}(\delta t^2)$ contribution. The matrix element is calcuted in detail in App. 3.A.3. Inserting this expression in the product of evolution functions and using a continuous time notation

$$U(x,t;x',t') = \int \mathcal{D}p \int_{x(t')=x'}^{x(t)=x} \mathcal{D}x\ \exp\left\{\frac{i}{\hbar}\int_{t'}^{t} dt''\left[p(t'')\dot{x}(t'') - \mathcal{H}(p(t''),x(t''))\right]\right\} \tag{3.85}$$

If the kinetic energy is quadratic in p, the two p-dependent terms in the exponential can be combined to form a Gaussian weight:

$$p\dot{x} - \frac{p^2}{2m} = -\frac{1}{2m}(p-m\dot{x})^2 + \frac{m}{2}\dot{x}^2\ . \tag{3.86}$$

After translation $p - m\dot{x} \mapsto p$, the momentum can be integrated out and yields a simple factor $m/(2\pi \mathrm{i}\hbar\delta t)^{N/2}$ which can be absorbed in the measure $\mathcal{D}x$ (similarly to what we have done in the stochastic case). Then,

$$U(x,t;x',t') = \int_{x(t')=x'}^{x(t)=x} \mathcal{D}x \ \exp\left\{\frac{\mathrm{i}}{\hbar}\int_{t'}^{t} dt'' \left[\frac{m}{2}\dot{x}^2(t'') - V(x(t''))\right]\right\} . \tag{3.87}$$

In the exponential we recognise the *classical action*,

$$S = \int_{t'}^{t} dt'' \ L(\dot{x},x) \ , \tag{3.88}$$

with $L(\dot{x},x)$ the *Lagrangian*.

3.2.3 Wick's rotation

Make now an analytic continuation from real to *imaginary time*

$$t \mapsto -\mathrm{i}\tau \tag{3.89}$$

This is also called a *Wick rotation*. The expression above becomes

$$U(x,-\mathrm{i}\tau;x',-\mathrm{i}\tau') = \int_{x(-\mathrm{i}\tau')=x'}^{x(-\mathrm{i}\tau)=x} \mathcal{D}x \ \exp\left\{\frac{\mathrm{i}}{\hbar}\int_{-\mathrm{i}\tau'}^{-\mathrm{i}\tau} d(-\mathrm{i}\tau'') \left[\frac{m}{2}\left(\frac{dx(-\mathrm{i}\tau'')}{d(-\mathrm{i}\tau'')}\right)^2 - V(x(-\mathrm{i}\tau''))\right]\right\}$$

Renaming $x(-\mathrm{i}\tau) \mapsto x(-\tau)$ and $U(x,-\mathrm{i}\tau;x',-\mathrm{i}\tau') \mapsto U(x,-\tau;x',-\tau')$, and noticing that

$$\int_{-\mathrm{i}\tau'}^{-\mathrm{i}\tau} d(-\mathrm{i}\tau'') \ f(-\tau'') = \mathrm{i}\int_{\tau'}^{\tau} d\tau'' \ f(\tau'') \tag{3.90}$$

$$\frac{dx(-\mathrm{i}\tau'')}{d(-\mathrm{i}\tau'')} = \frac{1}{(-\mathrm{i})}\frac{dx(-\mathrm{i}\tau'')}{d\tau''} \mapsto \mathrm{i}\,\frac{dx(\tau'')}{d\tau''} = \mathrm{i}\,\dot{x}(\tau'') \tag{3.91}$$

one derives

$$U(x,\tau;x',\tau') = \int_{x(\tau')=x'}^{x(\tau)=x} \mathcal{D}x \ \exp\left\{-\frac{1}{\hbar}\int_{\tau'}^{\tau} d\tau'' \left[\frac{m}{2}\left(\dot{x}(\tau'')\right)^2 + V(x(\tau''))\right]\right\}$$

and the expression in the exponential is just the classical energy integrated over time (times $-1/\hbar$). This form is also called the *Euclidean action*

$$S_E = \int_{\tau'}^{\tau} d\tau'' \left[\frac{m}{2}\left(\dot{x}(\tau'')\right)^2 + V(x(\tau''))\right] \tag{3.92}$$

(in contrast with a Minkowskian one in which temporal and spatial contributions come with different signs). Tracing over states

$$\int dx \int_{x(\tau')=x}^{x(\tau)=x} \mathcal{D}x \ \exp\left\{-\frac{1}{\hbar}\int_{\tau'}^{\tau} d\tau'' \left[\frac{m}{2}\left(\dot{x}(\tau'')\right)^2 + V(x(\tau''))\right]\right\} . \tag{3.93}$$

That is, we must use boundary conditions such that the initial and final states are the same state, and we need to sum over all such states. This is the reason why we integrate over dx after setting $x(\tau') = x(\tau) = x$. We are getting closer to finding a representation of the partition sum. But what about the times τ and τ'?

- The choice of the "initial" time τ' is arbitrary. We can simply set it to zero, $\tau' = 0$.
- What about the "final" time τ? We started by representing elements of the evolution operator $e^{-i\hat{\mathcal{H}}t/\hbar}$. If we want to obtain the partition function $e^{-\beta_q \hat{\mathcal{H}}}$ we need the imaginary time $\tau = it$ to be related to the inverse temperature β_q as $\tau = \beta_q \hbar$.

The *partition function* is therefore

$$\mathcal{Z} = \int dx \int_{x(\tau')=x}^{x(\tau)=x} \mathcal{D}x \, \exp\left\{-\frac{1}{\hbar}\int_0^{\beta_q\hbar} d\tau'' \left[\frac{m}{2}\left(\dot{x}(\tau'')\right)^2 + V(x(\tau''))\right]\right\} . \tag{3.94}$$

This problem is equivalent to the classical mechanics of an *elastic string* with $x(\tau)$ the transverse displacement with respect to the internal coordinate along the string represented by τ. The length of the string is $\tau - \tau'$ and its ends are forced to be at $x(\tau') = x$ and $x(\tau) = x$, but otherwise the string can fluctuate. Its elastic energy is

$$E_{\text{elast}} = m\int_{\tau'}^{\tau} d\tau'' \left\{\left[1 + \left(\frac{dx(\tau'')}{d\tau''}\right)^2\right]^{1/2} - 1\right\} \approx \frac{m}{2}\int_{\tau'}^{\tau} d\tau'' \left(\frac{dx(\tau'')}{d\tau''}\right)^2 , \tag{3.95}$$

and it is added to the external potential V to get the full potential energy. Thus, the analytic continuation to imaginary time has transformed the quantum mechanical problem of a single particle moving in a one dimensional space into the statistical physics one of a one dimensional object with transverse displacements. The generalisation to higher dimensions is straightforward. This is another way of deriving the

> d-dimensional quantum mechanics – $d+1$ dimensional statistical physics correspondence with the association $t \mapsto -i\tau$ and $\beta \leftrightarrow 1/\hbar$

One can always interpret the imaginary time generating functional of the quantum problem in d dimensions as the equilibrium Gibbs-Boltzmann partition function of the classical model at finite inverse temperature in $d+1$ dimensions. The classical model, though, is *anisotropic*, since the direction associated to the imaginary time has different interactions from the truly spatial ones.

Mathematically, the imaginary time path integral is a better behaved object than its real time counterpart, since it is a sum of positive quantities, the statistical weights.

In practice, the sum over trajectories which are periodic in imaginary time, can only be done exactly for simple systems. In general, one has to resort to some form of perturbation theory or other approximation scheme.

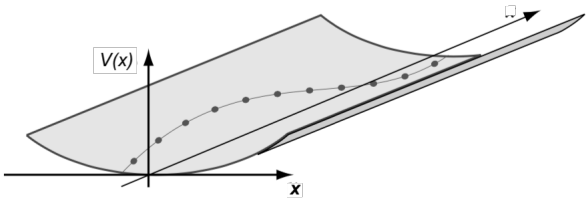

Figure 3.2 A string held under tension and confined to a potential well V.

Figure 3.3: Figure copied from [9], representing the elastic string (think of a polymer made of individual beads labelled by τ). The translation is such that the coordinate along the string is τ. The displacement of each "bead" is $x(\tau)$.

The Euclidean action is usually non-negative, which implies that if the action corresponding to some $x(\tau)$ is large, its contribution is very small. This fact dramatically improves the convergence of the path integral. The classical path is the one with the maximal contribution since it yields the minimal value to the action.

3.2.4 The ground state

Take a quantum system with Hamiltonian $\hat{\mathcal{H}}$ in canonical equilibrium at inverse temperature β_q (to keep the notation we were using so far). The elements of the (un-normalized) density matrix are

$$\langle x|e^{-\beta_q\hat{\mathcal{H}}}|x'\rangle \ . \tag{3.96}$$

Inserting a complete set of energy eigenstates $|n\rangle$,

$$\begin{aligned}\langle x|e^{-\beta_q\hat{\mathcal{H}}}|x'\rangle &= \sum_{n=0}^{\infty}\langle x|e^{-\beta_q\hat{\mathcal{H}}}|n\rangle\langle n|x'\rangle = \sum_{n=0}^{\infty} e^{-\beta_q E_n}\langle x|n\rangle\langle n|x'\rangle \\ &= \sum_{n=0}^{\infty} e^{-\beta_q E_n}\psi_n^*(x)\psi_n(x')\end{aligned} \tag{3.97}$$

with E_n the energy of the nth state and $\psi_n(x)$ its wave function. Taking the limit $\beta_q \to \infty$ the sum is dominated by the ground state contribution. One can then use

$$\lim_{\beta_q\to\infty}\mathcal{Z} = \int dx \lim_{\beta_q\to\infty}\langle x|e^{-\beta_q\hat{\mathcal{H}}}|x\rangle = e^{-\beta_q E_0}\int dx\ |\psi_0(x)|^2 = e^{-\beta_q E_0} \tag{3.98}$$

which implies

$$E_0 = -\lim_{\beta_q\to\infty}\frac{1}{\beta_q}\ln \mathrm{Tr}\, e^{-\beta_q\hat{\mathcal{H}}} \ . \tag{3.99}$$

We can now use the path integral expression for the trace of the density operator or partition function, Eq. (3.94), and therefore get the ground state energy in this way.

3.2.5 Classical Limit

In the correspondence limit, $\hbar \to 0$, the only history (or possibly histories) that contribute significantly to the path integral must be those that leave the action S stationary. Otherwise, the rapidly oscillating contributions would add up to zero. Thus, in the classical limit there is only one history $x_{\rm cl}(t)$ linking $x_{\rm cl}(t') = x'$ and $x_{\rm cl}(t) = x$ which contributes and it is the one that makes $\delta S = 0$, the *least action principle*. The classical trajectory satisfies the *Euler-Lagrange equation*

$$\left.\frac{\delta S}{\delta x(t'')}\right|_{x_{\rm cl}(t'')} = \frac{\partial L}{\partial x(t'')} - \frac{d}{dt''}\frac{\partial L}{\partial \dot{x}(t'')} = 0 \tag{3.100}$$

with the condition

$$\left.\frac{\delta^2 S}{\delta x(t'')\delta x(t''')}\right|_{x_{\rm cl}(t)} \quad \text{positive definite .} \tag{3.101}$$

3.2.6 Quantum corrections

Since the classical action satisfies $\delta S/\delta x = 0$ by construction, the action of an arbitrary trajectory satisfies

$$\begin{aligned} S[x(t)] &= S[x_{\rm cl}(t) + \delta x(t)] \\ &= S[x_{\rm cl}(t)] + \int dt'' \left.\frac{\delta S}{\delta x(t'')}\right|_{x_{\rm cl}} \delta x(t'') + \frac{1}{2}\int dt'' \int dt''' \left.\frac{\delta^2 S}{\delta x(t'')\delta x(t''')}\right|_{x_{\rm cl}} \delta x(t'')\delta x(t''') + \dots \\ &\simeq S[x_{\rm cl}(t)] + \frac{1}{2}\int dt'' \int dt''' \left.\frac{\delta^2 S}{\delta x(t'')\delta x(t''')}\right|_{x_{\rm cl}} \delta x(t'')\delta x(t''') \ . \end{aligned} \tag{3.102}$$

In the last line we cut the expansion at the second order. The Gaussian integral characterises the *quantum quadratic fluctuations* and it can be calculated interpreting the Hessian as a *differential operator* acting in the space of functions $y(t)$ with boundary conditions $\delta x(0) = \delta x(\tau) = 0$, since the boundary conditions are imposed on the classical solution. The quadratic term can then be integrated over and the final calculation is put in the form of the evaluation of a functional determinant:

$$\left[\det \left.\frac{\delta^2 S}{\delta x(t'')\delta x(t''')}\right|_{x_{\rm cl}}\right]^{-1/2} \tag{3.103}$$

We will not carry out this calculation here since it goes beyond the scope of these lectures.

3.2.7 The harmonic oscillator

We now derive the quantum partition function of the harmonic oscillator using the path integral formalism.

Take the quantum harmonic oscillator

$$\hat{\mathcal{H}} = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{x}^2 \tag{3.104}$$

with Lagrangian

$$L(\dot{x}, x) = K(\dot{x}) - V(x) = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2 \ . \tag{3.105}$$

The classical equation of motion is

$$\ddot{x}_{\rm cl} + \omega^2 x_{\rm cl} = 0 \ . \tag{3.106}$$

A generic trajectory is $x(t) = x_{\rm cl}(t) + \delta x(t)$. We impose the boundary conditions on the classical trajectory $x_{\rm cl}(t') = x'$ and $x_{\rm cl}(t) = x$. Therefore $\delta x(t') = \delta x(t) = 0$.

For the harmonic oscillator, terms of higher than quadratic order vanish and

$$S[x(t)] = S[x_{\rm cl}(t)] + S[\delta x(t)] \tag{3.107}$$

with the second term being identical to the original action, but evaluated on the perturbation of the classical trajectory. Then,

$$U(x,t;x',0) = e^{\frac{\rm i}{\hbar}S[x_{\rm cl}]} \int_{\delta x(t')=0}^{\delta x(t)=0} \mathcal{D}\delta x \ \exp\left\{\frac{\rm i}{\hbar}\int_{t'}^{t} dt'' \left[\frac{m}{2}\left(\frac{d\delta x(t'')}{dt''}\right)^2 - \frac{m\omega^2}{2}(\delta x(t''))^2\right]\right\} \ .$$

The calculation of the remaining functional integral can be found in the Feynman-Hibbs book, for example, or other traditional references on path integrals. The real time propagator reads

$$U(x,t|x',t') = \sqrt{\frac{m\omega}{2\pi{\rm i}\hbar\sin(\omega t)}} \ \exp\left\{\frac{{\rm i}m\omega}{2\hbar\sin(\omega t)}\left[(x^2+x'^2)\cos(\omega t) - 2xx'\right]\right\} \tag{3.108}$$

where we already set $t' = 0$. We now set $x' = x$, $t' = 0$ and $t = -{\rm i}\tau$, and we use $\sin(-{\rm i}z) = \frac{1}{2{\rm i}}(e^{-{\rm i}{\rm i}z} - e^{{\rm i}{\rm i}z}) = -\frac{\rm i}{2}(e^z - e^{-z}) = -{\rm i}\sinh z$ and $\cos(-{\rm i}z) = \frac{1}{2}(e^{-{\rm i}{\rm i}z} + e^{{\rm i}{\rm i}z}) = \frac{1}{2}(e^z + e^{-z}) = \cosh z$ to obtain

$$U(x,-{\rm i}\tau|x,0) = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\omega\tau)}} \ \exp\left\{-\frac{m\omega}{\hbar\sinh(\omega\tau)}\left[\cosh(\omega\tau)-1\right]x^2\right\} \ . \tag{3.109}$$

Finally, at $\tau = \beta\hbar$,

$$U(x,-{\rm i}\beta\hbar|x,0) = \sqrt{\frac{m\omega}{2\pi\hbar\sinh(\omega\beta\hbar)}} \ \exp\left\{-\frac{m\omega}{\hbar\sinh(\omega\beta\hbar)}\left[\cosh(\omega\beta\hbar)-1\right]x^2\right\} \ . \tag{3.110}$$

The integral over x needed to calculate the partition sum $\mathcal{Z}_q$ is just a Gaussian integral

$$\begin{aligned}\mathcal{Z}_q &= \int dx\, U(x, -\mathrm{i}\beta\hbar|x, 0) \\ &= \frac{1}{\sqrt{2[\cosh(\beta\hbar\omega) - 1]}} \\ &= \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}} \\ &= \sum_{n=0} e^{-\beta(n+1/2)\hbar\omega} \end{aligned} \tag{3.111}$$

and we recover the well-known result.

3.2.8 Tunneling and instantons

Consider a quantum particle in a double well potential $V(x)$ as the one sketched in Fig. 3.4. A particular formula with this form is the familiar $\lambda\phi^4$,

$$V(x) = \frac{r^2}{4u} + \frac{r}{2}x^2 + \frac{u}{4}x^4 \ , \tag{3.112}$$

with $r < 0$. The minima and the maximum are at

$$x_{\min} = \pm(-r/u)^{1/2} \equiv \pm x_0 \qquad\qquad x_{\max} = 0 \ . \tag{3.113}$$

For convenience, we added the constant $r^2/(4u)$ so that $V(\pm x_0) = 0$. Consequently, $V(x_{\max}) = r^2/(4u)$. We note that r^2/u controls the height of the barrier and $(-r/u)^{1/2}$ the distance between the two minima, that is, the thickness of the barrier. If one compares the two, one sees that the larger r the "steeper" the barrier.

Some quantum mechanics

Classically, if the total energy of the particle is lower than the height of the barrier, the particle's motion is oscillatory within the well where it is placed initially. The minimal energy configuration is doubly degenerate, and static at the bottom of each well, with vanishing kinetic and potential energies.

Quantum mechanically, if there were no coupling across the barrier, the Hamiltonian would have two independent, oscillator-like sets of low-lying eigenstates sitting in the two local minima, see the parabola approximating the left well and the equidistant levels in the sketch in Fig. 3.4, with energies $E_n = (n + 1/2)\hbar\omega$, as in (3.111). Allowing for a weak inter-barrier coupling, the oscillator ground states (like all higher states) split into a *doublet* of a symmetric and an antisymmetric eigenstate, $|S\rangle$ and $|A\rangle$ with energies E_S and E_A, respectively. In this case, there is a small tunnelling probability and the particle can be found with non-vanishing probability in the well where it was not initially. The

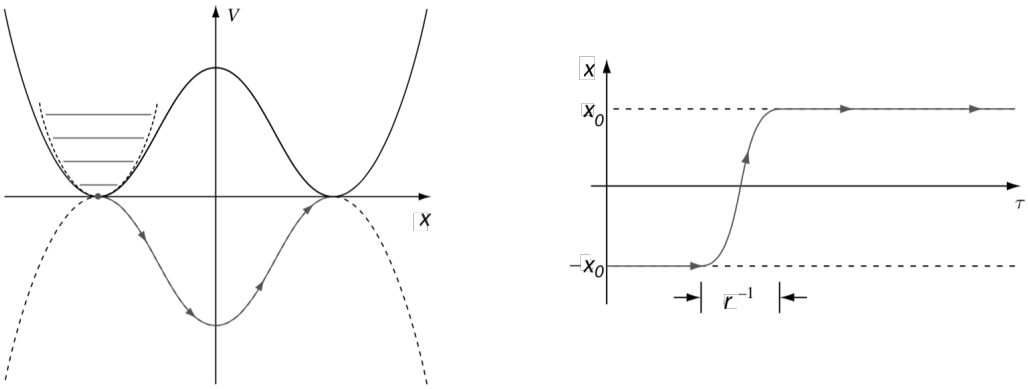

Figure 3.4: Figures copied from [9]. The left panel represents the double well potential $V(x)$ and its reversed $-V(x)$. The minima/maxima have $V = 0$. The right panel plots a typical instanton, with width $|r|^{-1}$ taking the particle from the left well (top of the left hill) to the right one (top of the right hill).

transition amplitudes between the left and the right well, and the one to remain in the right well, from time 0 to an imaginary time $-\mathrm{i}\tau$ are

$$\begin{aligned} U(x_0, -\mathrm{i}\tau, \pm x_0, 0) &= \langle x_0 | e^{-\hat{\mathcal{H}}\tau/\hbar} | \pm x_0 \rangle \\ &\sim \langle x_0 | \left(|S\rangle e^{-E_S\tau/\hbar} \langle S| + |A\rangle e^{-E_A\tau/\hbar} \langle A| \right) | \pm x_0 \rangle \end{aligned} \tag{3.114}$$

Setting

$$E_{A/S} = \frac{\omega\hbar}{2} \pm \frac{\Delta}{2} \,, \tag{3.115}$$

with Δ the energy splitting between the symmetric and anti-symmetric states, and using the symmetry properties $|\langle x_0|S\rangle|^2 = |\langle -x_0|S\rangle|^2 = C/2$ and $\langle x_0|A\rangle\langle A| - x_0\rangle = -|\langle x_0|A\rangle|2 = -C/2$,

$$\begin{aligned} U(x_0, -\mathrm{i}\tau, \pm x_0, 0) &\sim \frac{C}{2} \left(e^{-(\hbar\omega - \Delta)\tau/(2\hbar)} \pm e^{-(\hbar\omega + \Delta)\tau/(2\hbar)} \right) \\ &= C e^{-\omega\tau/2} \begin{cases} \cosh(\Delta\tau/\hbar) \\ \sinh(\Delta\tau/\hbar) \end{cases} \end{aligned} \tag{3.116}$$

The splitting between the ground and first excited states Δ determines the *tunnelling rate*.

The path integral calculation

In the path integral calculation, we go to imaginary time in part because the evaluation of the path integral by saddle point is better controled.

The transition amplitude between a point x' at (imaginary) time τ' and another point x at (imaginary) time τ is given by

$$U(x,\tau;x',\tau') = \int_{x(\tau')=x'}^{x(\tau)=x} \mathcal{D}x \; \exp\left\{-\frac{1}{\hbar}\int_{\tau'}^{\tau} d\tau'' \left[\frac{m}{2}\left(\dot{x}(\tau'')\right)^2 + V(x(\tau''))\right]\right\} \tag{3.117}$$

and one has to sum over all possible paths in imaginary time. In the literature one does not write the $(-\mathrm{i})$ in front of the time τ so we will henceforth not do it and follow the usual notation, as already done above. For "thick" enough barriers, the leading contributions can be obtained by a *semi-classical $\hbar \to 0$ approximation*, which corresponds to a quadratic expansion around the trajectories with *minimal action*:

$$\left.\frac{\delta S[x(\tau'')]}{\delta x(\tau)}\right|_{x_{\rm cl}(\tau)} = 0 \qquad \text{and} \qquad \left.\frac{\delta^2 S[x(\tau'')]}{\delta x(\tau)\delta x(\tau')}\right|_{x_{\rm cl}(\tau)} \quad \text{positive definite .} \tag{3.118}$$

Note that here there is no ambiguity about the need to look for a minimum of the action. Writing $x(\tau) = x_{\rm cl}(\tau) + y(\tau)$, the result is

$$\begin{aligned} U &\approx \underbrace{e^{-\frac{1}{\hbar}S[x_{\rm cl}(\tau)]}}_{U_{\rm cl}} \underbrace{\int \mathcal{D}y \; \exp\left\{-\frac{1}{2\hbar}\int_{\tau'}^{\tau} d\tau'' \int_{\tau'}^{\tau} d\tau''' \, y(\tau'') \left.\frac{\delta^2 S[x(\tau)]}{\delta x(\tau'')\delta x(\tau''')}\right|_{x_{\rm cl}} y(\tau''')\right\}}_{U_{\rm q}} \\ &= U_{\rm cl} \times U_{\rm q} \end{aligned} \tag{3.119}$$

and it is written as the product of a classical contribution $U_{\rm cl}$ and a quantum one $U_{\rm q}$. The Gaussian integral yields the one over the square root of the *determinant* of the Hessian operator:

$$U_{\rm q} \propto \left[\det \left.\frac{\delta^2 S[x(\tau)]}{\delta x(\tau'')\delta x(\tau''')}\right|_{x_{\rm cl}}\right]^{-1/2} . \tag{3.120}$$

The first equation in (3.118) imposes the extreme condition on the trajectory and yields

$$-m\frac{d^2 x_{\rm cl}(\tau'')}{d\tau''^2} + V'(x_{\rm cl}(\tau'')) = 0 \qquad \tau'' \in [\tau',\tau] . \tag{3.121}$$

with the boundary conditions $x_{\rm cl}(\tau') = x'$ and $x_{\rm cl}(\tau) = x$.

Equation (3.121) is identical to:

- The equation for a *domain wall* in the Ginzburg-Landau field theoretical approach to the one dimensional Ising model (with τ representing the spatial direction). We see, once again, a connection between a quantum problem in $d = 0$ spatial dimensions in this case with a classical one in $d = 0+1$ dimension. The domain wall corresponds to a trajectory describing the tunnelling of the particle from one to the other potential well.

– The saddle-point equation (3.121) describes the classical trajectory of a particle moving in the *inverted potential* $-V(x)$, see Fig. 3.4. At the initial instant the particle is, say, at the top of the left hill. At the final time τ it should arrive at, and stay there ever after, the top of the right hill. This classical trajectory should let the particle roll down the hill to the right and climb up the second hill with just enough kinetic energy to reach the top and stay there.

Note that this equation represents energy conservation in a system with potential energy $-V$:

$$E = \frac{m}{2}\left(\frac{dx_{\rm cl}(\tau'')}{d\tau''}\right)^2 - V(x_{\rm cl}(\tau'')) = \text{const} \qquad \tau'' \in [\tau', \tau] \; . \tag{3.122}$$

The procedure to obtain this condition is the following. Multiply the saddle-point equation $d^2x_{\rm cl}(\tau'')/d\tau''^2 = V'(x_{\rm cl}(\tau''))$ by $dx_{\rm cl}(\tau'')/d\tau''$. Then, $(1/2)\, d(dx_{\rm cl}(\tau'')/d\tau'')^2/d\tau'' = dV(x_{\rm cl}(\tau''))/d\tau''$. Integrate now over τ'' to find Eq. (3.122). Now, we set the additive integration constant to zero since $\dot{x}_{\rm cl} = V(x_{\rm cl}) = 0$ at the extremes of integration, where $x_{\rm cl} = -x_0$ and $x_{\rm cl} = x_0$, for the problem we want to study. Thus

$$\frac{m}{2}\left(\frac{dx_{\rm cl}(\tau'')}{d\tau''}\right)^2 = V(x_{\rm cl}(\tau'')) \; . \tag{3.123}$$

This is equivalent to stating that we are interested in classical trajectories with $E = 0$ in the mechanical problem with inverted potential. Note that Eq. (3.123) is a *first order differential equation* while the Euler-Lagrange, or Newton equations, are second order ones.

Another way to obtain Eq. (3.123) - and in general first order differential equations - for topological configurations in field theories, is the so-called *Bogomol'nyi trick* [12]. The idea is to re-write the action as (possibly a sum of) square(s) plus a constant and then minimize it by requiring that what is squared vanishes. In this problem, this method amounts to rewriting the imaginary time action as

$$\begin{aligned} S &= \int_{\tau'}^{\tau} d\tau'' \left[\frac{m}{2}\left(\dot{x} \mp \sqrt{\frac{2V(x)}{m}}\right)^2 \pm m\dot{x}\sqrt{\frac{2V(x)}{m}}\right] \\ &= \int_{\tau'}^{\tau} d\tau'' \, \frac{m}{2}\left(\dot{x} \mp \sqrt{\frac{2V(x)}{m}}\right)^2 \pm \sqrt{m}\int_{-x_0}^{x_0} dx \, \sqrt{2V(x)} \; . \end{aligned} \tag{3.124}$$

The last term yields a constant which depends on the potential energy form but not on the trajectory. The first one is set to zero by the condition (3.123) when the upper sign is selected which corresponds to the boundary conditions chosen.

A trivial solution to Eq. (3.123) would be the constant $x_{\rm cl}(\tau) = \pm x_0$, but it does not respect the boundary conditions $x_{\rm cl}(\tau') = -x_0$ and $x_{\rm cl}(\tau) = x_0$.

Another solution is one in which $x_{\rm cl}(\tau)$ smoothly connects $x_{\rm cl}(\tau') = -x_0$ and $x_{\rm cl}(\tau) = x_0$ with $dx_{\rm cl}(\tau)/d\tau = 0$ at τ' and τ. This so-called *instanton* is a *topological* trajectory, in the sense that it interpolates between two inequivalent ground states $-x_0$ and x_0 and it cannot be smoothly deformed to the trivial constant situations x_0 or $-x_0$.

From Eq. (3.123) the non-trivial trajectories are explicitly given by

$$\int_{x'}^{x} \frac{dx_{\rm cl}}{[2V(x_{\rm cl})/m]^{1/2}} = \tau - \tau' \; . \tag{3.125}$$

They have action

$$S_{\rm cl} = S[x_{\rm cl}] = \int_{\tau'}^{\tau} d\tau'' \left[\frac{m}{2} \left(\frac{dx_{\rm cl}(\tau'')}{d\tau''} \right)^2 + V(x_{\rm cl}(\tau'')) \right] \tag{3.126}$$

with $x_{\rm cl}$ solving the classical equation of motion. We have already shown that the first and second terms are identical, thanks to Eq. (3.123). We then uncover that the classical instanton action is

$$\begin{aligned} S_{\rm cl} &= m \int d\tau'' \left(\frac{dx_{\rm cl}(\tau'')}{d\tau''} \right) \left(\frac{dx_{\rm cl}(\tau'')}{d\tau''} \right) = m \int d\tau'' \left(\frac{dx_{\rm cl}(\tau'')}{d\tau''} \right) \left(\frac{2V(x_{\rm cl}(\tau''))}{m} \right)^{1/2} \\ &= m^{1/2} \int_{-x_0}^{x_0} dx_{\rm cl} \, [2V(x_{\rm cl})]^{1/2} = m^{1/2} \int_{-x_0}^{x_0} du \, [2V(u)]^{1/2} \; , \end{aligned} \tag{3.127}$$

which is the same as the last term in Eq. (3.124) and is fully determined by the form of the potential. Surprisingly enough, it does not depend on the particular form of the trajectory $x_{\rm cl}$, and it is *finite*.

For a generic double well potential $V(x)$ one cannot find an explicit solution $x_{\rm cl}$. Still, one can derive some generic features of it. Taylor expanding $V(x)$ close to its minima, $V(x) \sim (1/2)V''(\pm x_0)(x - x_0)^2 \equiv m\omega^2(x - x_0)^2/2$, with ω the oscillator frequency of the (symmetric) minima. When the particle is close to any of these minima the equation of motion becomes $dx_{\rm cl}/d\tau \sim -\omega(x_{\rm cl} - x_0)$ and the solution is $x_{\rm cl}(\tau) \sim x_0 - e^{-\omega\tau}$. Thus, the *duration* of the instanton is determined by $\omega^2 = V''(\pm x_0)/m$. The instanton is therefore confined to a narrow interval of time, $\tau_W \sim 1/\omega = [m/V''(\pm x_0)]^{1/2}$. (We have already seen some similar when studying the domain wall width in the Landau theory.)

For a quartic potential, Eq. (3.125) is solved exactly by

$$x_{\rm cl}(\tau) = \pm x_0 \tanh[(\tau - \tau_0)/\tau_W] \qquad\qquad \tau_W \propto (m/r)^{1/2} \; , \tag{3.128}$$

with $x_0 > 0$, taking sign opposed values at the two limits $\tau \to \pm\infty$. One such solution, with positive sign is shown in the right panel in Fig. 3.4. τ_W is the *width* of the *instanton* which decreases with the *thickness* of the barrier, and is proportional to $|r|^{-1/2}$. We note that $V''(\pm x_0) = 2r + 3ux_0^2 = 2r + 3u(-r/u) = -r$, in agreement with the argument for the generic potential, $\tau_W \sim 1/[V''(\pm x_0)]^{1/2}$. The instanton can occur at any imaginary

time τ_0. Such parameters are called *zero modes*, as they do not change the zero energy character of the trajectory.

The density in the classical action for a quartic potential can be evaluated explicitly. It is

$$\left(\frac{dx_{\rm cl}(\tau'')}{d\tau''}\right)^2 = \frac{x_0^2}{\tau_W^2}\,\mathrm{sech}^4[(\tau''-\tau_0)/\tau_W]\;. \tag{3.129}$$

It is located around the center of the instanton and rapidly vanishes away from it. The total action, in the limit $\tau' \to -\infty$ and $\tau \to \infty$, reads

$$S_{\rm cl} = \frac{x_0^2}{\tau_W^2}\int_{-\infty}^{\infty} d\tau''\,\mathrm{sech}^4[(\tau''-\tau_0)/\tau_W] = \frac{x_0^2}{\tau_W}\int_{-\infty}^{\infty} du''\,\mathrm{sech}^4 u'' = \frac{4x_0^2}{3\tau_W}\;. \tag{3.130}$$

Note that a naïve perturbation theory around one of the two minima of the double well potential would never show the non-perturbative tunneling effect.

If one has to impose periodic boundary conditions, one has to combine this configuration with the *anti-instanton* in which the particle transits back from x_0 to $-x_0$. This, of course, can occur an even number of times in the considered time interval. Having noticed the possibility of getting (approximate) solutions of the saddle-point equations, one can build a gas of instantons and sum all possible combinations of them to evaluate the full instantonic contribution to the partition sum. The detailed evaluation will be carried out in TD6, see also [9, 13].

The Arrhenius law

Going back to classical stochastic dynamics as described by, for example, a Langevin process, a similar question can be asked: what is the probability of a particle, initialized in a well of a double well potential, to jump over the barrier and move to the other well? If temperature is non-zero, the thermal noise will kick the particle and increase its energy until an eventual sufficiently strong one takes it to the other well. The time needed to do is the so-called Arrhenius time which scales exponentially with the height of the barrier, $t_A \sim t_0 e^{B/T}$. This time-scale can be estimated with an analysis of the path-integral for the stochastic process similar to the one described above for the quantum one [14].

3.2.9 The reduced system

Imagine that you take a system of interest, say a quantum particle, in contact with an ensemble of independent quantum harmonic oscillators, which could represent phonons. One can be interested in, for example, calculating the partition function in sequential way, in the sense of first integrating the degrees of freedom of the "bath", that is to say, the phonons, and only later the ones of the particle [15].

We follow the same route as in the derivation of the classical Langevin equation by coupling the system to an ensemble of quantum harmonic oscillators,

$$[\hat{\pi}_a, \hat{q}_b] = -i\hbar\delta_{ab}\;. \tag{3.131}$$

The equilibrium density matrix reads

$$\rho_{\rm tot}(x,q_a;x',q_a') = \frac{1}{Z_{\rm tot}}\langle x,q_a|\ e^{-\beta\hat{\mathcal{H}}_{tot}}\ |x',q_a'\rangle\ , \tag{3.132}$$

with the partition function given by $Z_{\rm tot} = {\rm Tr}e^{-\beta\hat{\mathcal{H}}_{\rm tot}}$ and the trace taken over all the states of the full system. (Note that here and it what follows q_a represents the ensemble of oscillators.) The density matrix can be represented by a functional integral in imaginary time,

$$\rho_{\rm tot}(x,q_a;x',q_a') = \frac{1}{Z_{\rm tot}}\int_{x(0)=x'}^{x(\hbar\beta)=x}\mathcal{D}x\int_{q_a(0)=q_a'}^{q_a(\hbar\beta)=q_a}\mathcal{D}q_a\ e^{-\frac{1}{\hbar}S_{\rm E}^{\rm tot}}\ . \tag{3.133}$$

The Euclidean action $S_{\rm E}^{\rm tot}$ has contributions from the system, the reservoir, the interaction and the counter-term: $S_{\rm E}^{\rm tot} = S_{\rm E}^{\rm syst} + S_{\rm E}^{\rm env} + S_{\rm E}^{\rm int} + S_{\rm E}^{\rm counter}$. The environment action is

$$S_{\rm E}^{\rm env} = \sum_{a=1}^{N}\int_0^{\beta\hbar} d\tau\ \left\{\frac{m_a}{2}[\dot{q}_a(\tau)]^2 + \frac{m_a\omega_a^2}{2}[q_a(\tau)]^2\right\}\ , \tag{3.134}$$

that is to say, we choose an ensemble of independent oscillators. For simplicity we take a linear coupling

$$S_{\rm E}^{\rm int} = \int_0^{\beta\hbar} d\tau\ x(\tau)\ \frac{1}{N^{1/2}}\sum_{a=1}^{N} c_a q_a(\tau) \tag{3.135}$$

but others, are also possible. The path integral over the oscillators' coordinates and positions is quadratic. The calculation of expectation values involves a trace over states of the full system. For operators that depend only on the particle, as $A(\hat{x})$, the trace over the oscillators can be done explicitly. Hence, if one constructs the *reduced equilibrium density operator* $\hat{\rho}_{\rm red} = {\rm Tr}_{\rm env}\ \hat{\rho}_{\rm tot}$ that acts on the system's Hilbert space, the expectation value of the observables of the system is given by

$$\langle A(\hat{x})\rangle = \frac{{\rm Tr}_{syst}\ A(\hat{x})\hat{\rho}_{\rm red}}{{\rm Tr}\hat{\rho}_{\rm tot}}\ . \tag{3.136}$$

In the path-integral formalism this amounts to performing the functional integral over periodic functions $q_a(\tau)$. From the point of view of the oscillators the system's coordinate is an external τ-dependent force. Using a Fourier representation,

$$q_a(\tau) = \sum_{n=-\infty}^{\infty} q_a^{(n)}\ e^{i\nu_n\tau} \tag{3.137}$$

with

$$\nu_n = \frac{2\pi n}{\beta\hbar} \tag{3.138}$$

the *Matsubara frequencies*, the integration over the $q_a(\tau)$ can be readily done. A long series of steps, very carefully explained in [16] allow one to obtain the reduced density matrix:

$$\begin{aligned}\rho_{\rm red}(x,x') &= \langle x|{\rm Tr}_{\rm env}\,\hat\rho_{\rm tot}\,|x\rangle \\ &= \frac{1}{Z_{\rm red}}\int_{x(0)=x'}^{x(\hbar\beta)=x}\mathcal{D}x\;\; e^{-\frac{1}{\hbar}S_{\rm E}^{\rm syst}-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\int_0^{\tau}d\tau'\,x(\tau)K(\tau-\tau')x(\tau')}\end{aligned} \tag{3.139}$$

where $Z_{\rm red}$ is the partition function of the reduced system, $Z_{\rm red} = Z_{\rm tot}/Z_{\rm env}$ and $Z_{\rm env}$ the partition function of the isolated ensemble of oscillators. The interaction with the reservoir generated a renormalization of the parameter in the quadratic in x^2 term of $S_{\rm E}^{\rm syst}$ – cancelled by the counter-term – but also a retarded interaction in the effective action controlled by the kernel

$$K(\tau) = \frac{2}{\pi\hbar\beta}\sum_{n=-\infty}^{\infty}\int_0^{\infty}d\omega\;\frac{S(\omega)}{\omega}\;\frac{\nu_n^2}{\nu_n^2+\omega^2}\,e^{i\nu_n\tau}\;, \tag{3.140}$$

with $S(\omega)$ the *spectral density* of the bath,

$$S(\omega) \equiv \frac{1}{N}\sum_{a=1}^{N}\frac{c_a^2}{m_a\omega_a}\;\delta(\omega-\omega_a) \tag{3.141}$$

Different choices of the environment are possible by selecting different ensembles of harmonic oscillators. A common choice is

$$\frac{S(\omega)}{\omega} = 2\gamma_0\left(\frac{|\omega|}{\tilde\omega}\right)^{\alpha-1}\;f_c\left(\frac{|\omega|}{\Lambda}\right)\;. \tag{3.142}$$

The function $f_c(x)$ is a high-frequency cut-off of typical width Λ and is usually chosen to be an exponential. The frequency $\tilde\omega \ll \Lambda$ is a reference frequency that allows one to have a coupling strength γ_0 with the dimensions of viscosity. If $\alpha = 1$, the friction is said to be *Ohmic*, $S(\omega)/\omega$ is constant when $|\omega| \ll \Lambda$ as for a white noise. When $\alpha > 1$ ($\alpha < 1$) the bath is *superOhmic* (*subOhmic*). The exponent α is taken to vary in the interval $(0, 2)$ to avoid divergencies.

The last retarded interaction in (3.139) remains. The imaginary time dependence of K varies according to $S(\omega)$. Power laws in S lead to power-law decays in K and thus to a long-range interaction in the imaginary-time direction.

The effect of the quantum bath is more cumbersome than in the classical case and it can lead to rather spectacular effects. A well-known example is the *localization transition*, as function of the coupling strength to an Ohmic bath in the behaviour of a quantum particle in a double well potential [17, 18, 19]. This means that quantum tunneling from the well in which the particle is initially located to the other one is completely suppressed by sufficiently strong couplings to the bath. In the context of interacting macroscopic

systems, *e.g.* ferromagnets or spin-glasses, the locus of the transition between the ordered and the disordered phase depends strongly on the coupling to the bath and on the type of bath considered.

3.3 Correlations & linear responses

In this Section we introduce correlation and linear response functions and we discuss several of their properties.

Linear response functions are especially important since they are measured experimentally. For example, the electrical conductivity is the response to a weak applied field, the thermal conductivity the response to a thermal gradient, etc.

Some correlation functions have analytic properties that do not depend on the microscopic model considered. It is very important to keep them in mind to check whether approximation schemes satisfy these exact properties and, when formulating phenomenological models, be sure that they are consistent. Approximate calculations do not always satisfy all known exact relations, and one then has to choose violating the less harmful ones.

A detailed discussion of linear response theory and the symmetry properties of correlations and Green functions can be found in [20].

Under equilibrium conditions linear response function are related to some correlation functions. These relations are called fluctuation-dissipation theorems, and they also have to be preserved in any treatment of model systems in equilibrium.

3.3.1 Expectation values and correlation functions

We focus on systems with time-independent Hamiltonians. Go to the Heisenberg picture in which the operators depend on time while states do not. A generic operator $\hat{A}$ in the Schödinger picture transforms into the Heisenberg one

$$\hat{A}(t) = e^{i\hat{\mathcal{H}}t/\hbar}\hat{A}e^{-i\hat{\mathcal{H}}t/\hbar} = \hat{U}^\dagger(t)\hat{A}\hat{U}(t)\ . \tag{3.143}$$

The expected value of $\hat{A}$ is

$$\langle\hat{A}(t)\rangle = \mathrm{Tr}[\hat{A}(t)\hat{\rho}_0] \tag{3.144}$$

where $\hat{\rho}_0$ is the (already normalised) initial density operator. In Boltzmann equilibrium at inverse temperature β,

$$\hat{\rho}_0 = \frac{e^{-\beta\hat{\mathcal{H}}}}{\mathrm{Tr}e^{-\beta\hat{\mathcal{H}}}}\ . \tag{3.145}$$

In these cases, the evolution operators $e^{\pm i\hat{\mathcal{H}}t/\hbar}$ in $\hat{A}(t)$ commute with $\hat{\rho}_0$ and using the cyclic property of the trace they cancel each other. Then,

$$\langle\hat{A}(t)\rangle = \mathrm{Tr}[\hat{A}\hat{\rho}_0]\ . \tag{3.146}$$

A bit more generally, *one-time observables* are *time-independent* in any system with $\hat{\rho}_0(\hat{\mathcal{H}})$.

The term *Green function* refers specifically to correlators of field operators or creation and annihilation operators. In this respect, *correlation functions* are more general as they correlate any kind of observables. Still, the two terms are sometimes used interchangeably. The *zero-temperature time-ordered self-correlation function* of an operator $\hat{A}$ is defined as

$$C_{AA}(t,t') \equiv \langle 0|\mathcal{T}[\hat{A}(t)\hat{A}(t')]|0\rangle \tag{3.147}$$

where $\hat{A}(t)$ and $\hat{A}(t')$ are time-dependent and $|0\rangle$ is the ground state of $\hat{\mathcal{H}}$ which does not depend on time. $\mathcal{T}$ is the time-ordering operator

$$\mathcal{T}[\hat{A}(t)\hat{A}(t')] = \hat{A}(t)\hat{A}(t')\theta(t-t') + \hat{A}(t')\hat{A}(t)\theta(t'-t) \tag{3.148}$$

($\theta(y) = 1$ for $y > 0$, $\theta(y) = 0$ for $y < 0$, and there is some freedom in the choice of $\theta(0)$ which we take to be $\theta(0) = 1/2$.)

The *finite-temperature time-ordered self-correlation function* of the operator $\hat{A}$ is defined as

$$C_{AA}(t,t') = \frac{\mathrm{Tr}\,\{\mathcal{T}[\hat{A}(t)\hat{A}(t')]e^{-\beta\hat{\mathcal{H}}}\}}{\mathrm{Tr}\,e^{-\beta\hat{\mathcal{H}}}} = \frac{\sum_n \langle n|\mathcal{T}[\hat{A}(t)\hat{A}(t')]e^{-\beta E_n}|n\rangle}{\sum_n e^{-\beta E_n}}\,, \tag{3.149}$$

where $|n\rangle$ is a complete set of eigenstates of $\hat{\mathcal{H}}$ and each matrix element is weighted with the corresponding Boltzmann factor.

Note that one could define time-ordered correlation functions in out of equilibrium systems by using a $\hat{\rho}_0$ which is not the Boltzmann one.

These definitions can be straightforwardly extended to cases with two (or more) different operators $\hat{A}$ and $\hat{B}$.

The (equilibrium) two-time correlation is *stationary,* that is, depends only on $t - t'$, as can be checked from its very definition. Take the generic case of two different operators $\hat{A}$ and $\hat{B}$, and choose $t > t'$. Then, replacing the Heisenberg operators by their expressions in terms of time-independent ones:

$$\begin{aligned} C_{AB}(t,t') &= \frac{\mathrm{Tr}[e^{i\hat{\mathcal{H}}t/\hbar}\hat{A}e^{-i\hat{\mathcal{H}}t/\hbar}e^{i\hat{\mathcal{H}}t'/\hbar}\hat{B}e^{-i\hat{\mathcal{H}}t'/\hbar}e^{-\beta\hat{\mathcal{H}}}]}{\mathrm{Tr}e^{-\beta\hat{\mathcal{H}}}} \\ &= \frac{\mathrm{Tr}[e^{i\hat{\mathcal{H}}(t-t')/\hbar}\hat{A}e^{-i\hat{\mathcal{H}}(t-t')/\hbar}\hat{B}e^{-\beta\hat{\mathcal{H}}}]}{\mathrm{Tr}e^{-\beta\hat{\mathcal{H}}}} \\ &= C_{AB}(t-t',0) \;=\; \overline{C}_{AB}(t-t')\,. \end{aligned} \tag{3.150}$$

(The overline is just to indicate that the functional form is different from the starting one, which was a function of two variables. This distinction is often ignored.) The cyclic property of the trace, and the commutation of the evolution operator with the Boltzmann factor (same $\hat{\mathcal{H}}$ involved) allowed one to rewrite all evolution operators as functions of $t - t'$. A similar procedure can be used in the case $t' > t$. One usually uses the same notation (C_{AB}) for the function of two times in the left-hand-side and the one of only

one time-difference in the right-hand-side though these are two different functions. The stationarity property is also called *time translation invariance* since

$$C_{AB}(t,t') = C_{AB}(t+\delta t, t'+\delta t) \qquad \text{for any} \quad \delta t \tag{3.151}$$

if C_{AB} depends only on the time difference.

We note that the very much studied *quantum quenches* - both theoretically and experimentally - consist in preparing an initial state with one Hamitonian, $\hat{\mathcal{H}}_1$, and evolving it with another Hamiltonian, $\hat{\mathcal{H}}_2$. in these cases, the correlation functions need not be stationary.

The term Green function, is usually reserved to the correlation of fields, or creation and annihilation operators. e.g. $\hat{c}(t)$ and $\hat{c}^\dagger(t')$, with the latter creating an excitation at t' and the former destroying it at t. At zero temperature the two-point Green function or *propagator* is

$$G(t,t') = i\langle 0|\mathcal{T}c(t)c^\dagger(t')|0\rangle \tag{3.152}$$

and the finite temperature generalisation is obvious. A good summary of the properties of Green functions is here
`https://en.wikipedia.org/wiki/Green%27s_function_(many-body_theory)`

3.3.2 Linear response and the Kubo formula

We start by giving the definition of the *instantaneous linear response* of an Hermitian observable $\hat{A}$ to a perturbation linearly coupled to another Hermitian observable $\hat{B}$, in such a way that $\hat{\mathcal{H}} \mapsto \hat{\mathcal{H}} - h\hat{B}$ between the instants t' and $t'+\epsilon$ with ϵ infinitesimal. We then calculate it by treating the strength of the change, h, as a perturbation, taking the full interacting Hamiltonian of the system $\hat{\mathcal{H}}$ as the unperturbed Hamiltonian.

First, we write $\langle \hat{A}(t)\rangle_B$ with the evolution generated by $\hat{\mathcal{H}}$ from time 0 to t', $\hat{\mathcal{H}} - h\hat{B}$ from t' to $t'+\epsilon$, and $\hat{\mathcal{H}}$ from $t'+\epsilon$ to t. Note that we are assuming $t \geq t'$. The full evolution operator is then

$$\begin{aligned} \hat{U}_h(t,0) &= e^{-i\hat{\mathcal{H}}(t-t'-\epsilon)/\hbar} e^{-i(\hat{\mathcal{H}}-h\hat{B})\epsilon/\hbar} e^{-i\hat{\mathcal{H}}t'/\hbar} \,, \\ \hat{U}_h^\dagger(t,0) &= e^{i\hat{\mathcal{H}}t'/\hbar} e^{i(\hat{\mathcal{H}}-h\hat{B})\epsilon/\hbar} e^{i\hat{\mathcal{H}}(t-t'-\epsilon)/\hbar} \,. \end{aligned} \tag{3.153}$$

Note that we used $\hat{B}^\dagger = \hat{B}$. We do not worry about the possible non-commutativity of $\hat{\mathcal{H}}$ and $\hat{B}$ since both $h \to 0$ and $\epsilon \to 0$ let us factorise the exponentials. Moreover, we can Taylor expand the exponential of $\hat{B}$ in the middle factor and get

$$\begin{aligned} \hat{U}_h(t,0) &\sim e^{-i\hat{\mathcal{H}}(t-t'-\epsilon)/\hbar} e^{-i\hat{\mathcal{H}}\epsilon/\hbar} [1 + i(h\epsilon/\hbar)\hat{B} + \mathcal{O}((\epsilon h)^2)] e^{-i\hat{\mathcal{H}}t'/\hbar} \\ &\sim e^{-i\hat{\mathcal{H}}(t-t')/\hbar} [1 + i(h\epsilon/\hbar)\hat{B} + \mathcal{O}((\epsilon h)^2)] e^{-i\hat{\mathcal{H}}t'/\hbar} \end{aligned} \tag{3.154}$$

and similarly for $\hat{U}_h^\dagger$. Then,

$$\begin{aligned}\frac{\delta}{\delta\epsilon h}\hat{U}_h(t,0)\Big|_{h=0} &= e^{-i\hat{\mathcal{H}}(t-t')/\hbar}\frac{i}{\hbar}\hat{B}e^{-i\hat{\mathcal{H}}t'/\hbar}\,,\\ \frac{\delta}{\delta\epsilon h}\hat{U}_h^\dagger(t,0)\Big|_{h=0} &= -e^{i\hat{\mathcal{H}}t'/\hbar}\frac{i}{\hbar}\hat{B}e^{i\hat{\mathcal{H}}(t-t')/\hbar}\,,\end{aligned} \tag{3.155}$$

where we already dropped higher order contributions in h which vanish for $h \to 0$. The *instantaneous linear response function* is defined as

$$R_{AB}(t,t') \equiv \frac{\delta\langle\hat{A}(t)\rangle_B}{\delta\epsilon h}\Big|_{h=0} = \frac{\delta}{\delta\epsilon h}\mathrm{Tr}[\hat{U}_h^\dagger(t,0)\hat{A}\hat{U}_h(t,0)\hat{\rho}_0]\Big|_{h=0}\,, \tag{3.156}$$

and the information about the coupling to $\hat{B}$ is in the $\hat{U}_h$ and $\hat{U}_h^\dagger$. The first contribution comes from the variation of the $\hat{U}_h^\dagger$:

$$\begin{aligned}&\mathrm{Tr}\left[\frac{\delta}{\delta\epsilon h}\left(\hat{U}_h^\dagger(t,0)\right)\hat{A}\hat{U}_0(t,0)\hat{\rho}_0\right]\Big|_{h=0} = -\frac{i}{\hbar}\mathrm{Tr}\left[e^{i\hat{\mathcal{H}}t'/\hbar}\hat{B}e^{i\hat{\mathcal{H}}(t-t')/\hbar}\hat{A}\hat{U}_0(t,0)\hat{\rho}_0\right]\\ &= -\frac{i}{\hbar}\mathrm{Tr}\left[e^{i\hat{\mathcal{H}}t'/\hbar}\hat{B}e^{i\hat{\mathcal{H}}(t-t')/\hbar}\hat{A}e^{-i\hat{\mathcal{H}}t/\hbar}\hat{\rho}_0\right] = -\frac{i}{\hbar}\langle\hat{B}(t')\hat{A}(t)\rangle\end{aligned} \tag{3.157}$$

and the second one from the variation of $\hat{U}_h$

$$\begin{aligned}&\mathrm{Tr}\left[\hat{U}_0^\dagger(t,0)\hat{A}\frac{\delta}{\delta\epsilon h}\left(\hat{U}_h(t,0)\right)\hat{\rho}_0\right]\Big|_{h=0} = \frac{i}{\hbar}\mathrm{Tr}\left[\hat{U}_0^\dagger(t,0)\hat{A}e^{-i\hat{\mathcal{H}}(t-t')/\hbar}\hat{B}e^{-i\hat{\mathcal{H}}t'/\hbar}\hat{\rho}_0\right]\\ &= \frac{i}{\hbar}\mathrm{Tr}\left[e^{i\hat{\mathcal{H}}t/\hbar}\hat{A}e^{-i\hat{\mathcal{H}}(t-t')/\hbar}\hat{B}e^{-i\hat{\mathcal{H}}t'/\hbar}\hat{\rho}_0\right] = \frac{i}{\hbar}\langle\hat{A}(t)\hat{B}(t')\rangle\,.\end{aligned} \tag{3.158}$$

In the end we have

$$R_{AB}(t,t') = \frac{i}{\hbar}\langle[\hat{A}(t),\hat{B}(t')]\rangle\theta(t-t') \tag{3.159}$$

where we introduced the θ function that ensures *causality*, since the system cannot respond to a perturbation which has not been applied yet. The square brackets denote the commutator of $\hat{A}$ and $\hat{B}$ and we stress the fact that the right-hand-side is calculated without the external perturbation. In cases in which the observables $\hat{A}$ and $\hat{B}$ are simply replaced by say creation and annihilation operators, the right-hand-side is related to the *retarded Green function*.

We note that this is a model independent *Kubo formula*. Nowhere in this derivation we used a particular form of $\hat{\rho}_0$. This relation is actually valid beyond any equilibrium hypothesis. The proof above can be applied to field theories, in which the perturbation can be localised in space.

Linear response theory implies that the influence of two subsequent kicks of time-length ϵ is equal to the one of a single kick of time-length 2ϵ, that is, the effect of the perturbations is *additive*. In this way, one derives the time-delayed *susceptibility*

$$\chi_{AB}(t,t') = \int_{t'}^{t} dt''\ R_{AB}(t,t'') \tag{3.160}$$

as the result of a perturbation applied during a finite (and not infinitesimal) time-interval going from t' to t.

Another way of writing the linear response relation is

$$\langle \hat{A}(t) \rangle_B = \int_{-\infty}^{\infty} dt''\ R_{AB}(t,t'')h(t'') \tag{3.161}$$

which is just the integral version of the instantaneous (3.156). If we focus on stationary situations, the right-hand-side is a time convolution. In Fourier

$$\tilde{R}_{AB}(\omega) = \int dt\, e^{i\omega t} R_{AB}(t)\ , \qquad R_{AB}(t) = \int \frac{d\omega}{2\pi}\, e^{-i\omega t} \tilde{R}_{AB}(\omega)\ , \tag{3.162}$$

the relation above then reads

$$\langle \tilde{A}(\omega) \rangle_B = \tilde{R}_{AB}(\omega)\tilde{h}(\omega) \tag{3.163}$$

and is *local in ω*: the response is at the same frequency as the external field. This feature does not survive if higher order terms in the perturbation are kept to calculate non-linear responses.

Under equilibrium conditions, $\hat{\rho}_0 \propto e^{-\beta\hat{\mathcal{H}}}$, one finds that the linear response is stationary, as any other correlation function.

3.3.3 Linear response and Onsager relations

The response function is expressed in terms of a commutator of Hermitian operators times a theta function that imposes causality. Let us focus on the first factor and define

$$\hbar R''_{AB}(t,t') \equiv \langle [\hat{A}(t), \hat{B}(t')] \rangle\ . \tag{3.164}$$

The response$''$ of the operator $\hat{B}$ to an external perturbation that couples to $\hat{A}$ is simply related to the response$''$ of $\hat{A}$ to a perturbation that couples to $\hat{B}$; in other words, the operators have reversed roles:

$$\left.\begin{aligned} \hbar R''_{AB}(t,t') &= \langle [\hat{A}(t), \hat{B}(t')] \rangle \\ \hbar R''_{BA}(t',t) &= \langle [\hat{B}(t'), \hat{A}(t)] \rangle \end{aligned}\right\} \implies R''_{AB}(t,t') = -R''_{BA}(t',t)\ . \tag{3.165}$$

These are *Onsager's reciprocity relations*.

3.3.4 Causality and the Kramers-Kronig relations

The causality of the real-time linear response is ensured by the analyticity of $\mathrm{Im}\tilde{R}_{AB}(\omega)$ in the upper half complex plane. This is proved as follows. Write

$$R_{AB}(t,t') = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \tilde{R}_{AB}(\omega) \tag{3.166}$$

where we assumed that the linear response is stationary.[2] Focus on $t - t' < 0$, extend $\omega \to z \in \mathbb{C}$ and close the contour in the upper half plane. The exponential $e^{-i\omega(t-t')} \propto e^{-iiz_I(t-t')} = e^{z_I(t-t')}$ falls off exponentially and, if we take $\tilde{R}_{AB}(z)$ to be analytic in this half plane, the resulting integral vanishes. This argument shows that analyticity is a sufficient condition to get $R_{AB}(t,t') \propto \theta(t-t')$. One can also argue for necessity (we will not show it here).

Assuming now that $\tilde{R}_{AB}(\omega)$ is analytic in the upper half plane, and hence $R_{AB}(t,t')$ is causal, one can derive the Kramers-Kronig relations which relate real and imaginary parts of the response functions and read

$$\begin{aligned} \mathrm{Re}\tilde{R}_{AB}(\omega) &= -P\int \frac{d\omega'}{\pi} \frac{\mathrm{Im}R_{AB}(\omega')}{\omega-\omega'} , \\ \mathrm{Im}\tilde{R}_{AB}(\omega) &= \quad P\int \frac{d\omega'}{\pi} \frac{\mathrm{Re}R_{AB}(\omega')}{\omega-\omega'} . \end{aligned} \tag{3.167}$$

The proof goes as follows. First,

$$\begin{aligned} \int \frac{d\omega'}{\pi} \frac{1}{\omega'-\omega-i\eta} \tilde{R}_{AB}(\omega') &= 2i \oint \frac{dz}{2\pi i} \frac{1}{z-\omega-i\eta} \tilde{R}_{AB}(z) \\ &= 2i\tilde{R}_{AB}(\omega+i\eta) \end{aligned} \tag{3.168}$$

where we assumed that $\tilde{R}_{AB}(z)$ falls to zero sufficiently fast at infinity.

Next, the identity

$$\begin{aligned} \lim_{\eta\to 0} \frac{1}{\omega \mp i\eta} &= \lim_{\eta\to 0} \frac{\omega \pm i\eta}{\omega^2+\eta^2} = \lim_{\eta\to 0} \left[\frac{\omega}{\omega^2+\eta^2} \pm \frac{i\eta}{\omega^2+\eta^2} \right] \\ &= P\frac{1}{\omega} \pm i\pi\delta(\omega) \end{aligned} \tag{3.169}$$

P is the *principal part*. (Take this as a definition of the principal part.)

[2] In non-stationary cases one can rewrite the two time dependence as a dependence on t' and $t-t'$ and Fourier transform with respect to the time difference. The results below also apply in these cases at fixed t'.

Now, applying (3.169) to (3.168) in the limit $\eta \to 0$, and taking the real part of the result of the lhs:

$$\begin{aligned} \text{lhs} &= \text{Re} \lim_{\eta\to 0} \int \frac{d\omega'}{\pi} \frac{1}{\omega' - \omega - i\eta} \tilde{R}_{AB}(\omega') \\ &= -P \int \frac{d\omega'}{\pi} \frac{1}{\omega - \omega'} \text{Re}\tilde{R}_{AB}(\omega') + \text{Im}\tilde{R}_{AB}(\omega) \end{aligned} \tag{3.170}$$

and of the rhs

$$\text{rhs} = 2\text{Im} \lim_{\eta\to 0} \tilde{R}_{AB}(\omega + i\eta) = 2\text{Im}\tilde{R}_{AB}(\omega) \; . \tag{3.171}$$

Thus, the equality between the two yields the first Kramers-Kronig relation in (3.167). The imaginary part of the same operation yields

$$\begin{aligned} \text{lhs} &= \text{Im} \lim_{\eta\to 0} \int \frac{d\omega'}{\pi} \frac{1}{\omega' - \omega - i\eta} \tilde{R}_{AB}(\omega') \\ &= -P \int \frac{d\omega'}{\pi} \frac{1}{\omega - \omega'} \text{Im}\tilde{R}_{AB}(\omega') + \text{Re}\tilde{R}_{AB}(\omega) \end{aligned} \tag{3.172}$$

and of the rhs

$$\text{rhs} = 2\text{Re} \lim_{\eta\to 0} \tilde{R}_{AB}(\omega + i\eta) = 2\text{Re}\tilde{R}_{AB}(\omega) \tag{3.173}$$

and hence the second Kramers-Kronig relation in (3.167).

For the *spectral representation* of the linear response see [20].

3.3.5 The KMS relations

The cyclic properties of the trace and a Boltzmann density operator yield the so-called KMS (Kadanoff-Martin-Schwinger) relations. Take a canonical equilibrium correlation between two operators measured at different times,

$$C_{AB}(t,t') = \langle \hat{A}(t)\hat{B}(t')\rangle = \frac{\text{Tr}[e^{i\hat{\mathcal{H}}t/\hbar}\hat{A}e^{-i\hat{\mathcal{H}}t/\hbar}e^{i\hat{\mathcal{H}}t'/\hbar}\hat{B}e^{-i\hat{\mathcal{H}}t'/\hbar}e^{-\beta\hat{\mathcal{H}}}]}{\text{Tr}e^{-\beta\hat{\mathcal{H}}}} \; . \tag{3.174}$$

Inserting identities and moving the factors around one can show

$$\langle \hat{A}(t)\hat{B}(t')\rangle = \langle \hat{B}(t')\hat{A}(t + i\beta\hbar)\rangle = \langle \hat{B}(-t - i\beta\hbar)\hat{A}(-t')\rangle \tag{3.175}$$

which can also be written as

$$C_{AB}(t,t') = C_{BA}(t', t + i\beta\hbar) = C_{BA}(-t - i\beta\hbar, -t') \; . \tag{3.176}$$

As way of example, let us prove the first of these expressions.

$$\begin{aligned} C_{AB}(t,t') &= \frac{\mathrm{Tr}[e^{i\hat{\mathcal{H}}t/\hbar}\hat{A}e^{-i\hat{\mathcal{H}}t/\hbar}e^{i\hat{\mathcal{H}}t'/\hbar}\hat{B}e^{-i\hat{\mathcal{H}}t'/\hbar}e^{-\beta\hat{\mathcal{H}}}]}{\mathrm{Tr}e^{-\beta\hat{\mathcal{H}}}} \\ &= \frac{\mathrm{Tr}[e^{i\hat{\mathcal{H}}t/\hbar}e^{-\beta\hat{\mathcal{H}}}e^{\beta\hat{\mathcal{H}}}\hat{A}e^{\beta\hat{\mathcal{H}}}e^{-\beta\hat{\mathcal{H}}}e^{-i\hat{\mathcal{H}}t/\hbar}e^{i\hat{\mathcal{H}}t'/\hbar}\hat{B}e^{-i\hat{\mathcal{H}}t'/\hbar}e^{-\beta\hat{\mathcal{H}}}]}{\mathrm{Tr}e^{-\beta\hat{\mathcal{H}}}} \\ &= \frac{\mathrm{Tr}[e^{i\hat{\mathcal{H}}(t+i\beta\hbar)/\hbar}\cancel{e^{\beta\hat{\mathcal{H}}}}\hat{A}e^{-i\hat{\mathcal{H}}(t+i\beta\hbar)/\hbar}e^{-\beta\hat{\mathcal{H}}}e^{i\hat{\mathcal{H}}t'/\hbar}\hat{B}e^{-i\hat{\mathcal{H}}t'/\hbar}\cancel{e^{-\beta\hat{\mathcal{H}}}}]}{\mathrm{Tr}e^{-\beta\hat{\mathcal{H}}}} \\ &= \frac{\mathrm{Tr}[e^{i\hat{\mathcal{H}}t'/\hbar}\hat{B}e^{-i\hat{\mathcal{H}}t'/\hbar}e^{i\hat{\mathcal{H}}(t+i\beta\hbar)/\hbar}\hat{A}e^{-i\hat{\mathcal{H}}(t+i\beta\hbar)/\hbar}e^{-\beta\hat{\mathcal{H}}}]}{\mathrm{Tr}e^{-\beta\hat{\mathcal{H}}}} \\ &= \langle\hat{B}(t')\hat{A}(t+i\beta\hbar)\rangle \ . \end{aligned} \tag{3.177}$$

The other relations follow from similar steps.

Having assumed equilibrium conditions the correlation functions are stationary, and depend only on the difference between the two times involved, e.g. $C_{AB}(t,t') = C_{AB}(t-t')$. They can then be Fourier transformed,

$$C_{AB}(t-t') = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')}\tilde{C}_{AB}(\omega) \tag{3.178}$$

as well as the full KMS relations (3.176), which in Fourier space read

$$\tilde{C}_{AB}(\omega) = e^{\beta\hbar\omega}\tilde{C}_{BA}(-\omega) \ . \tag{3.179}$$

3.3.6 The fluctuation-dissipation theorem

Let us define *symmetrized and anti-symmetrized* correlation functions

$$\begin{aligned} C_{[A,B]}(t,t') &= \frac{1}{2}\langle[\hat{A}(t),\hat{B}(t')]\rangle \ , \\ C_{\{A,B\}}(t,t') &= \frac{1}{2}\langle\{\hat{A}(t),\hat{B}(t')\}\rangle \ , \end{aligned} \tag{3.180}$$

which we assume are also *time-translational invariant*. Fourier transforming

$$\begin{aligned} 2\tilde{C}_{[A,B]}(\omega) &= [1-e^{-\beta\hbar\omega}]\tilde{C}_{AB}(\omega) \ , \\ 2\tilde{C}_{\{A,B\}}(\omega) &= [1+e^{-\beta\hbar\omega}]\tilde{C}_{AB}(\omega) \ . \end{aligned} \tag{3.181}$$

Taking the ratio between these two,

$$\tilde{C}_{[A,B]}(\omega) = \tanh\left(\frac{\beta\hbar\omega}{2}\right)\tilde{C}_{\{A,B\}}(\omega) \ . \tag{3.182}$$

We go back to the Kubo relation to replace the commutator by the linear response. However, one has to be careful, because these two, though proportional to each other in

the time domain, have in front the theta function which ensures causality. Therefore, the Fourier transform has to be taken with care. One can replace in the right-hand-side of Eq. (3.159) the Fourier representation of the commutator, taken to be stationary since in equilibrium,

$$\begin{aligned} R_{AB}(t,t') &= \frac{i}{\hbar}\,\theta(t-t')\int\frac{d\omega}{2\pi}\,e^{-i\omega(t-t')}\,2\tilde{C}_{[A,B]}(\omega) \\ &= \frac{i}{\hbar}\,\theta(t-t')\int\frac{d\omega}{2\pi}\,e^{-i\omega(t-t')}\tanh\left(\frac{\beta\hbar\omega}{2}\right)2\tilde{C}_{\{A,B\}}(\omega)\;. \end{aligned} \tag{3.183}$$

This is the *quantum fluctuation-dissipation theorem* in a mixed time-frequency domain. Applying now

$$\int_0^\infty dt\,e^{i\omega t} = \lim_{\epsilon\to 0^+}\frac{i}{\omega+i\epsilon} = \pi\delta(\omega)+i\frac{P}{\omega} \tag{3.184}$$

with P the principal part, we deduce

$$\tilde{R}_{AB}(\omega) = -\frac{1}{\hbar}\lim_{\epsilon\to 0^+}\int\frac{d\omega'}{\pi}\frac{1}{\omega-\omega'+i\epsilon}\tanh\left(\frac{\beta\hbar\omega'}{2}\right)2C_{\{A,B\}}(\omega') \tag{3.185}$$

from which we derive the imaginary and real parts

$$\begin{aligned} \mathrm{Im}\tilde{R}_{AB}(\omega) &= \frac{1}{\hbar}\tanh\left(\frac{\beta\hbar\omega}{2}\right)\tilde{C}_{\{A,B\}}(\omega)\;, \\ \mathrm{Re}\tilde{R}_{AB}(\omega) &= -\frac{1}{\hbar}P\int\frac{d\omega'}{\pi}\frac{1}{\omega-\omega'}\tanh\left(\frac{\beta\hbar\omega'}{2}\right)\tilde{C}_{\{A,B\}}(\omega')\;. \end{aligned} \tag{3.186}$$

This is the statement of the *fluctuation-dissipation theorem*, linking a linear response to its associated correlation function, in this case written in Fourier space. This relation is valid under equilibrium conditions only.

One can now take the limit $\beta\hbar\to 0$ to recover the classical limit. Let us focus on Eq. (3.183)

$$\begin{aligned} R_{AB}(t-t') &\to \frac{i}{\hbar}\theta(t-t')\int\frac{d\omega}{\pi}e^{-i\omega(t-t')}\frac{\beta\hbar\omega}{2}\tilde{C}_{AB}(\omega) \\ &= -\beta\frac{dC_{AB}(t-t')}{d(t-t')}\theta(t-t')\;. \end{aligned} \tag{3.187}$$

Another way of writing the fluctuation dissipation theorem, in the complex time domain, is

$$C_{\{A,B\}}(t_c)+C_{[A,B]}(t_c) = C_{\{A,B\}}(t_c^*)-C_{[A,B]}(t_c^*) \tag{3.188}$$

where $t_c = t+i\beta\hbar/2$.

The fluctuation dissipation theorem is a model independent relation between two-time correlation and linar response, written in the form of the expectation of the commutator of two operators, which extend to the quantum realm the fluctuation dissipation relations of classical statistical physics. It does not depend on the particular Hamiltonian of the system but it does on the equilibrium assumption.

3.4 Quantum phase transitions

At zero temperature thermal fluctuations are frozen but *quantum fluctuations* (due to Heisenberg's uncertainty principle) are still active. Tuning their strength with a non-thermal control parameter, that we called g in Fig. 3.5, one can drive an infinite size system through a *quantum phase transition*. A system in equilibrium at zero temperature is always in its lowest-energy state (or an equally weighted superposition if the lowest-energy is degenerate). Thus, a quantum phase transition is the result of competing *ground state phases* and it is identified from the non-analyticity of the *ground state energy*. A quantum critical point typically separates an ordered from a disordered phase, see Fig. 3.5, which is a modified version of a figure in `Wikipedia`. As in the classical case, quantum phase transitions can be of different order. We will focus here on second order ones.

Experiments in cuprate superconductors, heavy-fermion compounds, organic conductors and related systems have launched a renewed interest in quantum phase transitions since the early 90s [23, 24].

The influence of quantum mechanics on macroscopic systems can be of two kinds:

- they can be essential to understand the ordered phase itself (e.g., superconductivity).
- the critical behavior could be modified.

We will see that the comparison between two energy scales, namely $\hbar\omega$, which is the typical energy of long-distance order parameter fluctuations, and the thermal energy k_BT, will be key. Let us start by discussing some generic issues.

Switching on and increasing thermal fluctuations, a transition line should detach from the horizontal axis and approach the classical critical point in the limit $p \to 0$. Around the classical phase transition, the system must be governed by classical thermal fluctuations.

One could complain, and claim that the impossibility of reaching $T = 0$ also inhibits the existence of quantum phase transitions in nature. However, characteristics of the transition can be detected in the system's low-temperature behavior near the quantum critical point. At non-zero temperatures, classical fluctuations with an energy scale k_BT compete with the quantum fluctuations of energy scale $\hbar\omega$, with ω the characteristic frequency of the quantum oscillations. Quantum fluctuations dominate the system's behavior in the *quantum critical region* where $\hbar\omega > k_BT$, and may lead to unconventional and unexpected physical behavior. This zone is sketched in Fig. 3.5 surrounded by two blue lines. Instead, close to the critical line that joins the quantum and classical critical points thermal fluctuations should dominate and render the critical properties thermal.

In the problems we will focus on, the energy of the ground state and first excited state are separated by a finite *gap* Δ for all finite size systems. In the infinite size limit, this minimal gap, associated to an avoided level crossing, can close at a particular value of the control parameter and thus allow for a transition. The transition corresponds to a

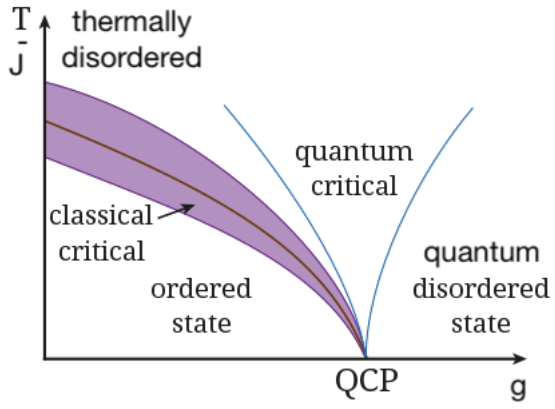

Figure 3.5: A quantum phase diagram. Say that p is the adimensional parameter that controls the strength of quantum fluctuations and T temperature, also adimensionalized by dividing it by some energy scale J.

strong change in the macroscopic properties of the ground state, and the (space and time) correlations suffer a qualitative change when going through it.

In a quantum problem the kinetic and potential terms in $\hat{\mathcal{H}}$ in general do not commute and, therefore, the quantum mechanical partition function does not factorize. Thus, the statics and dynamics are always coupled in a quantum system. An order parameter needs to be formulated in terms of space and time dependent operators.

In a classical phase transition, in addition to the long-range correlations in space there are analogous long-range correlations of the order parameter fluctuations in time. The typical time scale for a decay of the fluctuations is the correlation (or equilibration) time t_c. As the critical point is approached the correlation time diverges as

$$t_c \sim \xi^z \tag{3.189}$$

where ξ is the spatial correlation length and z is the dynamic critical exponent which links times to lengths. At a second order phase transition, fluctuations occur on all length and time scales, and the system is scale-invariant in both. As a consequence, all observables depend via power laws on the external parameters.

We have already seen that a d dimensional quantum problem can be mapped on a classical model in $d+1$ space dimensions, with the additional coordinate, which originates in time, having length $\beta\hbar$ and hence diverging at $T \to 0$. Time scales like the z-th power of a length. (Note that $z = 1$ for many transitions in clean insulators, however, in general other values of z including fractional ones can occur.)

We will study *second order* quantum phase transitions, in which the gap closes as

$$\Delta \sim J|g - g_c|^{z\nu} \tag{3.190}$$

with J the energy scale of the microscopic coupling and g the adimensional parameter

driving the transition.[3] $z\nu$ is a critical exponent. The correlation length diverges

$$\xi \sim \Lambda |g - g_c|^{-\nu} \tag{3.191}$$

with Λ a microscopic length scale typically of the order of the lattice spacing and z a *dynamic critical exponent* characterising the behaviour of time dependent correlations and

$$\Delta \sim \xi^{-z} \ . \tag{3.192}$$

These transitions concern the properties of the ground state. It is thus also very important to understand the implications of a very weak temperature on the ideal zero temperature ones, since in experiments there are always some thermal effects.

When both thermal and quantum fluctuations are active one has to quantify the importance of ones with respect to the other ones and decide whether the theory of classical phase transitions is enough to describe the critical phenomenon or some new features arise due to the quantum fluctuations. The hand-waving argument to decide, which was already mentioned above, is to compare the energy scales

$$\hbar\omega \quad vs. \quad k_B T \tag{3.193}$$

When the thermal energy dominates a classical description is appropriate. Otherwise, it is not.

A magnetic realisation of a quantum phase transition is achieved in the *insulator* $LiHoF_4$. The Ho ions can fluctuate between two states. At $T = 0$ the dipolar interactions between these ions puts them in a ferromagnetically ordered state. A field transverse to the preferred Ising-like direction can then be applied, and for a sufficiently strong strength leading to a too high tunnelling rate, disorder the samples towards a *quantum paramagnet*. Besides, thermal fluctuations can also be switched on and disorder the sample towards a *classical paramagnet*. Other experimental examples can be found in [23].

In the rest of this Section we deal with the quantum Ising chain, the simplest example with such a phase transition. In TD7 the Ising model defined on a fully connected graph with be analysed with different methods.

3.4.1 The quantum Ising chain

The quantum Ising chain or *transverse field Ising model* is the simplest quantum model with a zero temperature phase transition. The Hamiltonian is

$$\hat{\mathcal{H}} = -J \sum_{i=1}^{L-1} \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z - Jg \sum_{i=1}^{L} \hat{\sigma}_i^x \equiv \hat{\mathcal{H}}_\ell + \hat{\mathcal{H}}_t \ , \tag{3.194}$$

[3] In this Section we shall follow the notation in [23]

with free boundary conditions but one can simply impose periodic boundary conditions as well. The spin operators

$$\hat{\sigma}_i^a = \underbrace{\mathbb{I} \otimes \mathbb{I} \cdots \otimes \hat{\sigma}^a \otimes \mathbb{I} \cdots \otimes \mathbb{I}}_{L}$$

are Pauli matrices at site i (see App. 3.A). The operators $\hat{\sigma}_i^a$ with $i \neq j$ commute with each other. We called $\hat{\mathcal{H}}_\ell$ the first term, for longitudinal, and $\hat{\mathcal{H}}_t$ the second one, for transverse.

The two terms in the Hamiltonian do not commute. $J > 0$ sets the energy scale and g is the dimensionless parameter that takes the system through the quantum phase transition since it measures the relevance of the second compared to the first term, and hence the non-commutation of terms in the Hamiltonian.

- For $g = 0$ the Hamiltonian involves only $\hat{\sigma}_i^z$ and reduces to the classical Ising model. The term proportional to J favours magnetic ordering.
- For $g \neq 0$ the Hamiltonian has a transverse field term which no longer commutes with $\hat{\sigma}^z$. The $\hat{\sigma}^x$ induce quantum tunnelling and flip the spins. At zero T there are no thermal fluctuations, but the term proportional to g can flip the spins and destroy the order.

The phase diagram and the critical behaviour of this model are known exactly since the work of Barouch and McCoy in 1971. The solution described below, based on a mapping on a free fermion model, is due to Lieb *et al.* [25, 26, 27]. It is a technique which has been successfully used to other one dimensional quantum models and it is worth learning it. We present now a detailed analysis of this case.

Symmetry

The Hamiltonian (3.194) commutes with the operator

$$\hat{P} \equiv \prod_i \hat{\sigma}_i^x \ . \tag{3.195}$$

$\hat{P}$ is *Hermitian* $\hat{P}^\dagger = \hat{P}$, *idempotent* $\hat{P}^2 = \mathbb{I}$, and also *unitary* $\hat{P}\hat{P}^\dagger = \mathbb{I}$. $\hat{P}$ transforms the operators as

$$\hat{P}^\dagger \, \hat{\sigma}_i^x \, \hat{P} = \hat{\sigma}_i^x \qquad\qquad \hat{P}^\dagger \, \hat{\sigma}_i^z \, \hat{P} = -\hat{\sigma}_i^z \tag{3.196}$$

and it flips all spins from $|\uparrow\rangle$ to $|\downarrow\rangle$ and *vice-versa*. It generates a *global $\mathbb{Z}_2$ symmetry*. Since they commute, $\hat{\mathcal{H}}$ and $\hat{P}$ can be diagonalised in the same basis,

$$\hat{\mathcal{H}}|\psi_n\rangle = E_n|\psi_n\rangle \qquad\qquad \hat{P}|\psi_n\rangle = \pm|\psi_n\rangle \ . \tag{3.197}$$

Exercise 3.6 Prove all the statements above.

This property generalizes the up-down symmetry of classical Ising models with no applied field.

Ground states and low-lying excitations

Let us consider separately the limits in which one or the other term in the Hamiltonian dominate.

Transverse field dominates

For $g \gg 1$ the transverse field term in the Hamiltonian dominates and the unique ground state is

$$|\,0\,\rangle_{g\gg 1} = \prod_i |\,\rightarrow\rangle_i \qquad \text{with} \qquad |\,\rightarrow\rangle_i = \frac{1}{\sqrt{2}}\left(|\,\uparrow\rangle_i + |\,\downarrow\rangle_i\right) \tag{3.198}$$

the eigenstate of $\hat{\sigma}_i^x$ with eigenvalue $+1$. The ground state has energy $E_0 = -gJL$.

This is a *quantum paramagnet*. In the z basis $|\,0\,\rangle_{g\gg 1}$ is a flat superposition on all up-down states

$$|\,0\,\rangle_{g\gg 1} = \frac{1}{2^{L/2}} \prod_i \otimes \sum_{\sigma=\uparrow,\downarrow} |\sigma\rangle_i \,. \tag{3.199}$$

Neglecting the effect of the first term in the Hamiltonian ($g \to \infty$) the lowest lying excitations are such that a single spin i changed from $|\,\rightarrow\rangle_i$ to the eigenstate of $\hat{\sigma}_i^x$ with eigenvalue -1,

$$|\,\leftarrow\rangle_i = \frac{1}{\sqrt{2}}\left(|\,\uparrow\rangle_i - |\,\downarrow\rangle_i\right) . \tag{3.200}$$

There are L degenerate such *single particle* states. They have energy $E_1 = E_0 + 2Jg$ and the gap is $\Delta = E_1 - E_0 = 2Jg$. To get a macroscopic energy different one needs to reverse a macroscopic number of spins.

One can see now what is the effect of the longitudinal term $\hat{\mathcal{H}}_\ell = -J\sum_i \hat{\sigma}_i^z \hat{\sigma}_{i+1}^z$ on these excited states in perturbation theory. Calling $|i\rangle$ the state with the reversed i spin, the matrix element of $\hat{\mathcal{H}}_\ell$ is

$$\langle j|\hat{\mathcal{H}}_\ell|i\rangle = -J(\delta_{j,i-1} + \delta_{j,i+1}) \tag{3.201}$$

so $\hat{\mathcal{H}}_\ell$ has the effect of moving the spin flips on the lattice.

With these excitations one builds the wave functions

$$|k\rangle = \frac{1}{\sqrt{L}} \sum_i e^{ikx_i} |i\rangle \tag{3.202}$$

with excess energy with respect to the one of the ground state

$$\Delta e_k = 2Jg\left[1 - \frac{1}{g}\cos(ka) + \mathcal{O}(1/g^2)\right] \tag{3.203}$$

above the ground state, where a is the lattice spacing. The minimum of this expression is achieved for $k = 0$, $\Delta e_k^{\min} = 2J(g-1) + \mathcal{O}(1/g)$, and the *gap closes* for $g = 1$. (The

analysis of "two particle" states and more details on the spectrum in the perturbative limit can be found in [23].)

One can check that there are no longitudinal correlation $\langle 0 | \hat{\sigma}_i^z \hat{\sigma}_j^z | 0 \rangle_{g \gg 1} = \delta_{ij}$ in the ground state. One can expect that perturbative corrections in $1/g$ will build correlations between distant spins and

$$\langle 0 | \hat{\sigma}_i^z \hat{\sigma}_j^z | 0 \rangle_{g \gg 1} \sim e^{-|x_i - x_j|/\xi} \tag{3.204}$$

for large $|x_i - x_j|$ where x_i is the position of the ith spin and $| 0 \rangle_{g \gg 1}$ is the exact ground state for large g. The correlation length ξ should diverge approaching $g = 1$ from above with the critical exponent ν.

Longitudinal alignement

In the opposite limit $g \ll 1$ the two degenerate $g = 0$ ground states are

$$| 0 \rangle_{g=0} = \prod_i | \uparrow \rangle_i \qquad \text{or} \qquad | 0 \rangle_{g=0} = \prod_i | \downarrow \rangle_i \tag{3.205}$$

with energy $E_0 = -JL$.

At finite g some spins will be flipped but the two ground states remain perfectly degenerate because of the global $\mathbb{Z}_2$ symmetry that we already discussed (one would need to reverse L spins to go from one state to the other).

The basic excitations are the states with *domain walls*, which can also be thought of as particles since they are localized in space. The Hamiltonian hops these particles from one site to their neighbour

$$\langle i | \hat{\mathcal{H}} | i + 1 \rangle = -Jg \ . \tag{3.206}$$

Constructing plane waves from these excitations, they have excess energy

$$\Delta e_k = 2J \left[1 - g \cos(ka) + \mathcal{O}(g^2) \right] \tag{3.207}$$

Once again, the minimum is $\Delta e_k^{\min} = 2J(1 - g) + \mathcal{O}(g^2)$ and the gap closes at $g = 1$.

As regards the correlation functions, one expects

$$\langle 0 | \hat{\sigma}_i^z \hat{\sigma}_j^z | 0 \rangle_{g \sim 0} \sim \langle 0 | \hat{\sigma}_i^z | 0 \rangle_{g \sim 0} \langle 0 | \hat{\sigma}_j^z | 0 \rangle_{g \sim 0} \sim m^2 \tag{3.208}$$

for large $|x_i - x_j|$ where x_i is the position of the ith spin and $| 0 \rangle$ is the exact ground state for $g \ll 1$. m is the spontaneous magnetisation of the ground state. The connected correlation - correlation of fluctuations - should give access to an exponential decay controlled by a correlation length, diverging at $g \to 1^-$.

Since there is no way to go from the exponentially decaying correlations for $g \gg 1$ to the constant limit for $g \ll 1$ in an analytic way, there must be (at least) a phase transition at some intermediate g, where the system changes ground state. The correlation length diverges at g_c and the correlations at this particular value of the control parameter decay as power laws. m plays the role of the order parameter and it vanishes algebraically at g_c.

3.4.2 Duality

The basic excitations are spin flips for $g \gg 1$ and domain walls for $g \ll 1$. The spin flips are located at a lattice site, while the domain walls one can think of as being located in between two sites.

The spins flips are created by $\hat{\sigma}^z$ and the domain walls by $\prod_{j\leq i}\hat{\sigma}^x_i$, since this operator flips all the spins from up to down or vice versa to the left of the site $i+1$. The spin flips and domain walls are counted by $\hat{\sigma}^x_i$ and $\hat{\sigma}^z_i\hat{\sigma}^z_{i+1}$, respectively.

Defining

$$\hat{\tau}^z_{\bar{i}} \equiv \prod_{j\leq i}\hat{\sigma}^x_i \,, \qquad \bar{i} = i+1/2 \tag{3.209}$$

$$\hat{\tau}^x_{\bar{i}} \equiv \hat{\sigma}^z_i\hat{\sigma}^z_{i+1} \,, \qquad \bar{i} = i+1/2 \tag{3.210}$$

These new operators are defined on the *dual lattice* (mid points of the original lattice, with the same lattice spacing a, say) and satisfy

$$\{\hat{\tau}^\alpha_{\bar{i}}, \hat{\tau}^\beta_{\bar{i}}\} = 2\delta^{\alpha\beta} \,, \tag{3.211}$$

the same algebra as the original Pauli matrices, and commute on different sites. Setting, for simplicity, periodic boundary conditions, the Hamiltonian can be rewritten in terms of the $\hat{\tau}$ operators as

$$\hat{\mathcal{H}} = -J\sum_{\bar{i}}\hat{\tau}^x_{\bar{i}} - Jg\sum_{\bar{i}}\hat{\tau}^z_{\bar{i}}\hat{\tau}^z_{\bar{i}+1} \,, \tag{3.212}$$

that is, it keeps the form of the original model with $g \leftrightarrow 1/g$. Since for every phase transition in one model there must be another one in the other model, if there is only one transition then it must occur at

$$g_c = 1 \,. \tag{3.213}$$

3.4.3 The Jordan-Wigner transformation

In classical physics, Ising spins are very similar to occupation numbers. Indeed, one can map $s_i = \pm 1$ to $n_i = 1, 0$ via $n_i = (s_i+1)/2$.

In quantum cases, spins $1/2$ are very similar to spin-less fermions (see App. 3.A). The connection can be expressed as

$$\hat{\sigma}^z_i = 1 - 2\hat{c}^\dagger_i\hat{c}_i \,. \tag{3.214}$$

Consider a basis vector with all spins down (in the z-direction) and use the notations $|0\rangle \equiv |\ldots\downarrow\ldots\rangle$ and $|1\rangle \equiv |\ldots\uparrow\ldots\rangle$. The state $|0\rangle$ is the vacuum destroyed by all the lowering operators $\hat{\sigma}^-_i$,

$$\hat{\sigma}^-_i|0\rangle = 0 \qquad \forall i$$

and from it, all other states can be built up by applying raising operators $\hat{\sigma}^+_i$.

The raising and lowering operators $\hat{\sigma}^{\pm} = (\sigma^x \pm i\sigma^y)/2$ would be candidates to identify with creation and annihilation operators. However, although they satisfy local anti-commutation relations

$$\{\hat{\sigma}_i^+, \hat{\sigma}_i^-\} = \mathbb{I} \qquad \text{for all } i\,,$$

they commute at different sites, differently from actual fermions, which also anti-commute on different sites. For future reference we recall that with these conventions $[\hat{\sigma}_i^+, \hat{\sigma}_i^-] = \hat{\sigma}_i^z$.

True fermionic operators $\hat{c}_i$ and $\hat{c}_i^+$ are constructed through a Jordan-Wigner transformation as follows. Define modified raising and lowering operators

$$\begin{aligned} \hat{\sigma}_i^+ &= \left[\prod_{j<i}(1-2\hat{c}_j^\dagger\hat{c}_j)\right]\hat{c}_i\,, \\ \hat{\sigma}_i^- &= \left[\prod_{j<i}(1-2\hat{c}_j^\dagger\hat{c}_j)\right]\hat{c}_i^\dagger\,, \end{aligned} \tag{3.215}$$

The *string operator* $\prod_{j<i}(1-2\hat{c}_j^\dagger\hat{c}_j)$ is Hermitian and takes values ± 1 depending on whether an even/odd number of fermions is present to the left of site i. With this definition, the modified $\hat{\sigma}_i^{\pm}$ commute at different sites. Take $i<k$; then,

$$\begin{aligned} \hat{\sigma}_i^+\hat{\sigma}_k^- &= \prod_{j<i}(1-2\hat{c}_j^\dagger c_j)\hat{c}_i \prod_{m<k}(1-2\hat{c}_m^\dagger\hat{c}_m)\hat{c}_k^\dagger \\ &= \prod_{m<k}(1-2\hat{c}_m^\dagger c_m)\hat{c}_k^\dagger \prod_{j<i}(1-2\hat{c}_j^\dagger\hat{c}_j)(-1)^2\hat{c}_i \\ &= \hat{\sigma}_k^-\hat{\sigma}_i^+\,. \end{aligned} \tag{3.216}$$

The inverse relations are

$$\hat{c}_i = \left(\prod_{j<i}\hat{\sigma}_j^z\right)\hat{\sigma}_i^+\,, \qquad \hat{c}_i^\dagger = \left(\prod_{j<i}\hat{\sigma}_j^z\right)\hat{\sigma}_i^-\,. \tag{3.217}$$

The relations

$$\{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij} \qquad \{\hat{c}_i, \hat{c}_j\} = \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = 0 \tag{3.218}$$

imply

$$[\hat{\sigma}_i^+, \hat{\sigma}_j^-] = \delta_{ij}\hat{\sigma}_i^z \qquad [\hat{\sigma}_i^z, \hat{\sigma}_j^\pm] = \pm 2\delta_{ij}\hat{\sigma}_i^\pm \tag{3.219}$$

and *vice versa*.

Let us now apply the Jordan Wigner transformation to the quantum Ising chain. Write the mapping as

$$\hat{\sigma}_i^x = \mathbb{I} - 2\hat{c}_i^\dagger\hat{c}_i \qquad \hat{\sigma}_i^z = -\prod_{j<i}(1-2\hat{c}_j^\dagger\hat{c}_j)(\hat{c}_i + \hat{c}_i^\dagger) \tag{3.220}$$

In terms of the fermionic operators the Hamiltonian takes a quadratic form

$$\hat{\mathcal{H}} = -J\sum_{i=1}^{L-1}[\hat{c}_i^\dagger \hat{c}_{i+1} + \hat{c}_i^\dagger \hat{c}_{i+1}^\dagger + h.c.] - gJ\sum_{i=1}^{L-1}(1 - 2\hat{c}_i^\dagger \hat{c}_i)\ . \tag{3.221}$$

The Hamiltonian is now one of *non-interacting fermions*. Particle number is non-conserved due to the $\hat{c}_i^\dagger \hat{c}_i^\dagger$ terms and their Hermitian conjugates. Still, the Hamiltonian can be diagonalised as we explain in the next Section. Parity is conserved.

3.4.4 The Bogoliubov transformation

The fermionic Hamiltonian can be diagonalised by introducing the plane wave basis

$$\hat{c}_k = \frac{1}{\sqrt{L}}\sum_j \hat{c}_j\, e^{-\mathrm{i}kx_j} \tag{3.222}$$

These are *collective operators*. By inserting these expressions,

$$\begin{aligned}
\hat{\mathcal{H}} &= J\sum_k \{2(g-\cos(ka))\hat{c}_k^\dagger \hat{c}_k - i\sin(ka)(\hat{c}_{-k}^\dagger \hat{c}_k^\dagger + \hat{c}_{-k}\hat{c}_k) - g\} \\
&= 2J\sum_{k>0}\left\{(\hat{c}_k^\dagger\ \ \hat{c}_{-k})\begin{pmatrix} g-\cos(ka) & i\sin(ka) \\ -i\sin(ka) & -g+\cos(ka)\end{pmatrix}\begin{pmatrix}\hat{c}_k \\ \hat{c}_{-k}^\dagger\end{pmatrix} - g + (g-\cos(ka)\right\} \\
&\quad +2J(g-1)\hat{c}_0^\dagger \hat{c}_0
\end{aligned} \tag{3.223}$$

The matrix in the $k>0$ part of the spectrum can be written as

$$\mathbb{A}_k = \begin{pmatrix} g-\cos(ka) & i\sin(ka) \\ -i\sin(ka) & -g+\cos(ka)\end{pmatrix} = [g-\cos(ka)]\sigma^z - \sin(ka)\sigma^y \tag{3.224}$$

and it can be diagonalised, $\mathbb{D}_k = U_k^\dagger \mathbb{A}_k U_k$, via the rotation matrix

$$U_k = e^{-i\theta_k\sigma^x/2} = \cos(\theta_k/2)\mathbb{I} - i\sin(\theta_k/2)\sigma^x \tag{3.225}$$

with the angle θ_k defined by

$$\tan\theta_k = \frac{\sin(ka)}{g-\cos(ka)}\ . \tag{3.226}$$

Expanding the product $U_k^\dagger \mathbb{A}_k U_k$, collecting all terms proportional to σ^z on the one hand and the ones proportional to σ^y on the other, one shows that the choice (3.226) kills the latter and makes the former yield

$$\mathbb{D}_k = U_k^\dagger \mathbb{A}_k U_k = \sqrt{(g-\cos(ka))^2 + \sin^2(ka)}\ \sigma^z\ . \tag{3.227}$$

Concerning the fermions

$$\begin{pmatrix}\hat{c}_k \\ \hat{c}_{-k}^\dagger\end{pmatrix} = \hat{U}_k\begin{pmatrix}\hat{\gamma}_k \\ \hat{\gamma}_{-k}^\dagger\end{pmatrix} = \begin{pmatrix}\cos(\theta_k/2) & -i\sin(\theta_k/2) \\ -i\sin(\theta_k/2) & cos(\theta_k/2)\end{pmatrix}\begin{pmatrix}\hat{\gamma}_k \\ \hat{\gamma}_{-k}^\dagger\end{pmatrix} \tag{3.228}$$

One can check that $\{\hat{c}_k, \hat{c}^\dagger_{k'}\} = \delta_{k,k'} \Leftrightarrow \{\hat{\gamma}_k, \hat{\gamma}^\dagger_{k'}\} = \delta_{k,k'}$. All in all,

$$\hat{\mathcal{H}} = \sum_k \epsilon_k \left(\hat{\gamma}_k \hat{\gamma}^\dagger_k - \frac{1}{2} \right) + \text{cst} \tag{3.229}$$

with

$$\epsilon_k = 2J\sqrt{(g - \cos(ka))^2 + \sin^2(ka)} \; . \tag{3.230}$$

We have *fully diagonalised* the Hamiltonian with these transformations. It became one of free fermions. The ground state has no fermions $\hat{\gamma}_k|0\rangle = 0$ for all k and the excited states are built by acting with $\hat{\gamma}^\dagger_k$ on $|0\rangle$.

The minimum of the spectrum (3.230) is

$$\min_k \epsilon_k = 2J|g-1| \qquad k_{\min} = 0 \; . \tag{3.231}$$

The limiting form in the two extremes of the control parameter are

$$\begin{aligned} g \ll 1 \quad &\Longrightarrow \quad \epsilon_k = 2J[1 - g\cos(ka)] + \mathcal{O}(g^2) \\ g \gg 1 \quad &\Longrightarrow \quad \epsilon_k = 2Jg[1 - (1/g)\cos(ka)] + \mathcal{O}(1/g^2) \end{aligned} \tag{3.232}$$

as found before.

A field theory, extending the Ginzburg-Landau ideas to the quantum real, can be constructed in the continuous and scaling limit [23].

The phase transition

Having derived the full spectrum $\epsilon_k(g)$ we can draw it, both for $g < 1$ and $g > 1$. In both cases the gap at $k = 0$ vanishes for $g_c = 1$, the critical point.

The critical point separates ferromagnetic phase, in which the ground state has symmetry broken $\mathbb{Z}_2$, from a paramagnetic ground state. In both phases there is a gap $|g - g_c|$.

At the critical point the correlation time diverges together with the correlation length

$$\tau > \frac{\hbar}{\Delta} \qquad \xi = \frac{c\hbar}{\Delta} \tag{3.233}$$

with $c = 2Ja/\hbar$ the speed of the gapless excitations at criticality. These divergent scales help one construct a field theory in $1 + 1$ dimensions.

Higher dimensions

Comment: a transformation from a spin model to a particle one can also be done in higher dimensions. The difference is that it is done with creation and annihilation operators which anti-commute on the same site but commute on different sites. The particle models thus derived are like classical lattice gas models with exclusion; there cannot be double (or higher) occupation of any site.

Classical-quantum mapping

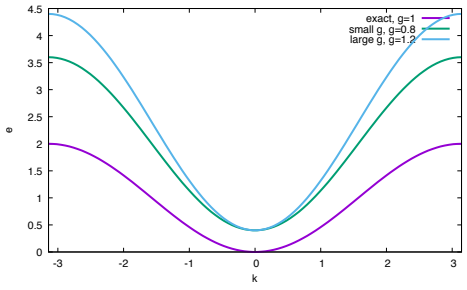

Figure 3.6: Spectra. Exact, and $g \gg 1$ and $g \ll 1$ approximations.

We have just solved the quantum Ising chain with essentially quantum methods. In the previous Section we discussed the quantum-classical mapping so, why not simply use it to obtain the same critical properties? The answer is yes, we could do it, but some properties of the quantum problem are better captured by the quantum formalism. For instance, linear response functions (which are measurable experimentally) are defined in real (and not imaginary) time. Performing the transformation from imaginary to real time is a difficult and some times ill-posed problem. Concepts like the phase coherence time have no classical analog. Finally, at finite temperature, the equivalent classical model is defined on a slab geometry in which the original d dimensions are infinite extent while the imaginary time one is finite. This makes the classical problem hard to deal with.

Appendices

3.A Appendices

We recall here definitions and properties of the spin 1/2 operators. You can find a very detailed description of this in [21].

3.A.1 The spin 1/2

The spin (angular momentum) is a quantum observable, which in three-dimensional Euclidean space is represented by a three component operator $\hat{\vec{S}} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$. The states are represented by two component spinors.

The commutation relation of spin 1/2 operators are

$$[\hat{S}_i^a, \hat{S}_j^b] = i\hbar\epsilon_{abc}\hat{S}_i^c\delta_{ij} \ , \tag{3.A.1}$$

with Latin indices taking values $1, 2, 3$ and corresponding to x, y, z. We stress that spin operators acting on different sites commute.

The spin 1/2 operators have eigenvalues $\pm\hbar/2$. For instance,

$$\hat{S}_z \,|\uparrow\rangle = \frac{\hbar}{2}\,|\uparrow\rangle \qquad\qquad \hat{S}_z \,|\downarrow\rangle = -\frac{\hbar}{2}\,|\downarrow\rangle \ , \tag{3.A.2}$$

and see the Pauli subsection to identify the eigenvectors of the other two operators, $\hat{S}_x$, and $\hat{S}_y$. The states $|\uparrow\rangle$ and $|\downarrow\rangle$ are also represented as $|+\rangle$ and $|-\rangle$.

The Hilbert space of a single spin is two-dimensional: for instance a basis is $\{|\uparrow\rangle, |\downarrow\rangle\}$, the two eigenstates of $\hat{S}_z$.

Raising and *lowering*, or *ladder* operators are defined as

$$\hat{S}_i^+ = \hat{S}_i^x + i\hat{S}_i^y \qquad\qquad \hat{S}_i^+ = \hat{S}_i^x - i\hat{S}_i^y \tag{3.A.3}$$

and act on the up and down state as

$$\begin{aligned} \hat{S}_i^+|-\rangle &= |+\rangle & \hat{S}_i^-|+\rangle &= |-\rangle \\ \hat{S}_i^+|+\rangle &= |-\rangle & \hat{S}_i^-|-\rangle &= |+\rangle \end{aligned} \tag{3.A.4}$$

Exercise 3.7 Show that

$$\{\hat{S}_i^+, \hat{S}_j^-\} = \delta_{ij} \tag{3.A.5}$$

with $\{\ ,\ \}$ the anti-commutator.

Equations (3.A.4) are thus similar to the action of creation and annihilation spinless fermionic operators

$$\begin{aligned} \hat{c}_i^\dagger|0\rangle &= |1\rangle & \hat{c}_i|1\rangle &= |0\rangle \\ \hat{c}_i^\dagger|1\rangle &= |0\rangle & \hat{c}_i|0\rangle &= |1\rangle \end{aligned} \tag{3.A.6}$$

On different sites the spin operators commute and are then different from fermion operators.

3.A.2 The Pauli matrices

The spin operators are often represented by 2×2 complex *Pauli matrices* and the states by two row columnar vectors. These matrices are labeled with numbers or directions, $\sigma^1 = \sigma^x$, $\sigma^2 = \sigma^y$, $\sigma^3 = \sigma^z$, with

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3.A.7}$$

In this representation $\hat{s}_a = \hbar/2\sigma_a$. We list below a number of important properties.

- They are Hermitian $(\sigma^a)^\dagger = \sigma^a$, for $a = 1, 2, 3$, with the † operation consisting in the combination of a transposition and complex conjugate operation.
- Together with the identity matrix $\mathbb{I}$ (sometimes noted σ^0) the Pauli matrices form a basis for the real vector space of 2×2 Hermitian matrices: any such matrix can be written in a unique way as a linear combination of them, with all coefficients being real numbers.
- Their inverses equal themselves, as they square to the identity, $(\sigma^a)^2 = \mathbb{I}$. In other words, they are nilpotent.
- Their traces vanish, $\mathrm{Tr}\,\sigma^a = 0$ and their determinants are all equal, $\det \sigma^a = -1$, for $a = 1, 2, 3$.
- Consequently, their eigenvalues are ± 1.
- Their normalized eigenvectors are

$$\sigma_z : \qquad |\uparrow\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad |\downarrow\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{3.A.8}$$

$$\sigma_y : \qquad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix} \qquad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix} \tag{3.A.9}$$

$$\sigma_x : \qquad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \tag{3.A.10}$$

  respectively.

- Their commutation relations are

$$[\sigma^a, \sigma^b] = 2\mathrm{i}\epsilon_{abc}\sigma^c \tag{3.A.11}$$

  with ϵ_{abc} the Levi-Civita symbol, $\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = 1$, $\epsilon_{132} = \epsilon_{321} = \epsilon_{213} = -1$, and zero in all cases in which two indices are equal.

- They anti-commute: $\{\sigma^a, \sigma^b\} = 2\delta_{ab}\mathbb{I}$.
- One readily checks $\sigma^a\sigma^b = \delta^{ab} + \mathrm{i}\epsilon^{abc}\sigma^c$.
- $\sigma^y \,|\uparrow\rangle = \begin{pmatrix} 0 \\ \mathrm{i} \end{pmatrix}$ and $\sigma^y \,|\downarrow\rangle = \begin{pmatrix} -\mathrm{i} \\ 0 \end{pmatrix}$.

3.A.3 The matrix element

Let us start recalling a number of basic properties of quantum mechanics.

The combination of exponentials of non-commuting operators is given by the *Baker-Campbell-Hausdorff formula*

$$e^{\hat{A}}\, e^{\hat{B}} = e^{\hat{A}+\hat{B}+\frac{1}{2}[\hat{A},\hat{B}]+\ldots}\,, \tag{3.A.1}$$

where higher-order repeated commutators are shown by the dots.

The *Trotter product formula* applies to arbitrary $n \times n$ complex matrices or operators and it reads

$$e^{\mathrm{i}(\hat{A}+\hat{B})} = \lim_{N\to\infty} (e^{\mathrm{i}\hat{A}/N} e^{\mathrm{i}\hat{B}/N})^N \tag{3.A.2}$$

At least formally, the evolution operator $\hat{U} = e^{-\mathrm{i}\hat{\mathcal{H}}t/\hbar}$ can be expressed in terms of the eigenstates $|n\rangle$ of $\hat{\mathcal{H}}$, $\hat{\mathcal{H}}|n\rangle = E_n|n\rangle$,

$$\hat{U} = e^{-\mathrm{i}\hat{\mathcal{H}}t/\hbar} = \sum_n |n\rangle\langle n| e^{-\mathrm{i}E_n t/\hbar}\,. \tag{3.A.3}$$

In the $|x\rangle$ basis,

$$\langle x|\hat{U}|x'\rangle = \sum_n \langle x|n\rangle\langle n|x'\rangle e^{-\mathrm{i}E_n t/\hbar} = \sum_n \psi_n(x)\psi_n^*(x') e^{-\mathrm{i}E_n t/\hbar}\,. \tag{3.A.4}$$

One can check that $U(x',t;x,0) \to \delta(x-x')$.

Exercise 3.8 Use the fact that for a free particle of mass m, the states $|n\rangle$ are just plane wave momentum states, and take the continuum limit of the sum over n (which becomes an integral over momenta) to show $U(x,t;x',0) = (m/2\pi\mathrm{i}\hbar t)^{1/2} \exp[\mathrm{i}m(x-x')^2/(2\hbar t)]$.

– Take an *orthonormal complete basis* of eigenstates, $|x\rangle$, of the position operator, $\hat{x}$, that is $\hat{x}|x\rangle = x|x\rangle$, with $\langle x'|x\rangle = \delta(x-x')$.

– Fourier transform each of these states,

$$|p\rangle = \int \frac{dx}{\sqrt{2\pi\hbar}}\, e^{\mathrm{i}xp/\hbar}\,|x\rangle\,, \tag{3.A.5}$$

and build another orthonormal complete basis of eigenstates, now of the momentum operator, $\hat{p}|p\rangle = p|p\rangle$. Indeed,

$$\begin{aligned}\langle p'|p\rangle &= \frac{1}{2\pi\hbar}\int dx \int dy\; e^{\mathrm{i}px/\hbar}e^{-\mathrm{i}p'y/\hbar}\,\langle y|x\rangle \\ &= \frac{1}{2\pi\hbar}\int dx \int dy\; e^{\mathrm{i}px/\hbar}e^{-\mathrm{i}p'y/\hbar}\,\delta(y-x) \\ &= \frac{1}{2\pi\hbar}\int dx\; e^{\mathrm{i}(p-p')x/\hbar} \\ &= \delta(p-p')\;. \end{aligned} \tag{3.A.6}$$

With these normalisations, two *resolutions of the identity* are

$$1 = \int dx\;|x\rangle\langle x| = \int dp\;|p\rangle\langle p|\;. \tag{3.A.7}$$

Because of the orthonormality of the elements $|x\rangle$, the bra-kets

$$\langle x|p\rangle = \frac{e^{\mathrm{i}xp/\hbar}}{\sqrt{2\pi\hbar}} \tag{3.A.8}$$

are *plane waves*. (As usual with Fourier transforms, there is some liberty in the placement of the $2\pi\hbar$ factor. We use this convention.)

In the rewriting of the finite time evolution function we encounter factors which are *matrix elements* of the kind

$$U(x_{k+1},t_{k+1};x_k,t_k) = \langle x_{k+1}|e^{-\mathrm{i}\,\hat{\mathcal{H}}\frac{\delta t}{\hbar}}|x_k\rangle\;. \tag{3.A.9}$$

This infinitesimal evolution operator can be factorised over the time-interval $\delta t \to 0$, since one can neglect the non-commutativity of the kinetic and potential energy terms (the higher order terms are proportional to higher powers of δt, which is infinitesimal[4]), and use Trotter's formula:

$$e^{-\mathrm{i}\hat{\mathcal{H}}\frac{\delta t}{\hbar}} \approx e^{-\mathrm{i}\,\frac{\hat{p}^2}{2m}\frac{\delta t}{\hbar}}e^{-\mathrm{i}\,V(\hat{x})\frac{\delta t}{\hbar}}\;. \tag{3.A.10}$$

Then,

$$U(x_{k+1},t_{k+1};x_k,t_k) = e^{-\mathrm{i}\,V(x_k)\frac{\delta t}{\hbar}}\;\langle x_{k+1}|e^{-\mathrm{i}\,\frac{\hat{p}^2}{2m}\frac{\delta t}{\hbar}}|x_k\rangle\;, \tag{3.A.11}$$

where the operator $V(\hat{x})$ acting on the right ket gave rise to the function V evaluated at the eigenvalue x_k. The remaining factor is the *free-particle propagator*. Inserting now the identity

$$\mathbb{I} = \int dp_k\;|p_k\rangle\langle p_k| \tag{3.A.12}$$

[4]While all this is fine for finite-dimensional matrices with finite matrix elements, it can be more delicate for operators in Hilbert space which could have large or even singular matrix elements. Still, we follow this route and neglect higher order terms in all the non-pathological cases we will deal with here.

we have

$$\begin{aligned} U(x_{k+1},t_{k+1};x_k,t_k) &= e^{-\mathrm{i}\,V(x_k)\frac{\delta t}{\hbar}} \int dp_k\ \langle x_{k+1}|e^{-\mathrm{i}\,\frac{\hat{p}^2}{2m}\frac{\delta t}{\hbar}}|p_k\rangle\ \langle p_k|x_k\rangle \\ &= e^{-\mathrm{i}\,V(x_k)\frac{\delta t}{\hbar}} \int dp_k\ e^{-\mathrm{i}\,\frac{p_k^2}{2m}\frac{\delta t}{\hbar}}\ \langle x_{k+1}|p_k\rangle\ \langle p_k|x_k\rangle \end{aligned} \tag{3.A.13}$$

Using now that the free-particle wave function is

$$\langle p_k|x_k\rangle = \frac{1}{\sqrt{2\pi\hbar}}\ e^{-\frac{\mathrm{i}}{\hbar}p_k x_k} \tag{3.A.14}$$

we have

$$U(x_{k+1},t_{k+1};x_k,t_k) = \int \frac{dp_k}{2\pi\hbar}\ e^{-\mathrm{i}\,\frac{p_k^2}{2m}\frac{\delta t}{\hbar}}\ e^{\mathrm{i}p_k\left(\frac{x_{k+1}-x_k}{\delta t}\right)\frac{\delta t}{\hbar}}\ e^{-\mathrm{i}\,V(x_k)\frac{\delta t}{\hbar}}\ . \tag{3.A.15}$$

(We note that one cannot evaluate this result from a Taylor series expansion in powers of δt of the exponential of the kinetic energy operator, the result is singular in the $\delta t \to 0$ limit.) The sign of the linear term in p_k in the exponential can be changed to minus, after a change of variables $p_k \to -p_k$. If one now performs the integral over the momentum p_k

$$U(x_{k+1},t_{k+1};x_k,t_k) = \left(\frac{-\mathrm{i}m}{2\pi\delta t\hbar}\right)^{1/2} e^{\mathrm{i}\,\frac{m}{2}\left(\frac{x_{k+1}-x_k}{\delta t}\right)^2\frac{\delta t}{\hbar}-\mathrm{i}\,V(x_k)\frac{\delta t}{\hbar}}\ . \tag{3.A.16}$$

The prefactor is included in the integral measure and no longer written.

3.A.4 Stationary phase approximation

The stationary phase approximation extends the steepest descent of Laplace method to integrals of rapidly varying imaginary exponentials. The idea is that sinusoids with rapidly varying phase cancel under the sum over all of them.

Calling $\hbar$ the small parameter, when a function f of a single real variable x has only one extreme x^*, $f'(x^*)=0$, the formula is

$$\lim_{\text{“}\hbar \ll f(x)\text{”}} \int dx\ e^{\mathrm{i}f(x)/\hbar} = e^{\mathrm{i}f(x^*)/\hbar}\ e^{\mathrm{i}\pi/4\ \mathrm{sign}f''(x^*)}\ \left(\frac{2\pi\hbar}{|f''(x^*)|}\right)^{1/2} \tag{3.A.1}$$

The idea to prove this equation is the same as for the usual steepest descent of saddle-point approximation. One expands the function in the exponential to second order in the distance from its extreme x^*:

$$\begin{aligned} f(x) &= f(x^*) + f'(x^*)(x-x^*) + \frac{1}{2}f''(x^*)(x-x^*)^2 + \mathcal{O}((x-x^*)^3) \\ &\sim f(x^*) + \frac{1}{2}f''(x^*)(x-x^*)^2 \end{aligned} \tag{3.A.2}$$

The first term is a constant with respect to x and comes out of integral. The quadratic corrections remain to be integrated over

$$\lim_{\text{“}\hbar \ll f(x)\text{”}} \int dx\; e^{\mathrm{i}f(x)/\hbar} = e^{\mathrm{i}f(x^*)/\hbar} \int dx\; e^{\mathrm{i}\frac{1}{2}f''(x^*)(x-x^*)^2/\hbar}\,. \tag{3.A.3}$$

When $\hbar$ is small compared to $f''(x^*)$, even a small difference $x - x^*$ will lead to rapid oscillations within the integral and cancellations. Then one can integrate over x going from $-\infty$ to ∞. The result is Eq. (3.A.1).

If the function f has several stationary points, then one separates the integral in non-overlapping intervals and approximates the result on each of them separately in the way described above.

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