From Path Integrals to Field Theory

Theoretical Chemistry and Spectroscopy Winter School

Domaine des Masures, Han-sur-Lesse, Belgium

Jean-Sébastien Caux

25-29 November 2019

Where and how I can be reached

Institute of Physics, University of Amsterdam, Room C4.262, Science Park 904, Amsterdam
email: j.s.caux@uva.nl or prof@jscaux.org   tel.: 020 525 5775

Suggested reading (to supplement class notes)

- [**BDFN**] J. J. Binney, N. J. Dowrick, A. J. Fisher and M. E. J. Newman, *The Theory of Critical Phenomena*, Oxford University Press, 1992.

- [**FH**] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals*, McGraw-Hill, New York, 1965.

- [**ID1**] C. Itzykson and J.-M. Drouffe, *Statistical Field Theory 1: From Brownian Motion to Renormalization and Lattice Gauge Theory*, Cambridge Monographs on Mathematical Physics, Cambridge University Press, 1991.

Prerequisites

Physics: classical mechanics, basic statistical and thermal physics, quantum mechanics, electromagnetism.

Mathematics: linear algebra, Fourier transforms, complex variables.

Plan of the course

- Classical paths: Brownian motion and random walks.

- Summing over paths. Exact solution of the two-dimensional Ising model.

- The path integral for a quantum particle

- Rudiments of field theory: from Ising to ϕ^4.

Fourier transformations

In the continuum. Let $f(x)$ be an integrable function of a real parameter x, which satisfies $\int_{-\infty}^{\infty} dx |f(x)| < \infty$. It can be represented as a Fourier transform:

$$f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} f(k) \qquad \text{with coefficients} \qquad f(k) = \int_{-\infty}^{\infty} dx e^{-ikx} f(x) \tag{1}$$

To go from one representation to the other, one uses the identity

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-x_0)} = \delta(x - x_0) \tag{2}$$

Continuum, finite interval. Let $f(x)$ be an integrable function defined on a finite interval $x \in [0, L[$. If we extend the definition of $f(x)$ to the whole real line by assuming (quasi-)periodicity $f(x + L) = e^{i2\pi\alpha} f(x)$ for some $\alpha \in [0, 1[$, we can represent $f(x)$ as the Fourier series

$$f(x) = \frac{1}{L} \sum_{n \in \mathbb{Z}} e^{ik_n x} f_{k_n}, \qquad f_{k_n} = \int_0^L dx e^{-ik_n x} f(x) \qquad \text{where} \qquad k_n \equiv \frac{2\pi}{L}(n + \alpha) \tag{3}$$

To go from one representation to the other, one uses the identities

$$\frac{1}{L} \sum_{n \in \mathbb{Z}} e^{ik_n(x-x_0)} = \sum_{m \in \mathbb{Z}} \delta(x - x_0 - mL), \qquad \int_0^L dx e^{i(k_n - k_m)x} = L\delta_{n,m} \tag{4}$$

The infinite-size limit is easily recovered by using the replacement $\frac{1}{L} \sum_n \to \int_{-\infty}^{\infty} \frac{dk}{2\pi}$.

Finite lattice. Consider a lattice of N points labeled by index $j = 1, ..., N$. We denote the lattice spacing by a. Let f_j be a number associated to site j. Assuming again some (quasi-)periodicity $f_{j+N} = e^{i2\pi\alpha} f_j$, the Fourier series can be defined as (other conventions are possible)

$$f_j = \frac{1}{N} \sum_{k_n \in \text{BZ}} e^{ik_n aj} f_{k_n}, \qquad f_{k_n} = \sum_{j=1}^{N} e^{-ik_n aj} f_j, \qquad k_n \equiv \frac{2\pi}{Na}(n + \alpha) \tag{5}$$

To go from one representation to the other, you can use the identities

$$\frac{1}{N} \sum_{k_n \in \text{BZ}} e^{ik_n a(j-l)} = \delta_{j,l}, \qquad \sum_{j=1}^{N} e^{-i(k_n - k_m)aj} = N\delta_{n,m} \tag{6}$$

The notation $k_n \in$ BZ means that we sum the momenta over one Brillouin zone, for example by convention by choosing $n = -N/2 + 1, -N/2 + 2, ..., N/2$ (for N even) or $n = 0, ..., N - 1$. In the continuum limit $a \to 0$, we simply redefine $Na \to L$, $aj \to x$ and use the rule $a \sum_{j=1}^{N}(...) \to \int_0^L dx(...)$ to fall back onto the earlier formulas.

Infinite lattice. When the lattice becomes infinite ($N \to \infty$ so now the lattice index $j \in \mathbb{Z}$), the momentum becomes a continuous variable $k \in]-\pi/a, \pi/a]$ (or equivalently $k \in [0, 2\pi/a[$ if you prefer). We then write

$$f_j = a \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi} e^{ikaj} f(k), \qquad f(k) = \sum_{j \in \mathbb{Z}} e^{-ikaj} f_j. \tag{7}$$

To go from one representation to the other, we use the identitites

$$a \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi} e^{ika(j-l)} = \delta_{jl}, \qquad \sum_{j\in\mathbb{Z}} e^{-i(k_1-k_2)aj} = \frac{2\pi}{a}\delta(k_1-k_2), \qquad k_i \in \left]-\frac{\pi}{a}, \frac{\pi}{a}\right]. \qquad (8)$$

This is a special case of the more general identity (which is worth remembering)

$$\sum_{n\in\mathbb{Z}} e^{2\pi i n y} = \sum_{\bar{n}\in\mathbb{Z}} \delta(y-\bar{n}). \qquad (9)$$

Note that very often, the prefactors $\frac{1}{2\pi}$, $\frac{1}{N}$ or $\frac{1}{L}$ are 'shared' between the direct and inverse Fourier transforms. You can then encounter expressions like

$$f_j = \frac{1}{\sqrt{N}} \sum_{k_n \in \text{BZ}} e^{ik_n aj} \tilde{f}_{k_n}, \qquad \tilde{f}_{k_n} = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{-ik_n aj} f_j. \qquad (10)$$

This is only a matter of convention, and should be clear from the context. The only important thing is that the *product* of prefactors equals $\frac{1}{N}$ (for the case of a finite lattice), $\frac{1}{L}$ (for the finite continuum interval) or $\frac{1}{2\pi}$ (for the infinite lattice or infinite continuum).

The multidimensional cases are straightforward generalizations of the above formulas.

Gaussian integration

Review of Gaussian integration   One-dimensional Gaussian integral:

$$I(a) \equiv \int_{-\infty}^{\infty} dx e^{-\frac{a}{2}x^2} = \sqrt{\frac{2\pi}{a}}, \qquad \Re a > 0. \tag{11}$$

First moment:

$$\int_{-\infty}^{\infty} dx x^2 e^{-\frac{a}{2}x^2} = -2\partial_a I(a) = \sqrt{\frac{2\pi}{a^3}}. \tag{12}$$

With linear piece:

$$\int_{-\infty}^{\infty} dx e^{-\frac{a}{2}x^2 + bx} = \int_{-\infty}^{\infty} dx e^{-\frac{a}{2}(x-b/a)^2 + \frac{b^2}{2a}} = \sqrt{\frac{2\pi}{a}} e^{\frac{b^2}{2a}}, \qquad b \in \mathbb{C}. \tag{13}$$

Generalization to complex arguments: for $z = x + iy$, $\int d(\bar{z}, z) = \int_{-\infty}^{\infty} dx dy$,

$$\int d(\bar{z}, z) e^{-\bar{z}wz} = \frac{\pi}{w}, \qquad \Re w > 0. \tag{14}$$

and

$$\int d(\bar{z}, z) e^{-\bar{z}wz + \bar{u}z + \bar{z}v} = \frac{\pi}{w} e^{\frac{\bar{u}v}{w}}, \qquad \Re w > 0. \tag{15}$$

Gaussian integration in more than one dimension: real case

$$\int d\mathbf{v} e^{-\frac{1}{2}\mathbf{v}^T \mathbf{A}\mathbf{v}} = (2\pi)^{N/2} \det \mathbf{A}^{-1/2} \tag{16}$$

where $\mathbf{A}$ is a positive definite real symmetric N-dimensional matrix and $\mathbf{v}$ is an N-component real vector.

Proof: can write $\mathbf{A} = \mathbf{O}^T \mathbf{D}\mathbf{O}$ with $\mathbf{O}$ an orthogonal matrix and $\mathbf{D}$ a diagonal matrix. Change of variables $\mathbf{v} \to \mathbf{O}\mathbf{v}$ having unit Jacobian $\det \mathbf{O} = 1$. Factorizes into product of one-dimensional Gaussian integrals, result $\prod_{i=1}^{N} \sqrt{\frac{2\pi}{d_i}}$. Replace product by determinant.

Multidimensional generalization of (13):

$$\int d\mathbf{v} e^{-\frac{1}{2}\mathbf{v}^T \mathbf{A}\mathbf{v} + \mathbf{j}^T \cdot \mathbf{v}} = (2\pi)^{N/2} \det \mathbf{A}^{-1/2} e^{\frac{1}{2}\mathbf{j}^T \mathbf{A}^{-1} \mathbf{j}} \tag{17}$$

This is important as a 'generator' of other useful identities.

Applying $\partial^2_{j_m j_n}|_{\mathbf{j}=0}$ to LHS of (17) gives $\int d\mathbf{v} e^{-\frac{1}{2}\mathbf{v}^T \mathbf{A}\mathbf{v}} v_m v_n = (2\pi)^{N/2} \det \mathbf{A}^{-1/2} A_{mn}^{-1}$ or

$$\langle v_m v_n \rangle = A_{mn}^{-1} \tag{18}$$

with

$$\langle ... \rangle \equiv (2\pi)^{-N/2} \det \mathbf{A}^{1/2} \int d\mathbf{v} e^{-\frac{1}{2}\mathbf{v}^T \mathbf{A}\mathbf{v}} (...) \tag{19}$$

This generalizes: differentiating four times,

$$\langle v_m v_n v_q v_p \rangle = A_{mn}^{-1} A_{qp}^{-1} + A_{mq}^{-1} A_{np}^{-1} + A_{mp}^{-1} A_{nq}^{-1} \tag{20}$$

$2n$-fold differentiation:

$$\langle v_{i_1} v_{i_2} ... v_{i_{2n}} \rangle = \sum_{pairings} A_{i_{k_1} i_{k_2}}^{-1} ... A_{i_{k_{2n-1}} i_{k_{2n}}}^{-1} \tag{21}$$

which is known as **Wick's theorem**, here for real bosonic fields. Total number of terms: $C_{2n} = \frac{(2n)!}{n! 2^n} = (2n-1)!!$, *i.e.* using pair exchange symmetry and exchange symmetry within each pair.

Gaussian integration in more than one dimension: complex case   Complex version of (16):

$$\int d(\mathbf{v}^\dagger, \mathbf{v}) e^{-\mathbf{v}^\dagger \mathbf{A} \mathbf{v}} = \pi^N \det \mathbf{A}^{-1} \tag{22}$$

with $\mathbf{v}$ an N-dimensional complex vector, $d(\mathbf{v}^\dagger, \mathbf{v}) \equiv \prod_{i=1}^{N} d\Re v_i d\Im v_i$, and $\mathbf{A}$ a complex matrix with positive definite Hermitian part.

Generalization of (22):

$$\int d(\mathbf{v}^\dagger, \mathbf{v}) e^{-\mathbf{v}^\dagger \mathbf{A} \mathbf{v} + \mathbf{w}^\dagger \cdot \mathbf{v} + \mathbf{v}^\dagger \cdot \mathbf{w}'} = \pi^N \det \mathbf{A}^{-1} e^{\mathbf{w}^\dagger \mathbf{A}^{-1} \mathbf{w}'} \tag{23}$$

with $\mathbf{w}, \mathbf{w}'$ independent vectors in general.

Averages of components: differentiating this twice, $\partial^2_{w'_m \bar{w}_n}(...)|_{\mathbf{w}=\mathbf{w}'=0}$ gives

$$\langle \bar{v}_m v_n \rangle = A^{-1}_{nm} \tag{24}$$

where $\langle ... \rangle \equiv \pi^{-N} \det \mathbf{A} \int d(\mathbf{v}^\dagger, \mathbf{v}) e^{-\mathbf{v}^\dagger \mathbf{A} \mathbf{v}}(...)$.

For $2n$ components: Wick's theorem for complex bosonic fields:

$$\langle \bar{v}_{i_1} \bar{v}_{i_2} ... \bar{v}_{i_n} v_{j_1} v_{j_2} ... v_{j_n} \rangle = \sum_P A^{-1}_{j_1 i_{P_1}} ... A^{-1}_{j_n i_{P_n}}. \tag{25}$$

Total number of terms: $C_n = n!$.

1   Classical wanderings

1.1   Brownian motion

Mankind has long been aware of the seemingly random motion of particles embedded within a fluid. For the historians among you, it might be interesting to remember that the Roman poet Lucretius described it in one of his scientific poems 'On the Nature of Things' (circa 60 BC). More importantly, it was qualitatively described in more scientific terms (through microscope observations) by Robert Brown in 1827. One of Albert Einstein's three famous papers of 1905 [1] is entirely devoted to precisely this subject, and helped establish Brownian motion as the definitive proof of the atomic hypothesis. Einstein was hereby able to determine the size of atoms, and Avogadro's number.

We will here focus on a somewhat simplified scenario which tends to Brownian motion in a certain limit. This is the problem of a random walker on a regular lattice. Besides Brownian motion, the random walker problem has extremely many applications besides physics, for example in ecology, biology or economics.

1.2   The random walker

Our objective in this section will be limited to making some quantitative statements about random walks. Being by definition random, such a walk of course cannot be described exactly, and our objectives will thus be limited to making probabilitic statements.

We will begin by considering the most easily treatable case of a random walker moving in a d-dimensional hypercubic lattice. Let us thus consider d-dimensional Euclidean space, with basis unit vectors

$$\hat{\boldsymbol{n}}_\mu, \quad \mu = 1, ..., d, \quad \text{such that} \quad \hat{\boldsymbol{n}}_\mu \cdot \hat{\boldsymbol{n}}_\nu \equiv \sum_{i=1}^d \hat{n}_\mu^i \hat{n}_\nu^i = \delta_{\mu\nu}. \tag{26}$$

Let us denote the lattice spacing as a. Our lattice is then defined by all points

$$\mathcal{L}_a \equiv \{\boldsymbol{r}\} \quad \text{such that} \quad \boldsymbol{r} = a \sum_{\mu=1}^d n^\mu \hat{\boldsymbol{n}}_\mu, \qquad n^\mu \in \mathbb{N}. \tag{27}$$

Each point has $2d$ neighbours; this is known as the **coordination number** of this lattice, and we will denote it as $c_{\mathcal{L}_a}$.

Let us now imagine that we are observing a walker obeying the following rules:[1]

- **rule 1**: at each time interval δt, the walker takes one step on the lattice;

- **rule 2**: the direction each step is taken in, is uniformly distributed between the $c_{\mathcal{L}_a}$ possible choices.

Examples of paths traced out by such a walker are provided in Fig. 1 for the case of a two-dimensional square lattice. Some comments are immediately in order. The meanderings of the walker away from the origin are slow: some sites are visited many times over (the number of times a site is visited is not visible in the plots, but can be imagined) and the path therefore tends to be divided into dense clusters where the wanderer keeps retracing his steps, linked by narrow bridges representing rarer chance instances where the wanderer follows more or less one direction for a while. Very occasionally, the walker wanders much further, as if a drift current was present (*e.g.* the bottom right instance of Fig. 1). These instances are rare events.

The second rule is an expression of the **Markov property** of the random walk, namely that the status of the system at a point in time is sufficient to determine its status at the next time

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[1]The commonly made analogy to a drunken wanderer is entirely inappropriate: our walker is a very predictable being, since it *certainly* makes one step at each unit of time with *perfectly uniformly random* choice of direction.
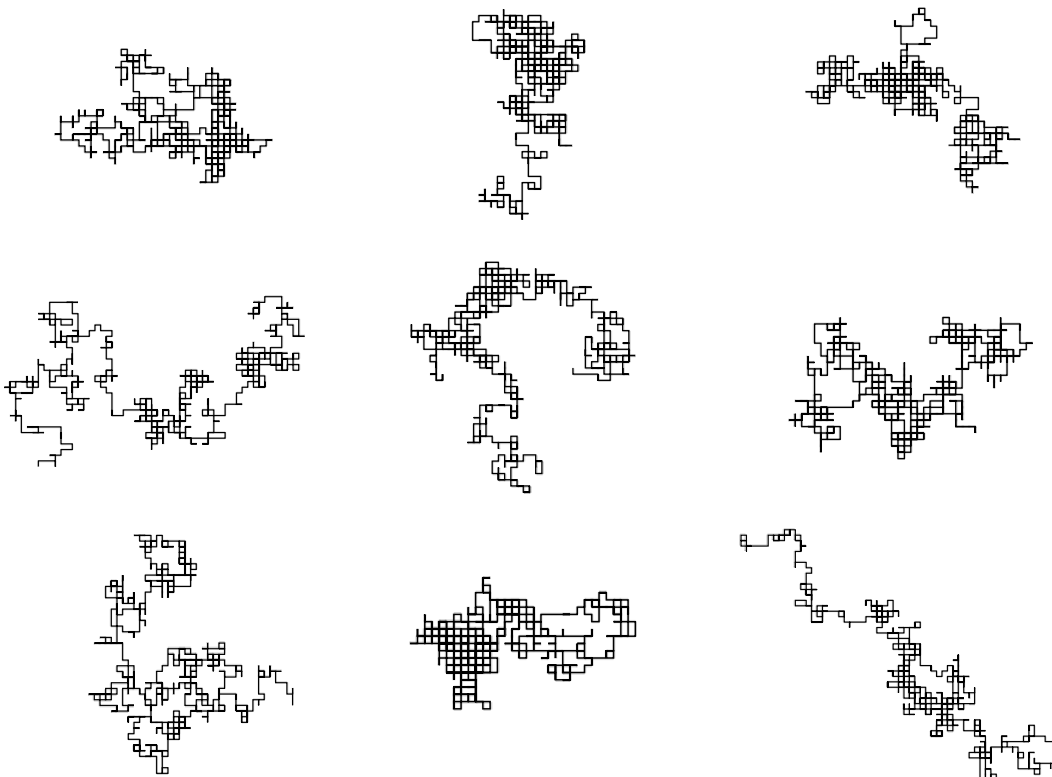
Figure 1: Examples of random walks on the square lattice. Each walk consists of 1000 steps.

increment. Processes with discrete time evolution obeying the Markov property are commonly referred to as **Markov chains.**

The random walker, despite following extremely simple rules, displays rather interesting behaviour (you can view this as an example of **emergence**: simple rules yield rich physics). We can ask ourselves very many questions about the walker. Most fundamental of all is:

- What is the conditional probability $P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0}$ of finding the walker at site $\boldsymbol{r}_1$ at time $t_1 = t_0 + s\delta t$ (s being the number of steps taken) given that it was at $\boldsymbol{r}_0$ at time t_0?

In theory, a detailed answer to this question is sufficient to answer all possible questions one might have about the random walker, since these will be expressible as functions of the $P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0}$.

We can state a few obvious facts. We consider a (spatial *and* time) translationally-invariant system, so the probabilities are unchanged by a constant shift of coordinates:

$$P_{\boldsymbol{r}_1-\boldsymbol{r}_2,t_1|\boldsymbol{r}_0-\boldsymbol{r}_2,t_0} = P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = P_{\boldsymbol{r}_1,t_1+t_2|\boldsymbol{r}_0,t_0+t_2}. \tag{28}$$

We can therefore view the origins $\boldsymbol{r}_0$, t_0 as being fixed from now on. By definition, at time t_0, our walker is standing at $\boldsymbol{r}_0$:

$$P_{\boldsymbol{r}_1,t_0|\boldsymbol{r}_0,t_0} = \delta_{\boldsymbol{r}_1,\boldsymbol{r}_0}. \tag{29}$$

Second, all probabilities are positive-definite and bounded:

$$0 \leq P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} \leq 1 \quad \forall\, \boldsymbol{r}_1, \quad \forall\, t_1 \geq t_0. \tag{30}$$

Third, the walker must be *somewhere*, so the probabilities obey the 'sum rule'

$$\sum_{\boldsymbol{r}_1\in\mathcal{L}_a} P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = 1 \quad \forall\, t_1 \geq t_0. \tag{31}$$

There are some further obvious facts that can be stated. For example, the probability must vanish if the time is not sufficient to go from $\boldsymbol{r}_0$ to $\boldsymbol{r}_1$ in time $t_1 - t_0$:

$$P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = 0 \quad \text{if} \quad |\boldsymbol{r}_1 - \boldsymbol{r}_0| > \frac{a}{\delta t}(t_1 - t_0) \tag{32}$$

(meaning that we can interpret $a/\delta t \equiv v_{\max}$ as an effective maximal (light) velocity), so the time dynamics in our system is causal: the walker will not be nonlocally teleported around the lattice under time evolution. As we will see, this effective light velocity is not very meaningful: the overwhelming majority of random walks will propagate at a diffusion velocity $v_d \ll v_{\max}$.

Another statement one could make is that since our hypercubic lattice is bipartite[2], the probability possesses a 'parity' feature whereby it is alternately (non)vanishing on each sublattice. This is an example of a **non-universal** statement: it relies on the microscopic features of the lattice considered here, and will not be true of other lattices. The most appealing way of thinking which we will pursue focuses of course on the universal features. What is meant by this? Things that do *not* depend on microscopic details, but rather apply to whole classes of situations. As a simple illustration here, consider the problem of the random walker but on different lattices, say the triangular and honeycomb ones. The triangular lattice is not bipartite; the honeycomb one is. Looking at Fig. 2, in which example paths are given for triangular, square and honeycomb lattices, one can observe a rather striking similarity. This similarity becomes exact in the so-called **scaling limit** taking the time interval (number of steps) and distance scale (lattice spacing) respectively to ∞ and zero in a meaningful way (which we will do later for the square lattice). The concept of scaling is illustrated in Fig. 3.

1.2.1   Time evolution

Let us now focus on the time dependence of the occupation probabilities. Our starting point is the implementation of the second rule of the walker, namely the one-time-step relation

$$P_{\boldsymbol{r}_1,t_1+\delta t|\boldsymbol{r}_0,t_0} = \frac{1}{c_{\mathcal{L}_a}} \sum_{\boldsymbol{r}'\text{n.n.}\boldsymbol{r}_1} P_{\boldsymbol{r}',t_1|\boldsymbol{r}_0,t_0} \tag{33}$$

where we write the requirement that $\boldsymbol{r}'$ be nearest neighbour to $\boldsymbol{r}_1$ as $\boldsymbol{r}'$n.n.$\boldsymbol{r}_1$. For our hypercubic lattice, this is specialized to

$$P_{\boldsymbol{r}_1,t_1+\delta t|\boldsymbol{r}_0,t_0} = \frac{1}{2d} \sum_{\sigma=\pm 1} \sum_{\mu=1}^{d} P_{\boldsymbol{r}_1+a\sigma\hat{\boldsymbol{n}}_\mu,t_1|\boldsymbol{r}_0,t_0}. \tag{34}$$

We here recognize the discretized version of the Laplacian operator, which we will denote ∇_a^2 and define as

$$\nabla_a^2 f_{\boldsymbol{r}} \equiv \frac{1}{a^2} \sum_{\mu=1}^{d} \left[f_{\boldsymbol{r}+a\hat{\boldsymbol{n}}_\mu} + f_{\boldsymbol{r}-a\hat{\boldsymbol{n}}_\mu} - 2f_{\boldsymbol{r}} \right]. \tag{35}$$

This scales to the usual Laplacian in the continuum limit: if the lattice-defined $f_{\boldsymbol{r}}$ scales to a differentiable function $f(\boldsymbol{r})$, then

$$\lim_{a\to 0} \nabla_a^2 f_{\boldsymbol{r}} = \nabla^2 f(\boldsymbol{r}). \tag{36}$$

We can thus rewrite our one-time-step relation as

$$P_{\boldsymbol{r}_1,t_1+\delta t|\boldsymbol{r}_0,t_0} - P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = \frac{a^2}{2d} \nabla_a^2 P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0}. \tag{37}$$

This is simply a lattice version of the continuum diffusion equation (in reality here: the heat equation)

$$\left(\frac{\partial}{\partial t} - D\,\nabla^2 \right) P(\boldsymbol{r},t) = 0, \tag{38}$$

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[2]That is: it can be divided into two sublattices A and B such that all nearest neighbours of $\boldsymbol{r} \in A$ are in B, and vice-versa.

Figure 2: Examples of random walks on the triangular (top), square (middle) and honeycomb (bottom) lattices. Each walk consists of 1000 steps. The similarity between these three instances is an illustration of the concept of universality.

Figure 3: Illustration of scaling in random walks. The top left walk has 125 steps of length 32 on the two-dimensional square lattice. Each subsequent curve has four times as many steps of half the length. The mean distance from the origin reached by the walker remains the same.

in which D (the **diffusion constant**) parametrizes the efficiency of the diffusion (the higher D is, the quicker an initial state diffuses). Here, this constant is taken as the limiting value (assumed to be finite, and thus choosing $a^2 \propto \delta t$ in the scaling limit)

$$D = \lim_{\substack{a \to 0 \\ \delta t \to 0}} \frac{a^2}{2d\delta t}. \tag{39}$$

Getting back to our problem of describing the random walker, given an initial configuration of probabilities

$$P_{\boldsymbol{r},t_0|\boldsymbol{r}_0,t_0} \equiv P_{\boldsymbol{r},t_0}, \tag{40}$$

the probability configuration at all times $t_1 > t_0$ is thus obtainable from the solution of (37), which can in turn easily be obtained by simple Fourier transformation. Adopting the convention

$$f_{\boldsymbol{r}} = a^d \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^d\boldsymbol{k}}{(2\pi)^d} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} f(\boldsymbol{k}), \qquad f(\boldsymbol{k}) = \sum_{\boldsymbol{r} \in \mathcal{L}_a} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} f_{\boldsymbol{r}}, \tag{41}$$

we can write our single-site-localized initial condition as

$$P_{\boldsymbol{r},t_0|\boldsymbol{r}_0,t_0} = \delta_{\boldsymbol{r},\boldsymbol{r}_0}, \qquad P_{\boldsymbol{k},t_0|\boldsymbol{r}_0,t_0} = e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_0}. \tag{42}$$

The one-time-step equation (37) becomes

$$P_{\boldsymbol{k},t_1+\delta t|\boldsymbol{r}_0,t_0} = \frac{1}{d} \sum_{\mu=1}^{d} \cos(k^\mu a) \; P_{\boldsymbol{k},t_1|\boldsymbol{r}_0,t_0}. \tag{43}$$

Using this, we can immediately solve (37) for arbitrary $t_1 \ge t_0$ as

$$P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = a^d \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^d\boldsymbol{k}}{(2\pi)^d} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_0)} \left[\frac{1}{d} \sum_{\mu=1}^{d} \cos(k^\mu a) \right]^{\frac{t_1-t_0}{\delta t}}. \tag{44}$$

This is the full, exact solution of our problem: no approximations have been made, so this equation is exact for all values of $\boldsymbol{r}_1$ and $t_1 \geq t_0$. In particular, the fact that all probabilities are positive can be easily verified.

This is all very nice, but the fact remains that (44) is a bit unwieldy and does not make the physics very transparent. The question thus now becomes: can this equation be further simplified, at least for the most likely paths that our walker can follow?

1.2.2   Continuum limit

Let us consider taking the limit $\delta t \to 0$. For a fixed time interval $t_1 - t_0$, the exponent of the square bracket in (44) becomes very large. This term would only survive in the limit $\delta t \to 0$ if we were to simultaneously scale $k^\mu a$ to zero. For finite momenta, this means taking the lattice spacing to zero (which justifies calling what we are doing here a 'continuum limit'). Expanding the cosine under this assumption gives

$$\left[\frac{1}{d}\sum_{\mu=1}^{d}\cos(k^\mu a)\right]^{\frac{t_1-t_0}{\delta t}} = \left[1 - \frac{a^2}{2d}\boldsymbol{k}^2 + ...\right]^{\frac{t_1-t_0}{\delta t}} \to e^{-(t_1-t_0)\frac{a^2}{2d\delta t}\boldsymbol{k}^2} \tag{45}$$

in which we now explicitly recognize our diffusion constant D (39). In this limit, the probability density (per unit volume) of finding the particle around $\boldsymbol{r}_1$ at time t_1 scales to a smooth function of space and time coordinates:

$$p(\boldsymbol{r}_1, t_1 | \boldsymbol{r}_0, t_0) \equiv \lim a^{-d} P_{\boldsymbol{r}_1, t_1 | \boldsymbol{r}_0, t_0} = \int_{-\infty}^{\infty} \frac{d^d\boldsymbol{k}}{(2\pi)^d} e^{-(t_1-t_0)D\boldsymbol{k}^2 + i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_0)}$$

$$= \frac{1}{[4\pi D(t_1-t_0)]^{\frac{d}{2}}} \exp\left[-\frac{|\boldsymbol{r}_1-\boldsymbol{r}_0|^2}{4D(t_1-t_0)}\right]. \tag{46}$$

From this equation, we immediately see that after a time interval $t_1 - t_0$, the typical distance from the origin at which we find our walker is

$$|\boldsymbol{r}_1 - \boldsymbol{r}_0| \sim (t_1 - t_0)^\nu, \qquad \nu = \frac{1}{2}. \tag{47}$$

This is our first example of a **critical exponent**. Here, it is the **Hausdorff dimension** of the curve: the path has total length $\sim t_1 - t_0$, but it is confined in a ball of radius $\sim (t_1 - t_0)^{\frac{1}{2}}$.

Summarizing, this probability density is a positive-definite symmetric kernel which satisfies the normalization condition

$$\int d^d\boldsymbol{r} \; p(\boldsymbol{r}, t | \boldsymbol{r}_0, t_0) = 1, \tag{48}$$

and the diffusion equation

$$\left(\frac{\partial}{\partial t} - D\nabla^2\right) p(\boldsymbol{r}, t | \boldsymbol{r}_0, t_0) = 0 \tag{49}$$

with initial condition

$$p(\boldsymbol{r}_1, t_0 | \boldsymbol{r}_0, t_0) = \delta^{(d)}(\boldsymbol{r}_1 - \boldsymbol{r}_0). \tag{50}$$

Another interesting equation obeyed by the kernel originates from the fact that at any intermediate time, the walker must be somewhere. This completely trivial statement translates into the following nontrivial composition property

$$\int d^d\boldsymbol{r}_1 \; p(\boldsymbol{r}_2, t_2 | \boldsymbol{r}_1, t_1) \; p(\boldsymbol{r}_1, t_1 | \boldsymbol{r}_1, t_0) = p(\boldsymbol{r}_2, t_2 | \boldsymbol{r}_0, t_0), \quad \forall \, t_1 \text{ such that } t_2 > t_1 > t_0. \tag{51}$$

Said otherwise, our walker has no memory whatsoever. The diffusion process is purely local in time (in other words: there are no retarded effects), as per the (microscopic) Markovian dynamics highlighted previously.

Exercise: rare events. We have seen before that the occupation probability vanishes outside of a 'light cone' defined by the maximal velocity $v_{max} = a/\delta t$. What is the probability of our wanderer diffusing to a distance $|\boldsymbol{r}_1 - \boldsymbol{r}_0| = v_{max}(t_1 - t_0)$, as a function of $t_1 - t_0$?[3]

Exercise: isotropy of the diffusion. One feature which is manifested by the diffusion kernel we have obtained is that it is **isotropic** in space, namely that the diffusion occurs in precisely the same way irrespective of direction. We however started from a hypercubic lattice, which manifestly has $2d$ preferred directions. Can you explain what is going on?

Exercise: one step towards universality. Solve the problem of the random walker on the triangular lattice explicitly. Show that the continuum limit you obtain is precisely the same as the one we obtained for the square lattice.

1.2.3   Green's function

A simple question we can now ask (and answer!) is the following: how much time does our walker spend on a given point $\boldsymbol{r}_1$? This is simply given by explicitly summing (44)

$$\sum_{n=0}^{\infty} P_{\boldsymbol{r}_1,t_0+n\delta t|\boldsymbol{r}_0,t_0} = a^d \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^d \boldsymbol{k}}{(2\pi)^d} \frac{e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_0)}}{1 - \frac{1}{d}\sum_{\mu=1}^{d}\cos(k^\mu a)} \equiv \mathcal{G}_{\boldsymbol{r}_1-\boldsymbol{r}_0}. \tag{52}$$

As can directly be seen from (34), this quantity obeys the equation

$$\mathcal{G}_{\boldsymbol{r}_1-\boldsymbol{r}_0} = \delta_{\boldsymbol{r}_1,\boldsymbol{r}_0} + \frac{1}{2d}\sum_{\mu=1}^{d}\left[\mathcal{G}_{\boldsymbol{r}_1+a\hat{\boldsymbol{n}}_\mu-\boldsymbol{r}_0} + \mathcal{G}_{\boldsymbol{r}_1-a\hat{\boldsymbol{n}}_\mu-\boldsymbol{r}_0}\right] \tag{53}$$

or more economically in terms of our lattice Laplacian

$$-\nabla_a^2 \mathcal{G}_{\boldsymbol{r}_1-\boldsymbol{r}_0} = \frac{2d}{a^2}\delta_{\boldsymbol{r}_1,\boldsymbol{r}_0}. \tag{54}$$

The kernel $\mathcal{G}$ is thus the **Green's function** of (a constant times) the Laplacian, namely it is the kernel which inverts this operator[4]. The physical interpretation of the Green's function is thus quite direct for our random walker: for an infinitely long walk, $\mathcal{G}_{\boldsymbol{r}_1-\boldsymbol{r}_0}$ is the total number of time steps spent by our walker at $\boldsymbol{r}_1$, given that it started at $\boldsymbol{r}_0$.

1.2.4   Divergences

Simply by looking at the integral representation (52) in the region of small momenta, we see that the Green's function is given by a convergent integral for $d > 2$. For $d = 2$, we see that we get a logarithmic divergence (in terms of a smallest allowable wavelength/infrared cutoff $k_{\min}$ which we would like to put identically to zero) of the form $\int \frac{d^2\boldsymbol{k}}{k^2} \sim -\ln k_{\min}$; the $d = 1$ case diverges like $1/k_{\min}$. This is simply a manifestation of the fact that in $d \leq 2$, the walker left to wander for an infinite time, will tend to spend an infinite amount of time at each point of the lattice.

Infinities make the interpretation of our results problematic, and we must find a way to deal with them. You will no doubt have heard that dealing with infinities is the main object of the theory of **renormalization**. Handling the simple infinities we encounter here can thus be seen as a warm-up for more advanced dealings with renormalization.

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[3]For your information: this is the simplest case of a more general statement known as the **Lieb-Robinson bound** [2], which states that in a system with local interactions, correlations between objects relatively positioned outside an effective light-cone (defined by a finite group velocity characteristic of the system) vanish exponentially with distance.

[4]The Green's function of an operator is of course only defined modulo a function which is in the null space of this operator. Consider here adding a (lattice) harmonic function $f_h(\boldsymbol{r})$ such that $\nabla_a^2 f_h = 0$.

Subtraction.   The first way to deal with infinities is to... get rid of them by subtracting them away. This is not as mindless as it may seem. Note first that, as a function of position, the total time spent in one point is maximal at the origin. In other words, our Green's function $\mathcal{G}$ is maximal at $\boldsymbol{r}_1 = \boldsymbol{r}_0$. We can thus consider a Green's function $\mathcal{G}^s$ (s for *subtracted*) which is finite for all d by simply subtracting the (d-dependent, possibly infinity) constant $\mathcal{G}_{\boldsymbol{0}}$:

$$\mathcal{G}^s_{\boldsymbol{r}_1-\boldsymbol{r}_0} = \mathcal{G}_{\boldsymbol{r}_1-\boldsymbol{r}_0} - \mathcal{G}_{\boldsymbol{0}} = a^d \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^d\boldsymbol{k}}{(2\pi)^d} \frac{e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_0)} - 1}{1 - \frac{1}{d}\sum_{\mu=1}^{d} \cos(k^\mu a)}. \tag{55}$$

Since we have merely subtracted a constant, this new kernel still obeys (54), but it is not positive definite anymore. If fact, it is now *negative definite*.

Exercise: Green's function in one dimension.   Show that the subtracted Green's function in one dimension is exactly given by

$$\mathcal{G}^s_{\boldsymbol{r}_1-\boldsymbol{r}_0} = -\frac{|\boldsymbol{r}_1 - \boldsymbol{r}_0|}{a}. \tag{56}$$

Derivation:

$$\mathcal{G}^s_r = a \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi} \frac{e^{ikr} - 1}{1 - \cos ka} = -a \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{dk}{2\pi} \frac{\sin^2 kr}{\sin^2 ka} \stackrel{\text{[GR] } 3.624.6}{=} -\frac{r}{a}.$$

Regularization.   Another way of dealing with infinities is to introduce some sort of deformation parameter in the theory which renders all sums or integrals finite. Here, the infinities came from the fact that we are considering an infinitely long duration of the walk, our walker never getting tired of hopping around. Let us thus add assume that our walker obeys the additional rule, to be enforced with **rule 1** and **rule 2**:

- **rule 3**: during each time step, with probability η, our walker gets exhausted, quits the game and disappears from the lattice.

A more physical interpretation of this 'exhaustible walker' problem is for example to imagine that our walker is a radioactive particle subject to decay.

Given such a finite probability of our walker disappearing at each time step, our probabilities (now denoted by a superscript η) are now simply given by a time-dependent rescaling of our earlier solution

$$P^{(\eta)}_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = (1-\eta)^{\frac{t_1-t_0}{\delta t}} P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0}. \tag{57}$$

Note that the sum rule now becomes

$$\sum_{\boldsymbol{r}_1} P^{(\eta)}_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = (1-\eta)^{\frac{t_1-t_0}{\delta t}} \quad \forall\, t_1 \geq t_0. \tag{58}$$

For this exhaustible walker, the Green's function becomes

$$\mathcal{G}^{(\eta)}_{\boldsymbol{r}_1-\boldsymbol{r}_0} \equiv \sum_{n=0}^{\infty} (1-\eta)^n P_{\boldsymbol{r}_1,t_0+n\delta t|\boldsymbol{r}_0,t_0}. \tag{59}$$

We obviously have that our earlier Green's function is given by the limit $\eta \to 0$ of the exhaustible walker Green's function:

$$\mathcal{G}_{\boldsymbol{r}_1-\boldsymbol{r}_0} = \lim_{\eta\to 0} \mathcal{G}^{(\eta)}_{\boldsymbol{r}_1-\boldsymbol{r}_0}. \tag{60}$$

Now however, the integral representation for $\mathcal{G}^{(\eta)}$ converges for all $\eta > 0$ (we by definition necessarily have $0 \leq \eta \leq 1$). This representation is

$$\mathcal{G}^{(\eta)}_{\boldsymbol{r}_1 - \boldsymbol{r}_0} = \frac{a^d}{1 - \eta} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^d \boldsymbol{k}}{(2\pi)^d} \frac{e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1 - \boldsymbol{r}_0)}}{\frac{1}{1-\eta} - \frac{1}{d}\sum_{\mu=1}^{d}\cos(k^\mu a)} \tag{61}$$

and obeys the equation

$$\left[-\nabla_a^2 + m^2\right] \mathcal{G}^{(m)}_{\boldsymbol{r}_1 - \boldsymbol{r}_0} = \frac{2d}{a^2(1-\eta)}\delta_{\boldsymbol{r}_1, \boldsymbol{r}_0} \tag{62}$$

where m can be interpreted as the **effective mass** (note that we now use the mass as superscript label for the Green's function). This is given here by

$$m^2 \equiv \frac{2d}{a^2}\frac{\eta}{1 - \eta} \tag{63}$$

(which is indeed a positive quantity since $0 \leq \eta \leq 1$) For our walker, the mass is thus related to the rate of exhaustion our walker displays as he wanders.

In the scaling limit, we will also take the mass to be finite (this means that we should scale $\eta \sim a^2 \sim \delta t$). The proper scaling of the Green's function is

$$\mathcal{G}_m(\boldsymbol{r}) \equiv \lim \frac{1}{2da^{d-2}}\mathcal{G}^{(m)}_{\boldsymbol{r}} = \int_{-\infty}^{+\infty} \frac{d^d \boldsymbol{k}}{(2\pi)^d}\frac{e^{i\boldsymbol{k}\cdot\boldsymbol{r}}}{\boldsymbol{k}^2 + m^2} \tag{64}$$

this function obeying the equation

$$\left[-\nabla^2 + m^2\right] \mathcal{G}_m(\boldsymbol{r} - \boldsymbol{r}_0) = \delta(\boldsymbol{r} - \boldsymbol{r}_0), \qquad \boldsymbol{r} \in \mathbb{R}^d. \tag{65}$$

Exercise: massive Green's functions in $d = 1, 2, 3$.

a)   Show that the 1d Green's function is

$$\mathcal{G}_m(r) = \frac{e^{-m|r|}}{2m} \tag{66}$$

so the correlation decays with distance on a scale given by the correlation length $\xi = 1/m$.

b)   show that in the 2d case, the Green's function becomes

$$\mathcal{G}_m(\boldsymbol{r})|_{d=2} = \int \frac{d^2 k}{(2\pi)^2}\frac{e^{-i\mathbf{k}\cdot\boldsymbol{r}}}{k^2 + m^2} = \frac{1}{2\pi}K_0(m|\boldsymbol{r}|) \tag{67}$$

(where K_0 is the modified Bessel function of the second kind), with limits

$$\mathcal{G}_m(\boldsymbol{r})|_{d=2} \simeq -\frac{1}{2\pi}\ln[\frac{m}{2}|\boldsymbol{r}|], \qquad |\boldsymbol{r}| \ll 1/m \tag{68}$$

and

$$\mathcal{G}_m(\boldsymbol{r})|_{d=2} \simeq \frac{1}{2}(2\pi m|\boldsymbol{r}|)^{-1/2}e^{-m|\boldsymbol{r}|}, \qquad |\boldsymbol{r}| \gg 1/m. \tag{69}$$

c)   show that in the 3d case, we get

$$\mathcal{G}_m(\boldsymbol{r})|_{d=3} = \int \frac{d^3 k}{(2\pi)^3}\frac{e^{-i\mathbf{k}\cdot\boldsymbol{r}}}{k^2 + m^2} = \frac{e^{-m|\boldsymbol{r}|}}{4\pi|\boldsymbol{r}|}. \tag{70}$$

In the $d = 2, 3$ cases, the Green's function thus diverges at short distance, but in all cases $d = 1, 2, 3$ it decays exponentially at large distances, with characteristic correlation length $\xi = 1/m$.

Derivation: Answers: Explicit calculations for the free propagators

a) 1d: By simple contour integration,

$$\mathcal{G}_m(r) = \int \frac{dk}{2\pi} \frac{e^{-ikr}}{(k+im)(k-im)} = \frac{e^{-m|r|}}{2m}.$$

b) 2d:

$$\mathcal{G}_m(\boldsymbol{r})|_{d=2} = \int \frac{d^2k}{(2\pi)^2} \frac{e^{-i\mathbf{k}\cdot\boldsymbol{r}}}{k^2+m^2} = \frac{1}{4\pi^2} \int_0^{2\pi} d\theta \int_0^\infty dk k \frac{e^{-ik|\boldsymbol{r}|\cos\theta}}{k^2+m^2}$$

$$= \frac{1}{2\pi^2} \int_0^\infty dk \frac{k}{k^2+m^2} \int_0^\pi d\theta \cos(k|\boldsymbol{r}|\cos\theta)$$

We can now use the identity (c.f. Gradshteyn & Ryzhik 3.715.18)

$$\int_0^\pi d\theta \cos(z\cos\theta) \cos n\theta = \pi \cos\frac{n\pi}{2} J_n(z)$$

where J_n is the n-th Bessel function of the first kind. Substituting, we get

$$\mathcal{G}_m(\boldsymbol{r})|_{d=2} = \frac{1}{2\pi} \int_0^\infty dk \frac{k J_0(k|\boldsymbol{r}|)}{k^2+m^2} = \frac{1}{2\pi} K_0(m|\boldsymbol{r}|)$$

in which we have used GR 6.532.4,

$$\int_0^\infty dk \frac{k J_0(kr)}{k^2+m^2} = K_0(mr)$$

in which K_n is the modified Bessel function of the second kind (here with $n=0$).

The limits for small and large values of $|\boldsymbol{r}|$ can be obtained from the asymptotic forms of Bessel functions at small argument,

$$K_0(z) = -\ln\frac{z}{2} I_0(z) + \sum_{k=0}^\infty z^{2k} 2^{2k} (k!)^2 \psi(k+1) \quad \text{GR 8.447.3,}$$

$$I_0(z) = \sum_{k=0}^\infty \frac{(z/2)^{2k}}{(k!)^2} \quad \text{GR 8.447.1,}$$

or at large argument

$$K_\nu(z) = \sqrt{\frac{\pi}{2z}} e^{-z} [1+...] \quad \text{GR 8.454.6.}$$

c) 3d:

$$\mathcal{G}_m(\boldsymbol{r})|_{d=3} = \frac{1}{(2\pi)^3} \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin\theta \int_0^\infty dk k^2 \frac{e^{-ik|\boldsymbol{r}|\cos\theta}}{k^2+m^2}.$$

Let $z = \cos\theta$. We get

$$\mathcal{G}_m(\boldsymbol{r})|_{d=3} = \frac{1}{4\pi^2} \int_0^\infty dk \frac{k^2}{k^2+m^2} \int_{-1}^1 dz e^{-ik|\boldsymbol{r}|z} = \frac{1}{2\pi^2|\boldsymbol{r}|} \int_0^\infty dk \frac{k\sin(k|\boldsymbol{r}|)}{k^2+m^2}$$

This integral is tabulated,

$$\int_{-\infty}^\infty dx \frac{r\sin(ax)}{x^2+b^2} = \pi e^{-ab} \qquad a>0, \Re b>0 \qquad \text{GR 3.723.4}$$

which gives the final result.

1.3 The path integral

It is straightforward to express the properties of the motion of our random walker in terms of sums over the paths which can be taken. We can immediately write

$$P_{\boldsymbol{r}_1,t_1|\boldsymbol{r}_0,t_0} = \frac{\text{Number of paths joining } \boldsymbol{r}_0 \text{ to } \boldsymbol{r}_1 \text{ with } \frac{t_1-t_0}{\delta t} \text{ steps}}{\text{Total number of paths out of } \boldsymbol{r}_0 \text{ with } \frac{t_1-t_0}{\delta t} \text{ steps}}. \tag{71}$$

Let us work directly in the scaling limit. From (46), we have that for initial and final positions and times $\boldsymbol{r}_i,t_i$ and $\boldsymbol{r}_f,t_f$, the probability density of finding the particle was given by the exact (in the scaling limit) expression

$$p(\boldsymbol{r}_f,t_f|\boldsymbol{r}_i,t_i) = \frac{1}{[4\pi D(t_f-t_i)]^{\frac{d}{2}}} \exp\left[-\frac{|\boldsymbol{r}_f-\boldsymbol{r}_i|^2}{4D(t_f-t_i)}\right]. \tag{72}$$

On the other hand, we have the composition property (51) which can be concatenated. Let us imagine that we split our time interval $t_f - t_i$ into N equal intervals of duration $\frac{t_f-t_i}{N} \equiv \Delta t$ (identifying $\boldsymbol{r}_0 \equiv \boldsymbol{r}_i, t_0 \equiv t_i$ and $\boldsymbol{r}_N \equiv \boldsymbol{r}_f, t_N \equiv t_f$), and apply (51) at each $N-1$ intermediate time step:

$$p(\boldsymbol{r}_f,t_f|\boldsymbol{r}_i,t_i) = \int \prod_{n=1}^{N-1} d^d\boldsymbol{r}_n p(\boldsymbol{r}_f,t_f|\boldsymbol{r}_{N-1},t_{N-1})p(\boldsymbol{r}_{N-1},t_{N-1}|\boldsymbol{r}_{N-2},t_{N-2})...p(\boldsymbol{r}_1,t_1|\boldsymbol{r}_i,t_i). \tag{73}$$

In the limit $N \to \infty$, the time steps Δt become infinitesimal (remember that we are working directly in the scaling limit: at each time step here, there are still infinitely many steps being taken on the original lattice, in other words we still have $\delta t/\Delta t = 0$). For an infinitesimal time step, we can write

$$p(\boldsymbol{r}_{n+1},t_{n+1}|\boldsymbol{r}_n,t_n) \underset{t_{n+1}-t_n=\Delta t\to 0^+}{\longrightarrow} \frac{1}{[4\pi\Delta t]^{\frac{d}{2}}} \exp\left[-\frac{\Delta t}{4D}\left|\frac{\Delta\boldsymbol{r}(t_n)}{\Delta t}\right|^2\right] \tag{74}$$

where

$$\frac{\Delta\boldsymbol{r}(t_n)}{\Delta t} \equiv \frac{\boldsymbol{r}_{n+1}-\boldsymbol{r}_n}{\Delta t} \to \frac{d\boldsymbol{r}(t)}{dt}. \tag{75}$$

We can thus write our probability as the **path integral**

$$p(\boldsymbol{r}_f,t_f|\boldsymbol{r}_i,t_i) = \int\limits_{\substack{\boldsymbol{r}(t_i)=\boldsymbol{r}_i \\ \boldsymbol{r}(t_f)=\boldsymbol{r}_f}} \mathcal{D}\boldsymbol{r}(t) \exp\left[-\frac{1}{4D}\int_{t_i}^{t_f} dt \left|\frac{d\boldsymbol{r}(t)}{dt}\right|^2\right] \tag{76}$$

where the **path integral measure** is here defined as

$$\int\limits_{\substack{\boldsymbol{r}(t_i)=\boldsymbol{r}_i \\ \boldsymbol{r}(t_f)=\boldsymbol{r}_f}} \mathcal{D}\boldsymbol{r}(t)F[\boldsymbol{r}(t)] \equiv \lim_{N\to\infty} \left[\frac{N}{4\pi D(t_f-t_i)}\right]^{Nd/2} \int \prod_{n=1}^{N-1} d\boldsymbol{r}_n F(\{\boldsymbol{r}_n\})\Bigg|_{\substack{\boldsymbol{r}_0=\boldsymbol{r}_i \\ \boldsymbol{r}_N=\boldsymbol{r}_f}} \tag{77}$$

where $F[\boldsymbol{r}(t)]$ is the functional corresponding to the function $F(\{\boldsymbol{r}_n\})$.

For the exhaustible walker, we simply use (57) and the limits (recalling (39))

$$\lim(1-\eta)^{\frac{t_f-t_i}{\delta t}} = \lim\left(1-\frac{a^2}{2d}m^2\right)^{\frac{t_f-t_i}{\delta t}} = e^{-(t_f-t_i)Dm^2} \tag{78}$$

so we simply have

$$p_m(\boldsymbol{r}_f,t_f|\boldsymbol{r}_i,t_i) = e^{-(t_f-t_i)Dm^2} p(\boldsymbol{r}_f,t_f|\boldsymbol{r}_i,t_i). \tag{79}$$

For the Green's function, we have

$$\mathcal{G}_m(\boldsymbol{r}) = \lim \frac{a^2}{2d} \sum_{n=0}^{\infty} p_m(\boldsymbol{r}, n\delta t|\boldsymbol{0}, 0) \tag{80}$$

and we therefore obtain the path integral representation

$$\mathcal{G}_m(\boldsymbol{r}) = D \int_0^{\infty} dt \int_{\substack{\boldsymbol{r}(0)=\boldsymbol{0} \\ \boldsymbol{r}(t)=\boldsymbol{r}}} \mathcal{D}\boldsymbol{r}(t') \exp\left[-\int_0^t dt' \left(Dm^2 + \frac{1}{4D} |\dot{\boldsymbol{r}}(t')|^2 \right) \right]. \tag{81}$$

A few comments are in order. Why did we even bother to define such a path integral, given that we had the exact solution for any initial/final positions in equation (46)? The reason is of course that while we were able to provide such an exact solution for this particular case, this is by no means the usual situation. In most circumstances, we cannot solve the time evolution equations exactly, and must be content with some form of approximation. The time evolution is implemented by an evolution equation of the form (49) but generically containing other terms whose effects cannot be tracked exactly. One then relies on approximations (for example that the relevant dynamics is restricted to some low-energy/slow-changing configurations). Dividing the time evolution into microscopic time steps as we have done here is then still meaningful: expressions corresponding to (81) can always be written down irrespective of how our time evolution occurs, whereas solutions like (46) are more often than not too much to wish for.

1.4   Visit and return probabilities

Let us now return to the random walker on the hypercubic lattice (before taking the scaling limit), and address a slightly different question: what is the probability $\Pi_{\boldsymbol{r},t}$ that the walker has trodden at least once on site $\boldsymbol{r}$ by time t, given that it started at $\boldsymbol{r}_0 \equiv \boldsymbol{0}$ at time $t_0 \equiv 0$? For the special case $\boldsymbol{r} = \boldsymbol{r}_0$, this is known as the **return probability**[5].

The probabilities $P_{\boldsymbol{r},t}$[6] are not exactly what we are looking for (though it is intimately related): summing these over all times would give the mean time spent at site $\boldsymbol{r}$. Instead, let us define the intermediate quantities $P_{\boldsymbol{r},t;i}$ of being at site $\boldsymbol{r}$ for the i-th time at time t. We then have that

$$P_{\boldsymbol{r},t} = \delta_{\boldsymbol{r},\boldsymbol{0}}\delta_{t,0} + \sum_{i=1}^{\infty} P_{\boldsymbol{r},t;i}. \tag{82}$$

Note that only a finite number of terms contribute to this sum, since $P_{\boldsymbol{r},t;i} = 0$ for $i > t/\delta t$. Note also that our definitions are such that $P_{\boldsymbol{r},0;i} = 0$. Since an $i+1$-th visit necessarily follows as i-th visit, we can write the recurrence relation (using homogeneity of the walk in space and time)

$$P_{\boldsymbol{r},t;i+1} = \sum_{t_1+t_2=t} P_{\boldsymbol{r},t_1;i} P_{\boldsymbol{0},t_2;1}. \tag{83}$$

The summation of this relation over $i = 1, ..., \infty$ then yields

$$P_{\boldsymbol{r},t} - P_{\boldsymbol{r},t;1} - \delta_{\boldsymbol{r},\boldsymbol{0}}\delta_{t,0} = \sum_{t_1+t_2=t} P_{\boldsymbol{r},t_1} P_{\boldsymbol{0},t_2;1} - \delta_{\boldsymbol{r},\boldsymbol{0}} P_{\boldsymbol{r},t;1}. \tag{84}$$

The probability of having visited site $\boldsymbol{r}$ at least once is then

$$\Pi_{\boldsymbol{r}} = \sum_{t=0}^{\infty} P_{\boldsymbol{r},t;1}. \tag{85}$$

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[5]In here and all further considerations, we assume that the walker has *left* the origin, so we exclude the initial state at the initial time.

[6]Dropping the $\boldsymbol{r}_0, t_0$ arguments for notational simiplicity. Remember that our random walk is homogeneous in space and (discrete) time.

Treating the more general case of the exhaustible walker, we can simply replace all the P by $P^{(\eta)}$, giving for example

$$P_{\boldsymbol{r},t}^{(\eta)} - P_{\boldsymbol{r},t;1}^{(\eta)} - \delta_{\boldsymbol{r},\boldsymbol{0}}\delta_{t,0} = \sum_{t_1+t_2=t} P_{\boldsymbol{r},t_1}^{(\eta)} P_{\boldsymbol{0},t_2;1}^{(\eta)} - \delta_{\boldsymbol{r},\boldsymbol{0}}P_{\boldsymbol{r},t;1}^{(\eta)}. \tag{86}$$

Using

$$\Pi_{\boldsymbol{r}}^{(\eta)} = \sum_{t=0}^{\infty} P_{\boldsymbol{r},t;1}^{(\eta)}, \qquad \Pi_{\boldsymbol{r}} = \lim_{\eta\to0}\Pi_{\boldsymbol{r}}^{(\eta)}, \tag{87}$$

and summing over time gives

$$\mathcal{G}_{\boldsymbol{r}}^{(\eta)} = \delta_{\boldsymbol{r},\boldsymbol{0}} + [1 - \delta_{\boldsymbol{r},\boldsymbol{0}}]\,\Pi_{\boldsymbol{r}}^{(\eta)} + \mathcal{G}_{\boldsymbol{r}}^{(\eta)}\Pi_{\boldsymbol{0}}^{(\eta)}. \tag{88}$$

This gives us two very aesthetic equations: first of all, the return probability is simply expressed in terms of the Green's function at zero distance:

$$\Pi_{\boldsymbol{0}}^{(\eta)} = 1 - \frac{1}{\mathcal{G}_{\boldsymbol{0}}^{(\eta)}}. \tag{89}$$

Second, the visit probability at site $\boldsymbol{r}$ is simply given by the ratio of the Green's function at that point to that at the origin:

$$\Pi_{\boldsymbol{r}}^{(\eta)} = \frac{\mathcal{G}_{\boldsymbol{r}}^{(\eta)}}{\mathcal{G}_{\boldsymbol{0}}^{(\eta)}}, \qquad \boldsymbol{r} \neq \boldsymbol{0}. \tag{90}$$

Some comments are in order. We know that for $d \leq 2$, $\lim_{\eta\to0}\mathcal{G}_{\boldsymbol{r}}^{(\eta)} \to \infty$ uniformly for any $\boldsymbol{r}$, so $\Pi(\boldsymbol{0}) \to 1$ and $\Pi(\boldsymbol{r}) \to 1$ for any $\boldsymbol{r}$. For $d > 2$ the return probability is less than one, and decreases as $1/d$ for large d.

Exercise: return probability for large d**.**   Obtain an explicit expansion in $1/d$ of the Green's function at the origin, and thus of the return probability, starting from the representation (52).

2   The Ising model

2.1   Historical bullet points

What has now come to be known as the Ising model was in fact formulated by W. Lenz in 1920 as a model for a ferromagnet. His student E. Ising treated the one-dimensional case in 1925 [3]. The two-dimensional case was solved (for zero field) by Lars Onsager in 1944 [4], this feat still being recognized as one of the towering achievements in classical statistical mechanics. Onsager's exact solution paved the way for the refinement of our understanding of critical phenomena in general. A.B. Zamolodchikov solved the two-dimensional, nonzero-field case in 1989. Amazingly, the three-dimensional Ising model remains unsolved, irrespective of whether the field vanishes or not.

The Ising model's Hamiltonian is arguably the simplest system of interacting spins on a lattice which one can imagine. Consider a generic lattice. Each lattice site i carries a spin variable s_i taking values $s_i = \pm 1$. Spins are pairwise coupled and subjected to an external field B:

$$H = \frac{1}{2} \sum_{i,j} \mathcal{J}_{ij} s_i s_j - B \sum_i s_i \tag{91}$$

where the spin couplings are assumed to be nonvanishing only for nearest neighbour pairs,

$$\mathcal{J}_{ij} = \left\{ \begin{array}{cc} \mathcal{J}, & i,j \ \text{nearest neighbours,} \\ 0 & \text{otherwise} \end{array} \right. \tag{92}$$

If $\mathcal{J} < 0$, the coupling induces ferromagnetic correlations between neighbouring spins. On the contrary, if $\mathcal{J} > 0$, antiferromagnetic configurations are preferred. The first fundamental question which we would like to ask is whether the system develops some form of spin order at low temperatures. Physically, we know that such spin ordering exists: consider for example the case of iron, which develops a spontaneous magnetization at low temperatures.

Such thermodynamic questions are best addressed using the standard tools of equilibrium statistical mechanics. We will thus work our way towards the evaluation of the partition function of the Ising model, which is given by the full configurational sum

$$Z_{\text{Ising}} = \sum_{\{s_i\}} \exp \left[\beta \left(B \sum_i s_i - \frac{1}{2} \sum_{ij} \mathcal{J}_{ij} s_i s_j \right) \right]. \tag{93}$$

The physics of the model will greatly depend on the dimensionality. We expect higher-dimensional versions of the model to be more 'rigid', namely that the tendency to order should be greater on higher-dimensional lattices. We will here consider the simplest cases of one- and two-dimensional lattices.

2.2 The one-dimensional Ising model

The evaluation of the partition function for the one-dimensional case is completely straightforward. Taking our lattice sites to be labelled by the integer $i = 0, ..., N-1$ and imposing periodic boundary conditions $s_N \equiv s_0$ and adopting the ferromagnetic convention

$$\mathcal{J} \equiv -\epsilon, \qquad \epsilon > 0, \tag{94}$$

we can write

$$H = \sum_{i=0}^{N-1} H_{s_i, s_{i+1}}, \qquad H_{s_i, s_j} = -\epsilon \ s_i s_j + \frac{B}{2}(s_i + s_j). \tag{95}$$

The partition function can then be written

$$Z = \sum_{\{s_i\}} \prod_{i=0}^{N-1} \exp\left[-\beta H(s_i, s_{i+1})\right] = \ \mathrm{Tr} \ T^N \tag{96}$$

where we have defined the **transfer matrix** (viewing the spin values as labels of the matrix coordinates)

$$T_{ss'} \equiv \exp\left[-\beta H_{s,s'}\right] = \begin{pmatrix} e^{\beta(\epsilon+B)} & e^{-\beta\epsilon} \\ e^{-\beta\epsilon} & e^{\beta(\epsilon-B)} \end{pmatrix}. \tag{97}$$

Since T is positive symmetric, it has real positive eigenvalues and can be diagonalized by an orthogonal transformation. Denoting the two eigenvalues as λ_0 and λ_1 with $\lambda_0 > \lambda_1$, we have

$$\lim_{N\to\infty} \frac{1}{N} \ln \ \mathrm{Tr} \ T^N = \lim_{N\to\infty} \frac{1}{N} \ln\left[\lambda_0^N + \lambda_1^N\right] = \ln\lambda_0. \tag{98}$$

This largest eigenvalue is easily shown to be

$$\lambda_0 = e^{\beta\epsilon}\left[\cosh\beta B + \sqrt{\cosh^2\beta B - (1 - e^{-4\beta\epsilon})}\right]. \tag{99}$$

This gives the free energy per site

$$f = -\epsilon - \frac{1}{\beta}\ln\left[\cosh\beta B + \sqrt{\cosh^2\beta B - (1 - e^{-4\beta\epsilon})}\right]. \tag{100}$$

The average magnetization per site is

$$\langle s \rangle = -\left(\frac{\partial f}{\partial B}\right)\bigg|_T = \frac{\sinh\beta B}{\sqrt{\cosh^2\beta B - (1 - e^{-4\beta\epsilon})}}. \tag{101}$$

In the zero field case, the partition function and free energy per site become

$$Z = 2^N \cosh^N(\beta\epsilon), \qquad f = -\frac{1}{\beta}\ln\left[2\cosh(\beta\epsilon)\right]. \tag{102}$$

The zero magnetic field limit is such that $\langle s \rangle = 0$ for any value of β, and the one-dimensional Ising model therefore never exhibits a phase transition to a ferromagnetic state (in other words: the one-dimensional Ising model never spontaneously magnetizes).[7]

The two-dimensional Ising model cannot be solved using the simple procedure we have just applied to the one-dimensional case. We will follow a diagrammatic route proposed by Kac and Ward [5] since it involves a nicely illustrative path summation-like logic. Note that this is not the method Onsager used, which was based on a fermionic representation of the problem. What we are about to do is inuitively much simpler to understand.

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[7]History says that this negative result had a severe impact on Ising, who never published another scientific paper.

2.3   High-temperature expansion and loop summations

Our reasonings will be based on the observation that at high temperatures (so small β), the partition function of the Ising model can be represented as the formal series

$$Z_{\text{Ising}} = \sum_{\{s_i\}} e^{-\beta H(\{s_i\})} = \sum_{\{s_i\}} \sum_{n=0}^{\infty} \frac{[-\beta H(\{s_i\})]^n}{n!} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \sum_{\{s_i\}} [\beta H(\{s_i\})]^n. \tag{103}$$

Specializing to the zero-field case, we can start from the representation

$$Z_{\text{Ising}} = \sum_{\{s_i\}} \prod_{\langle i,j \rangle} e^{\beta \epsilon s_i s_j}, \qquad \epsilon \equiv -\mathcal{J}. \tag{104}$$

Using the simple identity

$$e^{\pm A} = \cosh A \pm \sinh A = \cosh A (1 \pm \tanh A) \tag{105}$$

then allows to rewrite the partition function as

$$Z_{\text{Ising}} = \sum_{\{s_i\}} \prod_{\langle i,j \rangle} \cosh(\beta \epsilon) \left[1 + s_i s_j \tanh(\beta \epsilon)\right] = [\cosh(\beta \epsilon)]^{Nz/2} \sum_{\{s_i\}} \prod_{\langle i,j \rangle} (1 + s_i s_j v) \tag{106}$$

where the parameter

$$v \equiv \tanh(\beta \epsilon) \tag{107}$$

will be our (small) expansion parameter. The polynomial

$$\prod_{\langle i,j \rangle} (1 + s_i s_j v) = 1 + v \sum_{\langle i,j \rangle} s_i s_j + v^2 \sum_{\langle i,j \rangle} \sum_{\langle k,l \rangle} s_i s_j s_k s_l + \dots \tag{108}$$

has terms which can be pictorially represented by drawing a line between sites i and j if $s_i s_j$ appears in the product of spins. The large temperature expansion thus becomes a summation over all possible line drawings which can be made on the lattice considered. Now the crucial fact is that upon performing the configurational sum $\sum_{\{s_i\}}$, a large number of terms in the expansion simply vanish, namely all those where at least one spin is appearing an odd number of times. Said otherwise, the only drawings which do not vanish upon performing the configurational sum are those associated to **closed loops** where each spin is 'visited' by an even (explicitly: 0, 2, ..., z) number of line segments. We thus obtain that the partition function of the Ising model (in arbitrary dimension) can be written as

$$Z_{\text{Ising}} = [\cosh(\beta \epsilon)]^{Nz/2} 2^N \sum_{l=0}^{\infty} g(l) v^l \tag{109}$$

where $g(l)$ is the number of loops of l segments which can be drawn on the lattice. We adopt the convention that $g(0) = 1$. Also, by definition, $g(l) = 0$ for $l > \frac{z}{2}N$.

2.4   The two-dimensional square lattice Ising model

Let us now obtain the partition function for the two-dimensional Ising model via the high-temperature expansion defined above. We specialize to a square lattice of width L in both directions. The total number of sites is thus simply $N = L^2$. For definiteness, we impose periodic boundary conditions in both directions.

2.4.1   Counting loops on the square lattice

First, a bit of terminology. A **closed path** of l links is an arrowed path going from one site back to the same site in l steps. A **loop** is a pattern of links, each lattice point seeing an even number of links. Example: a ring of l links represents $2l$ closed paths, but is only one loop.

A closed path is called **connected** if it is formed by a single body of links, and is otherwise called **disconnected**. Let us write the number of closed, connected paths of length l as $h(l)$. For convenience, we define a function (whose aim is to give us the number of distinct connected loops) $D(l)$ as

$$D(l) \equiv \frac{1}{2l} h(l). \tag{110}$$

The total number of loops should be expressible in terms of the number of distinct connected loops. We should be able to write something like

$$g(l) \stackrel{?}{=} \sum_{n=1}^{l} \frac{1}{n!} \sum_{l_1+...+l_n=l} D(l_1)...D(l_n). \tag{111}$$

There is however a problem with this simple construction. Namely, some configurations are overcounted. Consider for example the paths shown in Fig. 4 which contribute to $g(8)$. These three distinct patterns should however be associated to a single loop contribution in a proper counting. Similarly, Fig. 5 shows four patterns contributing to a forbidden loop in the sum for $g(8)$.
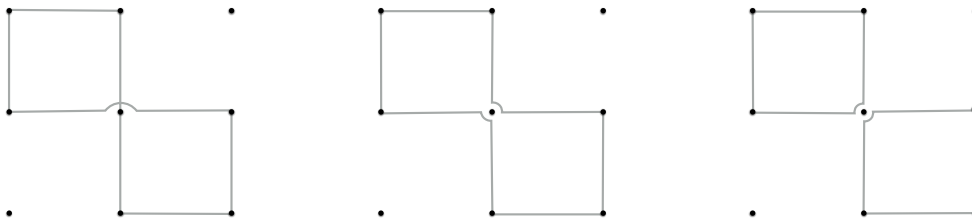

Figure 4: Three patterns contributing to $g(8)$ and which should really be associated to a single loop (this loop being allowed in the expansion of the partition function). The total phases associated to each are respectively $+1$ (closed loop, one crossing), -1 (one closed loop, no crossings) and $+1$ (two closed loops). The sum of these three thus gives a contribution of total weight 1.

To correct for this overcounting, we will modify our definition of $D(l)$ in such a way that different closed paths obtain an amplitude which will effectively 'cancel off' the extraneous terms. Explicitly, we will associate a left turn with a phase $e^{i\frac{\pi}{4}}$, and a right turn with a phase $e^{-i\frac{\pi}{4}}$. The amplitude of a given path is then the product of the phase factors at each turn of the path. A non-crossing closed loop therefore obtains a phase -1, whereas a single-crossing path (like a 'figure-of-eight' one) gets phase $+1$. This generalizes: paths with even/odd numbers of crossings get $-1/+1$ phases.

This idea is implemented in the actual calculation by introducing a matrix $\boldsymbol{M}$ with elements M_{ij} being nonzero if it is possible to link sites $\boldsymbol{i}$ and $\boldsymbol{j}$ by a single line segment. Going further, $(\boldsymbol{M}^l)_{ij}$ will be nonzero only if it is possible to link sites $\boldsymbol{i}$ and $\boldsymbol{j}$ by l line segments. Conveniently,
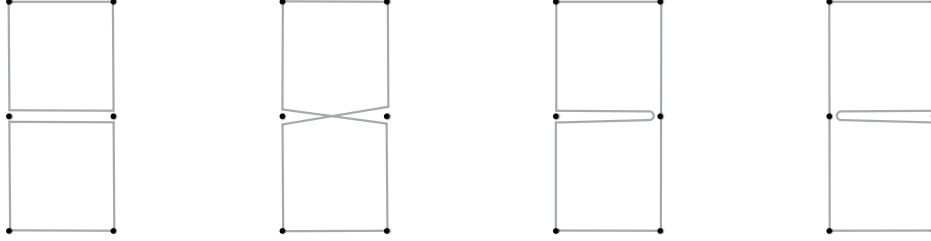
Figure 5: Four contributions to the same loop (this loop is forbidden in the partition function expansion). The phases are here respectively $+1$, $+1$, -1 and -1. The total contribution thus cancels.

the rules for matrix multiplication mean that if we give weight 1 to each path, the matrix element $(\boldsymbol{M}^l)_{\boldsymbol{ij}}$ will be proportional to the number of paths linking sites $\boldsymbol{i}$ and $\boldsymbol{j}$ by l line segments. We have to include our phases however; since there are four different directions for getting to and leaving a site, we view each element of matrix $\boldsymbol{M}$ as a 4×4 matrix $\boldsymbol{m}_{\boldsymbol{ij}}^{\alpha\beta}$ with $\alpha, \beta = 0, ..., 3$ labelling the entry/exit directions. Labelling $0 \equiv E$, $1 \equiv N$, $2 \equiv W$, $3 \equiv S$, we have (using our phase conventions, and using $\boldsymbol{i} - \boldsymbol{j}$ as subindex)

$$\boldsymbol{m}_{(-1,0)} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ e^{-i\frac{\pi}{4}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ e^{i\frac{\pi}{4}} & 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{m}_{(1,0)} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & e^{i\frac{\pi}{4}} & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & e^{-i\frac{\pi}{4}} & 0 \end{pmatrix},$$

$$\boldsymbol{m}_{(0,-1)} = \begin{pmatrix} 0 & e^{i\frac{\pi}{4}} & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & e^{-i\frac{\pi}{4}} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{m}_{(0,1)} = \begin{pmatrix} 0 & 0 & 0 & e^{-i\frac{\pi}{4}} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{i\frac{\pi}{4}} \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{112}$$
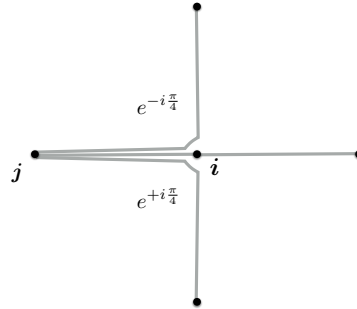
An example of these is illustrated in Fig. 6.

Figure 6: Illustration of the construction of the $\boldsymbol{m}_{(1,0)}$ matrix.

Now the diagonal elements $(\boldsymbol{M}^l)_{\boldsymbol{ii}}^{\alpha\alpha}$ involve a summation of terms each representing a distinct closed path going from/to site $\boldsymbol{i}$ in l steps (with entering direction α). The number of distinct

connected loops we are looking for is thus

$$D(l) \equiv -\frac{1}{2l} \text{ Tr } \boldsymbol{M}^l = -\frac{1}{2l} \sum_{\boldsymbol{i}} \text{ Tr } \boldsymbol{m}_{\boldsymbol{i}\boldsymbol{i}}^{(l)} \tag{113}$$

(where the first trace is over the $4N$ indices of the $\boldsymbol{M}$ matrix, and the second one over the 4 indices of the $\boldsymbol{m}$ matrices), where we have included a factor -1 to correct for the fact that a simple closed loop comes with this factor.

The partition function can be written in terms of $D(l)$ as

$$Z_{\text{Ising}} = [\cosh(\beta\epsilon)]^{Nz/2} 2^N \left[1 + \sum_{l=1}^{\infty} v^l \sum_{n=1}^{l} \frac{1}{n!} \sum_{l_1+...+l_n=l} D(l_1)...D(l_n) \right]$$

$$= [\cosh(\beta\epsilon)]^{Nz/2} 2^N \left[1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left[\sum_{l=1}^{\infty} D(l)v^l \right]^n \right] = [\cosh(\beta\epsilon)]^{Nz/2} 2^N \exp\left[\sum_{l=1}^{\infty} D(l)v^l \right], \tag{114}$$

with $D(0) \equiv 1$. Since $\boldsymbol{M}$ is diagonalizable, we can express $D(l)$ in terms of its eigenvalues,

$$D(l) = -\frac{1}{2l} \sum_{\boldsymbol{i}} \text{ Tr } \boldsymbol{M}^l = -\frac{1}{2l} \sum_{\alpha=0}^{4N-1} \lambda_\alpha^l. \tag{115}$$

This result in turn allows us to write the partition function as

$$Z_{\text{Ising}} = [\cosh(\beta\epsilon)]^{Nz/2} 2^N \exp\left[-\sum_{\alpha=0}^{4N-1} \sum_{l=1}^{\infty} \frac{\lambda_\alpha^l v^l}{2l} \right] = [\cosh(\beta\epsilon)]^{Nz/2} 2^N \prod_{\alpha} (1 - v\lambda_\alpha)^{\frac{1}{2}}. \tag{116}$$

Our last step thus consists in finding the eigenvalues of $\boldsymbol{M}$. Because of translational invariance, we have that each of its elements depends on the coordinate difference vector,

$$\boldsymbol{m}_{\boldsymbol{ij}} \equiv m_{\boldsymbol{i}-\boldsymbol{j}}. \tag{117}$$

Its Fourier coefficients are

$$\boldsymbol{M_q} = \sum_{\boldsymbol{j}} m_{\boldsymbol{j}} e^{-i\boldsymbol{q}\cdot\boldsymbol{j}}, \qquad \boldsymbol{q} = \frac{2\pi}{L}\boldsymbol{n}, \qquad n_i = 0, ..., L-1. \tag{118}$$

Explicitly, the $\boldsymbol{M}$ matrix becomes block diagonal in momentum, each momentum block being given by

$$\boldsymbol{M_q} = \begin{pmatrix} Q_{(1,0)}^{-1} & Q_{(0,1)}^{-1} e^{i\frac{\pi}{4}} & 0 & Q_{(0,1)} e^{-i\frac{\pi}{4}} \\ Q_{(1,0)}^{-1} e^{-i\frac{\pi}{4}} & Q_{(0,1)}^{-1} & Q_{(1,0)} e^{i\frac{\pi}{4}} & 0 \\ 0 & Q_{(0,1)}^{-1} e^{-i\frac{\pi}{4}} & Q_{(1,0)} & Q_{(0,1)} e^{i\frac{\pi}{4}} \\ Q_{(1,0)}^{-1} e^{i\frac{\pi}{4}} & 0 & Q_{(1,0)} e^{-i\frac{\pi}{4}} & Q_{(0,1)} \end{pmatrix}, \qquad Q_{\boldsymbol{j}} \equiv e^{-i\boldsymbol{q}\cdot\boldsymbol{j}}. \tag{119}$$

Instead of calculating the eigenvalues one by one and substituting them in the expression for the partition function, let us instead directly calculate the product: in each momentum sector,

$$\prod_{\alpha=0}^{3} (1 - v\lambda_{\boldsymbol{q},\alpha}) = \text{ Det } [v\boldsymbol{M_q} - \boldsymbol{1}] = (1 + v^2)^2 - 2v(1 - v^2) \Re\left(Q_{(1,0)} + Q_{(0,1)} \right). \tag{120}$$

This gives us the explicit exact expression

$$Z_{\text{Ising}} = [\cosh(\beta\epsilon)]^{Nz/2} 2^N \prod_{\boldsymbol{q}} \left((1 + v^2)^2 - 2v(1 - v^2) [\cos q_1 + \cos q_2] \right)^{\frac{1}{2}} \tag{121}$$

for the partition function of the two-dimensional Ising model.

Exercise: thermodynamic properties of the two-dimensional Ising model.
   Show that in the thermodynamic limit, the free energy per site is:

$$\beta f = -\ln 2 - \frac{1/2}{(2\pi)^2} \int_{-\pi}^{\pi} dk_1 dk_2 \ln\left[\cosh^2(2\beta\epsilon) - \sinh(2\beta\epsilon)(\cos k_1 + \cos k_2)\right]. \qquad (122)$$

Show that this gives the internal energy per site ($u = \frac{d(\beta f)}{d\beta}$) is

$$u = -\epsilon \coth(2\beta\epsilon)\left(1 - \left[1 - 2\tanh^2(2\beta\epsilon)\right]\frac{2}{\pi}K(k)\right) \qquad (123)$$

where K is the complete elliptic integral of the first kind

$$K(k) \equiv \int_0^{\frac{\pi}{2}} d\phi \frac{1}{\sqrt{1 - k^2 \sin^2\phi}} \qquad (124)$$

with elliptic modulus

$$k \equiv 2\frac{\sinh(2\beta\epsilon)}{\cosh^2(2\beta\epsilon)}. \qquad (125)$$

   Going further, show that the specific heat $c = -\beta^2 \frac{du}{d\beta}$ is

$$c = \frac{4k_B}{\pi}(\beta\epsilon \coth(2\beta\epsilon))^2 \left(K(k) - E(k) - \text{sech}^2(2\beta\epsilon)\left[\frac{\pi}{2} - (1 - 2\tanh^2(2\beta\epsilon))K(k)\right]\right) \qquad (126)$$

in which $E(k)$ is the complete elliptic integral of the second kind

$$E(k) \equiv \int_0^{\frac{\pi}{2}} d\phi \sqrt{1 - k^2 \sin^2\phi}. \qquad (127)$$

Exercise: phase transition and critical exponents.
   The complete elliptic integral of the first kind $K(k)$ diverges when $k \to 1$. Show that this yields the critical temperature

$$\beta_c = \frac{1}{2\epsilon}\ln(1 + \sqrt{2}). \qquad (128)$$

Show that as the temperature approaches the critical value, the specific heat c diverges. What kind of divergence is it?

Exercise: correlation functions of the one-dimensional Ising model.
   Using the logic of transfer matrices, show that the spin-spin correlation function of the one-dimensional Ising model is

$$\langle s_0 s_n \rangle = \tanh^n(\beta\epsilon).$$

Rederive the same result using the high-temperature expansion.

3   The Dirac-Feynman path integral

Let us now move to the realm of quantum mechanics. Instead of the time evolution being driven by a stochastic process as in the case of Brownian motion, our system will now obey the deterministic Schrödinger equation.

The path integral formulation of quantum mechanics was initiated by P.A.M. Dirac, but pushed to new heights by R. P. Feynman. The book by Feynman & Hibbs contains a detailed exposition of the method.

The path integral formulation of quantum mechanics possesses a number of advantages over the standard formulation.

1. the classical limit ($\hbar \to 0$) is clear

2. it provides road towards non-perturbative methods

3. it serves as a prototype for the functional field integral

4. it has many direct applications for systems with one degree of freedom.

Our starting point to formulate the path integral is to perform a formal integration of the time-dependent Schrödinger equation:

$$i\hbar\partial_t|\Psi\rangle = \hat{H}|\Psi\rangle \quad \to \quad |\Psi(t')\rangle = \hat{U}(t',t)|\Psi(t)\rangle, \qquad \hat{U}(t',t) = e^{-\frac{i}{\hbar}\hat{H}(t'-t)}. \tag{129}$$

Considering the simplest situation in which we have a single particle evolving in a continuum interval (with the position labeled by q), we can write the wavefunction in the real space representation as

$$\Psi(q',t') = \langle q'|\Psi(t')\rangle = \langle q'|\hat{U}(t',t)|\Psi(t)\rangle = \int dq\, U(q',t';q,t)\Psi(q,t) \tag{130}$$

where the time-evolution operator has matrix elements

$$U(q',t';q,t) = \langle q'|e^{-\frac{i}{\hbar}\hat{H}(t'-t)}|q\rangle \tag{131}$$

Since this matrix element represents the probability amplitude for a particle to propagate from points q to point q' in a time $t'-t$, this is known as the **propagator** of the theory.

The basic idea behind Feynman's path integral is to split the finite time interval into infinitesimal chunks Δt, such that $t = N\Delta t$ with $N \gg 1$. The time evolution operator then factorizes into a product of time-step operators,

$$e^{-\frac{i}{\hbar}\hat{H}t} = \left[e^{-\frac{i}{\hbar}\hat{H}\Delta t}\right]^N. \tag{132}$$

Assuming that the Hamiltonian takes the form of the sum of a kinetic and a potential part, $\hat{H} = \hat{T} + \hat{V}$, we can factorize the time-step operator according to

$$e^{-\frac{i}{\hbar}\hat{H}\Delta t} = e^{-\frac{i}{\hbar}\hat{T}\Delta t}e^{-\frac{i}{\hbar}\hat{V}\Delta t} + O(\Delta t^2) \tag{133}$$

in which the $O(\Delta t^2)$ error is proportional to the commutator of $\hat{T}$ and $\hat{V}$. The truncation of this power-series expansion in Δt thus makes sense if Δt is much smaller than the reciprocal of the matrix elements of this commutator. Since our number N of time slices can be chosen to be arbitrarily large, the expansion formally converges.

The propagator can then be approximated by

$$\langle q_f|\left[e^{-\frac{i}{\hbar}\hat{H}\Delta t}\right]^N|q_i\rangle \simeq \langle q_f|\mathbf{1}_N e^{-\frac{i}{\hbar}\hat{T}\Delta t}e^{-\frac{i}{\hbar}\hat{V}\Delta t}\mathbf{1}_{N-1}...\mathbf{1}_1 e^{-\frac{i}{\hbar}\hat{T}\Delta t}e^{-\frac{i}{\hbar}\hat{V}\Delta t}|q_i\rangle \tag{134}$$

in which **1** are fixed time-slice resolutions of the identity operator, each being the product of resolutions of the identity in q and p space,

$$\mathbf{1}_n = \mathbf{1}_{q_n}\mathbf{1}_{p_n} = \int dq_n|q_n\rangle\langle q_n|\int dp_n|p_n\rangle\langle p_n| = \int dq_ndp_n|q_n\rangle\langle p_n|(\langle q_n|p_n\rangle)$$

$$= \int dq_ndp_n|q_n\rangle\langle p_n|\frac{e^{\frac{i}{\hbar}q_np_n}}{\sqrt{2\pi\hbar}} \tag{135}$$

in which we have used the convention $\langle p|q\rangle = \langle q|p\rangle^* = e^{-\frac{i}{\hbar}qp}/\sqrt{2\pi\hbar}$. Assuming that $\hat{T}$ is diagonalized by states $|p\rangle$, and $\hat{V}$ by states $|q\rangle$), we obtain

$$\langle q_f|e^{-\frac{i}{\hbar}\hat{H}t}|q_i\rangle \simeq \int \prod_{n=1}^{N}\frac{dq_ndp_n}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}q_np_n}\langle q_f|q_N\rangle\langle p_N|e^{-\frac{i}{\hbar}T(p_N)\Delta t}e^{-i\frac{i}{\hbar}V(q_{N-1})\Delta t}|q_{N-1}\rangle \times$$

$$\times \langle p_{N-1}|e^{-\frac{i}{\hbar}T(p_{N-1})\Delta t}e^{-i\frac{i}{\hbar}V(q_{N-2})\Delta t}|q_{N-2}\rangle \times ... \times |q_i\rangle. \tag{136}$$

The T and V exponentials are now simple numbers, and can be taken out of the bra-ket inner products. Substituting again the projection coefficients $\langle p_n|q_{n-1}\rangle = e^{-\frac{i}{\hbar}p_nq_{n-1}}/\sqrt{2\pi\hbar}$ in this equation, we get

$$\langle q_f|e^{-\frac{i}{\hbar}\hat{H}t}|q_i\rangle \simeq \int \prod_{n=1}^{N-1}dq_n\prod_{n=1}^{N}\frac{dp_n}{2\pi\hbar}e^{-i\frac{\Delta t}{\hbar}\sum_{n=0}^{N-1}(T(p_{n+1})+V(q_n)-p_{n+1}\frac{q_{n+1}-q_n}{\Delta t})}|_{q_N=q_F,q_0=q_i}. \tag{137}$$

This is exact up to corrections of order $[\hat{T},\hat{V}]\Delta t^2/\hbar^2$.

The remarkable thing about (137) is that the left-hand side, a quantum-mechanical transition amplitude, is expressed purely in terms of (an integration over) classical phase-space variables $x_n = (q_n, p_n)$. The constant $\hbar$, and the fact that we are summing a complex-valued integrand, are the only leftovers of the original Schrødinger time evolution equation.

Let us now briefly discuss the behaviour of the integral (137). The first thing to notice is that rapid fluctuations of the arguments x_n as a function of n are strongly inhibited (since the integrand is oscillatory). Contributions for which $(q_{n+1}-q_n)p_{n+1} > O(\hbar)$ tend to cancel each other because of destructive interference. The only contributions which survive are from paths which are smooth in space-time, which allows us to take the limit $N \to \infty$ (keeping $t = N\Delta t$ fixed) and rewrite the product of phase-space integrals in terms of a path integral: the set of points $\{x_n\}$ becomes a curve $x(t)$, and

$$\Delta t\sum_{n=0}^{N-1} \to \int_0^t dt', \qquad \frac{q_{n+1}-q_n}{\Delta t} \to \partial_{t'}q|_{t'=t_n} \equiv \dot{q}|_{t'=t_n},$$

$$T(p_{n+1}) + V(q_n) \to T(p|_{t'=t_n}) + V(q|_{t'=t_n}) \equiv H(x|_{t'=t_n}) \tag{138}$$

i.e. the *classical* Hamiltonian. Then,

$$\lim_{N\to\infty}\int\prod_{n=1}^{N-1}dq_n\prod_{n=1}^{N}\frac{dp_n}{2\pi\hbar}(...)|_{q_N=q_f,q_0=q_i} \equiv \int \mathcal{D}x(...)|_{q(t)=q_f,q(0)=q_i} \tag{139}$$

defines the path integral measure. Finally, one gets for the propagator

$$\langle q_f|e^{-\frac{i}{\hbar}\hat{H}t}|q_i\rangle = \int \mathcal{D}x\,\exp\left[\frac{i}{\hbar}\int_0^t dt'(p\dot{q} - H(p,q))\right]|_{q(t)=q_f,q(0)=q_i} \tag{140}$$

which is the **Hamiltonian formulation of the path integral**.

In the specific case of free dynamics, $\hat{T} = \frac{\hat{p}^2}{2m}$, we can explicitly perform the (functional) Gaussian integral over momentum and obtain

$$\langle q_f | e^{-\frac{i}{\hbar}\hat{H}t} | q_i \rangle = \int \mathcal{D}x \; e^{-\frac{i}{\hbar}\int_0^t dt' V(q)} \times e^{-\frac{i}{\hbar}\int_0^t dt' (\frac{p^2}{2m} - p\dot{q})}|_{q(t)=q_f, q(0)=q_i} \tag{141}$$

$$= \int \mathcal{D}q \, \exp\left[\frac{i}{\hbar}\int_0^t dt' L(q,\dot{q})\right]|_{q(t)=q_f, q(0)=q_i} = \int \mathcal{D}q \, \exp\left[\frac{i}{\hbar}S[q,\dot{q}]\right]|_{q(t)=q_f, q(0)=q_i} \tag{142}$$

with $L(q,\dot{q}) = \frac{m}{2}\dot{q}^2 - V(q)$ is the classical Lagrangian, $S[q,\dot{q}]$ is the action functional, and

$$\mathcal{D}q = \lim_{N \to \infty} \left(\frac{Nm}{it2\pi\hbar}\right)^{N/2} \prod_{n=1}^{N-1} dq_n \tag{143}$$

is the functional measure of the remaining integral.

Therefore: a *quantum mechanical* transition amplitude has been expressed in terms of a *path integral* through phase space or coordinate space, weighed by the classical action. This is Dirac's 'sum over histories' idea, pushed by Feynman.

Gaussian functional integration [supplement to PRELIMINARIES on Gaussian integration]   Starting from (17), suppose that the vector **v** parametrizes the weight of a real scalar field on the sites of a one-dimensional lattice. In continuum limit: set $\{v_i\}$ becomes a function $v(x)$ and the matrix A_{ij} becomes an **operator kernel** or **propagator** $A(x, x')$. Natural generalization of (17):

$$\int \mathcal{D}v(x) \, \exp\left[-\frac{1}{2}\int dxdx' v(x)A(x,x')v(x') + \int dxj(x)v(x)\right]$$
$$= (\det \frac{A}{2\pi})^{-1/2} \exp\left[\frac{1}{2}\int dxdx' j(x)A^{-1}(x,x')j(x')\right] \tag{144}$$

where the inverse kernel satisfies

$$\int dx' A(x,x')A^{-1}(x',x'') = \delta(x - x'') \tag{145}$$

so $A^{-1}(x, x')$ is the **Green function** of the operator $A(x, x')$.

Equation (18) generalizes to

$$\langle v(x)v(x')\rangle = A^{-1}(x, x') \tag{146}$$

and (21) generalizes to

$$\langle v(x_1)v(x_2)...v(x_{2n})\rangle = \sum_{pairings} A^{-1}(x_{k_1}, x_{k_2})...A^{-1}(x_{k_{2n-1}}, x_{k_{2n}}). \tag{147}$$

The path integral for a free particle

For a free particle $\hat{H} = \frac{\hat{p}^2}{2m}$, $\hat{L} = \frac{m}{2}\hat{q}^2$, we have

$$G_{\text{free}}(q_f, q_i; t) \equiv \langle q_f | e^{-\frac{i}{\hbar}\frac{\hat{p}^2}{2m}t} | q_i \rangle = \lim_{N \to \infty} \left(\frac{Nm}{it2\pi\hbar} \right)^{N/2} \int \prod_{n=1}^{N-1} dq_n e^{\frac{i}{\hbar}\int_0^t dt' \frac{m}{2}(\frac{dq}{dt'})^2}. \tag{148}$$

We choose $q_0 = q_i$ and $q_N = q_f$, with $t = N\Delta t$. The action can be written

$$\frac{m}{2} \int_0^t dt' (\frac{dq}{dt'})^2 = \frac{m}{2}\Delta t \sum_{n=1}^{N} (\frac{q_n - q_{n-1}}{\Delta t})^2 = \frac{m}{2\Delta t} \sum_{n=1}^{N} (q_n - q_{n-1})^2. \tag{149}$$

Look at the integral for q_1:

$$\int_{-\infty}^{\infty} dq_1 e^{\frac{im}{2\hbar\Delta t}((q_2 - q_1)^2 + (q_1 - q_0)^2)} = \int_{-\infty}^{\infty} dq_1 e^{\frac{im}{2\hbar\Delta t}(2q_1^2 - 2q_1(q_0 + q_2) + q_2^2 + q_0^2)}$$

$$= \int_{-\infty}^{\infty} dq_1 e^{\frac{im}{2\hbar\Delta t}*2((q_1 - \frac{q_0 + q_2}{2})^2 - (\frac{q_0 + q_2}{2})^2 + \frac{q_2^2 + q_0^2}{2})} = I(-\frac{2im}{\hbar\Delta t})e^{\frac{im}{2\hbar\Delta t}\frac{(q_2 - q_0)^2}{2}}$$

$$= \left(\frac{2\pi i\hbar\Delta t}{2m} \right)^{1/2} e^{\frac{im}{2\hbar\Delta t}\frac{(q_2 - q_0)^2}{2}} \tag{150}$$

Now look at the integral for q_2:

$$\int_{-\infty}^{\infty} dq_2 e^{\frac{im}{2\hbar\Delta t}((q_3 - q_2)^2 + \frac{1}{2}(q_2 - q_0)^2)} = \int_{-\infty}^{\infty} dq_2 e^{\frac{im}{2\hbar\Delta t}(\frac{3}{2}q_2^2 - q_2(2q_3 + q_0) + q_3^2 + \frac{q_0^2}{2})}$$

$$= \int_{-\infty}^{\infty} dq_2 e^{\frac{im}{2\hbar\Delta t}(\frac{3}{2}(q_2 - \frac{2q_3 + q_0}{3})^2 - \frac{3}{2}(\frac{2q_3 + q_0}{3})^2 + q_3^2 + \frac{q_0^2}{2})}$$

$$= \left(\frac{2\pi\hbar i\Delta t}{m} * \frac{2}{3} \right)^{1/2} e^{\frac{im}{2\hbar\Delta t}(-\frac{2}{3}(q_3 + q_0/2)^2 + q_3^2 + \frac{q_0^2}{2})}. \tag{151}$$

But we have $-\frac{2}{3}(q_3 + q_0/2)^2 + q_3^2 + \frac{q_0^2}{2} = \frac{(q_3 - q_0)^2}{3}$ so after the q_2 integral, we have

$$\left(\frac{2\pi\hbar i\Delta t}{m} * \frac{1}{2} \right)^{1/2} \left(\frac{2\pi\hbar i\Delta t}{m} * \frac{2}{3} \right)^{1/2} e^{\frac{im}{2\hbar\Delta t}\frac{(q_3 - q_0)^2}{3}}. \tag{152}$$

Carrying on with the $q_3, ..., q_{N-1}$ integrals then gives

$$\left(\frac{2\pi\hbar i\Delta t}{m} \right)^{\frac{N-1}{2}} * \left(\frac{1}{N} \right)^{1/2} e^{\frac{im}{2\hbar\Delta t}\frac{(q_N - q_0)^2}{N}}. \tag{153}$$

By using $t = N\Delta t$ and $q_f = q_N, q_i = q_0$, we thus finally get

$$G_{\text{free}}(q_f, q_i; t) = \left(\frac{m}{2\pi\hbar it} \right)^{1/2} e^{\frac{im}{2\hbar t}(q_f - q_i)^2}. \tag{154}$$

The path integral for a free particle: alternative derivation using matrix Gaussian integration

The action can be written using

$$\sum_{n=1}^{N}(q_n - q_{n-1})^2 = q_0^2 + q_N^2 + \boldsymbol{q}^T \boldsymbol{M}_{N-1} \boldsymbol{q} - 2\boldsymbol{J}^T \cdot \boldsymbol{q} \tag{155}$$

where we have defined the $N-1$-dimensional vectors

$$\boldsymbol{q}^T \equiv \begin{pmatrix} q_1 & ... & q_{N-1} \end{pmatrix}, \qquad \boldsymbol{J}^T \equiv \begin{pmatrix} q_0 & 0 & ... & 0 & q_N \end{pmatrix}, \tag{156}$$

and the matrix (the supindex giving its dimension)

$$\boldsymbol{M}^{(\text{N-1})} = \begin{pmatrix} 2 & -1 & 0 & ... & 0 \\ -1 & 2 & -1 & 0 & ... \\ 0 & -1 & 2 & -1 & ... \\ ... & 0 & -1 & ... & -1 \\ 0 & ... & ... & -1 & 2 \end{pmatrix}. \tag{157}$$

We can calculate the determinant of $\boldsymbol{M}$ easily by for example putting all elements below the diagonal to zero, adding $1/2$ times row 1 to row 2, etc.:

$$\text{Det}\boldsymbol{M} = \text{Det} \begin{pmatrix} 2 & -1 & 0 & ... & ... \\ 0 & 2-\frac{1}{2} & -1 & 0 & ... \\ 0 & -1 & 2 & -1 & ... \end{pmatrix} = \text{Det} \begin{pmatrix} d_1 & -1 & 0 & ... \\ 0 & d_2 & -1 & ... \\ 0 & 0 & d_3 & ... \end{pmatrix} \tag{158}$$

where

$$d_1 \equiv 2, \qquad d_{n+1} = 2 - \frac{1}{d_n} \qquad \Rightarrow \qquad d_n = \frac{n+1}{n}, \tag{159}$$

and thus

$$\text{Det}\boldsymbol{M}_{N-1} = N. \tag{160}$$

The free propagator can be written as

$$G_{\text{free}}(q_f, q_i; t) = \lim_{N \to \infty} \left(\frac{Nm}{it2\pi\hbar}\right)^{N/2} e^{\frac{im}{2\hbar\Delta t}(q_0^2 + q_N^2)} \int \left[\prod_{n=1}^{N-1} dq_n\right] e^{-\frac{1}{2}\boldsymbol{q}^T \boldsymbol{A}\boldsymbol{q} + \boldsymbol{j}^T \cdot \boldsymbol{q}} \tag{161}$$

where

$$\boldsymbol{A} \equiv \frac{m}{i\hbar\Delta t}\boldsymbol{M}, \qquad \boldsymbol{j} \equiv \frac{m}{i\hbar\Delta t}\boldsymbol{J}. \tag{162}$$

The multivariable Gaussian integration can be performed using rule (17), yielding

$$(2\pi)^{\frac{N-1}{2}} \text{ Det } \mathbf{A}^{-1/2} e^{\frac{1}{2}\mathbf{j}^T \mathbf{A}^{-1}\mathbf{j}}. \tag{163}$$

In view of the structure of $\boldsymbol{J}$, the only inverse matrix elements we need are

$$(\boldsymbol{M}^{(\text{N-1})})_{1,1}^{-1} = (\boldsymbol{M}^{(\text{N-1})})_{N-1,N-1}^{-1} = \frac{\text{Det}\boldsymbol{M}^{(\text{N-2})}}{\text{Det}\boldsymbol{M}^{(\text{N-1})}} = \frac{N-1}{N},$$

$$(\boldsymbol{M}^{(\text{N-1})})_{1,N-1}^{-1} = (\boldsymbol{M}^{(\text{N-1})})_{N-1,1}^{-1} = \frac{1}{\text{Det}\boldsymbol{M}^{(\text{N-1})}} = \frac{1}{N}, \tag{164}$$

and thus

$$\boldsymbol{J}^T \boldsymbol{M}^{-1} \boldsymbol{J} = \frac{N-1}{N}(q_0^2 + q_N)^2 + \frac{2}{N}q_0 q_N = q_0^2 + q_N^2 - \frac{1}{N}(q_N - q_0)^2. \tag{165}$$

Collecting all factors then gives back the previous answer,

$$G_{\text{free}}(q_f, q_i; t) = \left(\frac{m}{2\pi\hbar it}\right)^{1/2} e^{\frac{im}{2\hbar t}(q_f - q_i)^2}. \tag{166}$$

3.1   Correspondence between classical and quantum propagators

There is one striking aspect which can be noticed upon careful comparison of the quantum free particle probability amplitude for propagation (154),

$$G_{\text{free}}(q_f, q_i; t) = \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{\frac{im}{2\hbar t}(q_f - q_i)^2} \tag{167}$$

with the classical one (46) (specialized to one dimension), using τ to denote the 'classical' time interval

$$p(r_f, \tau | r_i, 0) = \frac{1}{[4\pi D\tau]^{1/2}} \exp\left[-\frac{(r_f - r_i)^2}{4D\tau}\right]. \tag{168}$$

Explicitly, these expressions coincide under the identification

$$\tau = it \times \left(\frac{\hbar}{2Dm}\right). \tag{169}$$

The factor in parentheses is simply a scale for our clocks. More importantly, what should be noticed here is that there is a correspondence between quantum propagation in real(respectively: imaginary) time and classical propagation in imaginary(respectively: real) time. This could have been anticipated immediately from the starting point, by comparing the diffusion equation (49)

$$\frac{\partial}{\partial\tau}p(r_f, \tau | r_i, 0) = D\nabla_f^2 p(r_f, \tau | r_i, 0)$$

with the Schrödinger equation for the free particle,

$$i\hbar\frac{\partial}{\partial t}U(q_f, t; q_i, 0) = \frac{-\hbar^2}{2m}\nabla_f^2 U(q_f, t; q_i, 0).$$

This correspondence will also manifest itself at the level of general field theory, which will be treated in the following chapters. The mnemonic trick is that when going from classical to quantum, one should take $\tau \to it$.

3.2 An integral approximation method

One of the great aspects of the path integral formulation of a problem is that it is readily adaptable to approximation schemes.

To illustrate the idea, we begin with a very simple case. Consider a function $f(x)$ and the integral

$$I[f] = \int_{-\infty}^{\infty} dx e^{-f(x)}. \tag{170}$$

Knowing some features of the function f, what can we say about the functional $I[f]$? Suppose that $f(x)$ has a global minimum at x_0. The integrand will be largest in the region where f has this minimum. Expanding f, we get

$$I[f] = \int_{-\infty}^{\infty} dx e^{-f(x_0) - \frac{a}{2}(x-x_0)^2 + \mathcal{O}((x-x_0)^3)} = e^{-f(x_0)} G_a(1 + ...) \tag{171}$$

in which $a \equiv \frac{d^2}{dx^2} f|_{x_0}$ (since x_0 represents a minimum, we assume $a > 0$), $G_a \equiv \int_{-\infty}^{\infty} dx e^{-\frac{a}{2}x^2} = \sqrt{\frac{2\pi}{a}}$ is the Gaussian integral and ... represent corrections (which can be systematically computed in terms of fundamental integrals of the form $G_{a,n} \equiv \int_{-\infty}^{\infty} dx x^n e^{-\frac{a}{2}x^2}$). Note that the integral limits can be adapted here: to a certain degree of accuracy, provided the minimum point x_0 sits in the bulk of the original integration interval and that $f(x)$ becomes sufficiently large away from x_0, the boundaries can be put to $\pm\infty$. Note that the steeper the minimum of $f(x)$ is, the more accurate the approximation is. Note also that if f has multiple minima, then one can simply sum over the Gaussian-like integrals over each of these minima to approximate the full integral.

As an example, we can consider the integral representation of the Gamma function

$$\Gamma(z+1) = \int_0^{\infty} dx x^z e^{-x}. \tag{172}$$

Following our procedure gives

$$\Gamma(z+1) = \int_0^{\infty} dx e^{-x+z\ln x}, \quad f(x) = x - z\ln x, \quad x_0 = z, \quad f(x_0) = z(1-\ln z),$$

$$a = d_x^2 f(x)|_{x_0} = z/x^2|_{x_0} = 1/z, \quad \sqrt{2\pi/a} = \sqrt{2\pi z}. \tag{173}$$

We thus directly obtain Stirling's approximation,

$$\Gamma(z+1) = \sqrt{2\pi z} e^{z(\ln z - 1)}(1 + ...). \tag{174}$$

This approximation method is also valid when dealing with a complex-valued argument in the integrand's exponential. It is generally known as the **stationary phase approximation**.

3.3   Stationary phase approximation of path integrals

Let us now adapt this idea to path integrals. Consider the functional integral $\int \mathcal{D}x e^{-F[x]}$ where $\mathcal{D}x = \lim_{N\to\infty} \prod_{n=1}^{N} dx_n$. As before, we are integrating over a set of fixed time-slice coordinates becoming a smooth function of time in the limit $N \to \infty$, $\{x_n\} \to x(t)$ with t playing the role of the former index n. The functional $F[x]$ depends on $x(t)$ at any t.

Evaluating this functional integral in the stationary phase approximation consists is performing the following steps:

1. Find the points of stationary phase, *i.e.* configurations $\bar{x}(t)$ such that the functional derivative of the action vanishes,

$$D_x F = 0 \Leftrightarrow \frac{\delta F[x]}{\delta x(t)} = 0 \ \forall t. \tag{175}$$

2. Perform a (functional) Taylor expansion of F to second order around $\bar{x}$:

$$F[x] = F[\bar{x} + y] = F[\bar{x}] + \frac{1}{2} \int dt dt' y(t') A(t, t') y(t) + ... \tag{176}$$

where $A(t, t') = \frac{\delta^2 F[x]}{\delta x(t)\delta x(t')}|_{x=\bar{x}}$. The first-order term is zero because of the stationarity condition.

3. Check that kernel $\hat{A} \equiv \{A(t, t')\}$ is positive definite (thereby guaranteeing the convergence of the Gaussian approximation to the functional integral). If so, perform the functional integral over y, yielding $\int \mathcal{D}x e^{-F[x]} \simeq e^{-F[\bar{x}]} \det \left(\frac{\hat{A}}{2\pi}\right)^{-1/2}$ (see eq. (144)).

4. Finally, if there are many stationary phase configurations $\bar{x}_i(t)$, simply sum over the individual contributions:

$$\int \mathcal{D}x e^{-F[x]} \simeq \sum_i e^{-F[\bar{x}_i]} \det \left(\frac{\hat{A}_i}{2\pi}\right)^{-1/2}. \tag{177}$$

To summarize, the stationary phase approximation is based on finding the dominant terms contributing to the functional integral, including the maximal points and their Gaussian approximation.

Let us now apply the stationary phase approximation to the Lagrangian form of the Feynman path integral for a single particle. In particular, this converges quickly in the semiclassical limit when we take $\hbar \to 0$. The dominant trajectory is the solution to the classical equations of motion, $\bar{q}(t) = q_{cl}(t)$. Defining deviations as $r(t) = q(t) - q_{cl}(t)$ (assuming that there is only one classical path) then leads to

$$\langle q_f|e^{-\frac{i}{\hbar}\hat{H}t}|q_i\rangle \simeq e^{\frac{i}{\hbar}S[q_{cl}]} \int_{r(0)=r(t)=0} \mathcal{D}r \exp\left[\frac{i}{2\hbar}\int_0^t dt'dt'' r(t') \frac{\delta^2 S[q]}{\delta q(t')\delta q(t'')}|_{q=q_{cl}} r(t'')\right] \tag{178}$$

which is the Gaussian approximation to the path integral.

For free Lagrangians $L(q, \dot{q}) = \frac{m}{2}\dot{q}^2 - V(q)$, the second functional derivative integral term is computed most easily by Taylor expanding the action:

$$\begin{aligned} S[q] &= \int dt L(q, \dot{q}) = \int dt \left(\frac{m}{2}\dot{q}^2 - V(q)\right) \\ &= \int dt \left(\frac{m}{2}(\dot{q}_{cl}^2 + 2\dot{q}_{cl}\dot{r} + \dot{r}^2) - V(q_{cl}) - V'(q_{cl})r - \frac{1}{2}V''(q_{cl})r^2\right) + ... \\ &= S[q_{cl}] + \int dt \left(-m\ddot{q}_{cl}r - V'(q_{cl})r - \frac{m}{2}\ddot{r}r - \frac{1}{2}V''(q_{cl})r^2\right) + ... \\ &= S[q_{cl}] - \frac{1}{2}\int dt \ r(t)[m\partial_t^2 + V''(q_{cl}(t))]r(t) + ... \end{aligned} \tag{179}$$

with $V''(q_{cl}(t)) \equiv \partial_q^2 V(q)|_{q_{cl}(t)}$, so

$$\frac{1}{2} \int_0^t dt' dt'' r(t') \frac{\delta^2 S[q]}{\delta q(t')\delta q(t'')}|_{q=q_{cl}} r(t'') = -\frac{1}{2} \int_0^t dt' r(t')[m\partial_{t'}^2 + V''(q_{cl}(t'))]r(t'). \qquad (180)$$

Doing the Gaussian integration finally yields the approximation

$$\langle q_f | e^{-\frac{i}{\hbar}\hat{H}t} | q_i \rangle \simeq e^{\frac{i}{\hbar}S[q_{cl}]} \int_{r(0)=r(t)=0} \mathcal{D}r \, \exp\left[-\frac{i}{2\hbar} \int dt' r(t')[m\partial_{t'}^2 + V''(q_{cl}(t'))]r(t')\right]$$

$$= e^{\frac{i}{\hbar}S[q_{cl}]} \det\left(\frac{i}{2\pi\hbar}[m\partial_t^2 + V''(q_{cl}(t))]\right)^{-1/2}. \qquad (181)$$

The path integral for the harmonic oscillator

Let us consider a particle in a harmonic potential, whose Hamiltonian and Lagrangian are respectively

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2, \qquad \hat{L} = \frac{m}{2}\dot{x}^2 - \frac{m\omega^2}{2}\hat{x}^2. \tag{182}$$

The propagator is then

$$G_{ho}(q_f, q_i; t) = \langle q_f | e^{-\frac{i}{\hbar}\hat{H}t} | q_i \rangle = \int \mathcal{D}q \, e^{\frac{i}{\hbar}S_{ho}[q]} \Big|_{q(t)=q_f, q(0)=q_i} \tag{183}$$

where

$$S_{ho}[q] = \int_0^t dt' L(q, \dot{q}) = \frac{m}{2} \int_0^t dt' \left(\dot{q}^2 - \omega^2 q^2 \right). \tag{184}$$

The classical path is determined as

$$q_{cl}(t') = q_i \cos\omega t' - \left(\frac{q_f}{\sin\omega t'} - q_i \cot\omega t' \right) \tag{185}$$

so the classical action takes the value

$$S_{ho}[q_{cl}] = \frac{m\omega}{2\sin\omega t} \left((q_f^2 + q_i^2)\cos\omega t - 2q_f q_i \right). \tag{186}$$

The path integral itself can be calculated most easily using our expression (181), which is exact since our Hamiltonian is quadratic ($V'' = m\omega^2$). The deviations from the classical path can be expanded in Fourier modes

$$r(t') = \sum_{n=1}^{\infty} r_n \sin\frac{n\pi t'}{t}, \tag{187}$$

so we have

$$\int dt' r(t') \left[m\partial_{t'}^2 + V'' \right] r(t') = \frac{mt}{2} \sum_{n=1}^{\infty} r_n^2 \left[\omega^2 - \frac{n^2\pi^2}{t^2} \right]. \tag{188}$$

The path integral over $r(t')$ then corresponds over a product of integrals over the r_n. To avoid dealing with the details of this transformation (Jacobian, etc), the easiest is to consider the ratio with the free propagator (so with $\omega = 0$) which we have already calculated:

$$\frac{\prod_n \int dr_n e^{-\frac{imt}{4\hbar}\left[\omega^2 - \frac{n^2}{\pi^2}t^2\right]}}{\prod_n \int dr_n e^{-\frac{imt}{4\hbar}\left[-\frac{n^2}{\pi^2}t^2\right]}} = \prod_{n=1}^{\infty} \left[1 - \frac{\omega^2 t^2}{n^2\pi^2} \right]^{-1/2} = \left[\frac{\sin\omega t}{\omega t} \right]^{-1/2}. \tag{189}$$

Using the explicit expression for our free propagator, we thus obtain the exact propagator for the quantum harmonic oscillator:

$$G_{ho}(q_f, q_i; t) = \left(\frac{m\omega}{2\pi i\hbar \sin\omega t} \right)^{1/2} e^{\frac{im\omega}{2\hbar \sin\omega t}\left((q_f^2 + q_i^2)\cos\omega t - 2q_i q_f \right)}. \tag{190}$$

4   Rudiments of field theory: from Ising to ϕ^4

We have up to now familiarized ourselves with the idea of path integrals, in the contexts of Brownian motion and single-particle quantum mechanics. We have also encountered a many-body (classical) model, namely the Ising model, which we managed to exactly solve using a high-temperature diagrammatic expansion.

This final section will bring many of these concepts together and lead you to your first genuine field theory. We will learn some new very useful tricks along the way.

4.1   Again the Ising model...

Let us go back a couple of chapters and consider our (temporarily) favourite model once more, but this time on a square lattice in d dimensions. Our notations are slightly different here, for convenience. On each lattice site lives an **Ising spin** $S_\mathbf{a}$, which is a *classical* spin variable taking only two possible values, $S_\mathbf{a} = \pm 1$. The vector $\mathbf{a}$ labels the lattice sites. The **Ising model** is defined by the classical Hamiltonian

$$H_I = -\sum_{\mathbf{a},\mathbf{b}} J_{\mathbf{ab}} S_\mathbf{a} S_\mathbf{b} - \sum_\mathbf{a} H_\mathbf{a} S_\mathbf{a},$$

where $H_\mathbf{a}$ is a magnetic field (which can vary from one position to another, hence the index), and the interaction coefficients $J_{\mathbf{ab}} \equiv J(|\mathbf{a} - \mathbf{b}|)$ fall off quickly with distance.

The classical partition function of the Ising model can be written as the sum over all possible Ising spin configurations,

$$\mathcal{Z}_I = \sum_{\{S_\mathbf{a}\}} e^{-\beta H_I} \equiv \sum_{\{S_\mathbf{a}\}} e^{\sum_{\mathbf{a},\mathbf{b}} S_\mathbf{a} K_{\mathbf{ab}} S_\mathbf{b} + \sum_\mathbf{a} h_\mathbf{a} S_\mathbf{a}}.$$

where we have defined $K_{\mathbf{ab}} \equiv \beta J_{\mathbf{ab}}$ and $h_\mathbf{a} \equiv \beta H_\mathbf{a}$.

Let's consider the noninteracting problem first: we thus temporarily set $K_{\mathbf{ab}} = 0$ everywhere. Using the simple identity $\sum_{S_\mathbf{a}} e^{h_\mathbf{a} S_\mathbf{a}} = 2 \cosh h_\mathbf{a}$, the classical partition function becomes

$$\mathcal{Z}_I|_{K_{\mathbf{ab}}=0} = \prod_\mathbf{a} 2 \cosh h_\mathbf{a}.$$

What makes solving this exactly difficult[8] is the presence of the interaction term. The annoying thing is that the spin variables take discrete values, and the exponential of their product isn't simple to sum up over all configurations.

4.2   On Hubbard and Stratonovich

One of the most important tools of field theory is a rather simple trick allowing to find equivalent representations to a given theory. Here, our difficulty is that we don't really like summing over discrete values of spin variables (the partition function becomes a thermodynamically large polynomial). What we like are Gaussian integrals, which we can more or less always handle. Can we thus, using some magic, transform our Ising theory into Gaussian-like integrals?

This is the point at which we can introduce the so-called Hubbard-Stratonovich transformation. The idea is as follows. We begin with a representation of the unit matrix as a field integral over an auxiliary (real, bosonic) field ψ,

$$\mathbf{1} \equiv \mathcal{N} \int \mathcal{D}\psi e^{-\frac{1}{4} \sum_{\mathbf{ab}} \psi_\mathbf{a} (K^{-1})_{\mathbf{ab}} \psi_\mathbf{b}}, \qquad \mathcal{D}\psi \equiv \prod_\mathbf{a} d\psi_\mathbf{a}$$

---

[8]We have already seen that the solution to the $d = 1$ Ising theory (in any field $h_\mathbf{a} = h$) is straightforward; in $d = 2$, Onsager offered the solution at zero field using a fermionic representation, but we derived it using a high-temperature expansion; the $d = 3$ case remains one of the most famous outstanding problems of classical statistical physics.

with K^{-1} the matrix inverse of K. According to our rules for Gaussian integration, the normalization is easily found to be

$$\mathcal{N} = \left[\det\left(4\pi K\right)\right]^{-1/2}. \tag{191}$$

For each lattice site $\mathbf{a}$, we thus have some 'dummy' integration variable $\psi_{\mathbf{a}}$. What use is that? Here is the trick. Consider this representation of unity, but with a shifted value of these dummy variables. This form is also valid:

$$\mathbf{1} \equiv \mathcal{N} \int \mathcal{D}\psi e^{-\frac{1}{4}\sum_{\mathbf{ab}}(\psi_{\mathbf{a}}+\theta_{\mathbf{a}})(K^{-1})_{\mathbf{ab}}(\psi_{\mathbf{b}}+\theta_{\mathbf{b}})}, \qquad \mathcal{D}\psi \equiv \prod_{\mathbf{a}} d\psi_{\mathbf{a}}$$

in which $\theta_{\mathbf{a}}$ are constants which can be put to whatever value we wish (the integration measure doesn't change under such shifts by constants). Written out explicitly,

$$\mathbf{1} \equiv \mathcal{N} \int \mathcal{D}\psi e^{-\frac{1}{4}\sum_{\mathbf{ab}}\psi_{\mathbf{a}}(K^{-1})_{\mathbf{ab}}\psi_{\mathbf{b}}-\frac{1}{2}\sum_{\mathbf{ab}}\theta_a(K^{-1})_{\mathbf{ab}}\psi_{\mathbf{b}}-\frac{1}{4}\sum_{\mathbf{ab}}\theta_{\mathbf{a}}(K^{-1})_{\mathbf{ab}}\theta_{\mathbf{b}}}$$

$$= e^{-\frac{1}{4}\sum_{\mathbf{ab}}\theta_{\mathbf{a}}(K^{-1})_{\mathbf{ab}}\theta_{\mathbf{b}}} \times \mathcal{N} \int \mathcal{D}\psi e^{-\frac{1}{4}\sum_{\mathbf{ab}}\psi_{\mathbf{a}}(K^{-1})_{\mathbf{ab}}\psi_{\mathbf{b}}-\frac{1}{2}\sum_{\mathbf{ab}}\theta_a(K^{-1})_{\mathbf{ab}}\psi_{\mathbf{b}}}$$

You can now see that by choosing $\theta_{\mathbf{a}} = -2\sum_{\mathbf{b}} K_{\mathbf{ab}} S_{\mathbf{b}}$, we obtain the equality

$$e^{\sum_{\mathbf{ab}} S_{\mathbf{a}} K_{\mathbf{ab}} S_{\mathbf{b}}} = \mathcal{N} \int \mathcal{D}\psi e^{-\frac{1}{4}\sum_{\mathbf{ab}}\psi_{\mathbf{a}}(K^{-1})_{\mathbf{ab}}\psi_{\mathbf{b}}+\sum_{\mathbf{a}} S_{\mathbf{a}}\psi_{\mathbf{a}}}.$$

It is worth pondering this equation somewhat. On the left-hand side, we have a partition function weight for spins interacting with each other. On the right-hand side, we have a functional integral over an additional object ψ which takes values at all lattice sites (since it's defined throughout our space, we call it a *field*); the spins are coupled to this field, and this field has self-couplings (given by the inverse matrix of the spin self-coupling matrix on the left-hand side) representing what can be interpreted as its elastic energy.

One can thus view a system of spins interacting with each other, as a system of spins interacting with an auxiliary field, this field having its own self-interactions. This is **exact**, in no way is it an approximation. These two viewpoints are completely equivalent.

Using this last identity, you can now see that the partition function of the interacting Ising theory can be written

$$\mathcal{Z}_I = \mathcal{N} \int \mathcal{D}\psi \sum_{\{S_{\mathbf{a}}\}} e^{-\frac{1}{4}\sum_{\mathbf{ab}}\psi_{\mathbf{a}}(K^{-1})_{\mathbf{ab}}\psi_{\mathbf{b}}+\sum_{\mathbf{a}}(\psi_{\mathbf{a}}+h_{\mathbf{a}})S_{\mathbf{a}}}$$

and thus the Ising model can be viewed as a model of spins coupled to a field, this field having elastic energy.

The next step is even more entertaining. Since the spins now enter linearly in the effective action, we can simply sum over all possible spin configurations ($\sum_{\{S_{\mathbf{a}}\}}$). After a redefinition of the field $\psi \to \phi$ according to

$$\phi_{\mathbf{a}} \equiv \frac{1}{2} \sum_{\mathbf{b}} (K^{-1})_{\mathbf{ab}}(\psi_{\mathbf{b}} + h_{\mathbf{b}}) \tag{192}$$

(this leads to a redefinition of the constant $\mathcal{N} \to \tilde{\mathcal{N}}$ which we won't care about here), we get to the representation of the Ising model's partition function as a **classical functional field integral**

$$\mathcal{Z}_I = \tilde{\mathcal{N}} \int \mathcal{D}\phi e^{-S[\phi]}, \tag{193}$$

with effective action

$$S[\phi] \equiv \sum_{\mathbf{ab}} \phi_{\mathbf{a}} K_{\mathbf{ab}} \phi_{\mathbf{b}} - \sum_{\mathbf{a}} \phi_{\mathbf{a}} h_{\mathbf{a}} - \sum_{\mathbf{a}} \ln \cosh(2 \sum_{\mathbf{b}} K_{\mathbf{ab}} \phi_{\mathbf{b}}). \tag{194}$$

I remind you that *we have not made any approximation whatsoever* to reach this point. The question becomes whether we can go much further. The last term should quickly temper your enthusiasm. Logarithms are generally hard to handle, and the case here is no exception.

4.3   Gradient expansion

We now make a low-temperature approximation, by assuming that the fluctuations of ϕ are small (for our purposes here, this translates into taking $|\phi_{\mathbf{a}}| \ll 1$). We first define the Fourier representations (N is the total number of Ising spins in the system, and we assume periodic boundary conditions in all directions for simplicity) of the field and interaction as

$$\phi_{\mathbf{a}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{a}} \phi_{\mathbf{k}}, \qquad K_{\mathbf{ab}} = \frac{1}{N} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot(\mathbf{a}-\mathbf{b})} K_{\mathbf{k}}. \tag{195}$$

We then assume that the interaction is mostly local in space, so that we can use a small-momentum expansion (also called the gradient expansion) of the interaction,

$$K_{\mathbf{k}} = K_0 + \frac{1}{2} \mathbf{k} \cdot \mathbf{k} \; K_0^{''} + \mathrm{O}(|\mathbf{k}|^4). \tag{196}$$

The nastily nonlinear function we have to deal with in the action can be expanded as

$$\ln\cosh x = \frac{1}{2} x^2 - \frac{1}{12} x^4 + \dots \tag{197}$$

Explicitly, we can write

$$x_{\mathbf{a}} = 2 \sum_{\mathbf{b}} K_{\mathbf{ab}} \phi_{\mathbf{b}} = \frac{2}{N^{3/2}} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\mathbf{b}} e^{-i\mathbf{k}\cdot(\mathbf{a}-\mathbf{b})-i\mathbf{k}'\cdot\mathbf{b}} K_{\mathbf{k}} \phi_{\mathbf{k}'} = \frac{2}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{a}} K_{\mathbf{k}} \phi_{\mathbf{k}}. \tag{198}$$

Similarly,

$$\sum_{\mathbf{a}} \frac{x_{\mathbf{a}}^2}{2} = \frac{2}{N} \sum_{\mathbf{k}_1,\mathbf{k}_2} K_{\mathbf{k}_1} K_{\mathbf{k}_2} \phi_{\mathbf{k}_1} \phi_{\mathbf{k}_2} \sum_{\mathbf{a}} e^{-i(\mathbf{k}_1+\mathbf{k}_2)\cdot\mathbf{a}} = 2 \sum_{\mathbf{k}} K_{\mathbf{k}} K_{-\mathbf{k}} \phi_{\mathbf{k}} \phi_{-\mathbf{k}} \tag{199}$$

and

$$\sum_{\mathbf{a}} \frac{x_{\mathbf{a}}^4}{12} = \frac{4}{3N^2} \sum_{\mathbf{k}_1 \dots \mathbf{k}_4} K_{\mathbf{k}_1} K_{\mathbf{k}_2} K_{\mathbf{k}_3} K_{\mathbf{k}_4} \phi_{\mathbf{k}_1} \phi_{\mathbf{k}_2} \phi_{\mathbf{k}_3} \phi_{\mathbf{k}_4} \sum_{\mathbf{a}} e^{-i(\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4)\cdot\mathbf{a}} \tag{200}$$

Doing the gradient expansion in each of these, and keeping only leading terms,

$$\sum_{\mathbf{a}} \frac{x_{\mathbf{a}}^2}{2} \simeq 2 \sum_{\mathbf{k}} (K_0 + \frac{1}{2}|\mathbf{k}|^2 K_0^{''} + \dots)^2 \phi_{\mathbf{k}} \phi_{-\mathbf{k}} \tag{201}$$

$$\sum_{\mathbf{a}} \frac{x_{\mathbf{a}}^4}{12} = \frac{4K_0^4}{3N} \sum_{\mathbf{k}_1 \dots \mathbf{k}_4} \phi_{\mathbf{k}_1} \phi_{\mathbf{k}_2} \phi_{\mathbf{k}_3} \phi_{\mathbf{k}_4} \delta_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4,0} \tag{202}$$

Putting things together, we get that the action has the form

$$S[\phi] = \sum_{\mathbf{k}} [\phi_{\mathbf{k}}(c_1 + c_2\mathbf{k}\cdot\mathbf{k})\phi_{-\mathbf{k}} + c_3\phi_{\mathbf{k}} h_{-\mathbf{k}}] + \frac{c_4}{N} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \phi_{\mathbf{k}_1} \phi_{\mathbf{k}_2} \phi_{\mathbf{k}_3} \phi_{\mathbf{k}_4} \delta_{\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4,0} + \dots \tag{203}$$

with coefficients

$$c_1 = K_0 - 2K_0^2, \qquad c_2 = \frac{1}{2} K_0^{''} - 2K_0 K_0^{''}, \qquad c_3 = -1, \qquad c_4 = \frac{4}{3} K_0^4. \tag{204}$$

Upon Fourier transforming back to real space (specializing to $h = 0$), the action becomes

$$S[\phi] = \int d^d x \left[c_2 (\partial\phi)^2 + c_1 \phi^2 + c_4 \phi^4 \right]. \tag{205}$$

A simple rescaling $\phi \to \frac{1}{\sqrt{2c_2}}\phi$ then gives the so-called ϕ^4 theory,

$$\mathcal{Z} = \int \mathcal{D}\phi \, e^{-S[\phi]}, \qquad S[\phi] = \int d^d x \left[\frac{1}{2}(\partial\phi)^2 + \frac{r}{2}\phi^2 + g\phi^4 \right], \qquad (206)$$

with $r = \frac{c_1}{c_2}$ and $g = \frac{c_4}{4c_2^2}$. The calculation of course only makes sense if $c_2 > 0$. Since we expect that $K_0'' < 0$, this means $K_0 > 1/4$.

For your information, the Ising model has a transition when r changes sign from positive values to negative ones, $i.e.$ when the potential becomes a 'Mexican hat' like potential. We can see that r changes sign when $c_1 = 0$ so $K_0 = 1/2$ and thus the critical temperature is given by the condition $\beta_c = \frac{1}{2J_0}$. For $\beta > \beta_c$, $r < 0$ and the system is in the ordered phase. For $\beta < \beta_c$, $r > 0$ and the system is in the disordered phase.

References

[1] A. Einstein. Über die von der molekularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen. *Ann. Physik*, 322(8):549–560, 1905.

[2] E. H. Lieb and D. W. Robinson. The finite group velocity of quantum spin systems. *Commun. Math. Phys.*, 28(3):251–257, 1972.

[3] E. Ising. Beitrag zur Theorie des Ferromagnetismus. *Zeitschrift für Physik*, 31:253–258, 1925.

[4] L. Onsager. Crystal Statistics. I. A Two-Dimensional Model with an Order-Disorder Transition. *Phys. Rev.*, 65:117–149, Feb 1944.

[5] M. Kac and J. C. Ward. A Combinatorial Solution of the Two-Dimensional Ising Model. *Phys. Rev.*, 88:1332–1337, 1952.