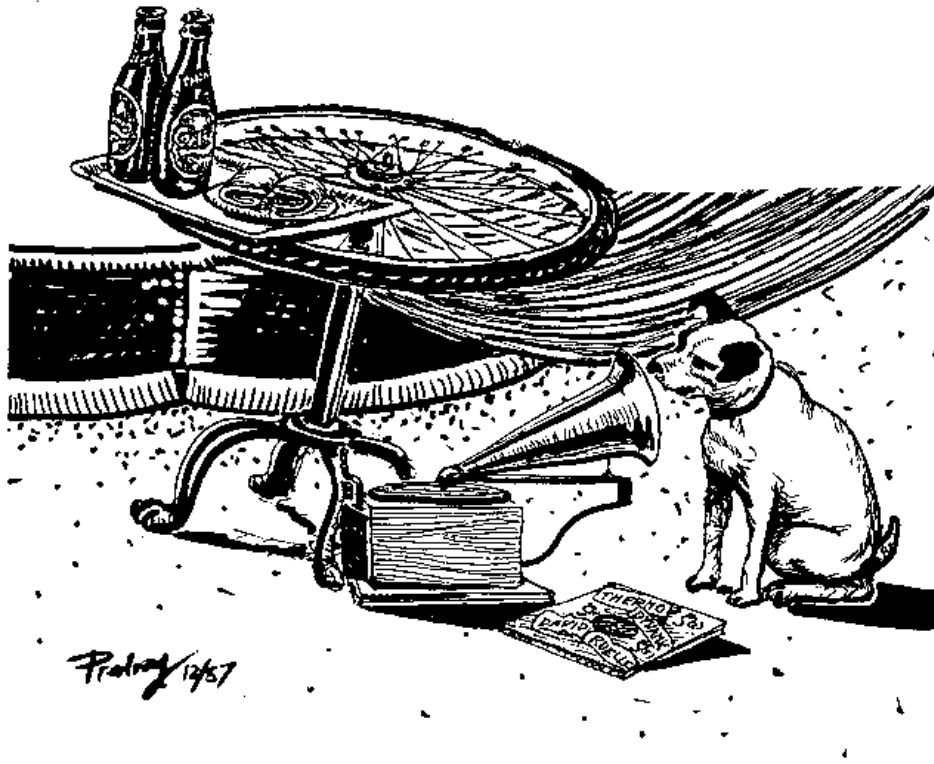# QUANTUM FIELD THEORY
a cyclist tour

Predrag Cvitanović

What reviewers say:

> N. Bohr: *"The most important work since that Schrödinger killed the cat."* ⋯
>
> R.P. Feynman: *"Great doorstop!"*

Contents

Preface

Ben Mottelson was the only physicist I personally knew who thought equally clearly quantum-mechanically and classically, the rest of us are not so lucky. Still, I have never understood why my colleagues say that "while we understand classical mechanics," quantum mechanics is mysterious. I never got the memo: to me it is equally magical that both classical and quantum mechanics follow variational principles.

The partition sum that accounts for all things allowed by quantum and statistical physics,

$$e^{\Gamma[\Phi]+J\cdot\Phi} = \int [d\phi]\, e^{S[\phi]+J\cdot\phi}, \tag{1}$$

expresses the quantum action $\Gamma[\Phi]$ of mid-20th century quantum field theory as a 'path integral' weighted by the work $S[\phi]$ of the late 17th century classical mechanics. That's The Law. All else - Hamilton's equations, Maxwell's equations, Schrödinger equation - is nipping at the edges. If you now join a hedge fund, steal a gazillion dollars, destroy the planet, go hide on Mars, and decide to reconstruct all of physics at your leisure, this is *all* you have to remember. This is the whole of physics; the rest is commentary. Isn't that aaaa-maaaa-zing?

Almost every single thing we learn about quantum mechanics and thus come to believe is quantum mechanics –operators, commutators, complex amplitudes, unitary evolution operators, Green's functions, Hilbert spaces, spectra, path integrals, spins, angular momenta– under a closer inspection has nothing quantum mechanical to it. It is machinery equally suited to classical, statistical and stochastic mechanics, which in ChaosBook.org are thought of together - in terms of evolution operators and their spectra. The common theme of the three theories is that things fall apart, and infinitely many fragments have to be pieced together to craft a theory. In the end it is only the $i/\hbar$ granularity of phase space that is the mystery of quantum mechanics; and why, a century later, quantum mechanics is still a theory that refuses to fail?

Over the years I have watched study group after study group of graduate students grovel in orgies of spacetime, spin and color indices, and have tried desperately to deprogram them through my ChaosBook.org/FieldTheory book [1], but all in vain: students *want* Quantum Field Theory to be mysterious and accessed only by pages of index summations. Or two-forms. Or Borcher classes. These notes are yet another attempt to demystify most of field theory, inspired by young Feynman driving yet younger Dyson across the continent to Los Alamos, hands off the steering wheel and gesticulating: "Path integrals are everything!" These lectures are about "everything." The theory is developed here at not quite the pedestrian level, perhaps at a cyclist level. We start out on a finite lattice, without any functional voodoo; all we have to know is how to manipulate finite dimensional vectors and matrices. Then we restart on a more familiar ground, by reformulating the old fashioned Schrödinger quantum mechanics as Feynman path integral in chapter 2. More of such stuff can be found in ref. [1].

This version of field theory presupposes some prior exposure to statistical mechanics, electromagnetism and quantum mechanics.

Who is the 3-legged dog reappearing throughout the book? Long ago, when I was innocent and knew not Borel measurable α to Ω sets, I asked V. Baladi a question about dynamical zeta functions, who then asked J.-P. Eckmann, who then asked D. Ruelle. The answer was transmitted back: "The master says: 'It is holomorphic in a strip'." Hence His Master's Voice (H.M.V.) logo, and the 3-legged dog is us, still eager to fetch the bone, or at least a missing figure, if a reader is kind enough to draw one for us. What is depicted on the cover? Roberto Artuso found the smørrebrød at the Niels Bohr Institute indigestible, so he digested H.M.V.'s wisdom on a strict diet of two Carlsbergs and two pieces of Danish pastry for lunch every day. Frequent trips down to Milano's ancestral home is what kept him alive.

Chapter 1

Lattice field theory

Be wise, discretize.
— [Mark Kac](#)

We motivate path integrals to come by formulating the simplest example of a propagator, Green's function for the random walk on a lattice, as a sum over paths. In order to set the stage for the continuum formulation, we then describe lattice derivatives and lattice Laplacians, and explain how symmetry under translations enables us to diagonalize the free propagator by means of a discrete Fourier transform.

5

1.1   Wanderings of a drunken snail

> Statistical mechanics is formulated in a Euclidean world in which there is no time, just space. Q. What do we mean by 'propagation' in such a space?

We have no idea what the structure of our space on distances much shorter than interatomic might be. The very space-time might be discrete rather than continuous, or it might have geometry different from the one we observe at the accessible distance scales. The formalism we use should reflect this ignorance. We deal with this problem by coarse-graining the space into small cells and requiring that our theory be insensitive to distances comparable to or smaller than the cell sizes.

Our next problem is that we have no idea why there are "particles," and why or how they propagate. The most we can say is that there is some probability that a particle steps from one cell to another cell. At the beginning of the century, the discovery of Brownian motion showed that matter was not continuous but was made up of atoms. In quantum physics we have no experimental indication of having reached the distance scales in which any new space-time structure is being sensed: hence for us this stepping probability has no direct physical significance. It is a phenomenological parameter which - in the continuum limit - is related to the "mass" of the particle.

Assume that the state of a particle is given by its position $i = (x_1, x_2, \cdots, x_d)$, and that the particle is a 'scalar', i.e., it has no further internal degrees of freedom, such as spin or color. What is it like to be free? A free particle exists only in itself and for itself; it neither sees nor feels the others; it is, in this chilly sense, free. But if it is not at once paralyzed by the vast possibilities opened to it, it soon becomes perplexed by the problems of realizing any of them alone. Born free, it is constrained by the very lack of constraint. Sitting in its cell, it is faced by a choice of doing nothing (s = stopping probability) or stepping into any of the $2d$ neighboring cells (h = stepping probability):

hop with
probability h
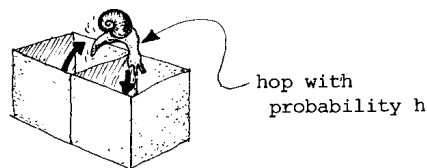
The number of neighboring cells defines the dimension of the space. The stepping and stopping probabilities are related by the probability conservation:

$$1 = s + 2dh, \qquad d = \text{ the dimension of spacetime } . \tag{1.1}$$

Taking the stepping probability to be the same in all directions means that we have assumed that the space is *isotropic*.

Our next assumption is that the space is *homogeneous*, i.e., that the stepping probability does not depend on the location of the cell; otherwise the propagation is not free, but is constrained by some external geometry. This can either mean

that the space is infinite, or that it is compact and periodic (a torus; a Lie group manifold). That is again something beyond our ken - we proceed in the hope that the predictions of our theory will be insensitive to very large distances.

The isotropy and homogeneity assumptions imply that at distances much larger than the lattice spacing, our theory should be invariant under rotations and translations. A theory that is insensitive to the very short and very long distances is said to be well behaved in the 'ultraviolet' and 'infrared' limits.

While counting continuum Brownian paths might be tricky, counting them in a discretized space is a breeze. Divade the space into little d-dimensional hypercubes ('cells', 'tiles'). Let the snail start in the cell z and hop along until it stops in the cell z'.

a Brownian walk: a walk on a lattice:
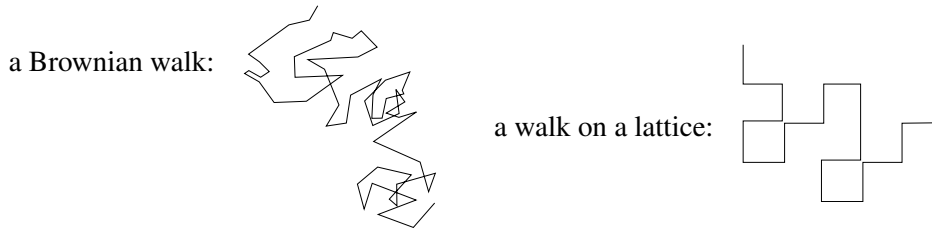
The probability of this path is $h^\ell s$, where ℓ is the number of steps. The total probability that a particle wanders from the zth cell and stops in the z'th cell is the sum of probabilities associated with all distinct paths between them:

$$\Delta_{zz'} = s \sum_{\ell=0}^{\infty} h^\ell T_{zz'}(\ell) \,, \tag{1.2}$$

where $T_{zz'}(\ell)$ is the number of all paths of ℓ steps connecting lattice sites z and z'. In order to compute $T_{zz'}(\ell)$, define a shift operator, and its inverse (also its transpose)

$$(\mathsf{r}_j)_{zz'} = \delta_{z+\mathbf{e}_j,z'} \,, \qquad (\mathsf{r}_j^{-1})_{zz'} = \delta_{z,z'+\mathbf{e}_j} \,, \tag{1.3}$$

where $\mathbf{e}_j$ is a unit step in direction j. If a particle is introduced into the z'th cell by a source $J_z = \delta_{z'z}$, the shift operator moves it into a neighboring cell:

$$(\mathsf{r}_j J)_z = \delta_{z'+\mathbf{e}_j,z} \qquad \Rightarrow \qquad \tag{1.4}$$

The hopping operator

$$T_{zz'} = \sum_{j=1}^{d} (\mathsf{r}_j + \mathsf{r}_j^{-1})_{zz'} \tag{1.5}$$

generates all steps of length 1:

$$TJ = \quad \text{} \quad , \tag{1.6}$$

(the examples are drawn in two dimensions, so the lattice does not look square as this is meant to be a sidewise view from above the lattice). The paths of length 2

are counted by

$$T^2 J = \text{[diagram]} \, .\tag{1.7}$$

There are 4 ways of returning, 2 ways of reaching a diagonal corner, and so on. Note –and this is the key observation– that the zth component of the vector $T^\ell J$ counts the number of paths of length ℓ connecting the zth and the z'th cells. The probability that the particle stops in the zth cell is given by the 'path sum'

$$\phi_z \;=\; s \sum_{\ell=0}^{\infty} h^\ell (T^\ell J)_z \,,\tag{1.8}$$

the sum of all paths connecting the two cells. The value of the field ϕ_z is the probability that the particle introduced into the cell z' by the source J ends in the cell z. According to (1.6), (1.7), the numbers of paths originating in cell z' are

$$\sum_z (TJ)_z = 2d \,, \quad \sum_z (T^2 J)_z = (2d)^2 \,, \quad \cdots$$

so, by the stepwise probability conservation (1.1), ϕ_z is a correctly normalized probability field (probability density on lattice site z),

$$\sum_z \phi_z \;=\; s\,(1 + 2dh + (2d)^2 h^2 + \cdots) \;=\; \frac{s}{1 - 2dh} = 1 \,.\tag{1.9}$$

Actually, the powers of the hopping operator (1.5) also form a geometric series, which we can sum up like we would sum up a matrix series,

$$\phi_z \;=\; \Delta J \,, \qquad \Delta_{zz'} = \left(\frac{s}{1 - hT} \right)_{zz'} \,,\tag{1.10}$$

yielding an explicit formula for the Euclidean free scalar particle propagator (1.2).

A. The probability $\Delta_{zz'}$ that a drunken snail starting out in the cell z ends up in the cell z' is given by the sum of all paths starting in z' and ending in z.

1.1.1 Fields

Let us set up some 'lattice field theory' notation, conventional in solid state physics and quantum field theory. We'll return to the evaluation of the Euclidean free massive scalar particle propagator (1.10) in sect. 1.4.7.

In a d-dimensional hypercubic discretization of a Euclidean space, the d continuous Euclidean coordinates $x \in \mathbb{R}^d$ are replaced by a hypercubic integer lattice

$$\mathcal{L} = \Big\{ \sum_{j=1}^{d} z_j \mathbf{e}_j \mid z \in \mathbb{Z}^d \Big\}, \qquad \mathbf{e}_j \in \{\mathbf{e}_1, \mathbf{e}_2, \cdots, \mathbf{e}_d\} \,,\tag{1.11}$$
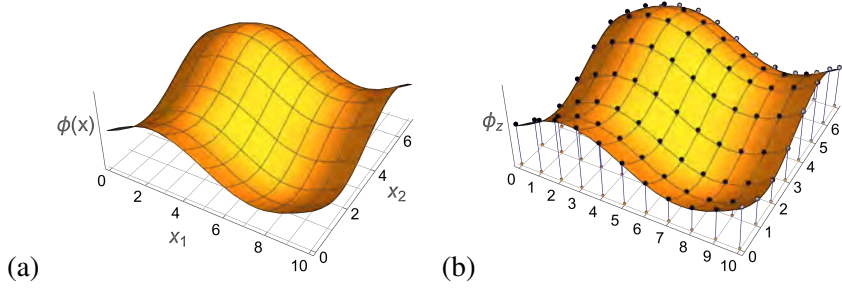
Figure 1.1: Discretization of a field over two-dimensional spacetime. (a) A periodic scalar field configuration $\phi(x)$ over a primitive cell of spatial period L, temporal period T, plotted as a function of continuous coordinates $x \in \mathbb{R}^2$. (b) The corresponding discretized field configuration (1.13) over $[10{\times}7]_0$ primitive cell, with the field value ϕ_z at the lattice site $z \in \mathbb{Z}^2$ indicated by a dot. (Han Liang [7].)

spanned by a set of orthogonal unit vectors $\mathbf{e}_j$, with lattice spacing $a_j = |\mathbf{e}_j| = \Delta x_j$ along the direction of unit vector $\mathbf{e}_j$. We shall use lattice units, always setting $a_j = 1$. A field $\phi(x)$ over d continuous coordinates x_j is represented by a discrete array of field values over lattice sites

$$\phi_z = \phi(x), \quad x_j = a_j z_j = \text{lattice site}, \qquad z \in \mathbb{Z}^d, \tag{1.12}$$

as sketched in figure 1.1. A lattice *field configuration* is a d-dimensional array of field values (in what follows, illustrative examples will be presented in one or two spatiotemporal dimensions)

$$\Phi = \begin{matrix} \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \phi_{-2,1} & \phi_{-1,1} & \phi_{0,1} & \phi_{1,1} & \phi_{2,1} & \cdots \\ \cdots & \phi_{-2,0} & \phi_{-1,0} & \phi_{0,0} & \phi_{1,0} & \phi_{2,0} & \cdots \\ \cdots & \phi_{-2,-1} & \phi_{-1,-1} & \phi_{0,-1} & \phi_{1,-1} & \phi_{2,-1} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{matrix} \; . \tag{1.13}$$

A field configuration is a *point* in system's *state space*

$$\mathcal{M} = \left\{ \Phi \mid \phi_z \in \mathbb{R}, \; z \in \mathbb{Z}^d \right\}, \tag{1.14}$$

the totality of states Φ, given by all possible values of site fields, where ϕ_z can be a single scalar field, or a multitplet of real or complex fields.

While we refer here to such discretization as a lattice field theory, the lattice might arise naturally from a many-body setting with the nearest neighbors interactions, such as many-body quantum chaos models, with a multiplet of fields at every site.

1.1.2   Periodic field configurations

> Q. What are these 'operators', such as the shift operator (1.3)? The hypercubic lattice $z \in \mathbb{Z}^d$ is infinite in all directions, so these are not matrices, they are infinite-dimensional objects. Our bridge to this infinity will be to tile the infinite lattice by repeats of finite tiles.

To get a grip on these 'operators', let's start small, and make the lattice 1-dimensional and finite, a chain of L lattice sites. For a hyper-cubic lattice the
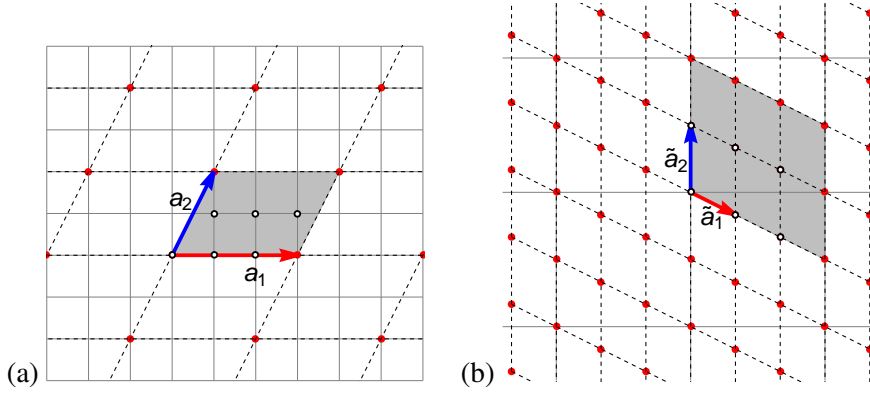
Figure 1.2: (a) The intersection points z of the light grey lines form the integer square lattice (1.12). The primitive vectors $\mathbf{a}_1 = (3, 0)$ and $\mathbf{a}_2 = (1, 2)$ form the primitive cell $\mathbb{A} = [3{\times}2]_1$ (see (1.17)), whose translations tile the Bravais lattice $\mathcal{L}_{\mathbb{A}}$ (red points). (b) The intersection points k of the light grey lines form the reciprocal square lattice. Translations of reciprocal primitive vectors $\tilde{\mathbf{a}}_1$ and $\tilde{\mathbf{a}}_2$ generate the reciprocal lattice $\mathcal{L}_{\tilde{\mathbb{A}}}$ (red points). (Shaded) The reciprocal primitive cell $\tilde{\mathbb{A}}$. A wave vector outside this region is equivalent to a wave vector within it by a reciprocal lattice translation. Note that the number of lattice sites within the reciprocal primitive cell $\tilde{\mathbb{A}}$ equals the number of sites within the spatiotemporal primitive cell $\mathbb{A}$. (Han Liang [7].)

translations in different directions commute, $\mathsf{r}_j \mathsf{r}_i = \mathsf{r}_i \mathsf{r}_j$, so it is sufficient to understand the action of a shift on a 1-dimensional lattice. So we can write down r (1.3) in its full $[L{\times}L]$ matrix glory. Writing the finite lattice shift operator as an 'upper shift' matrix

$$
\mathsf{r} = \begin{pmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & \ddots & \ddots & \\ & & & 0 & 1 \\ 0 & & & & 0 \end{pmatrix},
$$

is no good, as r so defined is nilpotent, and after L steps the particle marches off the lattice edge, and nothing is left, $\mathsf{r}^L = 0$. The smart way to approximate an infinite lattice by a finite one is to insist that the discretization preserve the translational invariance, and represent the *periodic* lattice operator. On a *periodic lattice* every point is equally far from the 'boundary' $L/2$ steps away, the 'surface' effects are equal for all points, and the shift operator $\mathsf{r}_{zz'} = \delta_{z+1,z'}$ acts as a cyclic permutation matrix

$$
\mathsf{r} = \begin{pmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & \ddots & \ddots & \\ & & & 0 & 1 \\ 1 & & & & 0 \end{pmatrix}, \tag{1.15}
$$

with '1' in the lower left corner assuring periodicity. Now, lets go back to the infinite lattice, by tiling the infinite lattice by repeats of a finite periodic field configuration.

A lattice field configuration is $\mathcal{L}_{\mathbb{A}}$-*periodic* if

$$
\phi_{z+\mathsf{r}} = \phi_z \tag{1.16}
$$

for any discrete translation $r = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + \cdots n_d\mathbf{a}_d$ in the *Bravais lattice*

$$\mathcal{L}_{\mathbb{A}} = \Big\{ \sum_{j=1}^{d} n_j\mathbf{a}_j \mid n_j \in \mathbb{Z} \Big\}, \tag{1.17}$$

where the $[d{\times}d]$ matrix $\mathbb{A} = [\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_d]$ formed from primitive lattice vectors $\{\mathbf{a}_j\}$ defines a d-dimensional *primitive cell* [2, 6] (see figure 1.2 (a)).

Primitive cell $\mathbb{A}$ field configuration lattice-site fields (1.13) take values in the $V_{\mathbb{A}}$-dimensional state space

$$\mathcal{M}_{\mathbb{A}} = \{ \Phi \mid \phi_z \in \mathbb{R} ,\ z \in \mathbb{A} \} . \tag{1.18}$$

The *volume* of Bravais lattice $\mathcal{L}_{\mathbb{A}}$ equals the number of lattice sites $z \in \mathbb{A}$ within the primitive cell (see figure 1.2 (a)):

$$V_{\mathbb{A}} = |\mathrm{Det}\,\mathbb{A}| . \tag{1.19}$$

For example, repeats of the $V_{\mathbb{A}} = 15$-dimensional $[5{\times}3]$ primitive cell field configuration

$$\Phi = \begin{bmatrix} \phi_{-2,1} & \phi_{-1,1} & \phi_{0,1} & \phi_{1,1} & \phi_{2,1} \\ \phi_{-2,0} & \phi_{-1,0} & \phi_{0,0} & \phi_{1,0} & \phi_{2,0} \\ \phi_{-2,-1} & \phi_{-1,-1} & \phi_{0,-1} & \phi_{1,-1} & \phi_{2,-1} \end{bmatrix} \tag{1.20}$$

tile periodically the doubly-infinite state space (1.13).

A. While an operator, such as the shift operator (1.3), is an infinite-dimensional object, periodic tilings of spacetime enable us to treat operators as though they were finite-dimensional matrices.

1.1.3   Orbits

These periodic field configurations are described by a finite number $V_{\mathbb{A}}$ of field values.
Q. Does the way they are laid out on the lattice matter?

Consider a one-dimensional primitive cell $\mathbb{A}$, defined by a single primitive vector $\mathbf{a}_1 = n$ in (1.17). One-lattice-spacing shift operator (6.13) is a cyclic permutation operator that translates a field configuration by one lattice site,

$$\begin{aligned} \Phi &= [\phi_0\,\phi_1\,\phi_2\,\phi_3\,\cdots\,\phi_{n-1}] \\ r\Phi &= [\phi_1\,\phi_2\,\phi_3\,\cdots\,\phi_{n-1}\,\phi_0] , \quad \text{or} \quad (r\Phi)_z = \phi_{z+1} , \\ &\cdots \\ r^{n-1}\Phi &= [\phi_{n-1}\,\phi_0\,\phi_1\,\phi_2\,\cdots\,\phi_3] , \\ r^n\Phi &= [\phi_0\,\phi_1\,\phi_2\,\phi_3\,\cdots\,\phi_{n-1}] , \quad \text{so} \quad r^n\Phi = \Phi . \end{aligned} \tag{1.21}$$

While each field configuration $r^j\Phi$ might be a distinct point in the primitive cell's state space (1.18), they are equivalent, in the sense that all consist of the same set of lattice site fields $\{\phi_z\}$, up to a cyclic relabelling of lattice sites.

In this way actions of a group of relabelling permutations $g \in G$ on field configurations over a multi-periodic primitive cell $\mathbb{A}$ foliate the state space into a union

$$\mathcal{M}_{\mathbb{A}} = \{\Phi\} = \cup_p \mathcal{M}_p \qquad (1.22)$$

of *orbits*,

$$\mathcal{M}_p = \{g\,\Phi_p \mid g \in G\} \qquad (1.23)$$

each a set of equivalent field configurations, labelled p, or perhaps by Φ_p, one of the configurations in the set. Each orbit is a fixed point of G, as any element $g\mathcal{M}_p = \mathcal{M}_p$ simply permutes the configurations within the set. The number of distinct field configurations in the orbit is known as the *index* of orbit $\mathcal{M}_p$. It can be as large as $|G|$, the number of elements in G, or as small as 1, if the field configuration is $\phi_z = \phi$, a constant (or a 'steady state').

A. While an operator, such as the shift operator (1.3), is an infinite-dimensional object, periodic tilings of spacetime enable us to treat operators as finite-dimensional matrices.

1.2 Lattice derivatives

In order to measure spatial variations of fields, we need to define *lattice derivatives*.

Consider a function $\phi(x)$ discretized on a d-dimensional lattice (1.12). Each set of field values ϕ -a vector ϕ_z- is a possible *field configuration*.

Assume the lattice is a hypercubic integer lattice (1.11), and let $\{\mathbf{e}_j\}$ be the unit lattice cell vectors pointing along the d positive directions. The forward *lattice derivative* is then

$$(\partial_j\phi)_z = \frac{\phi(x + a\mathbf{e}_j) - \phi(x)}{a} = \frac{\phi_{z+\mathbf{e}_j} - \phi_z}{a} . \qquad (1.24)$$

The backward *lattice derivative* is its transpose

$$(\partial_j\phi)_z^\top = \frac{\phi(x - a\mathbf{e}_j) - \phi(x)}{a} = \frac{\phi_{z-\mathbf{e}_j} - \phi_z}{a} . \qquad (1.25)$$

Anything else with the correct $a \to 0$ limit would do, but this is the simplest choice. We can rewrite the lattice derivative as a linear operator, by introducing the *shift operator* (or *stepping operator*) (1.3) in the direction j. The partial lattice derivative (1.25) can now be written as a multiplication by the operator:

$$\partial_j\phi_z = \frac{1}{a}\left(\mathsf{r}_j - \mathbf{1}\right)_{zz'}\phi_{z'} .$$

In the 1-dimensional case the [$L{\times}L$] matrix representation of the lattice derivative is:

$$\partial = \frac{1}{a}\begin{pmatrix} -1 & 1 & & & & \\ & -1 & 1 & & & \\ & & -1 & 1 & & \\ & & & \ddots & & \\ & & & & & 1 \\ 1 & & & & & -1 \end{pmatrix} . \qquad (1.26)$$

To belabor the obvious: On a finite lattice of L points a derivative is simply a finite $[L \times L]$ matrix. Continuum field theory is a world in which the lattice is so fine that it looks smooth to us. Whenever someone calls something an "operator," think "matrix." For finite-dimensional spaces a linear operator *is* a matrix; things get subtler for infinite-dimensional spaces.

Looking forward, the continuum limit of this operator will be related to what field theorists call particle 'momentum', so we find it convenient to refer to the forward lattice difference operator in jth lattice direction as the 'lattice momentum' operator

$$\mathsf{p}_j = \mathsf{r}_j - \mathbb{1}, \tag{1.27}$$

where the lattice spacing is set to $a = 1$ (easily reinstated, if needed).

1.2.1   Lattice Laplacian

> I'm the field ϕ_z on lattice site z.
> Q. What's up with my neighbors?

In lattice field theory 'locality' means that a field at site z interacts only with its neighbors. To keep the exposition as simple as possible, we shall -for time being- treat the spatial and temporal directions on equal footing, with the graph Laplace operator [4, 8, 14, 18]

$$\Box \, \phi_z = \sum_{z'}^{\|z'-z\|=1} (\phi_{z'} - \phi_z) \quad \text{for all } z, z' \in \mathbb{Z}^d \tag{1.28}$$

comparing the field on lattice site z to its $2d$ nearest neighbors.

On the d-dimensional hyper-cubic lattice, Laplacian is the centered, reflection symmetric second lattice derivative,

$$\Box = \sum_{j=1}^{d} (\mathsf{r}_j - 2\,\mathbb{1} + \mathsf{r}_j^{-1}). \tag{1.29}$$

For example, the two-dimensional square lattice Laplace operator is given by

$$\Box = \mathsf{r}_1 + \mathsf{r}_2 - 4\,\mathbb{1} + \mathsf{r}_2^{-1} + \mathsf{r}_1^{-1}, \tag{1.30}$$

and in the 1-dimensional finite periodic chain case the $[L \times L]$ matrix representation of the lattice Laplacian is

$$\Box = \frac{1}{a^2} \begin{pmatrix} -2 & 1 & & & & 1 \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & 1 & & \ddots & \\ & & & & & 1 \\ 1 & & & & 1 & -2 \end{pmatrix}. \tag{1.31}$$

The lattice Laplacian measures the second variation of a field ϕ_z across three neighboring sites: it is spatially *non-local*. You can easily check that it does what the second derivative is supposed to do by applying it to a parabola restricted to the

lattice, $\phi_z = \phi(az)$, where $\phi(az)$ is defined by the value of the continuum function $\phi(x) = \phi^2$ at the lattice point $x = az$.

We can write it in terms of the 'lattice momentum' operator (1.27), and relate it to T, the hopping operator (1.5),

$$\begin{aligned}
\Box &= -\sum_{j=1}^{d} \mathsf{p}_j^\top \mathsf{p}_j = -\sum_{j=1}^{d} \left(\mathsf{r}_j^{-1} - \mathbf{1}\right)\left(\mathsf{r}_j - \mathbf{1}\right) \\
&= \frac{1}{a^2}\left(T - 2d\mathbf{1}\right) .
\end{aligned}$$ (1.32)

The Euclidean free scalar particle propagator (1.10) can thus be written as

$$\Delta = \frac{1}{\mathbf{1} - \frac{h}{s}a^2 \Box} .$$ (1.33)

In what follows it will be convenient to reinterpret and rescale this drunken-walk propagator Δ (1.4) together with the probability density fields ϕ_z in (1.10), and consider instead the "free field action" (**??**) of form

$$S[\phi] = -\frac{1}{2}\phi^\top \cdot \mathcal{J}^{-1} \cdot \phi .$$ (1.34)

where the "free" or "bare" massive scalar propagator $\mathcal{J}$ is parametrized as

$$\mathcal{J} = \frac{1}{p^2 + \mu^2} .$$ (1.35)

What this parametrization says is that the mass squared m^2 of the Euclidean scalar particle is proportional to $m^2 \sim s/h$: the heavier the particle, the less likely it is to hop, the more likely is it to stop.

> A. Laplacian measures local curvature, how much I stick out among my neighbors.

1.2.2 Integration by parts

(Please skip this and all other bits marked 'cyclist' on the first reading - not essential at this time.)

In the continuum, integration by parts moves ∂ around,

$$\int [dx]\phi^\top \partial^2 \phi \to -\int [dx]\partial\phi^\top \cdot \partial\phi ;$$

on a lattice this amounts to a matrix transposition

$$\left[\left(\mathsf{r}_j - \mathbf{1}\right)\phi\right]^\top \cdot \left[\left(\mathsf{r}_j - \mathbf{1}\right)\phi\right] = \phi^\top \cdot \left(\mathsf{r}_j^{-1} - \mathbf{1}\right)\left(\mathsf{r}_j - \mathbf{1}\right)\phi .$$

If you are wondering where the "integration by parts" minus sign is, it is there in discrete case at well. It comes from the identity

$$\partial^\top = \frac{1}{a}\left(\mathsf{r}^{-1} - \mathbf{1}\right) = -\mathsf{r}^{-1}\frac{1}{a}\left(\mathsf{r} - \mathbf{1}\right) = -\mathsf{r}^{-1}\partial .$$

Integrating by parts is now "summing by parts." Let a_i and b_i be n-periodic vectors, and $(\partial a)_i = a_i - a_{i-1}$ be the difference operator. Then

$$\sum_{i=1}^{n}(\partial a)_i b_i = -\sum_{i=1}^{n} a_i(\partial b)_{i+1} .$$ (1.36)

1.2.3   Inverting the Laplacian

Evaluation of perturbative corrections to be undertaken in (5.29) requires that we come to grips with the "free" or "bare" propagator $\mathcal{J}$. While the Laplacian is a simple difference operator (1.31), the propagator is a messier object. A way to compute is to start expanding the propagator $\mathcal{J}$ as a power series in the Laplacian

$$\mathcal{J} = \frac{1}{p^2 + \mu^2} = \frac{1}{m^2} \sum_{k=0}^{\infty} \frac{1}{m^{2k}} \Box^k \, . \tag{1.37}$$

As $\Box$ is a finite matrix, the expansion is convergent for sufficiently large m^2. To get a feeling for what is involved in evaluating such series, evaluate $\Box^2$ in the 1-dimensional case:

$$\Box^2 = \frac{1}{a^4} \begin{pmatrix} 6 & -4 & 1 & & & & 1 & -4 \\ -4 & 6 & -4 & 1 & & & & 1 \\ 1 & -4 & 6 & -4 & 1 & & & \\ & 1 & -4 & \ddots & & & & 1 \\ 1 & & & & & & 6 & -4 \\ -4 & 1 & & & & 1 & -4 & 6 \end{pmatrix} . \tag{1.38}$$

What $\Box^3$, $\Box^4$, $\cdots$ contributions look like is now clear; as we include higher and higher powers of the Laplacian, the propagator matrix fills up; while the *inverse* propagator is differential operator connecting only the nearest neighbors, the propagator is integral, *non-local* operator, connecting every lattice site to any other lattice site. Due to the periodicity, these are all Toeplitz matrices, meaning that each successive row is a one-step cyclic shift of the preceding one. In statistical mechanics, $\mathcal{J}$ is the (bare) 2-point correlation. In quantum field theory, it is called a propagator.

These matrices can be evaluated as is, on the lattice, and sometime it is evaluated this way, but in case at hand a wonderful simplification follows from the observation that the lattice action is translationally invariant. We show how this works in sect. 1.3.

1.3   Periodic lattices

Our task now is to transform $\mathcal{J}$ into a form suitable to evaluation of Feynman diagrams. The theory we will develop in this section is applicable only to *translationally invariant* saddle point configurations; i.e., if no translation invariance, no diagonalization by Fourier transforms, and even a propagator might be hard to evaluate.

Consider the effect of a lattice translation $\phi \rightarrow r\phi$ on the matrix polynomial

$$S[r\phi] = -\frac{1}{2}\phi^\top \left(r^\top \mathcal{J}^{-1} r \right) \phi \, .$$

As $\mathcal{J}^{-1}$ is constructed from r and its inverse, $\mathcal{J}^{-1}$ and r commute, and $S[\phi]$ is invariant under translations,

$$S[r\phi] = S[\phi] = -\frac{1}{2}\phi^\top \cdot \frac{1}{\mathcal{J}} \cdot \phi \, . \tag{1.39}$$

If a function defined on a vector space commutes with a linear operator r, then the eigenvalues of r can be used to decompose the ϕ vector space into invariant subspaces. For a hyper-cubic lattice the translations in different directions commute, $r_j r_i = r_i r_j$, so it is sufficient to understand the spectrum of the 1-dimensional shift operator (6.13).

To develop a feeling for how this reduction to invariant subspaces works in practice, let us proceed cautiously, by expanding the scope of our deliberations to a lattice consisting of 2 points.

1.3.1 A 2-point lattice diagonalized

The action of the shift operator r (6.13) on a 2-point lattice $\phi = (\phi_0, \phi_1)$ is to permute the two lattice sites

$$\mathsf{r} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

As exchange repeated twice brings us back to the original state, $\mathsf{r}^2 = \mathbf{1}$, the characteristic polynomial of r is

$$(\mathsf{r} + 1)(\mathsf{r} - 1) = 0,$$

with eigenvalues $\omega_0 = 1, \omega_1 = -1$. The symmetrization, antisymmetrization projection operators are

$$P_0 \quad = \quad \frac{\mathsf{r} - \omega_1 \mathbf{1}}{\omega_0 - \omega_1} \quad = \quad \frac{1}{2}(\mathbf{1} + \mathsf{r}) \quad = \quad \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \tag{1.40}$$

$$P_1 \quad = \quad \frac{\mathsf{r} - \mathbf{1}}{-1 - 1} \quad = \quad \frac{1}{2}(\mathbf{1} - \mathsf{r}) \quad = \quad \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}. \tag{1.41}$$

Noting that $P_0 + P_1 = \mathbf{1}$, we can project a lattice state ϕ onto the two normalized eigenvectors of r:

$$\phi \quad = \quad \mathbf{1}\,\phi \;=\; P_0 \cdot \phi \;+\; P_1 \cdot \phi,$$

$$\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} \quad = \quad \frac{(\phi_0 + \phi_1)}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} + \frac{(\phi_0 - \phi_1)}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \tag{1.42}$$

$$= \quad \tilde{\phi}_0 \, \varphi_0 + \tilde{\phi}_1 \, \varphi_1. \tag{1.43}$$

As $P_0 P_1 = 0$, the symmetric and the antisymmetric states transform separately under any linear transformation constructed from r and its powers.

In this way the characteristic equation $\mathsf{r}^2 = \mathbf{1}$ enables us to reduce the 2-dimensional lattice state to two 1-dimensional ones, on which the value of the shift operator r is a number, $\omega_j \in \{1, -1\}$, and the normalized eigenvectors are $\varphi_0 = \frac{1}{\sqrt{2}}(1, 1)$, $\varphi_1 = \frac{1}{\sqrt{2}}(1, -1)$. As we shall now see, $(\tilde{\phi}_0, \tilde{\phi}_1)$ is the 2-site periodic lattice discrete Fourier transform of the field (ϕ_1, ϕ_2).

1.4 Discrete Fourier transforms

Let us generalize this reduction to a 1-dimensional periodic lattice with L sites.

1.4.1 Reciprocal primitive cell

Translation invariance of orbits suggests reformulating the theory in a discrete Fourier basis, a discretization approach that goes all the way back to Hill's 1886 paper [9].

   The n consecutive shifts (1.21) return a period-n field configuration to itself, so acting on an one-dimensional periodic primitive cell, shift operator satisfies the characteristic equation

$$\mathsf{r}^n - \mathbb{1} = \prod_{m=0}^{n-1} (\mathsf{r} - e^{\mathrm{i}k}\,\mathbb{1}) = 0\,, \tag{1.44}$$

with the n-th roots of unity eigenvalues $\{e^{\mathrm{i}k}\}$ indexed by integers m

$$k = \frac{2\pi}{n}m\,, \quad m = 0, 1, \cdots, n-1\,, \tag{1.45}$$

and n eigenvectors

$$\mathsf{r}\,\varphi(k) = e^{\mathrm{i}k}\varphi(k)\,, \quad [\varphi(k)]_z = e^{\mathrm{i}\,kz}\,. \tag{1.46}$$

The shift (1.21)

$$[\mathsf{r}\varphi(k)]_z = [\varphi(k)]_{z+1} = e^{\mathrm{i}\,k(z+1)} = e^{\mathrm{i}k}[\varphi(k)]_z$$
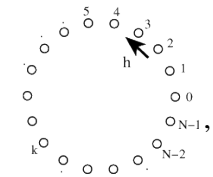
acts by rotating the eigenvector's overall phase.

   Wave numbers k form a one-dimensional *reciprocal lattice*,

$$\mathcal{L}_{\tilde{\mathbb{A}}} = \left\{ m\tilde{\mathbf{a}}_1 \mid m \in \mathbb{Z} \right\}\,, \quad \tilde{\mathbf{a}}_1 \cdot \mathbf{a}_1 = 2\pi\,,$$

with the primitive reciprocal lattice vector $\tilde{\mathbf{a}}_1 = 2\pi/n$, and the reciprocal primitive cell –the interval $[0, 2\pi)$– that contains n distinct wave numbers (1.45).

   Each application of r translates the lattice one step; in L steps the lattice is back in the original state

$$\mathsf{r}^L = \mathbf{1} \tag{1.47}$$

so the eigenvalues of r are the L distinct Lth roots of unity

$$\mathsf{r}^L - \mathbf{1} = \prod_{k=0}^{L-1} (\mathsf{r} - \omega^k \mathbf{1}) = 0\,, \qquad \omega = e^{i2\pi/L}\,. \tag{1.48}$$

As the eigenvalues are all distinct and L in number, the space is decomposed into L 1-dimensional subspaces.

1.4.2 Projection operators

(Please skip this and all other bits marked 'cyclist' on the first reading - not essential at this time.)

The general theory (expounded in appendix A1.1) associates with the kth eigenvalue of r a projection operator that projects a state ϕ onto kth eigenvector of r,

$$P_k = \prod_{j \neq k} \frac{\mathsf{r} - \omega^j \mathbf{1}}{\omega^k - \omega^j} \,. \tag{1.49}$$

A factor $(\mathsf{r} - \omega^j \mathbf{1})$ kills the jth eigenvector φ_j component of an arbitrary vector in expansion $\phi = \cdots + \tilde{\phi}_j \varphi_j + \cdots$. The above product kills everything but the eigen-direction φ_k, and the factor $\prod_{j \neq k} (\omega^k - \omega^j)$ ensures that P_k is normalized as a projection operator. The set of the projection operators is complete,

$$\sum_k P_k = \mathbf{1} \,, \tag{1.50}$$

and orthonormal

$$P_k P_j = \delta_{kj} P_k \qquad (\text{no sum on } k) \,. \tag{1.51}$$

In the case of discrete translational invariance, or cyclic group C_L, it is customary to write out the projection operator (1.49) as a character-weighted sum, see example 1.4.4.

As any matrix function $\mathcal{J} = \mathcal{J}(\mathsf{r})$ of the translation generator r takes a scalar value on the kth subspace,

$$\mathcal{J}(\mathsf{r}) P_k = \mathcal{J}(\omega^k) P_k \,, \tag{1.52}$$

the projection operators *diagonalize* the matrix $\mathcal{J}$, $P_j \mathcal{J}(\mathsf{r}) P_k = \mathcal{J}(\omega^k) P_k \delta_{jk}$.

The $[L \times L]$ projection operator matrix elements can be expressed in terms of the eigenvectors (1.55), (1.56) as

$$(P_k)_{\ell \ell'} = (\varphi_k)_\ell (\varphi_k^\dagger)_{\ell'} = \frac{1}{L} e^{i \frac{2\pi}{L}(\ell - \ell')k} \,, \qquad (\text{no sum on } k) \,. \tag{1.53}$$

The completeness (1.50) follows from (1.58), and the orthonormality (1.51) from (1.57).

$\tilde{\phi}_k$, the projection of the L-dimensional state (i.e., vector) ϕ on the kth subspace is given by

$$
\begin{aligned}
(P_k \cdot \phi)_\ell &= \tilde{\phi}_k (\varphi_k)_\ell \,, \qquad (\text{no sum on } k) \\
\tilde{\phi}_k &= \varphi_k^\dagger \cdot \phi = \frac{1}{\sqrt{L}} \sum_{\ell=0}^{L-1} e^{-i \frac{2\pi}{L} k \ell} \phi_\ell
\end{aligned} \tag{1.54}
$$

1.4.3   Eigenvectors of the translation operator

While constructing explicit eigenvectors is usually not a the best way to fritter one's youth away, as choice of basis is largely arbitrary, and all of the content of the theory is in the projection operators (see appendix A1.1), in case at hand the eigenvectors are so simple that we can construct and verify the solutions of the eigenvalue condition

$$\mathsf{r}\, \varphi_k = \omega^k \varphi_k \tag{1.55}$$

by hand:

$$\frac{1}{\sqrt{L}}\begin{bmatrix} 0 & 1 & & & & \\ & 0 & 1 & & & \\ & & 0 & 1 & & \\ & & & \ddots & & \\ & & & & 0 & 1 \\ 1 & & & & & 0 \end{bmatrix}\begin{bmatrix} 1 \\ \omega^k \\ \omega^{2k} \\ \omega^{3k} \\ \vdots \\ \omega^{(L-1)k} \end{bmatrix} = \omega^k \frac{1}{\sqrt{L}}\begin{bmatrix} 1 \\ \omega^k \\ \omega^{2k} \\ \omega^{3k} \\ \vdots \\ \omega^{(L-1)k} \end{bmatrix}$$

In words: the cyclic translation generator r shifts all components by one, and the original vector is recovered by factoring out the common factor ω^k. The $1/\sqrt{L}$ factor normalizes φ_k to a complex unit vector,

$$\varphi_k^\dagger \cdot \varphi_k = \frac{1}{L}\sum_{k=0}^{L-1} 1 = 1, \qquad \text{(no sum on } k)$$

$$\varphi_k^\dagger = \frac{1}{\sqrt{L}}\left(1, \omega^{-k}, \omega^{-2k}, \cdots, \omega^{-(L-1)k}\right). \tag{1.56}$$

The eigenvectors are orthonormal

$$\varphi_k^\dagger \cdot \varphi_j = \delta_{kj}, \tag{1.57}$$

as the explicit evaluation of $\varphi_k^\dagger \cdot \varphi_j$ yields the *Kronecker (circular) delta function for a periodic lattice*

$$\delta_{kj} = \frac{1}{L}\sum_{\ell=0}^{L-1} e^{i\frac{2\pi}{L}(k-j)\ell}. \tag{1.58}$$

The sum is over the L unit vectors pointing at a uniform distribution of points on the complex unit circle,
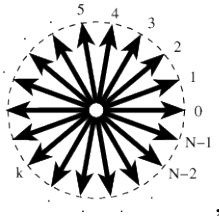
they cancel each other unless $k = j \pmod{L}$, in which case each term in the sum equals 1.

By the eigenvector condition (1.55), any matrix function $\mathcal{J} = \mathcal{J}(\mathsf{r})$ of the translation generator r takes a scalar value on the kth subspace,

$$\mathcal{J}(\mathsf{r})\varphi_k = \mathcal{J}(\omega^k)\varphi_k, \tag{1.59}$$

i.e., in the eigenvector basis, $\mathcal{J}$ is a diagonal matrix.

The L-dimensional vector $\tilde{\phi}$ of "wavenumbers" (discretized spatial coordinates), or "frequencies," "eigen-energies" (discretized time evolution steps) $\tilde{\phi}_k$ is the *discrete Fourier transform* of state (vector) ϕ. Hopefully rediscovering it this way helps you a little toward understanding why Fourier transforms are full of $e^{ix\cdot p}$ factors (they are eigenvalues of generators of translations; r for a discrete lattice, $\partial/\partial x$ for continuum), and that they are the natural set of basis functions when a theory is translationally invariant.

1.4.4 Cyclic group projection operators AKA discrete Fourier transform

(It's OK to skip this example on the first reading - the explicit Fourier eigenvectors and eigenvalues (1.55) are all that we need to carry out discrete Fourier transforms.)

Consider a cyclic group

$$C_N = \{e, g, g^2, \cdots g^{N-1}\}, \quad g^N = e.$$

If $M = D(g)$ is a $[d \times d]$ matrix representation of the one-step shift g, it must satisfy $M^N - \mathbf{1} = 0$, with eigenvalues given by the zeros of the characteristic polynomial

$$G(x) = x^N - 1 = (x - \lambda_0)(x - \lambda_1)(x - \lambda_2) \cdots (x - \lambda_{N-1}). \tag{1.60}$$

For the cyclic group the N distinct eigenvalues are the Nth roots of unity $\lambda_n = \omega^n$, $\omega = \exp(i\, 2\pi/N)$, $n = 0, \ldots N - 1$.

In the projection operator formulation (A1.3), they split the d-dimensional space into d/N-dimensional subspaces by means of projection operators

$$P_n = \prod_{m \neq n} \frac{M - \omega^m I}{\omega^n - \omega^m} = \frac{1}{\prod_{m=1}^{N-1}(1 - \omega^m)} \prod_{m=1}^{N-1} (\omega^{-n} M - \omega^m I), \tag{1.61}$$

where we have multiplied all denominators and numerators by ω^{-n}.

The denominator is a polynomial of form $G(x)/(x - \lambda_0)$, with the zeroth root $(x - \omega^0) = (x - 1)$ quotiented out from the characteristic polynomial,

$$\frac{x^N - 1}{x - 1} = (x - \omega)(x - \omega^2) \cdots (x - \omega^{N-1}).$$

Consider a sum of the first N terms of a geometric series, multiplied by $(x-1)/(x-1)$:

$$1 + x + \cdots + x^{N-1} = \sum_{m=0}^{N-1} x^m = \frac{1}{x-1} \sum_{m=0}^{N-1} (x-1)\, x^m = \frac{x^N - 1}{x - 1}. \tag{1.62}$$

So, the products in (1.61) can be written as sums

$$(x - \omega)(x - \omega^2) \cdots (x - \omega^{N-1}) = 1 + x + \cdots + x^{N-1}. \tag{1.63}$$

The P_n projection operator (1.61) denominator is evaluated by substituting $x \to 1$ into (1.63); that adds up to N. The numerator is evaluated by substituting $x \to \omega^{-n} M$. We obtain the projection operator as a discrete Fourier weighted sum of matrices M^m,

$$P_n = \frac{1}{N} \sum_{m=0}^{N-1} e^{-i\frac{2\pi}{N} nm}\, M^m, \tag{1.64}$$

instead of the product form (1.61).

This is the simplest example of the key group theory tool, the projection operator expressed as a sum over characters,

$$P_n = \frac{1}{|G|} \sum_{g \in G} \bar{\chi}_n(g) D(g).$$

As C_N irreps are all 1-dimensional, for the discrete Fourier transform all characters are simply $\bar{\chi}_n(g^m) = \omega^{-nm}$, the Nth complex roots of unity.

(B. Gutkin and P. Cvitanović)

1.4.5 Discrete Fourier transform operator

The $[L \times L]$ matrix $\mathcal{F}_{jk} = L^{-\frac{1}{2}} \omega^{jk}$, $j, k = 0, 1, 2, \cdots, L - 1$, formed from column eigenvectors (1.55),

$$
\mathcal{F} = \frac{1}{\sqrt{L}}
\begin{bmatrix}
1 & 1 & 1 & \ldots & 1 & 1 \\
1 & \omega & \omega^2 & \ldots & \omega^{L-2} & \omega^{L-1} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
1 & \omega^k & \omega^{2k} & \ldots & \omega^{(L-2)k} & \omega^{(L-1)k} \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
1 & \omega^{L-2} & \omega^{2(L-2)} & \ldots & \omega^{(L-2)(L-2)} & \omega^{(L-1)(L-2)} \\
1 & \omega^{L-1} & \omega^{2(L-1)} & \ldots & \omega^{(L-2)(L-1)} & \omega^{(L-1)(L-1)}
\end{bmatrix},
\qquad (1.65)
$$

is the *discrete Fourier transform operator* (remember, in the discretized world 'operator' is a synonym for 'matrix'). From the orthogonality of eigenvectors (1.57) it follows that $\mathcal{F}$ is a unitary matrix, with det $\mathcal{F} = 1$, and

$$
\mathcal{F}\mathcal{F}^\dagger = \mathbf{1} . \qquad (1.66)
$$

The operator $\mathcal{F}^\dagger$ is thus the *inverse Fourier transform*. The discrete Fourier transform (1.54) of a state (vector) ϕ is given by

$$
\tilde{\phi} = \mathcal{F}^\dagger \phi , \qquad (1.67)
$$

i.e., Fourier transformation rearranges components of vector ϕ into averages over all components (1.54), weighted by complex phases $\exp(i2\pi\ell/L)$ in all possible ways.

1.4.6 'Configuration-momentum' Fourier space duality

shift

What does a projection on the kth Fourier subspace mean? The discrete Fourier transform (1.64) of a state (vector) ϕ rearranges components of vector ϕ into averages over all its components, weighted by complex phases $\exp(i2\pi\ell/L)$ in all possible ways.

Consider first the projection on the 0th Fourier mode

$$
P_0 = \frac{1}{L} \sum_{m=0}^{L-1} \mathsf{r}^m .
$$

Applied to a lattice state $\phi = (\phi_1, \phi_2, \cdots, \phi_L)$, the shift matrix r translates the state by one site, $\mathsf{r}\phi = (\phi_2, \phi_3, \cdots, \phi_L, \phi_1)$, and so on for all powers r^m. The result is the space average (here correctly normalized, so that $\langle 1 \rangle = 1$) over all values of the periodic lattice field ϕ_m,

$$
\frac{1}{\sqrt{L}} \tilde{\phi}_0 = \frac{1}{L} \sum_{\ell=0}^{L-1} \phi_\ell = \langle \phi \rangle ,
$$

see (1.47) and (1.58). Every finite discrete group has such fully-symmetric representation, and in statistical mechanics and quantum mechanics this is often the most important state (the 'ground' state).

$\tilde{\phi}_1$ is the average weighted by one oscillation over the L-periodic lattice, and $\tilde{\phi}_k$, the projection of the L-dimensional state (i.e., vector) ϕ on the kth subspace

$$\tilde{\phi}_k = P_k \cdot \phi = \frac{1}{\sqrt{L}} \sum_{\ell=0}^{L-1} \omega^{k\ell} \phi_\ell \,, \tag{1.68}$$

is the average weighted by complex rotating phase ω^{km} which advances by ω^k in every step, and pulls out oscillating feature $\tilde{\phi}_k$ out of the field ϕ. For large L, modes $\tilde{\phi}_k$ with $k \ll L$ (or $(L-k) \ll L$, that is just a counter-rotation)) are called *hydrodynamic modes*, corresponding to "configuration" lattice fields ϕ which vary slowly and smoothly over many lattice spacings. Modes with $k \simeq L/2$ are suspect, they are lattice discretization artifacts.

If the lattice state is ϕ is localized, its Fourier transform will be global, and vice versa for a localized Fourier state $\tilde{\phi}$. For example, if the field ϕ is concentrated on the first site, $\phi_0 = 1$, rest zero, its Fourier transform will be uniformly distributed over all Fourier modes, $\tilde{\phi}_k = 1/\sqrt{L}$.

The complex function $\tilde{\phi}$ is can sometimes be interpreted as an 'amplitude function', with the square of its magnitude ($\tilde{\phi}^\dagger \cdot \tilde{\phi}$) then interpreted as the corresponding 'total probability'

$$\phi^\dagger \cdot \phi = \tilde{\phi}^\dagger \cdot \tilde{\phi} \,. \tag{1.69}$$

The fact that this is the same if evaluated with ϕ or with its Fourier transform $\tilde{\phi}$ is known as the "Parseval's identity."

Furthermore, by (1.59), discrete Fourier transform diagonalizes every translationally invariant matrix function $\mathcal{J}$, i.e., any matrix that commutes with the translation operator, $[\mathrm{r}, \mathcal{J}] = 0$. To show that, sandwich $\mathcal{J}$ with the identity $\mathbf{1} = \mathcal{F}\mathcal{F}^\dagger$:

$$\mathcal{J} = \mathbf{1}\mathcal{J}\mathbf{1} = \mathcal{F}\left(\mathcal{F}^\dagger \mathcal{J}\mathcal{F}\right)\mathcal{F}^\dagger = \mathcal{F}\tilde{\mathcal{J}}\mathcal{F}^\dagger \,.$$

The matrix

$$\tilde{\mathcal{J}} = \mathcal{F}^\dagger \mathcal{J}\mathcal{F} \tag{1.70}$$

is the Fourier transform of $\mathcal{J}$. No need to stop here - the terms in the action (1.39) that couple four (and, in general, 3, 4, $\cdots$) fields also have the Fourier space representations

$$
\begin{aligned}
\gamma_{\ell_1 \ell_2 \cdots \ell_n} \, \phi_{\ell_1}\phi_{\ell_2}\cdots\phi_{\ell_n} &= \tilde{\gamma}_{k_1 k_2 \cdots k_n} \, \tilde{\phi}_{k_1}\tilde{\phi}_{k_2}\cdots\tilde{\phi}_{k_n} \,, \\
\tilde{\gamma}_{k_1 k_2 \cdots k_n} &= \gamma_{\ell_1 \ell_2 \cdots \ell_n}(\varphi_{k_1})_{\ell_1}(\varphi_{k_2})_{\ell_2}\cdots(\varphi_{k_n})_{\ell_n} \\
&= \frac{1}{L^{n/2}} \sum_{\ell_1 \cdots \ell_n} \gamma_{\ell_1 \ell_2 \cdots \ell_n} \, e^{-i\frac{2\pi}{L}(k_1\ell_1 + \cdots + k_n\ell_n)} \,. \tag{1.71}
\end{aligned}
$$

The form of any translation-invariant function, such as (1.69), or the path integral (5.8) does not change under $\phi \to \tilde{\phi}$ transformation, and it does not matter whether we compute in the Fourier space, or in the configuration space that we started out with. For example, the trace of $\mathcal{J}$ is the same in either representation

$$\mathrm{tr}\,\mathcal{J} = \mathrm{tr}\,\mathcal{F}\tilde{\mathcal{J}}\mathcal{F}^\dagger = \mathrm{tr}\,\tilde{\mathcal{J}}\mathcal{F}^\dagger\mathcal{F} = \mathrm{tr}\,\tilde{\mathcal{J}} \,,$$

but, if $\mathcal{J}$ commutes with the translation operator r, the Fourier transform $\mathrm{tr}\,\tilde{\mathcal{J}}$ is diagonal and trivial to compute. By same reasoning it follows that $\mathrm{tr}\,\mathcal{J}^n = \mathrm{tr}\,\tilde{\mathcal{J}}^n$, and from the tr ln = ln tr relation that $\det\mathcal{J} = \det\tilde{\mathcal{J}}$. In fact, any scalar combination of ϕ's, J's and couplings, such as the partition function $Z[J]$, has exactly the same form in the configuration and the Fourier space.

Suppose you have two translationally invariant matrices A, B. Evaluating their product AB is a matrix computation. However, evaluating the product in the Fourier space is a simple scalar multiplication of their diagonal elements:

$$(\tilde{AB})_{kk'} = (\mathcal{F}^\dagger A\, B\mathcal{F})_{kk'} = \tilde{A}_k \tilde{B}_k \delta_{kk'} \tag{1.72}$$

The continuum Fourier transform version of this relation is called the "convolution theorem."

OK. But what's the payback?

1.4.7 Lattice Laplacian diagonalized

We can now use the Fourier transform (1.70) to convert matrix functions of the r matrix into scalars. As $\mathcal{J}$ *commutes* with r, then $(\tilde{\mathcal{J}})_{kk'} = \tilde{\mathcal{J}}_k \delta_{kk'}$ is a diagonal matrix, where the matrix $\mathcal{J}$ acts as a multiplication by the scalar $\tilde{\mathcal{J}}_k$ on the kth subspace. For example, for the 1-dimensional version of the lattice Laplacian matrix (1.32), the eigenvalue condition (1.55) yields the diagonalized Laplacian in the Fourier space,

$$\begin{aligned} \mathcal{J}_{\mathbb{A}}\varphi_k &= (-\Box + \mu^2\,\mathbb{1})\,\varphi_k = (\mathsf{p}^2 + \mu^2)\,\varphi_k \\ \mathsf{p} &= 2\sin(k/2)\,, \qquad k = \tfrac{2\pi}{n}m\,, \quad m = 0, 1, \cdots, n-1\,, \end{aligned} \tag{1.73}$$

expresses the Fourier-diagonalized lattice Laplacian as the square of the lattice momentum p,

$$(\tilde{\mathcal{J}}_{\mathbb{A}})_{mm'} = (\mathsf{p}^2 + \mu^2)\,\delta_{mm'}\,, \tag{1.74}$$

with n eigenvalues $\Lambda_m = p^2 + \mu^2$ indexed by the integer m. The 'cord function' $\mathrm{crd}(\theta) = 2\sin(\theta/2)$ was used already by Hipparchus cc. 130 BC in the same context, as a discretization of a circle by approximating n arcs by n cords [3, 23].

In the kth subspace the bare propagator is simply a number, and, in contrast to the mess generated by the configuration space inversion (1.37), there is nothing to inverting $\mathcal{J}$ to $\mathcal{J}^{-1}$:

$$(\varphi_{\mathbf{k}}^\dagger \cdot \mathcal{J}^{-1} \cdot \varphi_{\mathbf{k}'}) = \frac{\delta_{\mathbf{kk}'}}{p^2 + \mu^2}\,, \tag{1.75}$$

where $\mathbf{k} = (k_1, k_2, \cdots, k_d)$ is a d-dimensional vector in the L^d-dimensional dual lattice, i.e., the discretized "momentum" or "frequency" space.

Example: Orbit Jacobian matrix eigenvalues for primitive cell of period 3.

The wave-number range in (1.73) is $k \in (0, 2\pi/3, 4\pi/3)$. The Laplacian part of the reciprocal lattice orbit Jacobian matrix (1.74) takes values (up to a sign)

$$p(0) = 0\,, \; p(2\pi/3) = \sqrt{3}\,, \; .$$

A typical reciprocal lattice site evaluation of p^2:

$$\mathsf{p}_1^2 = p(2\pi/3)^2 = 3\,.$$

The eigenvalues of the Laplacian p^2 in (1.74), evaluated on the $V_{\mathbb{A}} = 3$ lattice sites of the reciprocal primitive cell, indexed by integer m, are

$$\boxed{\mathsf{p}_0^2 \;\vdots\; \mathsf{p}_1^2 \;\vdots\; \mathsf{p}_2^2} = \boxed{0 \;\vdots\; 3 \;\vdots\; 3}\,, \tag{1.76}$$

so, for example, the $(\tilde{\mathcal{J}}_{\mathbb{A}})_1$ eigenvalue is

$$\Lambda_2 = 3 + \mu^2\,,$$

and so on.

Going back to the partition function (5.29) and sticking in the factors of $\mathbf{1}$ into the bilinear part of the interaction, we replace the spatial source field J by its Fourier transform $\tilde{J}$, and the spatial propagator $\mathcal{J}$ by the diagonalized Fourier transformed $\tilde{G}_0$

$$J^\dagger \cdot \mathcal{J} \cdot J = J^\dagger \cdot \mathcal{F}\left(\mathcal{F}^\dagger \mathcal{J}\mathcal{F}\right)\mathcal{F}^\dagger \cdot J = \tilde{J}^\dagger \cdot \tilde{G}_0 \cdot \tilde{J}\,. \tag{1.77}$$

What's the price? The interaction term $S_I[\phi]$ (which in (5.29) was local in the configuration space) now has a more challenging k dependence in the Fourier transform version (1.71). For example, the locality of the quartic term leads to the 4-vertex *momentum conservation* in the Fourier space

$$
\begin{aligned}
S_I[\phi] &= \frac{1}{4!}\gamma_{\ell_1\ell_2\ell_3\ell_4}\,\phi_{\ell_1}\phi_{\ell_2}\phi_{\ell_3}\phi_{\ell_4} = -\beta u \sum_{\ell=1}^{L^d}(\phi_\ell)^4 \;\Rightarrow\\
&= -\beta u \frac{1}{L^d}\sum_{\{\mathbf{k}_i\}}^{L}\delta_{0,\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4}\,\tilde{\phi}_{\mathbf{k}_1}\tilde{\phi}_{\mathbf{k}_2}\tilde{\phi}_{\mathbf{k}_3}\tilde{\phi}_{\mathbf{k}_4}\,.
\end{aligned}
\tag{1.78}
$$

1.5 Lattice action

The number of *admissible periodic points* of period n, i.e., points on loops, or walks that return to the starting lattice point is given by $\operatorname{tr} T^n$. By spatial translations invariance, all L sites of a periodic lattice ($L_1 L_2 \cdots L_d$ for spatial dimension d) are equivalent, so one should study walks that start in a given site and return to it ("rooted lattice loop?"), i.e., in one spatial dimension $N_n = \operatorname{tr} T^n/\operatorname{tr}\mathbf{1} = \frac{1}{L}\operatorname{tr} T^n$. For example, in one spatial dimension we can enumerate all distinct walks by treating hopping matrices (1.5) as free (not using the inverse = transpose)

$$
\begin{aligned}
T^2 &= (\sigma + \sigma^\top)^2 = \sigma^2 + \sigma\sigma^\top + \sigma^\top\sigma + \sigma^{\top 2}\\
T^4 &= (\sigma^2 + \sigma\sigma^\top + \sigma^\top\sigma + \sigma^{\top 2})^2\\
&= \sigma^4 + (\sigma\sigma^\top)^2 + (\sigma^\top\sigma)^2 + \sigma^{\top 4}\\
&\quad + \sigma^3\sigma^\top + \sigma^2\sigma^\top\sigma + \sigma^2\sigma^{\top 2}\\
&\quad + \sigma\sigma^\top\sigma^2 + \sigma\sigma^{\top 2}\sigma + \sigma\sigma^{\top 3}\\
&\quad + \sigma^\top\sigma^3 + \sigma^\top\sigma^2\sigma^\top + \sigma^\top\sigma\sigma^{\top 2}\\
&\quad + \sigma^{\top 2}\sigma^2 + \sigma^{\top 2}\sigma\sigma^\top + \sigma^{\top 3}\sigma\,.
\end{aligned}
\tag{1.79}
$$

The returning walks (red) have equal numbers of left and right steps, so they multiply out to **1** (clearly, that can be counted combinatorially), and

$$N_2 = \frac{1}{L}\text{tr}\,T^2 = 2\,, \quad N_4 = \frac{1}{L}\text{tr}\,T^4 = 4 + N_2\,, \tag{1.80}$$

where N_4 includes 2 repeats of 2-cycles, and 4 prime 4-cycles.

tr T^{n_p} picks up contributions from all repeats of prime cycles, with each cycle contributing n_p periodic points, so N_n, the total number of periodic points of period n is given by

$$z^n N_n = z^n \text{tr}\,T^n = \sum_{n_p|n} n_p t_p^{n/n_p} = \sum_p n_p \sum_{r=1}^{\infty} \delta_{n_p r, n} t_p^r\,. \tag{1.81}$$

Here $m|n$ means that m is a divisor of n. In order to get rid of the awkward divisibility constraint $n = n_p r$ in the above sum, we introduce the generating function for numbers of periodic points (only cycles of even length can close into loops):

$$\sum_{n=1}^{\infty} z^{2n} N_{2n} = \text{tr}\,\frac{z^2 T^2}{1 - z^2 T^2}\,. \tag{1.82}$$

where we maybe should have used $T = a^2\square - 2\mathbf{1}$ from (1.32).

The right hand side is the geometric series sum of $N_n = \text{tr}\,T^n$. Substituting (1.81) into the left hand side, and replacing the right hand side by the eigenvalue sum tr $T^n = \sum \omega_\alpha^n$, we obtain our first example of a trace formula, the *topological trace formula*

$$\sum_{\alpha=0} \frac{z\omega_\alpha}{1 - z\omega_\alpha} = \sum_p \frac{n_p t_p}{1 - t_p}\,. \tag{1.83}$$

the free, non-interacting partition function

$$Z = \det\left(\square - m_0^2 \mathbf{1}\right)^{-1/2} = e^{-\frac{1}{2}\text{tr}\,\ln(\square - m_0^2 \mathbf{1})} \tag{1.84}$$

is the sum over all loops (returning walks), i.e., related to the trace of the propagator (1.2).

1.6 Continuum field theory

The lattice Laplacian kth Fourier component (**??**) is

$$\begin{aligned}
\tilde{\square}_{kk} &= \frac{2}{a^2}\left(\cos\left(\frac{2\pi}{L}k\right) - 1\right) \\
&= -\left(\frac{2\pi}{aL}\right)^2 k^2 + \frac{1}{12}\left(\frac{2\pi}{aL}\right)^4 a^2 k^4 - O(k^6)\,. \tag{1.85}
\end{aligned}$$

The quartic term can be neglected for low wave numbers $k \ll L$, i.e., low momenta, $p_\mu = 2\pi k_\mu/LL$, where $aL = LL$ is the lattice size.

In the continuum limit the probability to land in the kth cell is replaced by a probability density, $\phi_k = a^d \phi(x_k) \to (dx)^d \phi(x)$. After rescaling the wave-number k into momentum p, we obtain the continuum version of the scalar propagator

$$\Delta(x, y) = \int \frac{d^d p}{(2\pi)^d} \frac{e^{ip\cdot(x-y)}}{m^2 + p^2}\,. \tag{1.86}$$

1.7 Collective excitations: from particles to fields

One-dimensional harmonic chain is discussed by Ben Simons, in Lecture I: *Collective Excitations: From Particles to Fields Free Scalar Field Theory: Phonons* of his online course.

In Lecture 23 of his MIT course, Mehran Kardar [12] discusses elastodynamic equilibria of two-dimensional solids. Consider a perfect solid at $T = 0$. The equilibrium configuration of atoms forms a lattice,

$$\vec{x}^0_{mn} = m\,\vec{e}_1 + n\,\vec{e}_2\,,$$

where $\vec{e}_1$ and $\vec{e}_2$ are basis vectors, $a_j = |\vec{e}_j|$ is the lattice spacing along the jth direction, and $\{m, n\}$ are integers. At finite temperatures, the atoms fluctuate away from their equilibrium position, moving to

$$\vec{x}_{mn} = \vec{x}^0_{mn} + \vec{u}_{mn}\,,$$

As the low temperature (small kinetic energy) displacements do not vary substantially over nearby atoms, one can define a coarse-grained displacement field $\vec{u}(\vec{x})$, where $\vec{x} = (x_1, x_2)$ is treated as continuous, with an implicit short distance cutoff of the lattice spacing a. Due to translational symmetry, the elastic energy depends only on the strain matrix,

$$u_{ij}(\vec{x}) = \tfrac{1}{2}\left(\partial_i u_j + \partial_j u_i\right).$$

Kardar picks the triangular lattice, as its elastic energy is isotropic, (invariant under lattice rotations, see Landau and Lifshitz [13]). In terms of the Lamé coefficients λ and μ,

$$
\begin{aligned}
\beta H &= \frac{1}{2}\int d^2\vec{x}\,(2\mu\,u_{ij}u_{ij} + \lambda\,u_{ii}u_{jj}) \\
&= -\frac{1}{2}\int d^2\vec{x}\,u_i[2\mu\,\square\,\delta_{ij} + (\mu + \lambda)\,\partial_i\partial_j]\,u_j\,.
\end{aligned}
\tag{1.87}
$$

(here we have assumed either infinite or doubly periodic lattice, so no boundary terms from integration by parts), with the equations of motion something like (FIX!)

$$\partial_t^2 u_i = [2\mu\,\square\,\delta_{ij} + (\mu + \lambda)\,\partial_i\partial_j]\,u_j\,.\tag{1.88}$$

In general, the number of independent elastic constants depends on the dimensionality and rotational symmetry of the lattice in question. The symmetry of a square lattice permits an additional term proportional to $\partial_x^2 u_x^2 + \partial_y^2 u_y^2$. Thus in two dimensions, square lattices have three independent elastic constants, but triangular lattices are "elastically isotropic" (i.e., elastic properties are independent of direction and thus are characterized by only two Lamé coefficients [13]).

The Goldstone modes associated with the broken translational symmetry are *phonons*, the normal modes of vibrations. Eq. (1.88) supports two types of lattice normal modes, transverse and longitudinal.

The *order parameter* describing broken translational symmetry is

$$\rho_{\vec{G}}(\vec{x}) = e^{i\vec{G}\cdot\vec{r}(\vec{x})} = e^{i\vec{G}\cdot\vec{u}(\vec{x})}\,,$$

where $\vec{G}$ is any reciprocal lattice vector, where we have used that, by definition, $\vec{G} \cdot \vec{r_0}$ is an integer multiple of 2π. $\rho_{\vec{G}} = 1$ at zero temperature. Due to the fluctuations,

$$\langle \rho_{\vec{G}}(\vec{x}) \rangle = \langle e^{i\vec{G} \cdot \vec{u}(\vec{x})} \rangle$$

decreases at finite temperatures, and its correlations decay as $\langle \rho_{\vec{G}}(\vec{x}) \rho^*_{\vec{G}}(\vec{0}) \rangle$. Kardar computes this in Fourier space by approximating $\vec{G} \cdot \vec{q}$ with its angular average $G^2 q^2 / 2$, ignoring the rotationally symmetry-breaking term $\cos \vec{q} \cdot \vec{x}$, and getting only the asymptotics of the correlations right (the decay is algebraic).

The translational correlations are measured in diffraction experiments. The scattering amplitude is the Fourier transform of $\rho_{\vec{G}}$, and the scattered intensity at a wave-vector q is proportional to the structure factor. At zero temperature, the structure factor is a set of delta-functions (Bragg peaks) at the reciprocal lattice vectors.

The orientational order parameter that characterizes the broken rotational symmetry of the crystal can be defined as

$$\Psi(\vec{x}) = e^{6i\theta(\vec{x})},$$

where $\theta(\vec{x})$ is the angle between local lattice bonds and a reference axis. The factor of 6 accounts for the equivalence of the 6 possible C_{3v} orientations of the triangular lattice. (Kardar says the appropriate choice for a square lattice is $\exp(4i\theta(\vec{x}))$ - shouldn't the factor be 8, the order of C_{4v}?) The order parameter has unit magnitude at $T = 0$, and is expected to decrease due to fluctuations at finite temperature. The displacement $u(\vec{x})$ leads to a change in bond angle given by

$$\theta(\vec{x}) = -\tfrac{1}{2} \left(\partial_x u_y - \partial_y u_x \right).$$

Commentary

Remark 1.1. Collective excitations: from particles to fields. One-dimensional harmonic chain is discussed by Altland and Simons [1] *Condensed Matter Field Theory*: see Chapter 1 *Collective Excitations: From Particles to Fields* . In Lecture 23 of his MIT course, Mehran Kardar discusses elastodynamic equilibria of two-dimensional solids. For taking the infinite lattice limit (the first Brillouin zone, etc.) of (1.75), see Kadanoff [11] derivation of the *Sect. 3.4 Lattice Green Function*, eq. (3.20), available online here.

Remark 1.2. Lattice field theory. In his 1983 *Six Lectures on Lattice Field Theory* Michael Stone explains that the free, non-interacting partition function (1.84) is the sum over all loop (returning walks), i.e., related to the trace of the propagator (1.2). This goes back to Symanzik, and is probably explained at length in Federico Camia *Brownian Loops and Conformal Fields*, arXiv:1501.04861.

Check Rosenfelder *Path Integrals in Quantum Physics*, arXiv:1209.1315.

Meyer [15] *Lattice QCD: A brief introduction*.

Jansen [10] *Lattice field theory*.

Check out also online Simons, Lecture I: Simons courses *Collective Excitations: From Particles to Fields Free Scalar Field Theory: Phonons*; and *Quantum Condensed*

Matter Field Theory; as well as Piers Coleman [5] *Introduction to Many-Body Physics* +
.

    Further reading on lattice field theories: Sommer [21] *Introduction to Lattice Gauge Theories*; Wiese [22] *An Introduction to Lattice Field Theory*; Rothe [19] *Lattice Gauge Theories*; Smit [20] *Introduction to Quantum Fields on a Lattice*; Münster and M. Walzl [17] *Lattice gauge theory - A short primer*, arXiv:hep-lat/0012005; Montvay and G. Münster [16] *Quantum Fields on a Lattice*; Jorge L. deLyra *The Gaussian Model: An Exploration into the Foundations of Quantum Field Theory*;

Exercises

1.1. **Euclidean free scalar particle propagator.** Derive the Euclidean free scalar particle propagator (1.10).

1.2. **Scalar propagator, discrete Fourier representation.** Derive Fourier transform representation (1.75) of free scalar particle propagator, but with prefactors correct for starting with (1.10). (The notes probably have wrong prefactors).

1.3. **Scalar propagator, continuum configuration space** Derive the derive the continuum limit of the propagator (1.75) in the Fourier representation, with prefactors correct for starting with (1.10).

1.4. $1D$ **lattice Laplacian for period-8 periodic state.** Compute the eigenvalues of the period-8 $1D$ lattice Laplacian

$$
\begin{pmatrix}
2 & -1 & 0 & 0 & 0 & 0 & 0 & -1 \\
-1 & 2 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 2 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & 2 & -1 & 0 & 0 & 0 \\
0 & 0 & 0 & -1 & 2 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 2 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & -1 & 2 & -1 \\
-1 & 0 & 0 & 0 & 0 & 0 & -1 & 2
\end{pmatrix}.
$$

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Chapter 2

Path integral formulation of quantum mechanics

We introduce Feynman path integral and construct semiclassical approximations to quantum propagators and Green's functions.

Have: the Schrödinger equation, i.e., the (infinitesimal time) evolution law for any quantum wavefunction:

$$i\hbar \frac{\partial}{\partial t}\psi(t) = \hat{H}\psi(t)\,. \tag{2.1}$$

Want: $\psi(t)$ at any finite time, given the initial wave function $\psi(0)$.

As the Schrödinger equation (2.1) is a linear equation, the solution can be written down immediately:

$$\psi(t) = e^{-\frac{i}{\hbar}\hat{H}t}\psi(0)\,, \qquad t \geq 0\,.$$

Fine, but what does this mean? We can be a little more explicit; using the configuration representation $\psi(q,t) = \langle q|\psi(t)\rangle$ and the configuration representation completeness relation

$$\mathbf{1} = \int dq^D \, |q\rangle\langle q| \tag{2.2}$$

we have

$$\psi(q,t) = \langle q|\psi(t)\rangle = \int dq' \, \langle q|e^{-\frac{i}{\hbar}\hat{H}t}|q'\rangle\langle q'|\psi(0)\rangle\,, \qquad t \geq 0\,. \tag{2.3}$$

In sect. 2.1 we will solve the problem and give the explicit formula (2.9) for the propagator. However, this solution is useless - it requires knowing all quantum eigenfunctions, i.e., it is a solution which we can implement provided that we have already solved the quantum problem. In sect. 2.4 we shall derive Feynman's path integral formula for $K(q,q',t) = \langle q|e^{-\frac{i}{\hbar}\hat{H}t}|q'\rangle$.

2.1 Quantum mechanics: a brief review

We start with a review of standard quantum mechanical concepts prerequisite to the derivation of the semiclassical trace formula: Schrödinger equation, propagator, Green's function, density of states.

In coordinate representation the time evolution of a quantum mechanical wave function is governed by the Schrödinger equation (2.1)

$$i\hbar \frac{\partial}{\partial t} \psi(q,t) = \hat{H}(q, \frac{\hbar}{i} \frac{\partial}{\partial q}) \psi(q,t), \tag{2.4}$$

where the Hamilton operator $\hat{H}(q, -i\hbar\partial_q)$ is obtained from the classical Hamiltonian by substitution $p \rightarrow -i\hbar\partial_q$. Most of the Hamiltonians we shall consider here are of form

$$H(q,p) = T(p) + V(q), \qquad T(p) = \frac{p^2}{2m}, \tag{2.5}$$

appropriate to a particle in a D-dimensional potential $V(q)$. If, as is often the case, a Hamiltonian has mixed terms such as $\dot{q}\,p$, consult any book on quantum mechanics. We are interested in finding stationary solutions

$$\psi(q,t) = e^{-iE_n t/\hbar}\phi_n(q) = \langle q|e^{-i\hat{H}t/\hbar}|n\rangle,$$

of the time independent Schrödinger equation

$$\hat{H}\psi(q) = E\psi(q), \tag{2.6}$$

where E_n, $|n\rangle$ are the eigenenergies, respectively eigenfunctions of the system. For bound systems the spectrum is discrete and the eigenfunctions form an orthonormal

$$\int dq^D\, \phi_n^*(q)\phi_m(q) = \int dq^D\, \langle n|q\rangle\langle q|m\rangle = \delta_{nm} \tag{2.7}$$

and complete

$$\sum_n \phi_n(q)\phi_n^*(q') = \delta(q-q'), \qquad \sum_n |n\rangle\langle n| = \mathbf{1} \tag{2.8}$$

set of Hilbert space functions. For simplicity we will assume that the system is bound, although most of the results will be applicable to open systems, where one has complex resonances instead of real energies, and the spectrum has continuous components.

A given wave function can be expanded in the energy eigenbasis

$$\psi(q,t) = \sum_n c_n e^{-iE_n t/\hbar}\phi_n(q),$$

where the expansion coefficient c_n is given by the projection of the initial wave function onto the nth eigenstate

$$c_n = \int dq^D\, \phi_n^*(q)\psi(q,0) = \langle n|\psi(0)\rangle.$$

Figure 2.1: Path integral receives contributions from all paths propagating from q' to q in time $t = t' + t''$, first from q' to q'' for time t', followed by propagation from q'' to q in time t''.

The evolution of the wave function is then given by

$$\psi(q,t) = \sum_n \phi_n(q) e^{-iE_n t/\hbar} \int dq'^D \phi_n^*(q')\psi(q',0).$$

We can write this as

$$
\begin{aligned}
\psi(q,t) &= \int dq'^D K(q,q',t)\psi(q',0), \\
K(q,q',t) &= \sum_n \phi_n(q)\, e^{-iE_n t/\hbar} \phi_n^*(q') \\
&= \langle q|e^{-\frac{i}{\hbar}\hat{H}t}|q'\rangle = \sum_n \langle q|n\rangle e^{-iE_n t/\hbar} \langle n|q'\rangle,
\end{aligned}
\tag{2.9}
$$

where the kernel $K(q,q',t)$ is called the quantum evolution operator, or the *propagator*. Applied twice, first for time t_1 and then for time t_2, it propagates the initial wave function from q' to q'', and then from q'' to q

$$K(q,q',t_1+t_2) = \int dq'' \, K(q,q'',t_2)K(q'',q',t_1) \tag{2.10}$$

forward in time, hence the name "propagator", see figure 2.1. In non-relativistic quantum mechanics the range of q'' is infinite, meaning that the wave can propagate at any speed; in relativistic quantum mechanics this is rectified by restricting the forward propagation to the forward light cone.

Since the propagator is a linear combination of the eigenfunctions of the Schrödinger equation, the propagator itself also satisfies the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}K(q,q',t) = \hat{H}(q,\frac{i}{\hbar}\frac{\partial}{\partial q})K(q,q',t). \tag{2.11}$$

The propagator is a wave function defined for $t \geq 0$ which starts out at $t = 0$ as a delta function concentrated on q'

$$\lim_{t\to 0_+} K(q,q',t) = \delta(q-q'). \tag{2.12}$$

This follows from the completeness relation (2.8).

The time scales of atomic, nuclear and subnuclear processes are too short for direct observation of time evolution of a quantum state. For this reason, in most physical applications one is interested in the long time behavior of a quantum system.

In the $t \to \infty$ limit the sharp, well defined quantity is the energy E (or frequency), extracted from the quantum propagator via its Laplace transform, the energy dependent Green's function

$$G(q, q', E + i\epsilon) = \frac{1}{i\hbar} \int_0^\infty dt \, e^{\frac{i}{\hbar}Et - \frac{\epsilon}{\hbar}t} K(q, q', t) = \sum_n \frac{\phi_n(q)\phi_n^*(q')}{E - E_n + i\epsilon} \, . \qquad (2.13)$$

Here ϵ is a small positive number, ensuring that the propagation is forward in time.

This completes our lightning review of quantum mechanics.

Feynman arrived to his formulation of quantum mechanics by thinking of figure 2.1 as a "multi-slit" experiment, with an infinitesimal "slit" placed at every q' point. The Feynman path integral follows from two observations:

1. Sect. 2.3: For short time the propagator can be expressed in terms of classical functions (Dirac).

2. Sect. 2.4: The group property (2.10) enables us to represent finite time evolution as a product of many short time evolution steps (Feynman).

2.2 Matrix-valued functions

How are we to think of the quantum operator

$$\hat{H} = \hat{T} + \hat{V}, \qquad \hat{T} = \hat{p}^2/2m, \qquad \hat{V} = V(\hat{q}), \qquad (2.14)$$

corresponding to the classical Hamiltonian (2.5)?

Whenever you are confused about an "operator", think "matrix". Expressed in terms of basis functions, the propagator is an infinite-dimensional matrix; if we happen to know the eigenbasis of the Hamiltonian, (2.9) is the propagator diagonalized. Of course, if we knew the eigenbasis the problem would have been solved already. In real life we have to guess that some complete basis set is good starting point for solving the problem, and go from there. In practice we truncate such matrix representations to finite-dimensional basis set, so it pays to recapitulate a few relevant facts about matrix algebra.

The derivative of a (finite-dimensional) matrix is a matrix with elements

$$A'(x) = \frac{dA(x)}{dx}, \qquad A'_{ij}(x) = \frac{d}{dx}A_{ij}(x). \qquad (2.15)$$

Derivatives of products of matrices are evaluated by the chain rule

$$\frac{d}{dx}(AB) = \frac{dA}{dx}B + A\frac{dB}{dx}. \qquad (2.16)$$

A matrix and its derivative matrix in general do not commute

$$\frac{d}{dx}A^2 = \frac{dA}{dx}A + A\frac{dA}{dx}. \qquad (2.17)$$

The derivative of the inverse of a matrix follows from $\frac{d}{dx}(AA^{-1}) = 0$:

$$\frac{d}{dx}A^{-1} = -\frac{1}{A}\frac{dA}{dx}\frac{1}{A}. \tag{2.18}$$

As a single matrix commutes with itself, any function of a single variable that can be expressed in terms of additions and multiplications generalizes to a matrix-valued function by replacing the variable by the matrix.

In particular, the exponential of a constant matrix can be defined either by its series expansion, or as a limit of an infinite product:

$$e^A = \sum_{k=0}^{\infty} \frac{1}{k!}A^k, \qquad A^0 = \mathbf{1} \tag{2.19}$$

$$= \lim_{N\to\infty}\left(\mathbf{1} + \frac{1}{N}A\right)^N \tag{2.20}$$

The first equation follows from the second one by the binomial theorem, so these indeed are equivalent definitions. For finite N the two expressions differ by order $O(N^{-2})$. That the terms of order $O(N^{-2})$ or smaller do not matter is easy to establish for $A \to x$, the scalar case. This follows from the bound

$$\left(1 + \frac{x-\epsilon}{N}\right)^N < \left(1 + \frac{x+\delta x_N}{N}\right)^N < \left(1 + \frac{x+\epsilon}{N}\right)^N,$$

where $|\delta x_N| < \epsilon$ accounts for extra terms in the binomial expansion of (2.20). If $\lim \delta x_N \to 0$ as $N \to \infty$, the extra terms do not contribute. I do not have equally simple proof for matrices - would probably have to define the norm of a matrix (and a norm of an operator acting on a Banach space) first.

The logarithm of a matrix is defined by the power series

$$\ln(1 - B) = -\sum_{k=1}^{\infty} \frac{B^k}{k}. \tag{2.21}$$

Consider now the trace

$$\text{tr } \ln(1 - B) = -\sum_{k=1}^{\infty} \frac{\text{tr}\,(B^k)}{k}.$$

To the leading order in $1/N$

$$\det\left(\mathbf{1} + A/N\right) = 1 + \frac{1}{N}\text{tr}\,A + O(N^{-2}).$$

hence

$$\det e^A = \lim_{N\to\infty}\left(1 + \frac{1}{N}\text{tr}\,A + O(N^{-2})\right)^N = e^{\text{tr}\,A} \tag{2.22}$$

Defining $M = e^A$ we can write this as

$$\ln \det M = \text{tr } \ln M. \tag{2.23}$$

Due to non-commutativity of matrices, generalization of a function of several variables to a function is not as straightforward. Expression involving several matrices depend on their commutation relations. For example, the Baker-Campbell-Hausdorff commutator expansion

$$e^{tA}Be^{-tA} = B + t[A, B] + \frac{t^2}{2}[A, [A, B]] + \frac{t^3}{3!}[A, [A, [A, B]]] + \cdots \quad (2.24)$$

sometimes used to establish the equivalence of the Heisenberg and Schrödinger pictures of quantum mechanics, follows by recursive evaluation of t derivaties

$$\frac{d}{dt}\left(e^{tA}Be^{-tA}\right) = e^{tA}[A, B]e^{-tA} .$$

Expanding $\exp(A + B)$, $\exp A$, $\exp B$ to first few orders using (2.19) yields

$$e^{(A+B)/N} = e^{A/N}e^{B/N} - \frac{1}{2N^2}[A, B] + O(N^{-3}) , \quad (2.25)$$

and the *Trotter product formula*: if B, C and $A = B + C$ are matrices, then

$$e^A = \lim_{N \to \infty} \left(e^{B/N}e^{C/N}\right)^N . \quad (2.26)$$

2.3 Short time propagation

Split the Hamiltonian into the kinetic and potential terms $\hat{H} = \hat{T} + \hat{V}$ and consider the short time propagator

$$K(q, q', \Delta t) = \langle q|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|q'\rangle = \langle q|e^{-\hat{T}\lambda}e^{-\hat{V}\lambda}|q'\rangle + O(\Delta t^2) . \quad (2.27)$$

where $\lambda = \frac{i}{\hbar}\Delta t$. The error estimate follows from (2.25). In the coordinate representation the operator

$$e^{-\hat{V}\lambda}|q\rangle = e^{-V(q)\lambda}|q\rangle$$

is diagonal (a "*c*-number"). In order to evaluate $\langle q|e^{-\hat{T}\lambda}|q'\rangle$, insert the momentum eigenstates sum in a D-dimensional configuration space

$$\mathbf{1} = \int dp^D |p\rangle\langle p| , \qquad \langle p|q\rangle = (2\pi\hbar)^{-D/2}e^{-\frac{i}{\hbar}p \cdot q} , \quad (2.28)$$

and evaluate the Gaussian integral

$$
\begin{aligned}
\langle q|e^{-\lambda\hat{T}}|q'\rangle &= \int dp^D \langle q|e^{-\hat{T}\lambda}|p\rangle\langle p|q'\rangle = \int \frac{dp^D}{(2\pi\hbar)^{D/2}}e^{-\lambda p^2/2m}e^{\frac{i}{\hbar}p \cdot (q-q')} \\
&= \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{D}{2}} e^{\frac{i}{\hbar}\frac{m}{2\Delta t}(q-q')^2} .
\end{aligned}
\quad (2.29)
$$

Replacement $(q - q')/\Delta t \to \dot{q}$ leads (up to an error of order of Δt^2) to a purely *classical* expression for the short time propagator

$$K(q, q', \Delta t) = \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{D/2} e^{\frac{i}{\hbar}\Delta t\, L(q,\dot{q})} + O(\Delta t^2) , \quad (2.30)$$

where $L(q, \dot{q})$ is the Lagrangian of classical mechanics

$$L(q, \dot{q}) = m\frac{\dot{q}^2}{2} - V(q) . \quad (2.31)$$

2.4   Path integral

Next we express the finite time evolution as a product of many short time evolution steps.

Splitting the Hamiltonian into the kinetic and potential terms $\hat{H} = \hat{T} + \hat{V}$ and using the Trotter product formula (2.26) we have

$$e^{-\frac{i}{\hbar}\hat{H}t} = \lim_{N \to \infty} \left(e^{-\frac{i}{\hbar}\hat{T}\Delta t} e^{-\frac{i}{\hbar}\hat{V}\Delta t} \right)^N , \qquad \Delta t = t/N \tag{2.32}$$

Turn this into matrix multiplication by inserting the configuration representation completeness relations (2.2)

$$K(q, q', t) = \langle q | e^{-\frac{i}{\hbar}\hat{H}t} | q' \rangle \tag{2.33}$$

$$= \int dq_1^D \cdots dq_{N-1}^D \langle q | e^{-\hat{H}\lambda} | q_{N-1} \rangle \cdots \langle q_1 | e^{-\hat{H}\lambda} | q' \rangle$$

$$= \lim_{N \to \infty} \int dq_1^D \cdots dq_{N-1}^D \langle q' | e^{-\hat{T}\lambda} e^{-\hat{V}\lambda} | q_{N-1} \rangle \cdots \langle q_1 | e^{-\hat{T}\lambda} e^{-\hat{V}\lambda} | q \rangle .$$

The next step relies on convolution of two Gaussians being a Gaussian. Substituting (2.30) we obtain that the total phase shift is given by the *Hamilton's principal function*, the integral of (2.31) evaluated along the given path p from $q' = q(0)$ to $q = q(t)$:

$$R[q] = \lim_{N \to \infty} \sum_{j=0}^{N-1} \Delta t \left(\frac{m}{2} \left(\frac{q_{j+1} - q_j}{\Delta t} \right)^2 - V(q_j) \right) , \qquad q_0 = q'$$

$$= \int d\tau \, L(q(\tau), \dot{q}(\tau)) , \tag{2.34}$$

where functional notation $[q]$ indicates that $R[q]$ depends on the vector $q = (q', q_1, q_2, \ldots, q_{N-1}, q)$ defining a given path $q(\tau)$ in the limit of $N \to \infty$ steps, and the propagator is given by

$$K(q, q', t) = \lim_{N \to \infty} \int [dq] \, e^{\frac{i}{\hbar} R[q]} \tag{2.35}$$

$$[dq] = \prod_{j=1}^{N-1} \frac{dq_j^D}{(2\pi i \hbar \Delta t/m)^{D/2}} .$$

We assume that the energy is conserved, and that the only time dependence of $L(q, \dot{q})$ is through $(q(\tau), \dot{q}(\tau))$.

Path integral receives contributions from all paths propagating forward from q' to q in time t, see figure 2.1. The usual, more compact notation is

$$K(q, q', t) = \int \mathcal{D}q \, e^{\frac{i}{\hbar} R[q]} , \qquad \text{or, more picturesquely}$$

$$= C \sum_p e^{\frac{i}{\hbar} R[q_p]} , \qquad q' = q_p(0), \, q = q_p(t) , \tag{2.36}$$

where $\int \mathcal{D}q$ is shorthand notation for the $N \to \infty$ limit in (2.35),

$$\int \mathcal{D}q = \lim_{N \to \infty} \int [dq] , \tag{2.37}$$

and the "sum over the paths $C \sum_p$" is whatever you imagine it to be.

What's good and what's bad about path integrals? First the virtues:

- conceptual unification of

  - quantum mechanics
  - statistical mechanics
  - chaotic dynamics

- yields analytic solutions to classes of quantum problems

- quantum-classical correspondence

  - semiclassical theory

- theory of perturbative corrections

  - Feynman diagrams

- relativistic quantum field theory

And now for the bad news:

- $N \to \infty$ continuum limit

  - fraught with perils - sides of the road are littered with corpses of the careless

Exercises

2.1. **Dirac delta function, Lorentzian representation.**
Derive the representation

$$\delta(E - E_n) = - \lim_{\epsilon \to +0} \frac{1}{\pi} \operatorname{Im} \frac{1}{E - E_n + i\epsilon} \qquad (2.38)$$

of a delta function as imaginary part of $1/x$.

(Hint: read up on principal parts, positive and negative frequency part of the delta function, the Cauchy theorem in a good quantum mechanics textbook).

2.2. **Green's function.** Verify Green's function Laplace transform (2.13),

$$\begin{aligned} G(q, q', E + i\varepsilon) &= \frac{1}{i\hbar} \int_0^\infty dt \, e^{\frac{i}{\hbar}Et - \frac{\varepsilon}{\hbar}t} K(q, q', t) \\ &= \sum \frac{\phi_n(q)\phi_n^*(q')}{E - E_n + i\varepsilon}, \end{aligned}$$

argue that positive ϵ is needed (hint: read a good quantum mechanics textbook).

2.3. **Scalar field propagator.** [M. Srednicki, Quantum Field Theory, Part I arXiv:hep-th/0409035, problem 8.2]

Starting with

$$\Delta(x - x') = \int \frac{d^4k}{(2\pi)^4} \frac{e^{ik(x-x')}}{k^2 + m^2 - i\epsilon}, \qquad (2.39)$$

verify

$$\begin{aligned} \Delta(x - x') &= i \int \tilde{d}k \, e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}') - i\omega|t-t'|} \qquad (2.40) \\ &= i\theta(t - t') \int \tilde{d}k \, e^{ik(x-x')} \\ &\quad + i\theta(t' - t) \int \tilde{d}k \, e^{-ik(x-x')}. \quad (2.41) \end{aligned}$$

There should be an i in eq. (2.40).

2.4. **Quantum mechanical path integrals.**

Consider a particle moving in one dimension with separable Hamiltonian:

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

If the particle is at a position q at time $t = 0$, what is the probability amplitude that it will be at position q' at a later time $t = T$?

a) Show that the propagator from the initial spacetime point $(q, 0)$ to the final point (q', T) is

$$A = \langle q' | \psi(T) \rangle \equiv K(q', T; q, 0) = \langle q' | e^{-iHT} | q \rangle \quad (2.42)$$

(set $\hbar$ to 1 throughout).

b) Split the time evolution into two intervals $T = (T - t_1) + t_1$, show that the amplitude can be written as

$$A = \int dq_1 \, K(q', T; q_1, t_1) K(q_1, t_1; q, 0) \,. \quad (2.43)$$

c) Split the time interval T into a large number N of short time intervals of duration $\epsilon = T/N$:

$$A = \langle q' | \left(e^{-iH\epsilon} \right)^N | q \rangle = \langle q' | \underbrace{e^{-iH\epsilon} e^{-iH\epsilon} \cdots e^{-iH\epsilon}}_{N \text{ times}} | q \rangle \,,$$

and show that the amplitude can be written as the sum over the amplitudes of all possible N-segment paths,

$$A = \sum_{\text{paths}} A_{\text{path}} \,,$$

where

$$\sum_{\text{paths}} = \int dq_1 \cdots dq_{N-1} \,,$$

$$A_{\text{path}} = K_{q_N, q_{N-1}} K_{q_{N-1}, q_{N-2}} \cdots K_{q_2, q_1} K_{q_1, q_0} \,.$$

d) Show that the short-time propagator for one subinterval is given by

$$K_{q_{j+1}, q_j} = \int \frac{dp_j}{2\pi} e^{ip_j(q_{j+1} - q_j)} e^{-i\epsilon H(p_j, \bar{q}_j)} (1 + o(\epsilon^2)) \,, \quad (2.44)$$

where $\bar{q}_j = \frac{1}{2}(q_j + q_{j+1})$.

e) Combine N such factors, show that to the order of $o(\epsilon^2)$ the amplitude of a path is

$$A_{\text{path}} = \int \prod_{j=0}^{N-1} \frac{dp_j}{2\pi} \exp i\epsilon \sum_{j=0}^{N-1} (p_j \dot{q}_j - H(p_j, \bar{q}_j)) \,. \quad (2.45)$$

f) Show that the propagator is given by

$$K = \int \prod_{j=1}^{N-1} dq_j \int \prod_{j=0}^{N-1} \frac{dp_j}{2\pi} \exp i\epsilon \sum_{j=0}^{N-1} (p_j \dot{q}_j - H(p_j, \bar{q}_j)) \quad (2.46)$$

with one momentum integral for each segment (N total), and one position integral for each intermediate position ($N - 1$ total). In the $N \to \infty$ limit, this is a *phase-space path integral* integral over all functions $p(t)$, $q(t)$:

$$K \equiv \int \mathcal{D}p(t) \mathcal{D}q(t) \exp i \int_0^T dt \, (p\dot{q} - H(p, q)) \,, \quad (2.47)$$

with fixed ends $q(0) = q$, $q(T) = q'$.

g) Show that if the Hamiltonian is separable, $H = p^2/2m + V(q)$, one can carry out the momentum integrals in (2.46), and the propagator becomes

$$\begin{aligned}
K &= \int \prod_{j=1}^{N-1} dq_j \exp -i\epsilon \sum_{j=0}^{N-1} V(\bar{q}_j) \prod_{j=0}^{N-1} \left(\sqrt{\frac{m}{2\pi i\epsilon}} \exp i\epsilon \frac{m\dot{q}_j^2}{2} \right) \\
&= \left(\frac{m}{2\pi i\epsilon} \right)^{N/2} \int \prod_{j=1}^{N-1} dq_j \exp i\epsilon \sum_{j=0}^{N-1} \left(\frac{m\dot{q}_j^2}{2} - V(\bar{q}_j) \right) \,. (2.48)
\end{aligned}$$

The argument of the exponential is the action of a path passing through the points $q_0 = q, q_1, \cdots, q_{N-1}, q_N = q'$. This is the *configuration space path integral*

$$K = \int \mathcal{D}q(t) e^{iS[q(t)]} \,. \quad (2.49)$$

Chapter 3

Generating functionals

See P. Cvitanović [1] *Field theory*, chapter 2. *Generating functionals*, yours for a click here.

References

[1] P. Cvitanović, *Field Theory*, Notes prepared by E. Gyldenkerne (Nordita, Copenhagen, 1983).

Exercises

3.1. **2.B.1 Continuous indices (self energy for QCD).**
The numbers refer to exercises in P. Cvitanović [1] *Field theory*, chapter 2. *Generating functionals* (click here).

3.2. **2.D.1 Combinatoric weights.**

3.3. **2.E.1 Functional derivatives.**

3.4. **2.E.2 Feynman rules.**

3.5. **2.E.3 Zero-dimensional field theory.**

Chapter 4

Path integrals

See P. Cvitanović [2] *Field theory*, chapter 3. *Path integrals*, yours for a click here. The rest of this chapter are notes on some related literature, safely ignored.

4.1 Bell polynomials

[2018-12-22 Predrag] Fiol, Martínez-Montoya and Fukelman [3], *Wilson loops in terms of color invariants* (2018), note in passing that the power series for the logarithm of the full $\langle W \rangle$ (the connected $\ln \langle W \rangle$ partition function) can be in terms of partial Bell polynomials $B_{n,k}$ (I do not remember ever seeing this formula). Defining $f_k = d_R^{a_1 a_1 \dots a_k a_k}/N_R$

$$\ln \langle W \rangle = \sum_{k=1}^{\infty} \frac{g^k}{k!} \sum_{j=1}^{k} (-1)^{j-1}(j-1)! B_{k,j}(f_1, f_2, \dots, f_{k-j+1}) \tag{4.1}$$

This expression for $\ln \langle W \rangle$ is, however, extremely inefficient, and obscures the fact that the perturbative expansion of $\ln \langle W \rangle$ is simpler than that of $\langle W \rangle$.

More useful, perhaps, is the 1927 Ursell function (see wiki). For other applications of cumulants, see ChaosBook remark A20.1.

4.2 Legendre transforms

In Cvitanović [2] *Field theory*, chapter 2. Generating functionals, the Legendre transform eq. (2.28) comes out for free, just by looking at the 1PI subset of the connected graphs (that's why $\Gamma[\phi]$ comes out with the same sign as $\Gamma[\phi]$, unlike the Hamiltonian / Lagrangian relation in classical mechanics).

Here is some, mostly undigested reading on the *meaning* of Legendre transforms.

Probably the most pedagogical exposition is Zia, Redish and McKay [4] *Making sense of the Legendre transform*. I have also found enjoyable several posts by Baez, starting with Classical Mechanics versus Thermodynamics: "It seems this whole subject is a monument of austere beauty... covered with minus signs, like bird droppings." He writes:

If we fix the temperature T and volume V, the system will choose a state that minimizes the Helmholtz free energy A(T,V).

If we fix the temperature T and pressure P, the system will choose a state that minimizes the Gibbs free energy G(T,P).

Consider the cotangent bundle T^*Q, which has local coordinates q^i (coming from the coordinates on Q) and p_i (the corresponding coordinates on each cotangent space). We then call p_i the conjugate variable of the coordinate q^i.

Note that this is a unified picture, it avoids the most common approaches to classical mechanics, which start with either a 'Hamiltonian'

$$H : T^*Q \to \mathbb{R}$$

or a 'Lagrangian'

$$L : TQ \to \mathbb{R}$$

Instead, we started with Hamilton's principal function

$$S : Q \to \mathbb{R}$$

where Q is not the usual configuration space describing possible positions for a particle, but the 'extended' configuration space, which also includes time. Only this way do Hamilton's equations, like the Maxwell relations, become a trivial consequence of the fact that partial derivatives commute."

Back to my Field Theory book: I present Legendre and Fourier transforms as totally distinct functional transformations; Fourier as a multiplication by a matrix, and Legendre as a subset and (recursive) additions to it. Still, I explain that path integrals / generating functionals are "Fourier" or "Laplace" transforms of each other, and in the process of understanding that, one gets that the Legendre transform of $W[J]$, so they are the same transformation in some sense. That is discussed by Markus Deserno in his Legendre Transforms lecture notes. For my taste he is a bit too taken by "How much information is contained in a function?" but the sect. B. *Relation to Laplace transforms and partition functions* is of interest to us; Legendre transform emerges from a Laplace saddle point calculation. In stackexchange Qmechanic says the same thing: "the Legendre transformation can be e.g. seen as the leading classical tree-level formula of a formal semiclassical Fourier transformation." Read also Dan Piponi.

In the same stackexchange Domino Valdano puts it this way: "The mathematical relationship between Fourier and Legendre conjugates is somewhat analogous to the relationship between Lie groups and Lie algebras."

4.3   Complex actions

[2022-11-01 Predrag] Alexanian, MacKenzie, Paranjape and Ruel [1] *Problems with complex actions* (2007), consider Euclidean functional integrals involving complex actions. In this case there do not exist critical points of the action on the space of real fields. The proper definition of the function integral then requires the analytic continuation of the functional integration into the space of complex fields so as to pass through the complex critical points according to the method of steepest descent.

References

[1]   G. Alexanian, R. MacKenzie, M. B. Paranjape, and J. Ruel, "Problems with complex actions", Can. J. Phys. **85**, 699–705 (2007).

[2]   P. Cvitanović, *Field Theory*, Notes prepared by E. Gyldenkerne (Nordita, Copenhagen, 1983).

[3]   B. Fiol, J. Martínez-Montoya, and A. Rios Fukelman, "Wilson loops in terms of color invariants", J. High Energy Phys. **2019**, 202 (2019).

[4]   R. K. P. Zia, E. F. Redish, and S. R. McKay, "Making sense of the Legendre transform", Am. J. Phys **77**, 614–622 (2009).

Exercises

4.1. **3.B.1 Gaussian integrals for complex field.**

The numbers refer to exercises in P. Cvitanović [2] *Field theory*, chapter 3. *Path integrals* (click here).

4.2. **3.C.1 Wick expansion.**

4.3. **3.C.2 Counting QED diagrams.**

4.4. **3.F.3 Counting QED diagrams.**

Chapter 5

Field theory path integrals

The path integral (2.35) is an ordinary multi-dimensional integral. In the classical $\hbar \to 0$, the action is large (high price of straying from the beaten path) almost everywhere, except for some localized regions of the q-space. Highly idealized, the action looks something like the sketch in figure 5.1 (in order to be able to draw this on a piece of paper, we have suppressed a large number of q_ℓ coordinates).

Such integral is dominated by the minima of the action. The minimum value $S[q]$ states q^c are determined by the zero-slope, saddle-point condition

$$\frac{d}{d\phi_\ell} S[q^c] + J_\ell = 0.$$
(5.1)

The term "saddle" refers to the general technique of evaluating such integrals for complex q; in the statistical mechanics applications q^c are locations of the minima of $S[q]$, not the saddles. If there is a number of minima, only the one (or the n_c minima related by a discrete symmetry) with the lowest value of $-S[q^c] - q^c \cdot J$ dominates the path integral in the low temperature limit. The zeroth order, classical approximation to the partition sum (2.35) is given by the extremal state alone

$$Z[J] = e^{W[J]} \to \sum_c e^{W_c[J]} = e^{W_c[J] + \ln n_c}$$

$$W_c[J] = S[q^c] + q^c \cdot J.$$
(5.2)
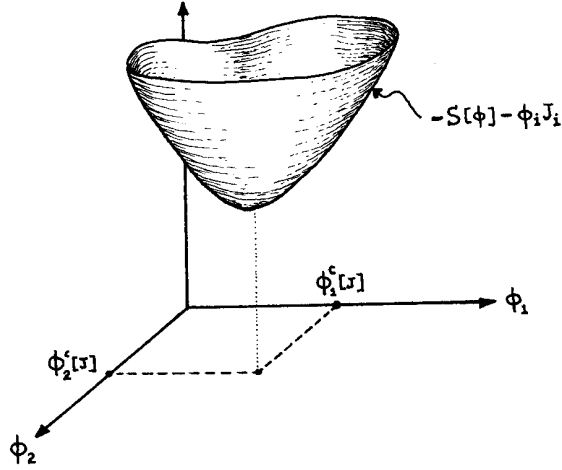
Figure 5.1: In the classical $\hbar \to 0$ limit (or the low temperature $T = 1/\beta$ limit) the path integral (5.8) is dominated by the minima of the integrand's exponent. The location ϕ^c of a minimum is determined by the extremum condition $\partial_\ell S[\phi^c] + J_\ell = 0$
.

In the *saddlepoint approximation* the corrections due to the fluctuations in the q^c neighborhood are obtained by shifting the origin of integration to

$$q_\ell \to q^c{}_\ell + q_\ell \,,$$

the position of the c-th minimum of $S[q] - q \cdot J$, and expanding $S[q]$ in a Taylor series around q^c.

For our purposes it will be convenient to separate out the quadratic part $S_0[q]$, and collect all terms higher than bilinear in q into an "interaction" term $S_I[q]$

$$
\begin{aligned}
S_0[q] &= -\sum_\ell q_\ell \left(M^{-1}\right)_{\ell\ell'} q_\ell \,, \\
S_I[q] &= -(\cdots)_{\ell\ell'\ell''} q_\ell q_{\ell'} q_{\ell''} + \cdots .
\end{aligned}
\tag{5.3}
$$

Rewrite the partition sum (2.35) as

$$e^{W[J]} = e^{W_c[J]} \int [dq]\, e^{-\frac{1}{2} q^\top \cdot M^{-1} \cdot q + S_I[q]} \,.$$

As the expectation value of any analytic function

$$f(q) = \sum f_{n_1 n_2 \ldots} q_1^{n_1} q_2^{n_2} \cdots / n_1! n_2! \cdots$$

can be recast in terms of derivatives with respect to J

$$\int [dq]\, f[q] e^{-\frac{1}{2} q^\top \cdot M^{-1} \cdot q} = f\left[\tfrac{d}{dJ}\right] \int [dq]\, e^{-\frac{1}{2} q^\top \cdot M^{-1} \cdot q + q \cdot J}\Big|_{J=0} \,,$$

we can move $S_I[q]$ outside of the integration, and evaluate the Gaussian integral in the usual way

$$
\begin{aligned}
e^{W[J]} &= e^{W_c[J]} e^{S_I[\frac{d}{dJ}]} \int [dq]\, e^{-\frac{1}{2} q^\top \cdot M^{-1} \cdot q + q \cdot J}\Big|_{J=0} \\
&= |\det M|^{\frac{1}{2}}\, e^{W_c[J]} e^{S_I[\frac{d}{dJ}]} e^{\frac{1}{2} J^\top \cdot M \cdot J}\Big|_{J=0} .
\end{aligned}
\tag{5.4}
$$

M is invertible only if the minima in figure 5.1 are isolated, and M^{-1} has no zero eigenvalues. The marginal case would require going beyond the Gaussian saddlepoints studied here, typically to the Airy-function type stationary points [1].

In the classical statistical mechanics $S[q]$ is a real-valued function, the extremum of $S[q]$ at the saddlepoint q^c is the minimum, all eigenvalues of M are strictly positive, and we can drop the absolute value brackets $|\cdots|$ in (5.4).

Expanding the exponentials and evaluating the $\frac{d}{dJ}$ derivatives in (5.4) yields the fluctuation corrections as a power series in $1/\beta = T$.

The first correction due to the fluctuations in the q^c neighborhood is obtained by approximating the bottom of the potential in figure 5.1 by a parabola, i.e., keeping only the quadratic terms in the Taylor expansion (5.3).

5.1   Field theory - setting up the notation

The partition sum for a lattice field theory defined by a Hamiltonian $\mathcal{H}[\phi]$ is

$$
\begin{aligned}
Z[J] &= \int [d\phi] e^{-\beta(\mathcal{H}[\phi] - \phi \cdot J)} \\
[d\phi] &= \frac{d\phi_1}{\sqrt{2\pi}} \frac{d\phi_2}{\sqrt{2\pi}} \cdots,
\end{aligned}
$$

where $\beta = 1/T$ is the inverse temperature, and J_ℓ is an external probe that we can twiddle at will site-by-site. For a theory of the Landau type the Hamiltonian

$$
\mathcal{H}_L[\phi] = \frac{r}{2}\phi_\ell\phi_\ell + \frac{c}{2}\partial_\mu\phi_\ell\partial_\mu\phi_\ell + u\sum_{\ell=1}^{N^d}\phi_\ell^4 \tag{5.5}
$$

is translationally invariant. Unless stated otherwise, we shall assume the repeated index summation convention throughout. We find it convenient to bury now some factors of $\sqrt{2\pi}$ into the definition of $Z[J]$ so they do not plague us later on when we start evaluating Gaussian integrals. Rescaling $\phi \to (\text{const})\phi$ changes $[d\phi] \to (\text{const})^N[d\phi]$, a constant prefactor in $Z[J]$ which has no effect on averages. Hence we can get rid of one of the Landau parameters r, u, and c by rescaling. The accepted *normalization convention* is to set the gradient term to $\frac{1}{2}(\partial\phi)^2$ by $J \to c^{1/2}J$, $\phi \to c^{-1/2}\phi$, and the $\mathcal{H}_L$ in (5.5) is replaced by

$$
\begin{aligned}
\mathcal{H}[\phi] &= \frac{1}{2}\partial_\mu\phi_\ell\partial_\mu\phi_\ell + \frac{m_0^2}{2}\phi_\ell\phi_\ell + \frac{g_0}{4!}\sum_\ell \phi_\ell^4 \\
m_0^2 &= \frac{r}{c}, \qquad g_0 = 4!\frac{u}{c^2}.
\end{aligned} \tag{5.6}
$$

Dragging factors of β around is also a nuisance, so we absorb them by defining the *action* and the *sources* as

$$
S[\phi] = -\beta\mathcal{H}[\phi], \qquad J_\ell = \beta J_\ell.
$$

The actions we learn to handle here are of form

$$
\begin{aligned}
S[\phi] &= -\frac{1}{2}(M^{-1})_{\ell\ell'}\phi_\ell\phi_{\ell'} + S_I[\phi], \\
S_I[\phi] &= \frac{1}{3!}\gamma_{\ell_1\ell_2\ell_3}\,\phi_{\ell_1}\phi_{\ell_2}\phi_{\ell_3} + \frac{1}{4!}\gamma_{\ell_1\ell_2\ell_3\ell_4}\,\phi_{\ell_1}\phi_{\ell_2}\phi_{\ell_3}\phi_{\ell_4} + \cdots.
\end{aligned} \tag{5.7}
$$

Why we chose such awkward notation M^{-1} for the matrix of coefficients of the $\phi_\ell\phi_{\ell'}$ term will become clear in due course (or you can take a peak at (5.12) now).

Our task is to compute the partition function $Z[J]$, the "free energy" $W[J]$, and the full n-point correlation functions

$$
\begin{aligned}
Z[J] &= e^{W[J]} = \int [d\phi] e^{S[\phi] + \phi \cdot J} \qquad\qquad (5.8)\\[4pt]
&= Z[0]\left(1 + \sum_{n=1}^{\infty} \sum_{\ell_1 \ell_2 \cdots \ell_n} G_{\ell_1 \ell_2 \cdots \ell_n} \frac{J_{\ell_1} J_{\ell_2} \ldots J_{\ell_n}}{n!}\right),\\[4pt]
G_{\ell_1 \ell_2 \cdots \ell_n} &= \langle \phi_{\ell_1} \phi_{\ell_2} \ldots \phi_{\ell_n} \rangle = \frac{1}{Z[0]} \frac{d}{dJ_{\ell_1}} \cdots \frac{d}{dJ_{\ell_n}} Z[J]\bigg|_{J=0}. \qquad (5.9)
\end{aligned}
$$

The "bare mass" m_0 and the "bare coupling" g_0 in (5.6) parameterize the relative strengths of quadratic, quartic fields at a lattice point vs. contribution from spatial variation among neighboring sites. They are called "bare" as the 2- and 4-point couplings measured in experiments are "dressed" by fluctuation contributions.

The action of discretized ϕ^4-theory can be written as

$$
S[\phi] = \sum_x a^d \left\{ \frac{1}{2} \sum_{\mu=1}^{4} (\partial_\mu \phi(x))^2 + \frac{m_0^2}{2} \phi(x)^2 + \frac{g_0}{4!} \phi(x)^4 \right\}.
$$

One usually starts with a finite hypercubic lattice with length $L_1 = L_2 = L_3 = L$ in every spatial direction and length $L_4 = T$ in Euclidean time,

$$
x_\mu = a n_\mu, \qquad n_\mu = 0, 1, 2, \ldots, L_\mu - 1,
$$

with finite volume $V = L^3 T$. A popular finite volume boundary conditions are periodic boundary conditions

$$
\phi(x) = \phi(x + a L_\mu \hat{n}_\mu),
$$

where $\hat{n}_\mu$ is the unit vector in the μ-direction.

In order to get rid of some of the lattice indices it is convenient to employ vector notation for the terms bilinear in ϕ, and keep the rest lumped into "interaction,"

$$
S[\phi] = -\frac{m^2}{2} \phi^\top \cdot \phi - \frac{C}{2} \left[(d_\mu - \mathbf{1}) \phi \right]^\top \cdot (d_\mu - \mathbf{1}) \phi + S_I[\phi]. \qquad (5.10)
$$

For example, for the discretized Landau Hamiltonian $m^2/2 = \beta m_0^2/2$, $C = \beta/a^2$, and the quartic term $S_I[\phi]$ is local site-by-site,

$$
\gamma_{\ell_1 \ell_2 \ell_3 \ell_4} = -4! \beta u \, \delta_{\ell_1 \ell_2} \delta_{\ell_2 \ell_3} \delta_{\ell_3 \ell_4},
$$

so this general quartic coupling is a little bit of an overkill, but by the time we get to the Fourier-transformed theory, it will make sense as a momentum conserving vertex (1.78).

Consider the action

$$
S[d\phi] = -\frac{1}{2} \phi^\top \cdot d^\top M^{-1} d \cdot \phi - \frac{\beta g_0}{4!} \sum_{\ell=1}^{N^d} (d\phi)_\ell^4.
$$

As M^{-1} is constructed from d and its inverse, M^{-1} and d commute, and the bilinear term is d invariant. In the quartic term d permutes cyclically the terms in the sum. The total action is translationally invariant

$$S[d\phi] = S[\phi] = -\frac{1}{2}\phi^\top \cdot M^{-1} \cdot \phi - \frac{\beta g_0}{4!} \sum_{\ell=1}^{N^d} \phi_\ell^4 \,. \tag{5.11}$$

5.2 Free propagation

In many field theory textbooks much time is spent on 'non-interacting fields', 'free propagation', etc... Attempts to 'derive' quantum mechanics from deeper principles often do not ever get to 'interacting fields'. Why is that?

Mathematical physics equals three tricks: 1) Gaussian integral, 2) integration by parts, and 3) (your own more sophisticated trick). As we shall now see, 1) suffices to solve free field theories.

5.3 Free field theory

There are field theory courses in which months pass while free non-interacting fields are beaten to pulp. This text is an exception, but even so we get our first glimpse of the theory by starting with no interactions, $S_I[\phi] = 0$. The free-field partition function (which sometimes ekes living under the name "Gaussian model") is

$$Z_0[J] = e^{W_0[J]} = \int [d\phi]e^{-\frac{1}{2}\phi^\top \cdot M^{-1} \cdot \phi + \phi \cdot J} = |\det M|^{\frac{1}{2}} e^{\frac{1}{2}J^\top \cdot M \cdot J}$$

$$W_0[J] = \frac{1}{2}J^\top \cdot M \cdot J + \frac{1}{2}\text{tr} \ln M \,. \tag{5.12}$$

The full n-point correlation functions (5.9) vanish for n odd, and for n even they are given by products of distinct combinations of 2-point correlations

$$G_{\ell\ell'} = (M)_{\ell\ell'}$$
$$G_{\ell_1\ell_2\ell_3\ell_4} = (M)_{\ell_1\ell_2}(M)_{\ell_3\ell_4} + (M)_{\ell_1\ell_3}(M)_{\ell_2\ell_4} + (M)_{\ell_1\ell_4}(M)_{\ell_2\ell_3}$$
$$G_{\ell_1\ell_2\cdots\ell_n} = (M)_{\ell_1\ell_2}\cdots(M)_{\ell_{n-1}\ell_n} + (M)_{\ell_1\ell_3}\cdots(M)_{\ell_{n-1}\ell_n} + \cdots \tag{5.13}$$

Keeping track of all these dummy indices (and especially when they turn into a zoo of of continuous coordinates and discrete indices) is a pain, and it is much easier to visualize this diagrammatically. Defining the propagator as a line connecting 2 lattice sites, and the probe J_ℓ as a source/sink from which a single line can originate

$$(M)_{\ell_1\ell_2} = \ell_1 \, \bullet\!\!-\!\!\bullet \, \ell_2 \,, \qquad J_\ell = \, \bullet\!\!-\!\!\circ \, \ell \,, \tag{5.14}$$

we expand the free-field theory partition function (5.12) as a Taylor series in $J^\top \cdot M^{-1} \cdot J$

$$\frac{Z_0[J]}{Z_0[0]} = 1 + \frac{1}{2}\circ\!\!-\!\!\circ + \frac{1}{2^3}\,\Big)\Big(+ \frac{1}{2^3}\frac{1}{3!}\,\Big)\Big(\Big) + \cdots \,. \tag{5.15}$$

In the diagrammatic notation the non-vanishing n-point correlations (5.13) are drawn as

$$G_{\varrho\varrho'} = \varrho \bullet\!\!-\!\!\bullet \varrho'$$

$$G_{\varrho_1\varrho_2\varrho_3\varrho_4} = \quad + \, \mathsf{X} + \,\smile\!\!\frown$$

$$G_{\varrho_1\varrho_2\varrho_3\varrho_4\varrho_5\varrho_6} = \quad + \mathsf{X}\,\mathsf{I} + \,\smile\!\!\frown\,\mathsf{I} + (11 \text{ terms}). \qquad (5.16)$$

The total number of distinct terms contributing to the noninteracting full n-point correlation is $1 \cdot 3 \cdot 5 \cdots (n-1) = (n-1)!!$, the number of ways that n source terms J can be paired into $n/2$ pairs M.

5.4 Feynman diagrams

For field theories defined at more than a single point the perturbative corrections can be visualized by means of Feynman diagrams. It is not clear that this is the intelligent way to proceed [4], as both the number of Feynman diagrams and the difficulty of their evaluation explodes combinatorially, but as most physicist stop at a 1-loop correction, for the purpose at hand this is a perfectly sensible way to proceed.

5.4.1 Hungry pac-men munching on fattened J's

The saddle-point expansion is most conveniently evaluated in terms of Feynman diagrams, which we now introduce. Expand both exponentials in (5.29)

$$e^{S_I[\frac{d}{dJ}]} e^{\frac{1}{2}J^\top \cdot M \cdot J} = \left\{ 1 + \frac{1}{4!}\mathsf{X} + \frac{1}{2}\frac{1}{(4!)^2}\mathsf{X}\,\mathsf{X} + \cdots \right\}$$

$$\times \left\{ 1 + \frac{1}{2}\circ\!\!-\!\!\circ + \frac{1}{2^2} \,\mathsf{II} + \frac{1}{2^3}\frac{1}{3!} \,\mathsf{III} + \cdots \right\} \qquad (5.17)$$

Here we have indicated $\frac{d}{dJ}$ as a pac-man that eats J, leaving a delta function in its wake

$$\frac{d}{dJ_j} J_\ell = \delta_{j\ell}$$

$$\overline{j}\,\mathcal{C}\!\circ\!\!-\!\!\circ_{\ell} = \overline{j \quad \ell}. \qquad (5.18)$$

For example, the rightmost pac-man in the $\sum_\ell (\frac{d}{dJ_\ell})^4$ interaction term quartic in derivative has four ways of munching a J from the free-field theory $\frac{1}{2}\left(\frac{1}{2}J^\top \cdot M \cdot J\right)^2$ term, the next pac-man has three J's to bite into in two distinct ways, and so forth:

$$\frac{1}{4!}\frac{1}{2^3}\mathsf{X}\,\mathsf{II} = \frac{1}{3!}\frac{1}{2^3}\mathsf{X}\,\mathsf{I} = \frac{1}{3!}\frac{1}{2^3}\left(\mathsf{X}\,\mathsf{I} + 2\,\mathsf{X}\right)$$

$$= \frac{1}{2^3}\,\mathsf{X} = \frac{1}{8}\,\infty. \qquad (5.19)$$

In field theory textbooks this process of tying together vertices by propagators is called the *Wick expansion*. Professionals have smarter ways of generating Feynman diagrams [3], but this will do for the problem at hand.

It is easy enough to prove this to all orders, but to this order you can simply check by expanding the exponential (5.8) that the free energy $W[J]$ perturbative corrections are the connected, diagrams with $J = 0$

$$W[0] = S[\phi^c] + \frac{1}{2}\text{tr}\,\ln M + \frac{1}{8}\,\infty + \frac{1}{16}\,\infty\infty + \frac{1}{48}\,\bigotimes. \qquad (5.20)$$

According to its definition, every propagator line M connecting two vertices carries a factor of $T = 1/\beta$, and every vertex a factor of $1/T$. In the ϕ^4 theory the diagram with n vertices contributes to the order T^n of the perturbation theory. In quantum theory, the corresponding expansion parameter is $\hbar$.

To proceed, we have to make sense of the propagator M of sect. 5.1, and learn how to evaluate diagrammatic perturbative corrections.

5.5 Saddle-point expansions

Good. You know how to evaluate a Gaussian integral, and now you would like to master path integrals. What to do? Simple - turn path integrals into Gaussian integrals, as follows:

Laplace method deals with integrals of form

$$I = \int_{-\infty}^{\infty} dx\, e^{-t\Phi(x)} \qquad (5.21)$$

where t and $\Phi(x)$ are real. If $\Phi(x)$ is bounded from below and smooth at minimal value $\Phi(x^*)$, $\Phi'(x^*) = 0$, $\Phi''(x^*) > 0$, I is dominated by the value of the integrand at $\Phi(x^*)$. For large values of t the Laplace estimate is obtained by expanding $\Phi(x^* + \delta x)$ to second order in δx and evaluting the resulting Gaussian integral,

$$I \approx \sum_{x^*} \sqrt{2\pi/t\Phi''(x^*)}\, e^{-t\Phi(x^*)}. \qquad (5.22)$$

Generalization to multidimensional integrals is straightforward. The Gaussian integral in d-dimensions is given by

$$\int [dx]e^{-\frac{1}{2}x^{\top}\cdot M^{-1}\cdot x + x\cdot J} = (\det M)^{\frac{1}{2}}\, e^{\frac{1}{2}J^{\top}\cdot M\cdot J}, \qquad (5.23)$$

$$[dx] = \frac{dx_1}{\sqrt{2\pi}}\frac{dx_2}{\sqrt{2\pi}}\cdots\frac{dx_d}{\sqrt{2\pi}},$$

where M is a real symmetric positive definite matrix, i.e., matrix with strictly positive eigenvalues.

The stationary phase estimate of (5.21) is

$$I \approx \sum_{x^*} (2\pi/t)^{d/2}\, |\det \mathbf{D}^2\Phi(x^*)|^{-1/2} A(x_n)\, e^{t\Phi(x^*) - \frac{i\pi}{4}m(x^*)},$$

where x^* are the stationary phase points

$$\frac{d}{dx_i}\Phi(x)\bigg|_{x=x^*} = 0,$$

$\mathbf{D}^2\Phi(x^*)$ denotes the matrix of second derivatives, and $m(x^*)$ is the number of its negative eigenvalues (when evaluated at the stationary phase point x^*).

These integrals is all that is needed for the semiclassical approximation, with the proviso that M^{-1} in (5.23) has no zero eigenvalues. If it has, the integral is not damped in direction of the associated eigenvector, and higher orders in Taylor expansion of $\Phi(x^* + \delta x)$ need to be retained (see (7.4) on Airy integral).

The "path integral" (5.8) is an ordinary multi-dimensional integral. In the $\beta \to \infty$ limit, or the $T \to 0$ low temperature limit, the action is large (high price of straying from the beaten path) almost everywhere, except for some localized regions of the ϕ-space. Highly idealized, the action looks something like the sketch in figure 5.1 (in order to be able to draw this on a piece of paper, we have suppressed a large number of ϕ_ℓ coordinates).

Such integral is dominated by the minima of the action. The minimum value $S[\phi]$ states ϕ^c are determined by the zero-slope, saddle-point condition

$$\frac{d}{d\phi_\ell} S[\phi^c] + J_\ell = 0. \tag{5.24}$$

The term "saddle" refers to the general technique of evaluating such integrals for complex ϕ; in the statistical mechanics applications ϕ^c are locations of the minima of $S[\phi]$, not the saddles. If there is a number of minima, only the one (or the n_c minima related by a discrete symmetry) with the lowest value of $-S[\phi^c] - \phi^c \cdot J$ dominates the path integral in the low temperature limit. The zeroth order, mean field approximation to the partition sum (5.8) is given by the extremal state alone

$$\begin{aligned} Z[J] &= e^{W[J]} \to \sum_c e^{W_c[J]} = e^{W_c[J] + \ln n_c} \\ W_c[J] &= S[\phi^c] + \phi^c \cdot J . \end{aligned} \tag{5.25}$$

In the *saddle-point approximation* the corrections due to the fluctuations in the ϕ^c neighborhood are obtained by shifting the origin of integration to

$$\phi_\ell \to \phi^c_\ell + \phi_\ell,$$

the position of the cth minimum of $S[\phi] - \phi \cdot J$, and expanding $S[\phi]$ in a Taylor series around ϕ^c. For our purposes it will be convenient to separate out the quadratic part $S_0[\phi]$, and collect all terms higher than bilinear in ϕ into an "interaction" term $S_I[\phi]$

$$\begin{aligned} S_0[\phi] &= -\sum_\ell \phi_\ell \left(\frac{\beta r}{2c} + 12\frac{\beta u}{c^2}(\phi^c_\ell)^2 \right) \phi_\ell + \frac{\beta}{2} \sum_{\ell,\ell'} \phi_\ell \Delta_{\ell\ell'} \phi_{\ell'} , \\ S_I[\phi] &= -\frac{\beta u}{c^2} \sum_{\ell=1}^{N^d} \phi_\ell^4 . \end{aligned} \tag{5.26}$$

Spatially nonuniform ϕ^c_ℓ are conceivable. The *mean field theory* assumption is that the translational invariance of the lattice is not broken, and ϕ^c_ℓ is independent of the lattice point, $\phi^c_\ell \to \phi^c$. In the ϕ^4 theory considered here, it follows from (5.24) that $\phi^c = 0$ for $r > 0$, and $\phi^c = \pm\sqrt{|r|/4u}$ for $r < 0$. There are at most $n_c = 2$ distinct ϕ^c states with the same $S[\phi^c]$, and in the thermodynamic limit we

can neglect the "mean field entropy" $\ln n_c$ in (5.25) when computing free energy density per site[1],

$$-\beta f[J] = \lim_{N \to \infty} W[J]/N^d \,. \tag{5.27}$$

We collect the matrix of bilinear ϕ coefficients in

$$(M^{-1})_{\ell\ell'} = \beta m_0'^2 \delta_{\ell\ell'} - \beta c \Delta_{\ell\ell'} \,, \qquad m_0'^2 = m_0^2 + 12u(\phi^c)^2 \tag{5.28}$$

in order to be able to rewrite the partition sum (5.8) as

$$e^{W[J]} = e^{W_c[J]} \int [d\phi] e^{-\frac{1}{2}\phi^\top \cdot M^{-1} \cdot \phi + S_I[\phi]} \,.$$

As the expectation value of any analytic function

$$g(\phi) = \sum g_{n_1 n_2 \dots} \phi_1^{n_1} \phi_2^{n_2} \cdots /n_1! n_2! \cdots$$

can be recast in terms of derivatives with respect to J

$$\int [d\phi] g[\phi] e^{-\frac{1}{2}\phi^\top \cdot M^{-1} \cdot \phi} = g\left[\frac{d}{dJ}\right] \int [d\phi] e^{-\frac{1}{2}\phi^\top \cdot M^{-1} \cdot \phi + \phi \cdot J}\bigg|_{J=0} \,,$$

we can move $S_I[\phi]$ outside of the integration, and evaluate the Gaussian integral in the usual way, as in (5.4),

$$\begin{aligned} e^{W[J]} &= e^{W_c[J]} e^{S_I[\frac{d}{dJ}]} \int [d\phi] e^{-\frac{1}{2}\phi^\top \cdot M^{-1} \cdot \phi + \phi \cdot J}\bigg|_{J=0} \\ &= |\det M|^{\frac{1}{2}} e^{W_c[J]} e^{S_I[\frac{d}{dJ}]} e^{\frac{1}{2}J^\top \cdot M \cdot J}\bigg|_{J=0} \,. \end{aligned} \tag{5.29}$$

M is invertible only if the minima in figure 5.1 are isolated, and M^{-1} has no zero eigenvalues. The marginal case would require going beyond the Gaussian saddle-points studied here, typically to the Airy-function type stationary points [1]. In the classical statistical mechanics $S[\phi]$ is a real-valued function, the extremum of $S[\phi]$ at the saddle-point ϕ^c is the minimum, all eigenvalues of M are strictly positive, and we can drop the absolute value brackets $|\cdots|$ in (5.29).

As we shall show in sect. 5.4, expanding the exponentials and evaluating the $\frac{d}{dJ}$ derivatives in (5.29) yields the fluctuation corrections as a power series in $1/\beta = T$.

The first correction due to the fluctuations in the ϕ^c neighborhood is obtained by approximating the bottom of the potential in figure 5.1 by a parabola, i.e., keeping only the quadratic terms in the Taylor expansion (5.26). For a single minimum the "free energy" is in this approximation

$$W[J]_{\text{1-loop}} = W_c[J] + \frac{1}{2}\text{tr} \ln M \,, \tag{5.30}$$

where we have used the matrix identity $\ln \det M = \text{tr} \ln M$, valid for any finite-dimensional matrix. This result suffices to establish the Ginzburg criterion (explained in many excellent textbooks) which determines when the effect of fluctuations is comparable or larger than the mean-field contribution alone.

---

[1] For classically chaotic field theories we will not be so lucky - there the number of contributing saddles grows exponentially with the lattice size.

5.6 Saddle-point expansions are asymptotic

The first trial ground for testing our hunches about field theory is the *zero-dimensional field theory*, the field theory of a lattice consisting of one point. As there are no neighbors, there are no derivatives to take, and the field theory is a humble 1-dimensional integral

$$Z[J] = \int \frac{d\phi}{\sqrt{2\pi}} e^{-\frac{\phi^2}{2M} - \beta u\phi^4 + \phi J} .$$

In zero-dimensional field theory M is a [1×1] matrix, i.e. just a number. As it is in good taste to get rid of extraneous parameters, we rescale $\phi^2 \to M\phi^2$, $\sqrt{M}J \to J$, and are left with one parameter which we define to be $g = 4\beta M^2 u$. As multiplicative constants do not contribute to averages, we will drop an overall factor of $\sqrt{M}$ and study the integral

$$Z[J] = \int \frac{d\phi}{\sqrt{2\pi}} e^{-\phi^2/2 - g\phi^4/4 + \phi J} . \tag{5.31}$$

Substituting M as defined by (5.28) we have $g = T/(r + 12u(\phi^c)^2)$, so the small g expansions is a *low temperature* expansion. However, as we approach the critical temperature, $r + 12u(\phi^c)^2 \to 0$, the perturbation theory fails us badly, and that is one of the reasons why we need the renormalization theory.

The idea of the saddle-point expansion (5.29) is to keep the Gaussian part $\int d\phi\, e^{-\phi^2/2 + \phi J}$ as is, expand the rest as a power series, and then compute the moments

$$\int \frac{d\phi}{\sqrt{2\pi}} \phi^n e^{-\phi^2/2} = \left(\frac{d}{dJ}\right)^n e^{J^2/2}\bigg|_{J=0} = (n-1)!! \quad \text{if } n \text{ even, 0 otherwise} .$$

We already know the answer. In this zero-dimensional theory we have taken $M = 1$, the n-point correlation is simply the number of terms in the diagrammatic expansion, and according to (5.16) that number is exploding combinatorially, as $(n-1)!!$. And here our troubles start.

To be concrete, let us work out the *exact* zero-dimensional ϕ^4 field theory in the saddle-point expansion to all orders:

$$
\begin{aligned}
Z[0] &= \sum_n Z_n g^n , \\
Z_n &= \frac{(-1)^n}{n!4^n} \int \frac{d\phi}{\sqrt{2\pi}} \phi^{4n} e^{-\phi^2/2} = \frac{(-1)^n}{16^n n!} \frac{(4n)!}{(2n)!} .
\end{aligned}
\tag{5.32}
$$

The Stirling formula $n! = \sqrt{2\pi}\, n^{n+1/2} e^{-n}$ yields for large n

$$g^n Z_n \approx \frac{1}{\sqrt{n\pi}} \left(\frac{4gn}{e}\right)^n . \tag{5.33}$$

As the coefficients of the parameter g^n are blowing up combinatorially, no matter how small g might be, the perturbation expansion is not convergent! Why? Consider again (5.32). We have tacitly assumed that $g > 0$, but for $g < 0$, the potential is unbounded for large ϕ, and the integrand explodes. Hence the partition function in not analytic at the $g = 0$ point.

exercise 5.2

Sterling grows up

scalar ϕ^4 theory

@MathMatize
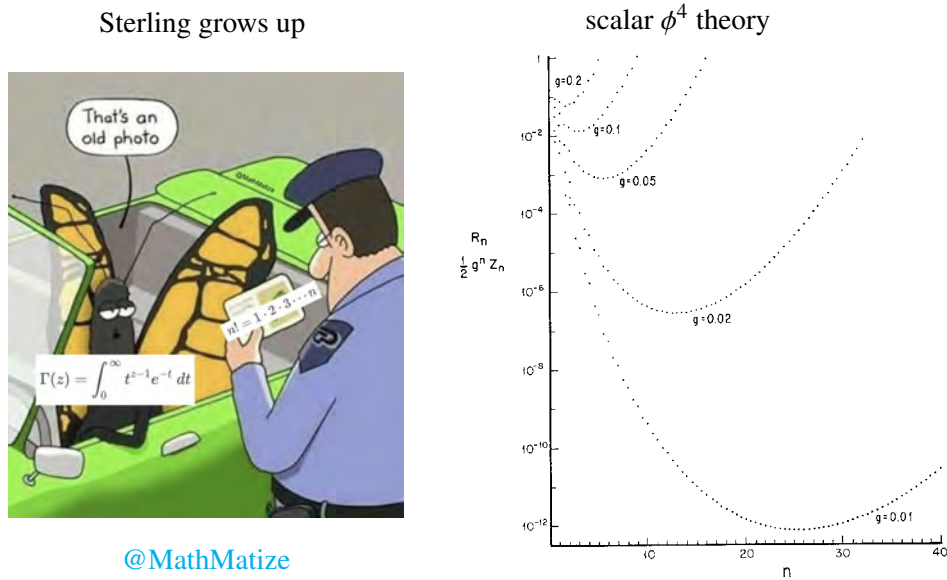
Figure 5.2: Plot of the saddle-point estimate of Z_n vs. the exact result (5.32) for $g = 0.2$, $g = 0.1$, $g = 0.05$, $g = 0.02$, $g = 0.01$.

Is the whole enterprise hopeless? As we shall now show, even though divergent, the perturbation series is an *asymptotic* expansion, and an asymptotic expansion can be extremely good [5]. Consider the residual error after inclusion of the first n perturbative corrections:

$$
\begin{aligned}
R_n &= \left| Z(g) - \sum_{m=0}^{n} g^m Z_m \right| \\
&= \int \frac{d\phi}{\sqrt{2\pi}} e^{-\phi^2/2} \left| e^{-g\phi^4/4} - \sum_{m=0}^{n} \frac{1}{m!} \left(-\frac{g}{4} \right)^m \phi^{4m} \right| \\
&\leq \int \frac{d\phi}{\sqrt{2\pi}} e^{-\phi^2/2} \frac{1}{(n+1)!} \left(\frac{g\phi^4}{4} \right)^{n+1} = g^{n+1} |Z_{n+1}| .
\end{aligned}
\tag{5.34}
$$

The inequality follows from the convexity of exponentials, a generalization of the inequality $e^x \geq 1 + x$. The error decreases as long as $g^n |Z_n|$ decreases. From (5.33) the minimum is reached at $4g\, n_{min} \approx 1$, with the minimum error

exercise 5.5

$$
g^n Z_n \big|_{min} \approx \sqrt{\frac{4g}{\pi}} \, e^{-1/4g} .
\tag{5.35}
$$

As illustrated by the figure 5.2, a perturbative expansion can be, for all practical purposes, very accurate. In QED such argument had led Dyson to suggest that the QED perturbation expansions are good to $n_{min} \approx 1/\alpha \approx 137$ terms. Due to the complicated relativistic, spinorial and gauge invariance structure of perturbative QED, there is not a shred of evidence that this is so. The very best calculations performed so far stop at $n \leq 5$.

Commentary

Remark 5.1. Gaussian integrals.   Kadanoff [6] has a nice discussion of Gaussian integrals, the central limit theorem and large deviations in *Chap. 3 Gaussian Distributions*, available online here.

Remark 5.2. Asymptotic series.

- The Taylor expansion in g fails, as g is precisely on the border of analyticity. The situation can sometimes be rescued by a *Borel re-summation*.

- If you really care, an asymptotic series can be improved by resumations "beyond all orders", a technically daunting task (see M. Berry's papers on such topics as re-summation of the Weyl series for quantum billiards).

- Pairs of nearby and coalescing saddles should be treated by uniform approximations, where the Airy integrals

$$Z_0[J] = \frac{1}{2\pi i} \int_C dx \, e^{-x^3/3! + Jx}$$

  play the role the Gaussian integrals play for isolated saddles [1]. In case at hand, the phase transition $\phi^c = 0 \to \pm\phi^c \neq 0$ is a quartic inflection of this type, and in the Fourier representation of the partition function one expects instead of $|\det M|^{1/2}$ explicit dependence on the momentum $k^{1/4}$. Whether anyone has tried to develop a theory of the critical regime in this way I do not know.

- If there are symmetries that relate terms in perturbation expansions, a perturbative series might be convergent. For example, individual Feynman diagrams in QED are not gauge invariant, only their sums are, and QED α^n expansions might still turn out to be convergent series [2].

- Expansions in which the field ϕ is replaced by N copies of the original field are called $1/N$ expansions. The perturbative coefficients in such expansions are convergent term by term in $1/N$.

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Exercises

5.1. **Free-field theory combinatorics.** Check that there indeed are no combinatorial prefactors in the expansion (5.16).

5.2. **Quality of asymptotic series.** Use the saddle-point method to evaluate Z_n

$$ Z_n = \frac{(-1)^n}{n! 4^n} \int \frac{d\phi}{\sqrt{2\pi}} \, e^{-\phi^2/2 + 4n \ln \phi} $$

Find the smallest error for a fixed g; plot both your error and the the exact result (5.32) for $g = 0.1$, $g = 0.02$, $g = 0.01$. The prettiest plot makes it into these notes as figure 5.2!

5.3. **Complex Gaussian integrals.** (A repeat of exercise 4.1.) Read sect. 3.B, do exercise 3.B.1 of ref. [3].

5.4. **Prove** $\ln \det = \operatorname{tr} \ln$**.** (link here the $\ln \det = \operatorname{tr} \ln$ problem sets, already done).

5.5. **Convexity of exponentials.** Prove the inequality (5.34). Matthias Eschrig suggest that a more general proof be offered, applicable to any monotone descreasing sequence with alternating signs.

5.6. **Wick expansion for ϕ^4 theories.** Derive (5.20), check the combinatorial signs.

5.7. **Wick expansions.** Read sect. 3.C and do exercise 3.C.2 of ref. [3].

Chapter 6

Chaotic field theory

We started out by laying down The Law (1). In *Field Theory* (1983) we arrived at it by going fishing: pulling out fishnets of Feynman diagrams (what pros call "iterating Dyson-Schwinger equations"). The action was split into 'kinetic' and 'potential' parts $S[\Phi] = -\frac{1}{2}\Phi^{\top}\Box\Phi + V[\Phi]$, with nonlinear, interaction terms collected into a local, site-wise z dependent potential

$$V[\Phi] = \sum_z V(\phi_z), \qquad V(\phi) = \frac{1}{2}\mu^2\phi^2 - \frac{g}{k!}\phi^k, \quad k \geq 3. \tag{6.1}$$

The lattice-discretized Laplacian is a sparse matrix, with neighbor-neighbor interaction given by matrix elements whose size is 1. A Feynman diagram expansion is then (for all practical purposes, see sect. 5.6) convergent, provided the interaction coupling constant or constants g are small, relative to 'kinetic' term.

At the opposite end, in the limit of very strong potentials, or the anti-integrability limit [2, 3], the interactions with neighbors is a small correction. That's best understood by another piece of classical, 19th century wave mechanics, the WKB approximation. That we here call deterministic field theory, with support of the partition sum restricted to the deterministic solutions Φ_c, only the configurations that strictly obey The Law,

$$Z[J]_c = e^{\Gamma[\Phi]+J\cdot\Phi} = \sum_c e^{S[\Phi_c]+J\cdot\Phi_c}. \tag{6.2}$$

harmonic field theory   chaotic field theory
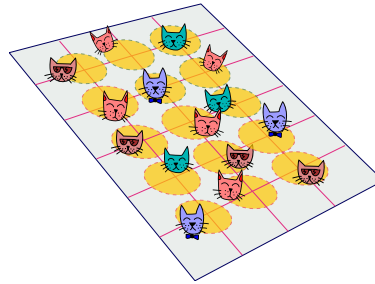
tight-binding model   Euclidean Klein-Gordon
(Helmholtz)   (damped Poisson)

Figure 6.1: (Color online)   The simplest of all chaotic field theories is the 'spatiotemporal cat', a deterministic Klein-Gordon field theory on a hypercubic lattice, with an unstable, "anti-harmonic" rotor at each lattice site, a cat that runs away rather than pushes back. In contrast to its elliptic sibling, the Helmholtz equation and its oscillatory solutions, spatiotemporal cat's periodic states are hyperbolic and unstable.

That, finally, puts us into the last quarter of 20th century: what one calls the 'chaos theory'.

When one refers to a physical phenomenon -such as motions of a Navier-Stokes fluid- as 'chaotic', or 'turbulent', one is told: We understand 'chaos' for a system such as Lorenz attractor, but what is a 'chaotic' field, a field with infinitely many degrees of freedom?

Our goal here is to answer this question pedagogically, as a sequence of pencil and paper calculations. We will explain what is 'deterministic chaos' by walking you through its simplest example, the coin toss or Bernoulli map, but reformulated as problem of determining admissible global solutions on an integer-time lattice.

What emerges is a spacetime which is very much like a big spring mattress, figure 6.1 (a), that obeys the familiar harmonic oscillator field theory equations, the discrete Helmholtz equation (or the tight-binding model), but instead of being 'springy', this metamaterial is a dicretization of the Euclidean Klein-Gordon equation, with a cat at every lattice site, that runs away, figure 6.1 (b), rather than pushing back, a theory formulated in terms of Hill determinants and zeta functions.

You might have gotten an impression that our field-theoretic formulation of spatiotemporal turbulence / chaos works only for Hamiltonian / Lagrangian systems, ie, for Euler, not Navier-Stokes. But our simplest example, the Bernoulli map, is a non-Hamiltonian dynamical system with infinite contraction ("dissipation") in one time step, and we have explored the '1d Navier-Stokes', ie., Kuramoto-Sivashinsky, in a great detail elsewhere (Matt Gudorf [17] and ChaosBook.org/overheads/spatiotemporal).

This is the simplest example of reformulating a space and time translationally invariant, exponentially unstable 'turbulent' field theory as a (D+1)-dimensional spatiotemporal system which treats space and time on equal footing. Here there is no 'evolution in time': there is only the determination of the repertoire of admissible tilings of spacetime by 'periodic orbits', very much as the partition function of the Ising model is a weighted sum formed by totality of its lattice states.
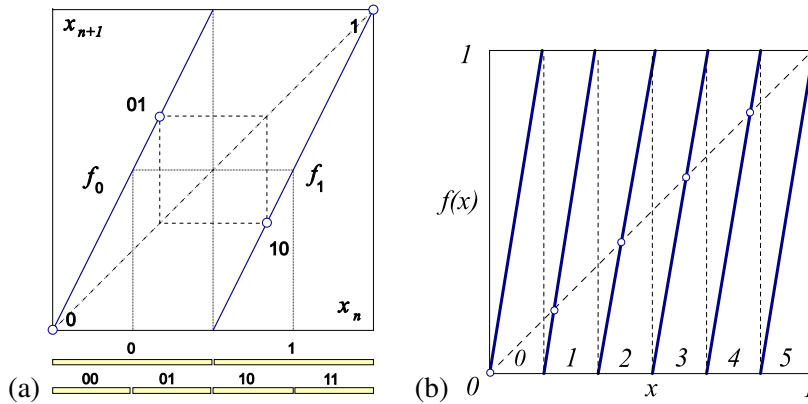
Figure 6.2: (Color online)   (a) The 'coin toss' map (6.3), together with the $\overline{0}$ fixed point, and the $\overline{01}$ 2-cycle. Preimages of the critical point $x_c = 1/2$ partition the unit interval into $\{\mathcal{M}_0, \mathcal{M}_1\}$, $\{\mathcal{M}_{00}, \mathcal{M}_{01}, \mathcal{M}_{10}, \mathcal{M}_{11}\}$, ..., subintervals. (b) The base-s Bernoulli map, here with the 'dice throw' stretching parameter $s = 6$, partitions the unit interval into 6 subintervals $\{\mathcal{M}_m\}$, labeled by the 6-letter alphabet (6.7). As the map is a circle map, $x_5 = 1 = 0 = x_0 \pmod 1$.

6.1   A fair coin toss

Remember? when we started this exposition with wanderings of a drunken snail (sect. 1.1), we generated all walks that build up the free propagator by assuming that the snail hops in all available directions with equal *probability* (1.1). In steps "chaos". Or "ergodicity". The Law is deterministic, and still we end up adding paths as though they were wanderings of a drunken snail.

The very simplest example of a deterministic law of evolution that gives rise to 'chaos' is the *Bernoulli* map, figure 6.2 (a), which models a coin toss. Starting with a random initial state, the map generates, deterministically, a sequence of tails and heads with 50-50% probability.

We introduce the model in its conventional, time-evolution dynamical formulation, than reformulate it as a lattice field theory, solved by determining all of admissible *periodic states*, field configurations that satisfy The Law (a global fixed point condition, really), and use this simple setting to illustrate (1) determination of periodic states from system's Euler–Lagrange equations, and (2) the evaluation of *Hill determinant*s, the stabilities of global solutions.

The base-2 *Bernoulli* shift map,

$$x_{t+1} = \begin{cases} f_0(x_t) = 2x_t\,, & x_t \in \mathcal{M}_0 = [0, 1/2) \\ f_1(x_t) = 2x_t \pmod 1\,, & x_t \in \mathcal{M}_1 = [1/2, 1) \end{cases}, \qquad (6.3)$$

is shown in figure 6.2 (a). If the linear part of such map has an integer-valued slope, or 'stretching' parameter $s \geq 2$,

$$x_{t+1} = s x_t \qquad (6.4)$$

that maps state x_t into a state outside the unit interval, the $\pmod 1$ operation results in the base-s Bernoulli circle map,

$$\phi_{t+1} = s\phi_t \pmod 1\,, \qquad (6.5)$$

sketched as a dice throw in figure 6.2 (b). The $\pmod 1$ operation subtracts $m_t = \lfloor s\phi_t \rfloor$, the integer part of $s\phi_t$, or the circle map *winding number*, to keep ϕ_{t+1} in

the unit interval $[0, 1)$, and partitions the unit interval into s subintervals $\{\mathcal{M}_m\}$,

$$\phi_{t+1} = s\phi_t - m_t, \qquad \phi_t \in \mathcal{M}_{m_t}, \tag{6.6}$$

where m_t takes values in the s-letter alphabet

$$m \in \mathcal{A} = \{0, 1, 2, \cdots, s-1\}. \tag{6.7}$$

The Bernoulli map is a highly instructive example of a hyperbolic dynamical system. Its symbolic dynamics is simple: the base-s expansion of the initial point ϕ_0 is also its temporal itinerary, with symbols from alphabet (6.7) indicating that at time t the orbit visits the subinterval $\mathcal{M}_{m_t}$. The map is a 'shift': a multiplication by s acts on the base-s representation of $\phi_0 = .m_1m_2m_3\cdots$ (for example, binary, if $s = 2$) by shifting its digits,

$$\phi_1 \quad = \quad f(\phi_0) = .m_2m_3\cdots. \tag{6.8}$$

Here we follow the 'future itinerary' labelling convention of ChaosBook sect. 14.6.

Periodic points can be counted by observing that the preimages of critical points $\{\phi_{c1}, \phi_{c2}, \cdots \phi_{c,s-1}\} = \{1/s, 2/s, \cdots, (s-1)/s\}$ partition the unit interval into s subintervals $\{\mathcal{M}_0, \mathcal{M}_1, \cdots, \mathcal{M}_{s-1}\}$, s^2 subintervals $\{\mathcal{M}_{m_1m_2}\}, \ldots, s^n$ subintervals, each containing *one* unstable period-n periodic point $\phi_{m_1m_2\cdots m_n}$, with stability multiplier s^n, see figure 6.2. The Bernoulli map is a full shift, in the sense that every itinerary is admissible, with one exception: on the circle, the rightmost fixed point is the same as the fixed point at the origin, $\phi_{s-1} = \phi_0 \pmod{1}$, so these fixed points are identified and counted as one, see figure 6.2. The total number of periodic points of period n is thus

$$N_n = s^n - 1. \tag{6.9}$$

6.2 Temporal Bernoulli

To motivate our formulation of a spatiotemporal deterministic field theory [11], we now recast the local initial value, time-evolution Bernoulli map problem as a *temporal lattice* fixed point condition, the problem of determining all global solutions.

'Temporal' here refers to the lattice site field ϕ_t and the source m_t taking their values on the lattice sites of a one-dimensional *temporal* integer lattice $t \in \mathbb{Z}$. Over a finite lattice segment, these can be written compactly as a *periodic state* and the corresponding *symbol block* (see sketch figure 1.1)

$$\Phi^\top = (\phi_{t+1}, \cdots, \phi_{t+n}), \quad \mathsf{M}^\top = (m_{t+1}, \cdots, m_{t+n}), \tag{6.10}$$

where $(\cdots)^\top$ denotes a transpose. The Bernoulli equation (6.6), rewritten as a first-order difference Euler–Lagrange equation

$$-\phi_{t+1} + (s\phi_t - m_t) = 0, \qquad \phi_t \in [0, 1), \tag{6.11}$$

takes the matrix form

$$\mathcal{J}\,\Phi - \mathsf{M} = 0, \qquad \mathcal{J} = -r + s\,\mathbb{1}, \tag{6.12}$$

where the $[n \times n]$ matrix

$$
r_{jk} = \delta_{j+1,k}, \qquad r = \begin{pmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & & \ddots & \\ & & & 0 & 1 \\ 1 & & & & 0 \end{pmatrix},
\tag{6.13}
$$

implements the shift operation (6.8), a cyclic permutation that translates forward-in-time periodic state Φ by one site, $(r\Phi)^\top = (\phi_2, \phi_3, \cdots, \phi_n, \phi_1)$. We refer to such local, lattice-site conditions as the Euler–Lagrange equations. The Euler–Lagrange equation (6.12) must be of the same form for all times, so the operator r has to be time-translation invariant, with $r_{n+1,n} = r_{1n} = 1$ matrix element enforcing its periodicity. After n shifts, a periodic state returns to the initial state,

$$
r^n = \mathbb{1}.
\tag{6.14}
$$

As the temporal Bernoulli condition (6.12) is a linear relation, a given block M, or 'code' in terms of alphabet (6.7), corresponds to a unique temporal periodic state Φ_M. That is why Percival and Vivaldi [20] refer to such symbol block M as a *linear code*. The temporal Bernoulli, however, is *not* a linear dynamical system figure 6.4. As illustrated by figure 6.2, it is a set of piecewise-linear s-stretching maps and their compositions, one for each state space region $\mathcal{M}_M$.

> System's Euler–Lagrange equations are the law everyone must obey: look at your left neighbor, right neighbor, remember who you were, make sure you fit in just right. The set $\{\Phi_c\}$ of all possible periodic states is system's 'Book of Life' - a catalogue of all possible 'lives', possible spatiotemporal patterns that the law allows, each life a *point* in system's infinite-dimensional state space, each life's likelihood given by its Hill determinant.

6.3   Determining periodic states

You might want to start here by computing period-2, period-3 periodic states by hand. You will then find the general case, eq. (6.17) easier.

As the temporal Bernoulli condition (6.12) is a linear relation, a given block M, or 'code' in terms of alphabet (6.7), corresponds to a unique temporal periodic state Φ given by the temporal lattice Green's function

$$
\Phi_M = g\,M, \qquad g = \frac{r/s}{\mathbb{1} - r/s}.
\tag{6.15}
$$

For an infinite lattice $t \in \mathbb{Z}$, this Green's function can be expanded as a series in

shited off-diagonals $(r/\Lambda)^k$,

$$
\mathsf{g} \;=\; \frac{r/\Lambda}{\mathbb{1} - r/\Lambda} = \sum_{k=1}^{\infty} \frac{r^k}{\Lambda^k}
$$

$$
= \begin{pmatrix}
0 & \Lambda^{-1} & \Lambda^{-2} & \Lambda^{-3} & \Lambda^{-4} & \Lambda^{-5} & \cdots \\
0 & 0 & \Lambda^{-1} & \Lambda^{-2} & \Lambda^{-3} & \Lambda^{-4} & \cdots \\
0 & 0 & 0 & \Lambda^{-1} & \Lambda^{-2} & \Lambda^{-3} & \cdots \\
0 & 0 & 0 & 0 & \ddots & & \\
0 & 0 & 0 & 0 & 0 & \Lambda^{-1} & \cdots \\
0 & 0 & 0 & 0 & 0 & 0 & \ddots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots
\end{pmatrix}, \tag{6.16}
$$

where $\Lambda = s$, the slope of the Bernoulli map figure 6.2, is the 1-time step stability multiplier for the Bernoulli system.

For a periodic state (6.10), the symbol block M repeats every n lattice sites, with an extra factor of $1/\Lambda^n$. Substituting $r^n = \mathbb{1}$ from (6.14) into (6.16), we can sum these prefactors as a geometric series, and obtain explicit formula for the field at any lattice site, as n-ary numbers in base $s = \Lambda$,

$$
\phi_0 = \frac{1}{1 - 1/\Lambda^n} \left(\frac{m_1}{\Lambda} + \frac{m_2}{\Lambda^2} + \cdots + \frac{m_{n-1}}{\Lambda^{n-1}} + \frac{m_n}{\Lambda^n} \right). \tag{6.17}
$$

For example, if $\Lambda = 2$ and $M = 011$, the corresponding lattice field is

$$
\phi_0 = \frac{8}{7} \left(\frac{1}{2} \cdot 0 + \frac{1}{4} \cdot 1 + \frac{1}{8} \cdot 1 \right) = \frac{1}{7} (2 + 1) = \frac{3}{7}.
$$

and the orbit $\mathcal{M}_M$ consists of the 3 translations / cyclic permutations $(\Phi_{011}, \Phi_{110}, \Phi_{101})$ of periodic state

$$
\Phi_{011} = \left(\frac{3}{7}, \frac{6}{7}, \frac{5}{7} \right).
$$

So we learn that the relation between finite-period periodic states and the ergodic periodic states is (her, for temporal Bernoulli, literally) like the relation between rational and real numbers: rationals have zero Lebesgue measure, but are dense in the unit interval, and serve as a perfectly fine marker to corsegrain the state space with.

6.4 Orbit stability

The Euler–Lagrange $F[\Phi_c] = 0$ condition turns out to be central to the theory of robust global methods for finding periodic states [5, 14, 16, 22–24]. One discretizes a periodic state into an n-sites temporal lattice configuration, and lists the field value at lattice sites

$$
\Phi^{\top} = (\phi_0, \phi_1, \cdots, \phi_{n-1}). \tag{6.18}
$$

Starting with an initial guess for Φ, a zero of the set of Euler–Lagrange equations $F[\Phi]_t = 0$, one per each lattice site t, can then be found by various methods [10,

12, 13, 18], for example, by Newton iteration, which requires an evaluation of the ▶
[$n \times n$] *orbit Jacobian matrix*

$$\mathcal{J}_{tt'} = \frac{\delta F[\Phi_c]_t}{\delta \phi_{t'}} \, . \tag{6.19}$$

The temporal Bernoulli Euler–Lagrange equation (6.12) can be viewed as a search for zeros of the vector of n functions

$$F[\Phi_M] = \mathcal{J}\Phi - M = 0 \tag{6.20}$$

$$\text{temporal Bernoulli:} \quad \mathcal{J} = -r + s\,\mathbb{1}, \tag{6.21}$$

with the entire periodic *periodic state* Φ_M treated as a single *point* $(\phi_0, \phi_1, \cdots, \phi_{n-1})$ in the n-dimensional state space unit hypercube $\Phi \in [0, 1)^n$.

For uniformly stretching systems, such as the temporal Bernoulli, [$n \times n$] orbit Jacobian matrix $\mathcal{J}$ (6.21) is a circulant, time-translation invariant matrix,

$$\mathcal{J} = \begin{pmatrix} s & -1 & 0 & 0 & \ldots & 0 & 0 \\ 0 & s & -1 & 0 & \ldots & 0 & 0 \\ 0 & 0 & s & -1 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \ldots & s & -1 \\ -1 & 0 & 0 & 0 & \ldots & 0 & s \end{pmatrix}, \tag{6.22}$$

While in classical mechanics matrices such as (6.19) are often called "Hessian", here we refer to them collectively as 'orbit Jacobian matrices', to emphasize that they describe the stability of any dynamical system, be it energy-conserving, or a dissipative system, with no Lagrangian formulation.

6.5 Hill determinants

Having shown that the inverse of Hill determinant $1/|\text{Det}\,\mathcal{J}_c|$ gives us the periodic state's probability weight in the deterministic partition function, our next task is to compute it. As we shall see in sect. 6.7.1, that is often best done on the reciprocal lattice. But first we show that on hypercubic lattices we can visualize a Hill determinant geometrically, as the volume of the associated fundamental parallelepiped.

6.5.1 Fundamental fact

Consider what the temporal Bernoulli Euler–Lagrange equation (6.12) means geometrically. The orbit Jacobian matrix $\mathcal{J}$ stretches the state space unit hypercube ▶
$\Phi \in [0, 1)^n$ into the n-dimensional *fundamental parallelepiped*, and maps each periodic state Φ_M into an integer lattice $\mathbb{Z}^n$ site, which is then translated by the winding numbers M into the origin, in order to satisfy the condition (6.20). Hence N_n, the total number of the solutions of the zero condition equals the number of integer lattice points within the fundamental parallelepiped, a number given by what Baake *et al.* [4] call the *'fundamental fact'*,

$$N_n = |\text{Det}\,\mathcal{J}|, \tag{6.23}$$

i.e., fact that the number of integer points in the fundamental parallelepiped is equal to its volume, or, what we refer to as its Hill determinant.
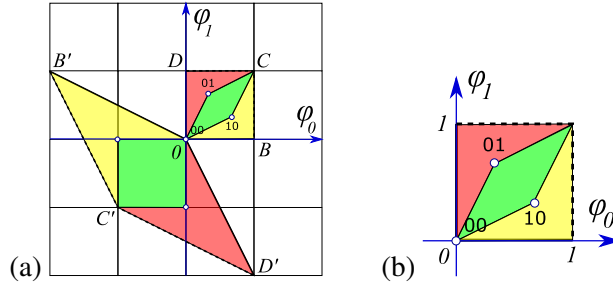
Figure 6.3: (Color online)   (a) The Bernoulli map (6.3) periodic states $\Phi_M = (\phi_0, \phi_1)$ of period 2 are the $\bar{0} = (0,0)$ point, and the two 2-cycle periodic states $\Phi_{01} = (1/3, 2/3)$ and Φ_{10}, see figure 6.2 (a). They all lie within the unit square $[0BCD]$, which is mapped by the orbit Jacobian matrix $-\mathcal{J}$ (6.25) into the fundamental parallelepiped $[0B'C'D']$. Periodic points Φ_M are mapped by $\mathcal{J}$ onto the integer lattice, $\mathcal{J}\Phi_M \in \mathbb{Z}^n$, and are sent back into the origin by integer translations M, in order to satisfy the root condition (6.20). Note that this fundamental parallelepiped is covered by 3 unit area quadrilaterals, hence $|\mathrm{Det}\,\mathcal{J}| = 3$. (b) Conversely, in the flow conservation sum rule (6.29) sum over all periodic states M of period n, the inverse of the Hill determinant defines the 'neighborhood' of a lattices state as the corresponding fraction of the unit hypercube volume.

The action of the orbit Jacobian matrix $\mathcal{J}$ for period-2 periodic states (periodic points) of the Bernoulli map of figure 6.2 (a), suffices to convey the idea. In this case, the $[2 \times 2]$ orbit Jacobian matrix (6.12), the unit square basis vectors, and their images are

$$\mathcal{J} = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix},$$

$$\Phi^{(B)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \rightarrow \Phi^{(B')} = \mathcal{J}\,\Phi^{(B)} = \begin{pmatrix} 2 \\ -1 \end{pmatrix},$$

$$\Phi^{(D)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \rightarrow \Phi^{(D')} = \mathcal{J}\,\Phi^{(D)} = \begin{pmatrix} -1 \\ 2 \end{pmatrix}, \tag{6.24}$$

i.e., the columns of the orbit Jacobian matrix are the edges of the fundamental parallelepiped,

$$\mathcal{J} = \left(\Phi^{(B')} \Phi^{(D')} \right), \tag{6.25}$$

drawn in figure 6.3, and $N_2 = |\mathrm{Det}\,\mathcal{J}| = 3$.

In general, the unit vectors of the state space unit hypercube $\Phi \in [0, 1)^n$ point along the n axes; orbit Jacobian matrix $\mathcal{J}$ stretches them into a fundamental parallelepiped basis vectors $\Phi^{(j)}$, each one a column of the $[n \times n]$ matrix

$$\mathcal{J} = \left(\Phi^{(1)} \Phi^{(2)} \cdots \Phi^{(n)} \right). \tag{6.26}$$

The Hill determinant

$$\mathrm{Det}\,\mathcal{J} = \mathrm{Det} \left(\Phi^{(1)} \Phi^{(2)} \cdots \Phi^{(n)} \right), \tag{6.27}$$

is then the volume of the fundamental parallelepiped whose edges are basis vectors $\Phi^{(j)}$. Note that the unit hypercubes and fundamental parallelepipeds are half-open, as indicated by dashed lines in figure 6.3 (a), so that their translates form a partition of the extended state space (6.4).

The interpretation of a Hill determinant as a fundamental parallelepiped applies only to linear Euler–Lagrange equations, basically Bernoulli. To compute it it in general, the right way to go is the reciprocal lattice, sect. 6.7.

6.6 Periodic orbit theory

For a general, nonlinear Euler–Lagrange equation root condition $F[\Phi] = 0$, the partition sum (5.2) is given by the sum over periodic states [1, 6, 9]. Ozorio de Almeida and Hannay [19] were the first to relate the periodic points to their Jacobian matrix generated volume; in 1984 they used such relation as an illustration of their 'principle of uniformity': "periodic points of an ergodic system, counted with their natural weighting, are uniformly dense in phase space." In periodic orbit theory [6, 8] this principle is stated as a flow conservation sum rule, where the sum is over all periodic states M of period n,

$$\sum_{|M|=n} \frac{1}{|\text{Det}\,\mathcal{J}_M|} = 1 \,. \tag{6.28}$$

For the Bernoulli system the 'natural weighting' takes a particularly simple form, as the Hill determinant of the orbit Jacobian matrix is the same for all periodic points of period n, $\text{Det}\,\mathcal{J}_M = \text{Det}\,\mathcal{J}$. For example, the sum over the $n = 2$ periodic states is,

$$\frac{1}{|\text{Det}\,\mathcal{J}_{00}|} + \frac{1}{|\text{Det}\,\mathcal{J}_{01}|} + \frac{1}{|\text{Det}\,\mathcal{J}_{10}|} = 1 \,, \tag{6.29}$$

see figure 6.3 (b). Furthermore, for any piece-wise linear system all curvature corrections [7] for orbits of periods $k > n$ vanish, leading to explicit periodic state formulas of kind displayed here. This is the 'periodic orbit theory'.

Actually, there is a bit more to it [9].

6.7 Reciprocal lattice

In the $\{\tilde{e}_k\}$ Fourier basis (1.46), a real n-dimensional periodic state vector Φ is mapped onto a n-dimensional complex reciprocal lattice vector

$$\tilde{\Phi} = (\tilde{u}_0, \tilde{u}_1, \tilde{u}_2, \ldots, \tilde{u}_{n-1}) \,, \tag{6.30}$$

with the kth Fourier mode of magnitude $|\tilde{u}_k|$ and phase $e^{i\theta_k}$.

On the reciprocal lattice, the shift matrix (6.13) is diagonal, $\tilde{r}_{jk} = \omega^k \delta_{jk}$, and the 'time' dynamics is breathtakingly simple: no matter what the dynamical system is, in one time step $\Phi \rightarrow r\Phi$, the kth Fourier mode phase is incremented by a fraction of the circle,

$$\begin{aligned}
(\tilde{u}_0, \tilde{u}_1, \tilde{u}_2, \ldots, \tilde{u}_{n-1}) &\rightarrow (\tilde{u}_0, \omega\tilde{u}_1, \omega^2\tilde{u}_2, \ldots, \omega^{n-1}\tilde{u}_{n-1}) \\
e^{i\theta_k} &\rightarrow e^{i(\theta_k + 2\pi k/n)} \,,
\end{aligned} \tag{6.31}$$

so reciprocal periodic states literally run in circles; for non-zero k and $|\tilde{u}_k|$, all reciprocal periodic states lie on vertices of regular complex plane n-gons, inscribed in circles of radius $|\tilde{u}_k|$, one circle for each orbit.

As a concrete example, consider the period-3 periodic states of the temporal Bernoulli (6.11) for stretching parameter $s = 2$. It is a linear problem and all periodic states are easily computed by hand, one for each symbol block M. There is always the point periodic state $(0, 0, 0)$ at the origin, and the remaining periodic

(a) (b) (c)
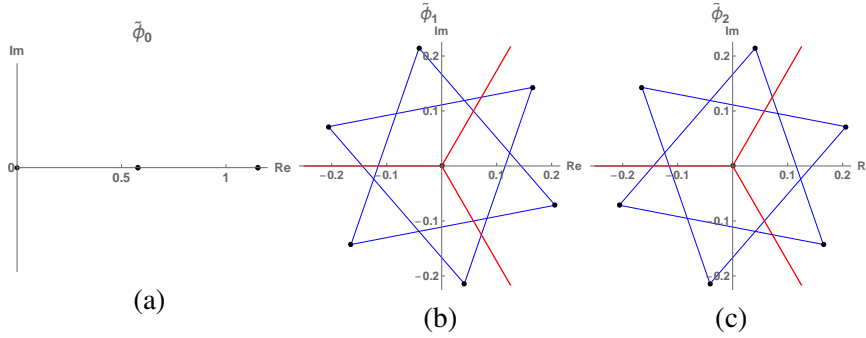
Figure 6.4: (Color online) The reciprocal lattice $(\tilde{u}_0, \tilde{u}_1, \tilde{u}_2)$ Fourier components of the seven C_3-equivariant period-3 periodic states, $s = 2$ temporal Bernoulli system (6.11). In $\tilde{u}_1$ and $\tilde{u}_2$ complex planes, reciprocal periodic states lie on vertices of the 2 equilateral triangles, one for each C_3 orbit, while the component at the origin is the point $\Phi = (0, 0, 0)$. The C_3 fundamental domain indicated by red border lines contains non-zero reciprocal periodic states whose phases lie in the $[-2\pi/6, 2\pi/6)$ wedge, one reciprocal periodic state for each distinct C_3 orbit.

states belong to $M_3 = 2$ period-3 orbits, where M_n is the number of prime orbits of period n. Discrete Fourier transform maps these 2 orbits into reciprocal lattice $(\tilde{u}_0, \tilde{u}_1, \tilde{u}_2)$ triangles, see figure 6.4. The time-step r acts on the $\tilde{u}_1, \tilde{u}_2$ components by complex 1/3-circle phase rotations $\exp(2\pi i/3)$ and $\exp(4\pi i/3)$, respectively: reciprocal periodic states connected by blue lines in figure 6.4 lie on a circle and belong to the same orbit. In this example the two orbits happen to lie on the same circle, as they are related by the *internal* $D_1 : \phi_i \rightarrow 1 - \phi_i$ symmetry of the Bernoulli system, see sect. **??**.

6.7.1 Hill determinant: Reciprocal lattice evaluation

Orbit Jacobian matrices of the temporal Bernoulli (6.22) consist of only identity matrix and cyclic shift matrix, whose eigenvectors are discrete Fourier basis (1.46), so they are diagonalized by discrete Fourier transform. In the space of reciprocal periodic states, orbit Jacobian matrices (6.21) are diagonal, each diagonal element an eigenvalue of an orbit Jacobian matrices, for the temporal Bernoulli

$$(s\,\mathbb{1} - r)\,\tilde{e}_k = (s - \omega^k)\,\tilde{e}_k\,. \tag{6.32}$$

Determinants are products of eigenvalues, so the temporal Bernoulli Hill determinant for any period-n periodic state is simply a polynomial whose roots are the nth roots of unity,

$$\text{Det}\,(s\,\mathbb{1} - r) = \prod_{k=0}^{n-1}(s - \omega^k) = s^n - 1\,, \tag{6.33}$$

in agreement with the time-evolution count (6.9).

6.8 Shadowing

From (6.15) it follows that the influence of a source $m_{t'}$ back in the past, at site t', falls off exponentially with the temporal lattice distance $t - t'$,

$$\phi_t = \sum_{t'=-\infty}^{t-1} g_{tt'} m_{t'}\,, \quad g_{tt'} = \frac{1}{\Lambda^{t-t'}}\,, \quad t > t'\,, \quad 0 \text{ otherwise}\,. \tag{6.34}$$

That means that an ergodic periodic state segment of length n (or a periodic state of a longer period) is shadowed by the periodic state (6.10) with the same first n sites symbol block M, with exponentially decreasing shadowing error of order $O(1/\Lambda^{n+1})$. The error is controlled by the weight $1/|\mathrm{Det}\,\mathcal{J}|$, with the Hill determinant (6.33) arising from inverting the orbit Jacobian matrix $\mathcal{J}$ to obtain the Green's function (6.12).

This error estimate is deeper than what it might seem at the first glance. In fluid dynamics, pattern recognition, neuroscience and other high or ∞-dimensional settings distances between 'close solutions' (let's say pixel images of two faces in a face recognition code) are almost always measured using some arbitrary yardstick, let's say a Euclidean L_2 norm, even though the state space is in no sense "Euclidean." Not so in the periodic orbit theory: here $1/|\mathrm{Det}\,\mathcal{J}|$ is the *intrinsic, coordinatization and norm independent* measure of the distance between neighboring spatiotemporal states.

6.9 Bernoulli as a first-order difference equation

🌶 The discrete time derivative of a lattice configuration Φ evaluated at the lattice site t is given by the 'lattice momentum' operator (1.27), $\mathsf{p} = r - \mathbb{1}$ (the difference operator [15]),

$$\dot{\phi}_t = \left[\frac{d\Phi}{dt}\right]_t = \frac{\phi_{t+1} - \phi_t}{\Delta t}\,. \tag{6.35}$$

The temporal Bernoulli condition (6.12) can be thus viewed as forward Euler method, a time-discretized, first-order difference equation

$$\frac{d\Phi}{dt} = \mathsf{p}\Phi + v(\Phi, \mathsf{M})\,, \tag{6.36}$$

where the 'velocity' vector field v is given by

$$v(\Phi, \mathsf{M}) = \mu\,\Phi - \mathsf{M}\,,$$

with the lattice spacing set to $\Delta t = 1$ (easily reinstated, if needed), and perturbations that grow (or decay) with rate $\mu = s - 1$. By inspection of figure 6.2 (a), it is clear that for *shrinking*, $\mu < 0$ parameter values the orbit is stable forward-in-time, with a single linear branch, 1-letter alphabet $\mathcal{A} = \{0\}$, and the only periodic states being the single point $\phi_0 = 0$, and its repeats $\Phi = (0, 0, \cdots, 0)$. However, for *stretching*, positive 'mass parameter' $\mu > 0$ values, the Bernoulli system (more generally, Rényi's beta transformations [21]) that we study here, every periodic state Φ_M is unstable, and there is a periodic state for each admissible symbol block M.

The temporal Bernoulli orbit Jacobian matrix $\mathcal{J} = d/dt - \mu\,r^{-1}$ is a difference operator whose determinant one can compute by a Fourier transform diagonalization (1.48). The eigenvalues of the temporal Bernoulli orbit Jacobian matrix (6.12) are (6.32), and its Hill determinant is the product of its eigenvalues, the nth roots of unity (6.33).

A fair coin toss, summarized.   We refer to the *global* temporal lattice condition (6.12) as the '*temporal* Bernoulli', in order to distinguish it from the 1-time step Bernoulli evolution *map* (6.5), in preparation for the study of *spatiotemporal* systems to be undertaken in ref. [11]. In the lattice formulation, a *global* temporal periodic state Φ_M is determined by the requirement that the *local* temporal lattice condition (6.11) is satisfied at every lattice site. In spatiotemporal formulation there is no need for forward-in-time, close recurrence searches for the returning periodic points. Instead, one determines each global temporal periodic state Φ_M at one go, by finding the zero of the Euler–Lagrange equation (6.12). The most importantly for what follows, the spatiotemporal field theory of ref. [11], this calculation requires no recourse to any *explicit coordinatization and partitioning of system's state space*.

And if you don't know, now you know.

Exercises

6.1. **Temporal Bernoulli periodic states.** Temporal Bernoulli (6.11) periodic states can be computed by hand. Set the stretching factor to $s = 2$, and determine periodic states Φ_M for all distinct symbol arrays M:

  (a) All steady states $\phi_t = \phi$. Explain why their number is *not* 2.

  (b) All periodic states of period 2, $\phi_t = \phi_{t+2}$. Explain why their number is *not* 4.

6.2. **Temporal Bernoulli periodic states, prime orbits.** Consider the temporal Bernoulli (6.11). The goal of this exercise is to demonstrate (i) that you can compute explicitly all of its periodic states, and (ii) you only need to compute prime orbits.

  (a) Given an n-sites symbol block M, derive the explicit formula (6.17) for the value of temporal Bernoulli field ϕ_0 at the latice site 0.

  (b) What now determines the field values $\phi_1, \phi_2, \cdots, \phi_{n-1}$?

  (c) List all $\Phi_M = (\phi_0, \phi_1, \phi_2, \cdots, \phi_{n-1})$ for periods $n = 1, 2, 3, 4$, stretching factor $s = 2$.

  (d) As you increase the period n, which periodic states are new, which ones you have already computed?

6.3. **Temporal Bernoulli Hill determinants.** Short periods temporal Bernoulli (6.11) Hill determinants are easily computed by hand.

  (a) What are Hill determinants of periodic states $M = 0, 1, 00, 01, 10$, arbitrary stretching parameter s?

  (b) What are Hill determinants of periodic states of periods $3, 4, n, \cdots$? (Hint: this is mostly a thinking exercise).

6.4. **Temporal Bernoulli prime orbits, Hill determinants.** Short periods temporal Bernoulli (6.11) Hill determinants are easily computed by hand. The goal of this exercise is to demonstrate (i) that you can compute explicitly all of its periodic states, and (ii) you only need to compute prime orbits.

  (a) XXX.

  (b) XXX

  (c) XXX

  (d) XXX

6.5. **Temporal Bernoulli 'path integral'.** I'm skating here on thin ice, so please help me, check it out.

  (a) XXX.

  (b) XXX

  (c) XXX

  (d) XXX

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Chapter 7

WKB quantization

The wave function for a particle of energy E moving in a constant potential V is

$$\psi = A e^{\frac{i}{\hbar} p q} \tag{7.1}$$

with a constant amplitude A, and constant wavelength $\lambda = 2\pi/k$, $k = p/\hbar$, and $p = \pm\sqrt{2m(E - V)}$ is the momentum. Here we generalize this solution to the case where the potential varies slowly over many wavelengths. This semiclassical (or WKB) approximate solution of the Schrödinger equation fails at deterministic turning points, configuration space points where the particle momentum vanishes. In such neighborhoods, where the semiclassical approximation fails, one needs to solve locally the exact quantum problem, in order to compute connection coefficients which patch up semiclassical segments into an approximate global wave function.

Two lessons follow. First, semiclassical methods can be very powerful - deterministic mechanics computations yield surprisingly accurate estimates of quantal spectra, without solving the Schrödinger equation. Second, semiclassical quantization does depend on a purely wave-mechanical phenomena, the coherent addition of phases accrued by all fixed energy phase space trajectories that connect pairs of coordinate points, and the topological phase loss at every turning point, a topological property of the deterministic flow that plays no role in classical mechanics.
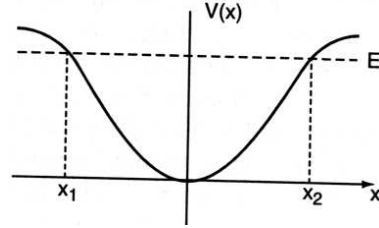
Figure 7.1: A 1-dimensional potential with two turning points at fixed energy E.

7.1 WKB ansatz

If the kinetic term $T(p)$ can be separated as in (2.5), the time-independent Schrödinger equation takes form

$$-\frac{\hbar^2}{2m}\psi''(q) + V(q)\psi(q) = E\psi(q)\,. \tag{7.2}$$

Consider a time-independent Schrödinger equation in 1 spatial dimension, with potential $V(q)$ growing sufficiently fast as $q \to \pm\infty$ so that the deterministic particle motion is confined for any E. Define the local momentum $p(q)$ and the local wavenumber $k(q)$ by

$$p(q) = \pm\sqrt{2m(E - V(q))}, \quad p(q) = \hbar k(q)\,. \tag{7.3}$$

The variable wavenumber form of the Schrödinger equation

$$\psi'' + k^2(q)\psi = 0 \tag{7.4}$$

sugests that the wave function be written as $\psi = Ae^{\frac{i}{\hbar}S}$, A and S real functions of q. Substitution yields two equations, one for the real and other for the imaginary part:

$$(S')^2 \;=\; p^2 + \hbar^2\frac{A''}{A} \tag{7.5}$$

$$S''A + 2S'A' \;=\; \frac{1}{A}\frac{d}{dq}(S'A^2) = 0\,. \tag{7.6}$$

The Wentzel-Kramers-Brillouin *(WKB)* or *semiclassical* approximation consists of dropping the $\hbar^2$ term in (7.5). Recalling that $p = \hbar k$, this amounts to assuming that $k^2 \gg \frac{A''}{A}$, which in turn implies that the phase of the wave function is changing much faster than its overall amplitude. So the WKB approximation can interpreted either as a short wavelength/high frequency approximation to a wave-mechanical problem, or as the semiclassical, $\hbar \ll 1$ approximation to quantum mechanics.

Setting $\hbar = 0$ and integrating (7.5) we obtain the phase increment of a wave function initially at q, at energy E

$$S(q, q', E) = \int_{q'}^{q} dq'' p(q'')\,. \tag{7.7}$$

This integral over a particle trajectory of constant energy, called the *action*, will play a key role in all that follows. The integration of (7.6) is even easier

$$A(q) = \frac{C}{|p(q)|^{\frac{1}{2}}}, \qquad C = |p(q')|^{\frac{1}{2}}\psi(q')\,, \tag{7.8}$$
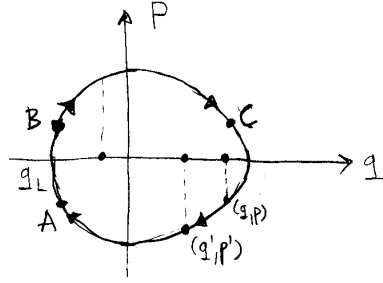
Figure 7.2: A 1-dof phase space trajectory of a particle moving in a bound potential.

where the integration constant C is fixed by the value of the wave function at the initial point q'. The *WKB* (or *semiclassical*) *ansatz* wave function is given by

$$\psi_{sc}(q, q', E) = \frac{C}{|p(q)|^{\frac{1}{2}}} e^{\frac{i}{\hbar}S(q,q',E)} . \tag{7.9}$$

In what follows we shall suppress dependence on the initial point and energy in such formulas, $(q, q', E) \to (q)$.

The WKB ansatz generalizes the free motion wave function (7.1), with the probability density $|A(q)|^2$ for finding a particle at q now inversely proportional to the velocity at that point, and the phase $\frac{1}{\hbar} q\, p$ replaced by $\frac{1}{\hbar} \int dq\, p(q)$, the integrated action along the trajectory. This is fine, except at any turning point q_0, figure 7.1, where all energy is potential, and

$$p(q) \to 0 \quad \text{as} \quad q \to q_0 , \tag{7.10}$$

so that the assumption that $k^2 \gg \frac{A''}{A}$ fails. What can one do in this case?

For the task at hand, a simple physical picture, due to Maslov, does the job. In the q coordinate, the turning points are defined by the zero kinetic energy condition (see figure 7.1), and the motion appears singular. This is not so in the full phase space: the trajectory in a smooth confining 1-dimensional potential is always a smooth loop (see figure 7.2), with the "special" role of the turning points q_L, q_R seen to be an artifact of a particular choice of the (q, p) coordinate frame. Maslov proceeds from the initial point (q', p') to a point (q_A, p_A) preceding the turning point in the $\psi(q)$ representation, then switch to the momentum representation

$$\widetilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int dq\, e^{-\frac{i}{\hbar}qp} \psi(q) , \tag{7.11}$$

continue from (q_A, p_A) to (q_B, p_B), switch back to the coordinate representation,

$$\psi(q) = \frac{1}{\sqrt{2\pi\hbar}} \int dp\, e^{\frac{i}{\hbar}qp} \widetilde{\psi}(p) , \tag{7.12}$$

and so on.

The only rub is that one usually cannot evaluate these transforms exactly. But, as the WKB wave function (7.9) is approximate anyway, it suffices to estimate these transforms to the leading order in $\hbar$ accuracy. This is accomplished by the method of stationary phase.

7.2 Method of stationary phase

All "semiclassical" approximations are based on saddle point evaluations of integrals of the type

$$I = \int dx\, A(x)\, e^{is\Phi(x)}, \qquad x, \Phi(x) \in \mathbb{R}, \tag{7.13}$$

where s is a real parameter, and $\Phi(x)$ is a real-valued function. In our applications $s = 1/\hbar$ will always be assumed large.

For large s, the phase oscillates rapidly and "averages to zero" everywhere except at the *extremal points* $\Phi'(x_0) = 0$. The method of approximating an integral by its values at extremal points is called the *method of stationary phase*. Consider first the case of a 1-dimensional integral, and expand $\Phi(x_0 + \delta x)$ around x_0 to second order in δx,

$$I = \int dx\, A(x)\, e^{is(\Phi(x_0) + \frac{1}{2}\Phi''(x_0)\delta x^2 + \dots)}. \tag{7.14}$$

Assume (for time being) that $\Phi''(x_0) \neq 0$, with either sign, $\mathrm{sgn}[\Phi''] = \Phi''/|\Phi''| = \pm 1$. If in the neighborhood of x_0 the amplitude $A(x)$ varies slowly over many oscillations of the exponential function, we may retain the leading term in the Taylor expansion of the amplitude, and approximate the integral up to quadratic terms in the phase by

$$I \approx A(x_0)\, e^{is\Phi(x_0)} \int dx\, e^{\frac{1}{2}is\Phi''(x_0)(x-x_0)^2}. \tag{7.15}$$

The one integral that we know how to integrate is the Gaussian integral $\int dx\, e^{-\frac{x^2}{2b}} = \sqrt{2\pi b}$ For for pure imaginary $b = i\,a$ one gets instead the *Fresnel integral formula*

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{-\frac{x^2}{2ia}} = \sqrt{ia} = |a|^{1/2}\, e^{i\frac{\pi}{4}\frac{a}{|a|}} \tag{7.16}$$

we obtain

$$I \approx A(x_0) \left| \frac{2\pi}{s\Phi''(x_0)} \right|^{1/2} e^{is\Phi(x_0) \pm i\frac{\pi}{4}}, \tag{7.17}$$

where $\pm$ corresponds to the positive/negative sign of $s\Phi''(x_0)$.

7.3 WKB quantization

We can now evaluate the Fourier transforms (7.11), (7.12) to the same order in $\hbar$ as the WKB wave function using the stationary phase method,

$$
\begin{aligned}
\widetilde{\psi}_{sc}(p) &= \frac{C}{\sqrt{2\pi\hbar}} \int \frac{dq}{|p(q)|^{\frac{1}{2}}}\, e^{\frac{i}{\hbar}(S(q)-qp)} \\
&\approx \frac{C}{\sqrt{2\pi\hbar}} \frac{e^{\frac{i}{\hbar}(S(q^*)-q^*p)}}{|p(q^*)|^{\frac{1}{2}}} \int dq\, e^{\frac{i}{2\hbar}S''(q^*)(q-q^*)^2},
\end{aligned}
\tag{7.18}
$$

where q^* is given implicitly by the stationary phase condition

$$0 = S'(q^*) - p = p(q^*) - p$$

and the sign of $S''(q^*) = p'(q^*)$ determines the phase of the Fresnel integral (7.16)

$$\widetilde{\psi}_{sc}(p) = \frac{C}{|p(q^*)p'(q^*)|^{\frac{1}{2}}} e^{\frac{i}{\hbar}[S(q^*)-q^*p]+\frac{i\pi}{4}\text{sgn}[S''(q^*)]} \,. \tag{7.19}$$

As we continue from (q_A, p_A) to (q_B, p_B), nothing problematic occurs - $p(q^*)$ is finite, and so is the acceleration $p'(q^*)$. Otherwise, the trajectory would take infinitely long to get across. We recognize the exponent as the Legendre transform

$$\tilde{S}(p) = S(q(p)) - q(p)p$$

which can be used to expresses everything in terms of the p variable,

$$q^* = q(p), \quad \frac{d}{dq}q = 1 = \frac{dp}{dq}\frac{dq(p)}{dp} = q'(p)p'(q^*) \,. \tag{7.20}$$

As the deterministic trajectory crosses q_L, the weight in (7.19),

$$\frac{d}{dq}p^2(q_L) = 2p(q_L)p'(q_L) = -2mV'(q_L) \,, \tag{7.21}$$

is finite, and $S''(q^*) = p'(q^*) < 0$ for any point in the lower left quadrant, including (q_A, p_A). Hence, the phase loss in (7.19) is $-\frac{\pi}{4}$. To go back from the p to the q representation, just turn figure 7.2 quarter-turn anticlockwise. Everything is the same if you replace $(q, p) \rightarrow (-p, q)$; so, without much ado we get the semiclassical wave function at the point (q_B, p_B),

$$\psi_{sc}(q) = \frac{e^{\frac{i}{\hbar}(\tilde{S}(p^*)+qp^*)-\frac{i\pi}{4}}}{|q^*(p^*)|^{\frac{1}{2}}} \widetilde{\psi}_{sc}(p^*) = \frac{C}{|p(q)|^{\frac{1}{2}}} e^{\frac{i}{\hbar}S(q)-\frac{i\pi}{2}} \,. \tag{7.22}$$

The extra $|p'(q^*)|^{1/2}$ weight in (7.19) is cancelled by the $|q'(p^*)|^{1/2}$ term, by the Legendre relation (7.20).

The message is that going through a smooth potential turning point the WKB wave function phase slips by $-\frac{\pi}{2}$. This is equally true for the right and the left turning points, as can be seen by rotating figure 7.2 by 180°, and flipping coordinates $(q, p) \rightarrow (-q, -p)$. While a turning point is not an invariant concept (for a sufficiently short trajectory segment, it can be undone by a 45° turn), for a complete period $(q, p) = (q', p')$ the total phase slip is always $-2 \cdot \pi/2$, as a loop always has $m = 2$ turning points.

The *WKB quantization condition* follows by demanding that the wave function computed after a complete period be single-valued. With the normalization (7.8), we obtain

$$\psi(q') = \psi(q) = \left|\frac{p(q')}{p(q)}\right|^{\frac{1}{2}} e^{i(\frac{1}{\hbar}\oint p(q)dq-\pi)}\psi(q') \,.$$

The prefactor is 1 by the periodic orbit condition $q = q'$, so the phase must be a multiple of 2π,

$$\frac{1}{\hbar}\oint p(q)dq = 2\pi\left(n + \frac{m}{4}\right) \,, \tag{7.23}$$
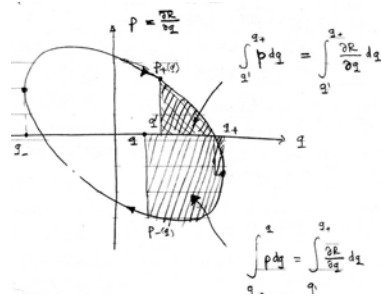
Figure 7.3: $S_p(E)$, the action of a periodic orbit p at energy E, equals the area in the phase space traced out by the 1-dof trajectory.

where m is the number of turning points along the trajectory - for this 1-dof problem, $m = 2$.

The action integral in (7.23) is the area (see figure 7.3) enclosed by the classical phase space loop of figure 7.2, and the quantization condition says that eigenenergies correspond to loops whose action is an integer multiple of the unit quantum of action, Planck's constant $\hbar$. The extra topological phase, which, although it had been discovered many times in centuries past, had to wait for its most recent quantum chaotic (re)birth until the 1970's. Despite its derivation in a noninvariant coordinate frame, the final result involves only canonically invariant deterministic quantities, the periodic orbit action S, and the topological index m.

7.3.1 Harmonic oscillator quantization

Let us check the WKB quantization for one case (the only case?) whose quantum mechanics we fully understand: the harmonic oscillator

$$E = \frac{1}{2m}\left(p^2 + (m\omega q)^2\right) .$$

The loop in figure 7.2 is now a circle in the $(m\omega q, p)$ plane, the action is its area $S = 2\pi E/\omega$, and the spectrum in the WKB approximation

$$E_n = \hbar\omega(n + 1/2) \tag{7.24}$$

turns out to be the *exact* harmonic oscillator spectrum. The stationary phase condition (7.18) keeps $V(q)$ accurate to order q^2, which in this case is the whole answer (but we were simply lucky, really). For many 1-dof problems the WKB spectrum turns out to be very accurate all the way down to the ground state. Surprisingly accurate, if one interprets dropping the $\hbar^2$ term in (7.5) as a short wavelength approximation.

7.4 Beyond the quadratic saddle point

We showed, with a bit of Fresnel/Maslov voodoo, that in a smoothly varying potential the phase of the WKB wave function slips by a $\pi/2$ for each turning point. This $\pi/2$ came from a $\sqrt{i}$ in the Fresnel integral (7.16), one such factor for every time we switched representation from the configuration space to the momentum space, or back. Good, but what does this mean?

The stationary phase approximation (7.14) fails whenever $\Phi''(x) = 0$, or, in our the WKB ansatz (7.18), whenever the momentum $p'(q) = S''(q)$ vanishes.
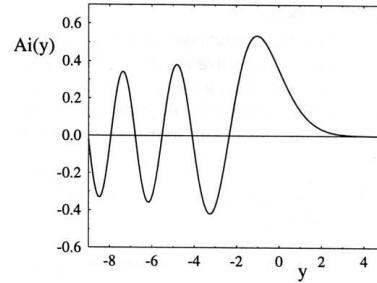
Figure 7.4: Airy function $Ai(q)$.

In that case we have to go beyond the quadratic approximation (7.15) to the first nonvanishing term in the Taylor expansion of the exponent. If $\Phi'''(x_0) \neq 0$, then

$$I \approx A(x_0)e^{is\Phi(x_0)} \int_{-\infty}^{\infty} dx \, e^{is\Phi'''(x_0)\frac{(x-x_0)^3}{6}} \,. \tag{7.25}$$

Airy functions can be represented by integrals of the form

$$Ai(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dy \, e^{i(xy-\frac{y^3}{3})} \,. \tag{7.26}$$

With a bit of Fresnel/Maslov voodoo we have shown that at each turning point a WKB wave function loses a bit of phase. Derivations of the WKB quantization condition given in standard quantum mechanics textbooks rely on expanding the potential close to the turning point

$$V(q) = V(q_0) + (q - q_0)V'(q_0) + \cdots ,$$

solving the Airy equation (with $V'(q_0) \rightarrow z$ after appropriate rescalings),

$$\psi'' = z\psi \,, \tag{7.27}$$

and matching the oscillatory and the exponentially decaying "forbidden" region wave function pieces by means of the *WKB connection formulas*. That requires staring at Airy functions (see (7.4)) and learning about their asymptotics - a challenge that we will have to eventually overcome, in order to incorporate diffraction phenomena into semiclassical quantization.

The physical origin of the topological phase is illustrated by the shape of the Airy function, figure 7.4. For a potential with a finite slope $V'(q)$ the wave function penetrates into the forbidden region, and accommodates a bit more of a stationary wavelength then what one would expect from the deterministic trajectory alone. For infinite walls (i.e., billiards) a different argument applies: the wave function must vanish at the wall, and the phase slip due to a specular reflection is $-\pi$, rather than $-\pi/2$.

Résumé

The WKB ansatz wave function for 1-degree of freedom problems fails at the turning points of the deterministic trajectory. While in the q-representation the WKB ansatz at a turning point is singular, along the p direction the deterministic

trajectory in the same neighborhood is smooth, as for any smooth bound potential the classical motion is topologically a circle around the origin in the (q, p) space. The simplest way to deal with such singularities is as follows; follow the deterministic trajectory in q-space until the WKB approximation fails close to the turning point; then insert $\int dp|p\rangle\langle p|$ and follow the deterministic trajectory in the p-space until you encounter the next p-space turning point; go back to the q-space representation, an so on. Each matching involves a Fresnel integral, yielding an extra $e^{-i\pi/4}$ phase shift, for a total of $e^{-i\pi}$ phase shift for a full period of a semi-classical particle moving in a soft potential. The condition that the wave-function be single-valued then leads to the 1-dimensional WKB quantization, and its lucky cousin, the Bohr-Sommerfeld quantization.

Alternatively, one can linearize the potential around the turning point a, $V(q) = V(a) + (q - a)V'(a) + \cdots$, and solve the quantum mechanical constant linear potential $V(q) = qF$ problem exactly, in terms of an Airy function. An approximate wave function is then patched together from an Airy function at each turning point, and the WKB ansatz wave-function segments in-between via the WKB connection formulas. The single-valuedness condition again yields the 1-dimensional WKB quantization. This a bit more work than tracking the deterministic trajectory in the full phase space, but it gives us a better feeling for shapes of quantum eigenfunctions, and exemplifies the general strategy for dealing with other singularities, such as wedges, bifurcation points, creeping and tunneling: patch together the WKB segments by means of exact QM solutions to local approximations to singular points.

Commentary

Remark 7.1. Bohr-Sommerfeld quantization.   Bohr-Sommerfeld quantization condition [2] was the key result of the old quantum theory, in which the electron trajectories were purely deterministically. They were lucky - the symmetries of the Kepler problem work out in such a way that the total topological index $m = 4$ amount effectively to numbering the energy levels starting with $n = 1$. They were unlucky - because the hydrogen $m = 4$ masked the topological index, they could never get the helium spectrum right - the semiclassical calculation had to wait for until 1980, when Leopold and Percival [1] added the topological indices.

References

[1]   J. G. Leopold and I. Percival, "The semiclassical two-electron atom and the old quantum theory", J. Phys. B **13**, 1037 (1980).

[2]   A. Sommerfeld, *Atombau und Spektrallinien* (Deutsch, Thun, Frankfurt/M, 1919).

Exercises

7.1. **WKB ansatz.** Try to show that no other ansatz other than

$$\psi(q,t) = A(q,t)\, e^{iR(q,t)/\hbar}, \qquad (7.28)$$

gives a meaningful definition of the momentum in the $\hbar \to 0$ limit.

7.2. **Fresnel integral.** Derive the Fresnel integral

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{-\frac{x^2}{2ia}} = \sqrt{ia} = |a|^{1/2} e^{i\frac{\pi}{4}\frac{a}{|a|}}.$$

7.3. **Sterling formula for $n!$.** Compute an approximate value of $n!$ for large n using the stationary phase approximation. Hint: $n! = \int_0^{\infty} dt\, t^n e^{-t}$.

7.4. **Airy function for large arguments.** Important contributions as stationary phase points may arise from extremal points where the first non-zero term in a Taylor expansion of the phase is of third or higher order. Such situations occur, for example, at bifurcation points or in diffraction effects, (such as waves near sharp corners, waves creeping around obstacles, etc.). In such calculations, one meets Airy functions integrals of the form

$$Ai(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dy\, e^{i(xy - \frac{y^3}{3})}. \qquad (7.29)$$

Calculate the Airy function $Ai(x)$ using the stationary phase approximation. What happens when considering the limit $x \to 0$. Estimate for which value of x the stationary phase approximation breaks down.

Chapter 8

Spin

> If I had had more time, I would have written less
>
> — Blaise Pascal, a remark made to a correspondent

8.1 Dirac Lagrangian

In a 3-semester QFT course we would study and understand in detail Weyl, Majorana and Dirac spinors. Here our focus is much narrower - get the tools needed to do one fundamental QED calculation that establishes the theory as a predictive description of observed quantum effects in interaction of matter and electromagnetic fields. For that we need the relativistically correct description of the free electron propagator.

I find these and these notes concise and non-nonsense discussion. The first thing to understand, perhaps unfamiliar to a student of non-relativistic quantum mechanics, is that the signature of the Minkowsky metric makes Lorentz transformations not unitary, and thus

(complex conjugate transpose spinor) × (complex spinor)

is *not* a scalar under Lorentz transformation, and thus *not* the correct definition of the "length" of the 4-component complex spinor. One has to use the appropriate Minkowsky metric on the spinor space as well.

The other deep thing to understand is that spinor fields are anticommuting, Grassmanian numbers. My own understanding is that such fields are imposing constraints ("negative dimensions"), in this case the *Pauli exclusion principle* that two or more identical fermions (particles with half-integer spin) cannot occupy the same quantum state, the principle that (almost literally) makes the world go round. As this will not impact our one-loop calculation, we will not discuss it further here.
Up to date version of these notes is P. Cvitanović [1] *Field theory*, chapter 7. *Spin*, yours for a click here.

References

[1] P. Cvitanović, *Field Theory*, Notes prepared by E. Gyldenkerne (Nordita, Copenhagen, 1983).

Exercises

8.1. **Dirac's γ matrices.**

   (a) Verify

   $$[S^{\kappa\lambda}, S^{\mu\nu}] = i(g^{\lambda\mu}S^{\kappa\nu} - g^{\lambda\nu}S^{\kappa\mu} - g^{\kappa\mu}S^{\lambda\nu} + g^{\kappa\nu}S^{\lambda\mu}).$$
   (8.1)

   (b) Verify

   $$M^{-1}(L)\gamma^\mu M(L) = L^\mu_\nu \gamma^\nu$$
   (8.2)

   for $L = \exp(\theta)$
   (i.e., $L^\mu_\nu = \delta^\mu_\nu + \theta^\mu_\nu + \frac{1}{2}\theta^\mu_\lambda \theta^\lambda_\nu + \cdots$) and

   $$M(L) = \exp(-\frac{i}{2}\theta_{\alpha\beta}S^{\alpha\beta}).$$
   (8.3)

   (c) Calculate

   $$\{\gamma^\rho, \gamma^\lambda\gamma^\mu\gamma^\nu\}, \qquad [\gamma^\rho, \gamma^\kappa\gamma^\lambda\gamma^\mu\gamma^\nu], \qquad (8.4)$$

   and $[S^{\rho\sigma}, \gamma^\lambda\gamma^\mu\gamma^\nu]$.

   (d) Show that

   $$\begin{aligned}
   \gamma^\alpha\gamma_\alpha &= 4 \\
   \gamma^\alpha\gamma^\nu\gamma_\alpha &= -2\gamma^\nu \\
   \gamma^\alpha\gamma^\mu\gamma^\nu\gamma_\alpha &= 4g^{\mu\nu} \\
   \gamma^\alpha\gamma^\lambda\gamma^\mu\gamma^\nu\gamma_\alpha &= -2\gamma^\nu\gamma^\mu\gamma^\lambda.
   \end{aligned}$$
   (8.5)

   Hint: use $\gamma^\alpha\gamma^\nu = 2g^{\nu\alpha} - \gamma^\nu\gamma^\alpha$ repeatedly.

8.2. **Continuous Lorentz transformations of spinors.**
   Under continuous Lorentz symmetries, Dirac spinor field $\Psi(x)$ transforms according to $\Psi'(x') = M(L)\Psi(x = L^{-1}x')$ where $M(L = e^\theta) = \exp(-\frac{i}{2}\theta_{\alpha\beta}S^{\alpha\beta})$.

   In the Dirac representation

   $$\gamma^0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

is hermitian, whereas the three γ^j are not. That, and the defining (anti-commutator) relation

$$\{\gamma^\mu, \gamma^\nu\} = \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\eta^{\mu\nu}I_4$$

is all we need to know, not the explicit forms of γ^μ. As we now check, γ^0 plays the role of the metric in the spinor space, via the *Dirac conjugate* defined as

$$\overline{\Psi} = \Psi^\dagger\gamma^0$$

Consider the transformation rules for the bilinears

$$S = \overline{\Psi}\Psi, \quad V^\mu = \overline{\Psi}\gamma^\mu\Psi, \quad T^{\mu\nu} = \overline{\Psi}\gamma^{[\mu}\gamma^{\nu]}\Psi.$$

Show that under *continuous* Lorentz symmetries, the S transforms as a scalar, the V^μ as a vector, and the $T^{\mu\nu}$ as an antisymmetric tensor.

The important thing to note is that due to the non-unitarity of Lorentz transformations the transpose (or a hermitian conjugate) of a Lorentz "rotation" is not its inverse, unlike what happens for 3-dimensional Euclidean rotations. Hence $\overline{\Psi}$ rather than the $\Psi^\dagger$ that shows up in bilinears of U(n, m).

8.3. **QED electron-electron-photon 1-loop Feynman-parametric integral.** Write down the QED electron-electron-photon vertex 1-loop Feynman integral in the Feynman-parametric form,

$$\Gamma^\mu_{(2)}(p', p) = -2ie^2 \iiint_0^1 dx\,dy\,dz\,\delta(x+y+z-1) \int \frac{d^4\ell}{(2\pi)^4} [\cdots]$$

8.4. **QED electron-electron-photon 1-loop numerator.** Simplify the gamma matrices in the numerator to the two form factors proportional to γ^μ and $\sigma^{\mu\nu}$.

Appendix A1

Group theory

A1.1   Invariants and reducibility

What follows is a bit dry, so we start with a motivational quote from Hermann Weyl on the "so-called first main theorem of invariant theory":

    "*All invariants are expressible in terms of a finite number among them. We cannot claim its validity for every group G; rather, it will be our chief task to investigate for each particular group whether a finite integrity basis exists or not; the answer, to be sure, will turn out affirmative in the most important cases.*"

    It is easy to show that any rep of a finite group can be brought to unitary form, and the same is true of all compact Lie groups. Hence, in what follows, we specialize to unitary and hermitian matrices.

A1.1.1   Projection operators

For $\mathbf{M}$ a hermitian matrix, there exists a diagonalizing unitary matrix $\mathbf{C}$ such that

$$\mathbf{CMC}^{\dagger} = \begin{bmatrix} \begin{array}{|ccc|} \hline \lambda_1 & \ldots & 0 \\ & \ddots & \\ 0 & \ldots & \lambda_1 \\ \hline \end{array} & 0 & 0 \\[2pt] 0 & \begin{array}{|cccc|} \hline \lambda_2 & 0 & \ldots & 0 \\ 0 & \lambda_2 & & \\ \vdots & & \ddots & \vdots \\ 0 & & \ldots & \lambda_2 \\ \hline \end{array} & 0 \\[2pt] 0 & 0 & \begin{array}{|cc} \hline \lambda_3 & \ldots \\ \vdots & \ddots \end{array} \end{bmatrix} . \qquad \text{(A1.1)}$$

Here $\lambda_i \neq \lambda_j$ are the r distinct roots of the minimal *characteristic* (or *secular*) polynomial

$$\prod_{i=1}^{r}(\mathbf{M} - \lambda_i \mathbf{1}) = 0. \tag{A1.2}$$

In the matrix $\mathbf{C}(\mathbf{M} - \lambda_2 \mathbf{1})\mathbf{C}^\dagger$ the eigenvalues corresponding to λ_2 are replaced by zeroes:

$$\begin{bmatrix} \lambda_1 - \lambda_2 & & & & \\ & \lambda_1 - \lambda_2 & & & \\ & & 0 & & \\ & & & \ddots & \\ & & & & 0 \\ & & & & & \lambda_3 - \lambda_2 \\ & & & & & & \lambda_3 - \lambda_2 \\ & & & & & & & \ddots \end{bmatrix},$$

and so on, so the product over all factors $(\mathbf{M} - \lambda_2 \mathbf{1})(\mathbf{M} - \lambda_3 \mathbf{1})\dots$, with exception of the $(\mathbf{M} - \lambda_1 \mathbf{1})$ factor, has nonzero entries only in the subspace associated with λ_1:

$$\mathbf{C}\prod_{j \neq 1}(\mathbf{M} - \lambda_j \mathbf{1})\mathbf{C}^\dagger = \prod_{j \neq 1}(\lambda_1 - \lambda_j) \begin{bmatrix} \begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix} & & & \\ & 0 & & \\ & & 0 & \\ 0 & & & 0 \\ & & & & \ddots \end{bmatrix}.$$

Thus we can associate with each distinct root λ_i a *projection operator* P_i,

$$P_i = \prod_{j \neq i} \frac{\mathbf{M} - \lambda_j \mathbf{1}}{\lambda_i - \lambda_j}, \tag{A1.3}$$

which acts as identity on the ith subspace, and zero elsewhere. For example, the projection operator onto the λ_1 subspace is

$$P_1 = \mathbf{C}^\dagger \begin{bmatrix} \begin{matrix} 1 & & \\ & \ddots & \\ & & 1 \end{matrix} & & \\ & 0 & \\ & & 0 \\ & & & \ddots \\ & & & & 0 \end{bmatrix} \mathbf{C}. \tag{A1.4}$$

The diagonalization matrix $\mathbf{C}$ is deployed in the above only as a pedagogical device. The whole point of the projector operator formalism is that we *never* need to carry such explicit diagonalization; all we need are whatever invariant matrices

M we find convenient, the algebraic relations they satisfy, and orthonormality and completeness of P_i: The matrices P_i are *orthogonal*

$$P_i P_j = \delta_{ij} P_j, \qquad \text{(no sum on } j), \tag{A1.5}$$

and satisfy the *completeness relation*

$$\sum_{i=1}^{r} P_i = \mathbf{1}. \tag{A1.6}$$

As $\text{tr}\,(\mathbf{C} P_i \mathbf{C}^\dagger) = \text{tr}\,P_i$, the dimension of the ith subspace is given by

$$d_i = \text{tr}\,P_i. \tag{A1.7}$$

It follows from the characteristic equation (A1.2) and the form of the projection operator (A1.3) that λ_i is the eigenvalue of **M** on P_i subspace:

$$\mathbf{M} P_i = \lambda_i P_i, \qquad \text{(no sum on } i). \tag{A1.8}$$

Hence, any matrix polynomial $f(\mathbf{M})$ takes the scalar value $f(\lambda_i)$ on the P_i subspace

$$f(\mathbf{M}) P_i = f(\lambda_i) P_i. \tag{A1.9}$$

This, of course, is the reason why one wants to work with irreducible reps: they reduce matrices and "operators" to pure numbers.

A1.1.2 Irreducible representations

Suppose there exist several linearly independent invariant $[d \times d]$ hermitian matrices $\mathbf{M}_1, \mathbf{M}_2, \ldots$, and that we have used $\mathbf{M}_1$ to decompose the d-dimensional vector space $V = V_1 \oplus V_2 \oplus \cdots$. Can $\mathbf{M}_2, \mathbf{M}_3, \ldots$ be used to further decompose V_i? Further decomposition is possible if, and only if, the invariant matrices commute:

$$[\mathbf{M}_1, \mathbf{M}_2] = 0, \tag{A1.10}$$

or, equivalently, if projection operators P_j constructed from $\mathbf{M}_2$ commute with projection operators P_i constructed from $\mathbf{M}_1$,

$$P_i P_j = P_j P_i. \tag{A1.11}$$

Usually the simplest choices of independent invariant matrices do not commute. In that case, the projection operators P_i constructed from $\mathbf{M}_1$ can be used to project commuting pieces of $\mathbf{M}_2$:

$$\mathbf{M}_2^{(i)} = P_i \mathbf{M}_2 P_i, \qquad \text{(no sum on } i).$$

That $\mathbf{M}_2^{(i)}$ commutes with $\mathbf{M}_1$ follows from the orthogonality of P_i:

$$[\mathbf{M}_2^{(i)}, \mathbf{M}_1] = \sum_j \lambda_j [\mathbf{M}_2^{(i)}, P_j] = 0. \tag{A1.12}$$

Now the characteristic equation for $\mathbf{M}_2^{(i)}$ (if nontrivial) can be used to decompose V_i subspace.

An invariant matrix $\mathbf{M}$ induces a decomposition only if its diagonalized form (A1.1) has more than one distinct eigenvalue; otherwise it is proportional to the unit matrix and commutes trivially with all group elements. A rep is said to be *irreducible* if all invariant matrices that can be constructed are proportional to the unit matrix.

An invariant matrix $\mathbf{M}$ commutes with group transformations $[G, \mathbf{M}] = 0$. Projection operators (A1.3) constructed from $\mathbf{M}$ are polynomials in $\mathbf{M}$, so they also commute with all $g \in \mathcal{G}$:

$$[G, P_i] = 0 \tag{A1.13}$$

Hence, a $[d \times d]$ matrix rep can be written as a direct sum of $[d_i \times d_i]$ matrix reps:

$$G = \mathbf{1}G\mathbf{1} = \sum_{i,j} P_i G P_j = \sum_i P_i G P_i = \sum_i G_i . \tag{A1.14}$$

In the diagonalized rep (A1.4), the matrix $\mathbf{g}$ has a block diagonal form:

$$\mathbf{CgC}^\dagger = \begin{bmatrix} \mathbf{g}_1 & 0 & 0 \\ 0 & \mathbf{g}_2 & 0 \\ 0 & 0 & \ddots \end{bmatrix}, \qquad \mathbf{g} = \sum_i \mathbf{C}^i \mathbf{g}_i \mathbf{C}_i . \tag{A1.15}$$

The rep $\mathbf{g}_i$ acts only on the d_i-dimensional subspace V_i consisting of vectors $P_i q$, $q \in V$. In this way an invariant $[d \times d]$ hermitian matrix $\mathbf{M}$ with r distinct eigenvalues induces a decomposition of a d-dimensional vector space V into a direct sum of d_i-dimensional vector subspaces V_i:

$$V \xrightarrow{\mathbf{M}} V_1 \oplus V_2 \oplus \ldots \oplus V_r . \tag{A1.16}$$

References

[1] N. Bleistein and R. A. Handelsman, *Asymptotic Expansions of Integrals* (Dover, New York, 1986).

Exercises

A1.1. Who ordered $\sqrt{\pi}$? Derive the Gaussian integral

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, e^{-\frac{x^2}{2a}} = \sqrt{a}, \qquad a > 0.$$

assuming only that you know to integrate the exponential function e^{-x}. Hint: x^2 is a radius-squared of something. π is related to the area or circumference of something.

A1.2. d-dimensional Gaussian integrals. Show that the Gaussian integral in d-dimensions is given by

$$\begin{aligned} Z[J] &= \int d^dx \, e^{-\frac{1}{2}x^\top \cdot M^{-1} \cdot x + x^\top \cdot J} \\ &= (2\pi)^{d/2} |\det M|^{\frac{1}{2}} \, e^{\frac{1}{2}J^\top \cdot M \cdot J}, \qquad \text{(A1.17)} \end{aligned}$$

where M is a real positive definite $[d \times d]$ matrix, i.e., a matrix with strictly positive eigenvalues, x and J are d-dimensional vectors, and $(\cdots)^\top$ denotes the transpose.

This integral you will see over and over in statistical mechanics and quantum field theory: it's called 'free field theory', 'Gaussian model', 'Wick expansion', etc.. This is the starting, 'propagator' term in any perturbation expansion.

Here we require that the real symmetric matrix M in the exponent is strictly positive definite, otherwise the integral is infinite. Negative eigenvalues can be accommodated by taking a contour in the complex plane [1], see exercise A1.4 *Fresnel integral*. Zero eigenvalues require stationary phase approximations that go beyond the Gaussian saddle point approximation, typically to the Airy-function type stationary points, see exercise A1.5 *Airy function for large arguments*.

A1.3. Convolution of Gaussians.

(a) Show that the Fourier transform of the convolution

$$[f * g](x) = \int d^dy \, f(x - y)g(y)$$

corresponds to the product of the Fourier transforms

$$[f * g](x) = \frac{1}{(2\pi)^d} \int d^dk \, F(k)G(k)e^{-ik \cdot x}, \quad \text{(A1.18)}$$

where

$$F(k) = \int \frac{d^dx}{(2\pi)^{d/2}} f(x) \, e^{-ik \cdot x}, \quad G(k) = \int \frac{d^dx}{(2\pi)^{d/2}} g(x) \, e^{-ik \cdot x}.$$

(b) Consider two normalized Gaussians

$$\begin{aligned} f(x) &= \frac{1}{N_1} e^{-\frac{1}{2}x^\top \cdot \frac{1}{\Delta_1} \cdot x}, \quad N_1 = \sqrt{\det(2\pi\Delta_1)} \\ g(x) &= \frac{1}{N_2} e^{-\frac{1}{2}x^\top \cdot \frac{1}{\Delta_2} \cdot x}, \quad N_2 = \sqrt{\det(2\pi\Delta_2)} \\ 1 &= \int d^dk \, f(x) = \int d^dk \, g(x). \end{aligned}$$

Evaluate their Fourier transforms

$$F(k) = \frac{1}{(2\pi)^{d/2}} e^{\frac{1}{2}k^\top \cdot \Delta_1 \cdot k}, \qquad G(k) = \frac{1}{(2\pi)^{d/2}} e^{\frac{1}{2}k^\top \cdot \Delta_2 \cdot k}.$$

Show that the convolution of two normalized Gaussians is a normalized Gaussian

$$[f * g](x) = \frac{(2\pi)^{-d/2}}{\sqrt{\det(\Delta_1 + \Delta_2)}} e^{-\frac{1}{2}x^\top \cdot \frac{1}{\Delta_1 + \Delta_2} \cdot x}.$$

In other words, covariances Δ_j add up. This is the d-dimenional statement of the familiar fact that cumulative error squared is the sum of squares of individual errors. When individual errors are small, and you are adding up a sequence of them in time, you get Brownian motion. If the individual errors are small and added independently to a solution of a deterministic equation, you get Langevin and Fokker-Planck equations.

A1.4. Fresnel integral.

(a) Derive the Fresnel integral

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, e^{-\frac{x^2}{2ia}} = \sqrt{ia} = |a|^{1/2} e^{i\frac{\pi}{4}\frac{a}{|a|}}.$$

Consider the contour integral $I_R = \int_{C(R)} \exp(iz^2) \, dz$, where $C(R)$ is the closed circular sector in the upper half-plane with boundary points 0, R and $R \exp(i\pi/4)$. Show that $I_R = 0$ and that $\lim_{R\to\infty} \int_{C_1(R)} \exp(iz^2) \, dz = 0$, where $C_1(R)$ is the contour integral along the circular sector from R to $R\exp(i\pi/4)$. [Hint: use $\sin x \geq (2x/\pi)$ on $0 \leq x \leq \pi/2$.] Then, by breaking up the contour $C(R)$ into three components, deduce that

$$\lim_{R\to\infty} \left(\int_0^R e^{ix^2} dx - e^{i\pi/4} \int_0^R e^{-r^2} dr \right)$$

vanishes, and, from the real integration $\int_0^{\infty} \exp(-x^2) \, dx = \sqrt{\pi}/2$, deduce that

$$\int_0^{\infty} e^{ix^2} dx = e^{i\pi/4} \sqrt{\pi}/2.$$

Now rescale x by real number $a \neq 0$, and complete the derivation of the Fresnel integral.

(b) In exercise A1.2 the exponent in the d-dimensional Gaussian integrals was real, so the real symmetric matrix M in the exponent had to be strictly positive definite. However, in quantum physics one often has to evaluate the d-dimenional Fresnel integral

$$\frac{1}{(2\pi)^{d/2}} \int d^d\phi \, e^{-\frac{1}{2i}\phi^\top \cdot M^{-1}\cdot\phi + i\,\phi\cdot J}\,,$$

with a hermitian matrix M. Evaluate it. What are conditions on its spectrum in order that the integral be well defined?

A1.5. **Airy function for large arguments.** Important contributions as stationary phase points may arise from extremal points where the first non-zero term in a Taylor expansion of the phase is of third or higher order. Such situations occur, for example, at bifurcation points or in diffraction effects, (such as waves near sharp corners, waves creeping around obstacles, etc.). In such calculations, one meets Airy functions integrals of the form

$$Ai(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dy \, e^{i(xy - \frac{y^3}{3})}\,. \qquad (A1.19)$$

Calculate the Airy function $Ai(x)$ using the stationary phase approximation. What happens when considering the limit $x \to 0$. Estimate for which value of x the stationary phase approximation breaks down.

A1.6. **Solving the Lyapunov differential equation.** Continuous time Lyapunov evolution equation for a covariance matrix $Q(t)$ is given by

$$\dot{Q} = A\,Q + Q\,A^\top + \Delta\,, \qquad (A1.20)$$

where $\{Q, A, \Delta\}$ are $[d\times d]$ matrices. The superscript $(\ )^\top$ indicates the transpose of the matrix. The stability matrix $A = A(\phi)$ and the noise covariance matrix $\Delta = \Delta(\phi)$ are given. They are evaluated on a trajectory $\phi(t)$, and thus vary in time, $A(t) = A(\phi(t))$ and $\Delta(t) = \Delta(\phi(t))$. Determine the covariance matrix $Q(t)$ for a given initial condition $Q(0)$, by taking the following steps:

(a) Write the solution in the form

$$Q(t) = J(t)[Q(0) + W(t)]J^\top(t)\,,$$

with the Jacobian matrix $J(t)$ satisfying

$$\dot{J}(t) = A(t)\,J(t)\,, \qquad J(0) = I\,, \qquad (A1.21)$$

with I the $[d\times d]$ identity matrix. The Jacobian matrix at time t,

$$J(t) = \hat{T}e^{\int_0^t d\tau\,A(\tau)}\,, \qquad (A1.22)$$

where $\hat{T}$ denotes the 'time-ordering' operation, can be evaluated by integrating (A1.21).

(b) Show that $W(t)$ satisfies

$$\dot{W} = \frac{1}{J}\,\Delta\,\frac{1}{J^\top}\,, \qquad W(0) = 0\,. \qquad (A1.23)$$

(c) Integrate (A1.20) to obtain

$$Q(t) = J(t)\left[Q(0) + \int_0^t d\tau\,\frac{1}{J(\tau)}\,\Delta(\tau)\,\frac{1}{J^\top(\tau)}\right]J^\top(t)\,. \qquad (A1.24)$$

(d) If $A(t)$ commutes with itself throughout the interval $0 \le \tau \le t$, the time-ordering operation is redundant, and we have the explicit solution $J(t, t') = \exp\int_{t'}^t d\tau\,A(\tau)$. Show that in this case the solution reduces to

$$\begin{aligned} Q(t) \;=\;& J(t)\,Q(0)\,J(t)^\top \qquad (A1.25) \\ &+ \int_0^t d\tau'\,J(t,\tau')\,\Delta(\tau')\,J(t,\tau')^\top\,. \end{aligned}$$

(e) It is hard to imagine a time dependent $A(t) = A(\phi(t))$ that would be commuting. However, in the neighborhood of an equilibrium point ϕ^* one can approximate the stability matrix with its time-independent linearization, $A = A(\phi^*)$. Show that in that case (A1.22) reduces to

$$J(t, t') = e^{(t-t')A}\,,$$

and (A1.25) to what?

A1.7. **Solving the Lyapunov differential equation.** Prove that if A is stable, the continuous Lyapunov equation

$$AQ + QA^\top = -\Delta < 0\,.$$

has a solution

$$Q = \int_0^\infty dt\, e^{tA}\Delta e^{tA^\top}\,, \qquad (A1.26)$$

and that this solution is unique. (P. Cvitanović)

A1.8. **Solving the discrete Lyapunov equation.** Prove that if M is contracting, the discrete Lyapunov equation

$$Q - MQM^\top = \Delta > 0$$

has a solution

$$Q = \sum_{k=0}^\infty M^k \Delta M^{k\top}\,, \qquad (A1.27)$$

and that this solution is unique. (P. Cvitanović)

A1.9. **Continuous vs. discrete time Lyapunov equation.** Show that the continuous Lyapunov equation solution (suited to a Laplace transform),

$$Q = \int_0^\infty dt\, e^{tA} \Delta e^{tA^\top}\,, \qquad A < 0\,,$$

is equivalent to the discrete Lyapunov equation solution (suited to a Z-transform),

$$Q = \sum_{k=0}^\infty M^k \bar{\Delta} M^{k\top}\,, \qquad |M| < 1\,,$$

where

$$M = e^A\,, \quad \bar{\Delta} = \int_0^1 dt\, e^{tA} \Delta e^{tA^\top}\,.$$

Parenthetically, often the notation does not distinguish $\bar{\Delta}$ from Δ. It should. (P. Cvitanović)

A1.10. **Lyapunov differential equation in resolvent form.** Show that the continuous Lyapunov equation solution,

$$Q = \int_0^\infty dt\, e^{tA} \Delta e^{tA^\top}\,, \qquad A < 0\,,$$

is equivalent to

$$Q = \frac{1}{2\pi} \int_{-\infty}^\infty d\omega\, \frac{1}{i\omega - A} \Delta \frac{1}{-i\omega - A^\top}\,.$$

(P. Cvitanović)

A1.11. **Discrete time Lyapunov equation in the resolvent form.** Show that the continuous Lyapunov equation solution,

$$Q = \int_0^\infty dt\, e^{tA} \Delta e^{tA^\top}\,, \qquad A < 0\,,$$

is equivalent to the discrete Lyapunov equation solution in resolvent form,

$$Q = \frac{1}{2\pi} \int_0^{2\pi} d\omega\, \frac{1}{1 - e^{-i\omega} M} \bar{\Delta} \frac{1}{1 - e^{i\omega} M^\top}\,.$$

(P. Cvitanović)

A1.12. **Noise covariance matrix for a discrete time periodic orbit.**

(a) Prove that the covariance matrix at a periodic point ϕ_a on a limit cycle p,

$$Q_a \quad = \quad M_{p,a} Q_a M_{p,a}^\top + \Delta_{p,a}\,, \qquad \text{(A1.28)}$$

where

$$\begin{aligned}
\Delta_{p,a} \quad = \quad & \Delta_a + M_{a-1}\Delta_{a-1}M_{a-1}^\top + M_{a-2}^2 \Delta_{a-2}(M_{a-2}^2)^\top \\
& + \cdots + M_{a-n_p+1}^{n_p-1} \Delta_{a-n_p+1}(M_{a-n_p+1}^{n_p-1})^\top \quad \text{(A1.29)}
\end{aligned}$$

is the noise accumulated per a single transversal of the periodic orbit, $M_{p,a} = M_p(\phi_a)$ is the cycle Jacobian matrix evaluated on the periodic point ϕ_a, and we have used the periodic orbit condition $\phi_{a+n_p} = \phi_a$.

(b) Derive the analogous formulas for the adjoint Fokker-Planck covariance matrix at a periodic point ϕ_a on a repelling cycle p.