QUANTUM FIELD THEORY
a cyclist tour

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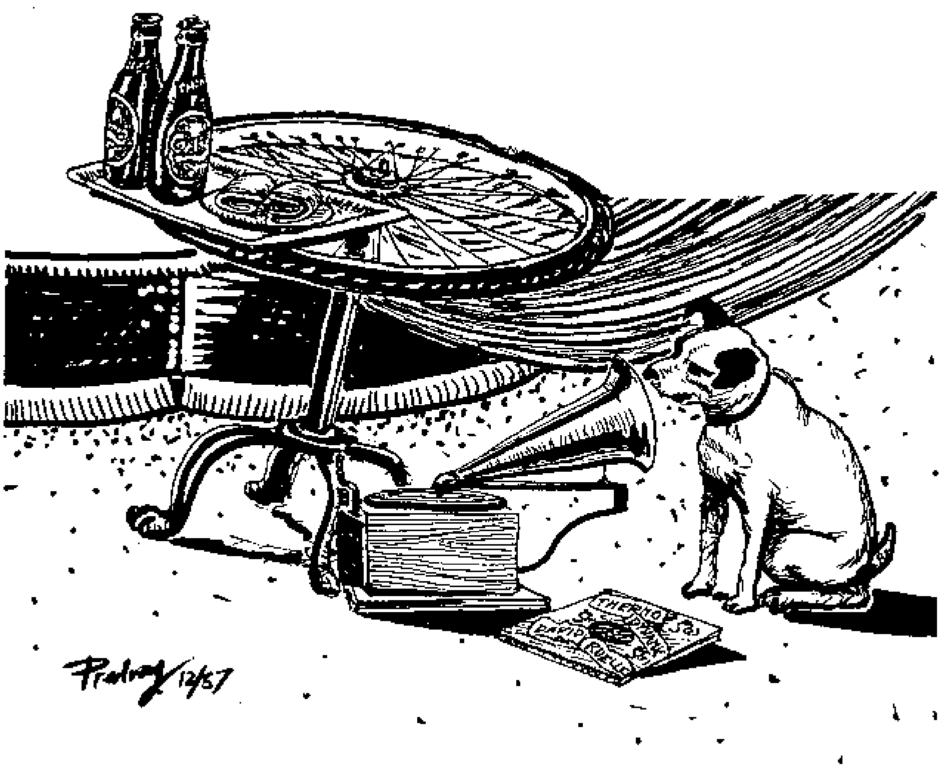

What reviewers say:

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

Incomplete notes for a
quantum field theory course

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Preface

Ben Mottelson is the only physicist I personally know who thinks 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 Newtonian and quantum mechanics follow from variational principles.

On the other hand, 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, spectra, path integrals, spins, angular momenta– under a closer inspection has nothing specifically 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 us?

Over the years I have watched in amazement study group after study group of graduate students grovel in orgies of Minkowski and spin indices, and tried in vain to deprogram them through my ChaosBook.org/FieldTheory book [2], but all in vain: students *want* Quantum Field Theory to be mysterious and accessed only by pages of indix summations. Or two-forms. 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 of the steering wheel and gesticulating: "Path integrals are everything!" These lectures are about of "everything." The theory is developed here at not quite the pedestrian level, perhaps a cyclist level. We do it mostly on a finite lattice, without any functional voodoo; all we have to know is how to manipulate finite dimensional vectors and matrices. More of such stuff can be found in ref. [2].

This version of field theory presupposes prior exposure to the Ising model and the Landau mean field theory of critical phenomena on the level of ref. [1], or any other decent introduction to critical phenomena.

Acknowledgments. These notes owe its existence to the Niels Bohr Institute's and Nordita's hospitable and nurturing environment, and the private, national and cross-national foundations that have supported the collaborators' research over a span of several decades. I am indebted to Benny Lautrup both for my first introduction to lattice field theory, and for the sect. 1.3 interpretation of the Fourier transform as the spectrum of the stepping operator. And last but not least– profound thanks to all the unsung heroes–students and colleagues, too numerous to list here–who have supported this project over many years in many ways, by surviving courses based on these notes, by providing invaluable insights, by teaching us, by inspiring us. I am thank the Carlsberg Foundation and Glen P. Robinson for partial support, and Dorte Glass, Tzatzilha Torres Guadarrama and Raenell Soller for typing parts of the manuscript.

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 grounds kept him alive.

Chapter 1

Lattice field theory

We motivate path integrals to come by formulating the simplest example of 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.

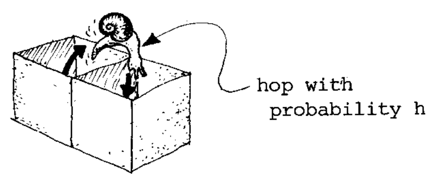
1.1 Wanderings of a drunken snail

Statistical mechanics is formulated in a Euclidean world in which there is no time, just space. 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 - might be related to the “mass” of the particle.

We assume that the state of a particle is specified by its position, and that it has no further internal degrees of freedom, such as spin or color: $i = (x_1, x_2, \cdots, x_d)$. 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):

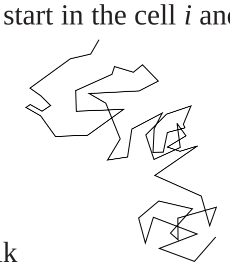


The number of neighboring cells defines the dimension of the space. The stepping and stopping probabilities are related by the probability conservation: $1 = s + 2dh$. Taking the stepping probability to be the same in all directions means that we have assumed that the space is *isotropic*.

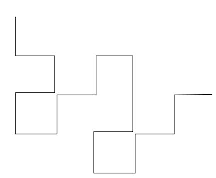
Our next assumption is that the space is *homogeneous*, i.e., that the stepping probability does not depend on the location of the cell; otherwise the propagation is not free, but is constrained by some external geometry. This can either mean that the space is infinite, or that it is compact and periodic (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. The requirement of insensitivity to the very short and very long distances means that the theory must have nice ultraviolet and infrared properties.

Let a particle start in the cell i and step along until it stops in the cell j.



a Brownian walk



a walk on a lattice

The probability of this process is $h^\ell s$, where ℓ is the number of steps in the corresponding path. The total probability that a particle wanders from the ith cell and stops in the jth cell is the sum of probabilities associated with all possible paths connecting the two cells:

$$\Delta_{ij} = s \sum_{\ell} h^{\ell} N_{ij}(\ell) \,, \tag{1.1}$$

where $N_{ij}(\ell)$ is the number of all paths of length ℓ connecting lattice sites i and j. In order to compute $N_{ij}(\ell)$, define a stepping operator

$$(\sigma^{\mu})_{ij} = \delta_{i+n_{\mu},j} \,, \tag{1.2}$$

where n_{μ} is a unit step in direction μ. If a particle is introduced into the ith cell by a source $J_k = \delta_{ik}$, the stepping operator moves it into a neighboring cell:

$$(\sigma^{\mu} J)_k = \delta_{i+n_{\mu},k} \to \text{[FieldTheory-p63a.ps]} \,.$$

The operator

$$(h \cdot \sigma)_{ij} = \sum_{\mu=1}^{d} h_{\mu}[(\sigma^{\mu})_{ij} + (\sigma^{\mu})_{ji}] \,, \qquad h_{\mu} = (h, h, \cdots, h) \tag{1.3}$$

generates all steps of length 1 with probability h:

$$(h \cdot \sigma) J = h \,\text{[FieldTheory-p63b.ps]} \,, \qquad i\text{th cell} \,.$$

(The examples are drawn in two dimensions). The paths of length 2 are generated by

$$(h \cdot \sigma)^2 J = h^2 \,\text{[FieldTheory-p63c.ps]} \,,$$

and so on. Note –and this is the key observation– that the ith component of the vector $(h \cdot \sigma)^{\ell} J$ counts the number of paths of length ℓ connecting the ith and the kth cells. The total probability that the particle stops in the kth cell is given by

$$\begin{aligned} \phi_k &= s \sum_{\ell=0}^{\infty} (h \cdot \sigma)^{\ell}_{kj} J_j \\ \phi &= \frac{s}{1 - h \cdot \sigma} J \,. \end{aligned} \tag{1.4}$$

The value of the field ϕ_k at a space point k measures the probability of observing the particle introduced into the system by the source J. The Euclidean free scalar particle propagator (1.1) is given by

$$\Delta_{ij} = \left(\frac{s}{1 - h \cdot \sigma} \right)_{ij} \,, \tag{1.5}$$

or, in the continuum limit (see sect. 1.5) by

exercise ??

$$\Delta(x, y) = \int \frac{d^d k}{(2\pi)^d} \frac{e^{ik\cdot(x-y)}}{k^2 + m^2} \,. \tag{1.6}$$

1.2 Lattice derivatives

In order to set up continuum field-theoretic equations which describe the evolution of spatial variations of fields, we need to define *lattice derivatives*.

Consider a smooth function $\phi(x)$ evaluated on an infinite d-dimensional lattice

$$\phi_\ell = \phi(x)\,, \qquad x = a\ell = \text{lattice point}\,, \quad \ell \in \mathbf{Z}^d\,, \tag{1.7}$$

where a is the lattice spacing. Each set of values of $\phi(x)$ (a vector ϕ_ℓ) is a possible lattice configuration. Assume the lattice is hyper-cubic, and let $\hat{n}_\mu \in \{\hat{n}_1, \hat{n}_2, \cdots, \hat{n}_d\}$ be the unit lattice cell vectors pointing along the d positive directions. The *lattice derivative* is then

$$(\partial_\mu \phi)_\ell = \frac{\phi(x + a\hat{n}_\mu) - \phi(x)}{a} = \frac{\phi_{\ell+\hat{n}_\mu} - \phi_\ell}{a}\,. \tag{1.8}$$

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 *stepping operator* in the direction μ

$$\left(\sigma_\mu\right)_{\ell j} = \delta_{\ell+\hat{n}_\mu, j}\,. \tag{1.9}$$

As σ will play a central role in what follows, it pays to understand what it does.

In computer dicretizations, the lattice will be a finite d-dimensional hypercubic lattice

$$\phi_\ell = \phi(x)\,, \qquad x = a\ell = \text{lattice point}\,, \quad \ell \in (\mathbf{Z}/N)^d\,, \tag{1.10}$$

where a is the lattice spacing and there are N^d points in all. For a hyper-cubic lattice the translations in different directions commute, $\sigma_\mu \sigma_\nu = \sigma_\nu \sigma_\mu$, so it is sufficient to understand the action of (1.9) on a 1-dimensional lattice.

Let us write down σ for the 1-dimensional case in its full $[N{\times}N]$ matrix glory. Writing the finite lattice stepping operator (1.9) as an 'upper shift' matrix,

$$\sigma = \begin{pmatrix} 0 & 1 & & & & \\ & 0 & 1 & & & \\ & & 0 & 1 & & \\ & & & & \ddots & \\ & & & & 0 & 1 \\ 0 & & & & & 0 \end{pmatrix}, \tag{1.11}$$

is no good, as σ so defined is nilpotent, and after N steps nothing is left, $\sigma^N = 0$. A sensible way to approximate an infinite lattice by a finite one is to replace it by a lattice periodic in each $\hat{n}_\mu$ direction. On a *periodic lattice* every point is equally far from the "boundary" $N/2$ steps away, the "surface" effects are equally negligible for all points, and the stepping operator acts as a cyclic permutation matrix

$$\sigma = \begin{pmatrix} 0 & 1 & & & & \\ & 0 & 1 & & & \\ & & 0 & 1 & & \\ & & & & \ddots & \\ & & & & 0 & 1 \\ 1 & & & & & 0 \end{pmatrix}, \tag{1.12}$$

with '1' in the lower left corner assuring periodicity.

Applied to the lattice configuration $\phi = (\phi_1, \phi_2, \cdots, \phi_N)$, the stepping operator translates the configuration by one site, $\sigma\phi = (\phi_2, \phi_3, \cdots, \phi_N, \phi_1)$. Its transpose translates the configuration the other way, so the transpose is also the inverse, $\sigma^{-1} = \sigma^T$. The partial lattice derivative (1.8) can now be written as a multiplication by a matrix:

$$\partial_\mu \phi_\ell = \frac{1}{a}\left(\sigma_\mu - \mathbf{1}\right)_{\ell j} \phi_j \,.$$

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

$$\partial = \frac{1}{a}\begin{pmatrix} -1 & 1 & & & & \\ & -1 & 1 & & & \\ & & -1 & 1 & & \\ & & & & \ddots & \\ & & & & & 1 \\ 1 & & & & & -1 \end{pmatrix}. \tag{1.13}$$

To belabor the obvious: On a finite lattice of N points a derivative is simply a finite $[N \times N]$ 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.

1.2.1 Lattice Laplacian

In the continuum, integration by parts moves ∂ around, $\phi^T \cdot \partial^2\phi \to -\partial\phi^T \cdot \partial\phi$; on a lattice this amounts to a matrix transposition

$$\left[\left(\sigma_\mu - \mathbf{1}\right)\phi\right]^T \cdot \left[\left(\sigma_\mu - \mathbf{1}\right)\phi\right] = \phi^T \cdot \left(\sigma_\mu^{-1} - \mathbf{1}\right)\left(\sigma_\mu - \mathbf{1}\right)\cdot\phi \,.$$

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

$$\partial^T = \frac{1}{a}\left(\sigma^{-1} - \mathbf{1}\right) = -\sigma^{-1}\frac{1}{a}\left(\sigma - \mathbf{1}\right) = -\sigma^{-1}\partial \,.$$

The symmetric (self-adjoint) combination $\Delta = -\partial^T\partial$

$$\Delta = -\frac{1}{a^2}\sum_{\mu=1}^{d}\left(\sigma_\mu^{-1} - \mathbf{1}\right)\left(\sigma_\mu - \mathbf{1}\right) = -\frac{2}{a^2}\sum_{\mu=1}^{d}\left(\mathbf{1} - \frac{1}{2}(\sigma_\mu^{-1} + \sigma_\mu)\right) \tag{1.14}$$

is the *lattice Laplacian*. We shall show below that this Laplacian has the correct continuum limit. In the 1-dimensional case the $[N \times N]$ matrix representation of the lattice Laplacian is:

$$\Delta = \frac{1}{a^2}\begin{pmatrix} -2 & 1 & & & & 1 \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & 1 & & \ddots & \\ & & & & & 1 \\ 1 & & & & 1 & -2 \end{pmatrix}. \tag{1.15}$$

The lattice Laplacian measures the second variation of a field ϕ_ℓ 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, $\phi_\ell = \phi(a\ell)$, where $\phi(a\ell)$ is defined by the value of the continuum function $\phi(x) = x^2$ at the lattice point $x_\ell = a\ell$.

1.2.2 Inverting the Laplacian

Evaluation of perturbative corrections in (2.20) requires that we come to grips with the "free" or "bare" propagator M. While the inverse propagator M^{-1} is a simple difference operator (2.19), the propagator is a messier object. A way to compute is to start expanding the propagator M as a power series in the Laplacian

$$\beta M = \frac{1}{m_0'^2 \mathbf{1} - \Delta} = \frac{1}{m_0'^2} \sum_{k=0}^{\infty} \left(\frac{1}{m_0'^2} \right)^k \Delta^k . \tag{1.16}$$

As Δ is a finite matrix, the expansion is convergent for sufficiently large $m_0'^2$. To get a feeling for what is involved in evaluating such series, evaluate Δ^2 in the 1-dimensional case:

$$\Delta^2 = \frac{1}{a^4} \begin{pmatrix} 6 & -4 & 1 & & & 1 & -4 \\ -4 & 6 & -4 & 1 & & & 1 \\ 1 & -4 & 6 & -4 & 1 & & \\ & 1 & -4 & \ddots & & & 1 \\ 1 & & & & & 6 & -4 \\ -4 & 1 & & & 1 & -4 & 6 \end{pmatrix} . \tag{1.17}$$

What Δ^3, Δ^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. In statistical mechanics, M is the (bare) 2-point correlation. In quantum field theory, it is called a propagator, for reasons explained in sect. 1.1. exercise ??

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 will show how this works in sect. 1.3.

1.3 Periodic lattices

Our task now is to transform M 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.

Consider the effect of a lattice translation $\phi \to \sigma\phi$ on the matrix polynomial

$$S[\sigma\phi] = -\frac{1}{2}\phi^T \left(\sigma^T M^{-1} \sigma\right) \phi .$$

As M^{-1} is constructed from σ and its inverse, M^{-1} and σ commute, and the function $S[\sigma\phi]$ is invariant under translations,

$$S[\sigma\phi] = S[\phi] = -\frac{1}{2}\phi^T \cdot M^{-1} \cdot \phi \,. \tag{1.18}$$

If a function (in this case, the function $S[\phi]$) defined on a vector space (in this case, the configuration ϕ) commutes with a linear operator σ, then the eigenvalues of σ can be used to decompose the ϕ vector space into invariant subspaces. For a hypercubic lattice the translations in different directions commute, $\sigma_\mu\sigma_\nu = \sigma_\nu\sigma_\mu$, so it is sufficient to understand the spectrum of the 1-dimensional stepping operator (1.12). To develop a feeling for how this reduction to invariant subspaces works in practice, let us continue humbly, 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 stepping operator σ (1.12) on a 2-point lattice $\phi = (\phi_1, \phi_2)$ is to permute the two lattice sites

$$\sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} .$$

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

$$(\sigma + 1)(\sigma - 1) = 0 \,,$$

with eigenvalues $\lambda_0 = 1, \lambda_1 = -1$. Construct now the symmetrization, antisymmetrization projection operators

$$P_0 = \frac{\sigma - \lambda_1 \mathbf{1}}{\lambda_0 - \lambda_1} = \frac{1}{2}(\mathbf{1} + \sigma) = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \tag{1.19}$$

$$P_1 = \frac{\sigma - \mathbf{1}}{-1 - 1} = \frac{1}{2}(\mathbf{1} - \sigma) = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} . \tag{1.20}$$

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

$$\begin{aligned} \phi &= \mathbf{1}\,\phi \;=\; P_0 \cdot \phi \;+\; P_1 \cdot \phi \,, \\ \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} &= \frac{(\phi_1 + \phi_2)}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{(\phi_1 - \phi_2)}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} && (1.21) \\ &= \tilde{\phi}_0 \hat{n}_0 + \tilde{\phi}_1 \hat{n}_1 \,. && (1.22) \end{aligned}$$

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

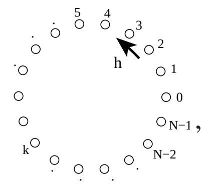
In this way the characteristic equation $\sigma^2 = \mathbf{1}$ enables us to reduce the 2-dimensional lattice configuration to two 1-dimensional ones, on which the value of the stepping operator σ is a number, $\lambda \in \{1, -1\}$, and the eigenvectors are $\hat{n}_0 = \frac{1}{\sqrt{2}}(1, 1)$, $\hat{n}_1 = \frac{1}{\sqrt{2}}(1, -1)$. We have inserted $\sqrt{2}$ factors for convenience, in order that the eigenvectors be normalized unit vectors. 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 N sites.

Each application of σ translates the lattice one step; in N steps the lattice is back in the original configuration

$$\sigma^N = \mathbf{1}$$



so the eigenvalues of σ are the N distinct N-th roots of unity

$$\sigma^N - \mathbf{1} = \prod_{k=0}^{N-1}(\sigma - \omega^k \mathbf{1}) = 0\,, \qquad \omega = e^{i\frac{2\pi}{N}}\,. \tag{1.23}$$

As the eigenvalues are all distinct and N in number, the space is decomposed into N 1-dimensional subspaces. The general theory (expounded in appendix A.1) associates with the k-th eigenvalue of σ a projection operator that projects a configuration ϕ onto k-th eigenvector of σ,

$$P_k = \prod_{j\neq k} \frac{\sigma - \lambda_j \mathbf{1}}{\lambda_k - \lambda_j}\,. \tag{1.24}$$

A factor $(\sigma - \lambda_j \mathbf{1})$ kills the j-th 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 $\prod_{j\neq k}(\lambda_k - \lambda_j)$ ensures that P_k is normalized as a projection operator. The set of the projection operators is complete,

$$\sum_k P_k = \mathbf{1}\,, \tag{1.25}$$

and orthonormal

$$P_k P_j = \delta_{kj} P_k \qquad \text{(no sum on } k)\,. \tag{1.26}$$

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 projection operators. However, in case at hand the eigenvectors are so simple that we can forget the general theory, and construct the solutions of the eigenvalue condition

$$\sigma\,\varphi_k \qquad = \qquad \omega^k \varphi_k \tag{1.27}$$

by hand:

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

The $1/\sqrt{N}$ factor is chosen in order that φ_k be normalized complex unit vectors

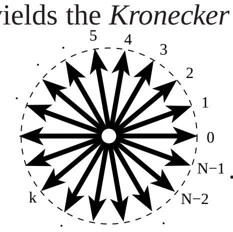
$$
\begin{aligned}
\varphi_k^\dagger \cdot \varphi_k &= \frac{1}{N}\sum_{k=0}^{N-1} 1 = 1\,, \qquad \text{(no sum on } k\text{)} \\
\varphi_k^\dagger &= \frac{1}{\sqrt{N}}\left(1, \omega^{-k}, \omega^{-2k}, \cdots, \omega^{-(N-1)k}\right).
\end{aligned}
\tag{1.28}
$$

The eigenvectors are orthonormal

$$
\varphi_k^\dagger \cdot \varphi_j = \delta_{kj}\,, \tag{1.29}
$$

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

$$
\delta_{kj} = \frac{1}{N}\sum_{\ell=0}^{N-1} e^{i\frac{2\pi}{N}(k-j)\ell} \tag{1.30}
$$



The sum is over the N unit vectors pointing at a uniform distribution of points on the complex unit circle; they cancel each other unless $k = j$ (mod N), in which case each term in the sum equals 1.

The projection operators can be expressed in terms of the eigenvectors (1.27), (1.28) as

$$
(P_k)_{\ell\ell'} = (\varphi_k)_\ell (\varphi_k^\dagger)_{\ell'} = \frac{1}{N} e^{i\frac{2\pi}{N}(\ell-\ell')k}\,, \qquad \text{(no sum on } k\text{)}\,. \tag{1.31}
$$

The completeness (1.25) follows from (1.30), and the orthonormality (1.26) from (1.29).

$\tilde{\phi}_k$, the projection of the ϕ configuration on the k-th subspace is given by

$$
\begin{aligned}
(P_k \cdot \phi)_\ell &= \tilde{\phi}_k\,(\varphi_k)_\ell\,, \qquad \text{(no sum on } k\text{)} \\
\tilde{\phi}_k &= \varphi_k^\dagger \cdot \phi = \frac{1}{\sqrt{N}}\sum_{\ell=0}^{N-1} e^{-i\frac{2\pi}{N}k\ell}\phi_\ell
\end{aligned}
\tag{1.32}
$$

We recognize $\tilde{\phi}_k$ as the *discrete Fourier transform* of ϕ_ℓ. 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 the generator of translations) and when are they the natural set of basis functions (only if the theory is translationally invariant).

1.4.1 Fourier transform of the propagator

Now insert the identity $\sum P_k = \mathbf{1}$ wherever profitable:

$$
\mathbf{M} = \mathbf{1}\mathbf{M}\mathbf{1} = \sum_{kk'} P_k \mathbf{M} P_{k'} = \sum_{kk'} \varphi_k (\varphi_k^\dagger \cdot \mathbf{M} \cdot \varphi_{k'}) \varphi_{k'}^\dagger\,.
$$

The matrix

$$
\tilde{M}_{kk'} = (\varphi_k^\dagger \cdot \mathbf{M} \cdot \varphi_{k'}) \tag{1.33}
$$

is the Fourier space representation of $\mathbf{M}$. No need to stop here - the terms in the action (1.18) that couple four (and, in general, 3, 4, $\cdots$) fields also have the Fourier space representations

$$\begin{aligned}
\gamma_{\ell_1\ell_2\cdots\ell_n}\,\phi_{\ell_1}\phi_{\ell_2}\cdots\phi_{\ell_n} &= \tilde{\gamma}_{k_1k_2\cdots k_n}\,\tilde{\phi}_{k_1}\tilde{\phi}_{k_2}\cdots\tilde{\phi}_{k_n}\,, \\
\tilde{\gamma}_{k_1k_2\cdots k_n} &= \gamma_{\ell_1\ell_2\cdots\ell_n}(\varphi_{k_1})_{\ell_1}(\varphi_{k_2})_{\ell_2}\cdots(\varphi_{k_n})_{\ell_n} \\
&= \frac{1}{N^{n/2}}\sum_{\ell_1\cdots\ell_n}\gamma_{\ell_1\ell_2\cdots\ell_n}\,e^{-i\frac{2\pi}{N}(k_1\ell_1+\cdots+k_n\ell_n)}\,.
\end{aligned} \tag{1.34}$$

According to (1.29) the matrix $U_{k\ell} = (\varphi_k)_\ell = \frac{1}{\sqrt{N}}e^{i\frac{2\pi}{N}k\ell}$ is a unitary matrix, so the Fourier transform is a linear, unitary transformation, $UU^\dagger = \sum P_k = \mathbf{1}$, with Jacobian $\det U = 1$. The form of the path integral (2.8) does not change under $\phi \to \tilde{\phi}_k$ transformation, and from the formal point of view, 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 $\mathbf{M}$ is the trace in either representation

$$\begin{aligned}
\mathrm{tr}\,\mathbf{M} &= \sum_\ell M_{\ell\ell} = \sum_{kk'}\sum_\ell (P_k\mathbf{M}P_{k'})_{\ell\ell} \\
&= \sum_{kk'}\sum_\ell (\varphi_k)_\ell(\varphi_k^\dagger\cdot\mathbf{M}\cdot\varphi_{k'})(\varphi_{k'}^\dagger)_\ell = \sum_{kk'}\delta_{kk'}\tilde{M}_{kk'} = \mathrm{tr}\,\tilde{\mathbf{M}}\,.
\end{aligned}$$

From this it follows that $\mathrm{tr}\,\mathbf{M}^n = \mathrm{tr}\,\tilde{\mathbf{M}}^n$, and from the $\mathrm{tr}\ln = \ln\mathrm{tr}$ relation that $\det\mathbf{M} = \det\tilde{\mathbf{M}}$. 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.

OK, a dizzying quantity of indices. But what's the payback?

1.4.2 Lattice Laplacian diagonalized

Now use the eigenvalue equation (1.27) to convert σ matrices into scalars. If $\mathbf{M}$ *commutes* with σ, then $(\varphi_k^\dagger\cdot\mathbf{M}\cdot\varphi_{k'}) = \tilde{M}_k\delta_{kk'}$, and the matrix $\mathbf{M}$ acts as a multiplication by the scalar $\tilde{M}_k$ on the kth subspace. For example, for the 1-dimensional version of the lattice Laplacian (1.14) the projection on the k-th subspace is

$$\begin{aligned}
(\varphi_k^\dagger\cdot\Delta\cdot\varphi_{k'}) &= \frac{2}{a^2}\left(\frac{1}{2}(\omega^{-k}+\omega^k)-1\right)(\varphi_k^\dagger\cdot\varphi_{k'}) \\
&= \frac{2}{a^2}\left(\cos\left(\frac{2\pi}{N}k\right)-1\right)\delta_{kk'}
\end{aligned} \tag{1.35}$$

In the k-th subspace the bare propagator is simply a number, and, in contrast to the mess generated by (1.16), there is nothing to inverting M^{-1}:

$$(\varphi_\mathbf{k}^\dagger\cdot M\cdot\varphi_{\mathbf{k}'}) = (\tilde{G}_0)_\mathbf{k}\delta_{\mathbf{k}\mathbf{k}'} = \frac{1}{\beta}\frac{\delta_{\mathbf{k}\mathbf{k}'}}{m_0'^2 - \frac{2c}{a^2}\sum_{\mu=1}^d\left(\cos\left(\frac{2\pi}{N}k_\mu\right)-1\right)}\,, \tag{1.36}$$

where $\mathbf{k} = (k_1, k_2, \cdots, k_\mu)$ is a d-dimensional vector in the N^d-dimensional dual lattice.

Going back to the partition function (2.20) and sticking in the factors of **1** into the bilinear part of the interaction, we replace the spatial J_ℓ by its Fourier transform $\tilde{J}_k$, and the spatial propagator $(M)_{\ell\ell'}$ by the diagonalized Fourier transformed $(\tilde{G}_0)_k$

$$J^T \cdot M \cdot J = \sum_{k,k'} (J^T \cdot \varphi_k)(\varphi_k^\dagger \cdot M \cdot \varphi_{k'})(\varphi_{k'}^\dagger \cdot J) = \sum_k \tilde{J}_k^\dagger (\tilde{G}_0)_k \tilde{J}_k \,. \tag{1.37}$$

What's the price? The interaction term $S_I[\phi]$ (which in (2.20) was local in the configuration space) now has a more challenging k dependence in the Fourier transform version (1.34). For example, the locality of the quartic term leads to the 4-vertex *momentum conservation* in the Fourier space

$$\begin{aligned} S_I[\phi] &= \frac{1}{4!}\gamma_{\ell_1\ell_2\ell_3\ell_4}\ \phi_{\ell_1}\phi_{\ell_2}\phi_{\ell_3}\phi_{\ell_4} = -\beta u \sum_{\ell=1}^{N^d} (\phi_\ell)^4 \ \Rightarrow \\ &= -\beta u \frac{1}{N^d} \sum_{\{\mathbf{k}_i\}}^{N} \delta_{0,\mathbf{k}_1+\mathbf{k}_2+\mathbf{k}_3+\mathbf{k}_4}\ \tilde{\phi}_{\mathbf{k}_1}\tilde{\phi}_{\mathbf{k}_2}\tilde{\phi}_{\mathbf{k}_3}\tilde{\phi}_{\mathbf{k}_4} \,. \end{aligned} \tag{1.38}$$

1.5 Continuum field theory

References

[1.1] P.M. Chaikin and T.C. Lubensky, *Principles of condensed matter physics* (Cambridge University Press, Cambridge 1995).

[1.2] P. Cvitanović, *Field theory*, notes prepared by E. Gyldenkerne (Nordita, Copenhagen, January 1983); ChaosBook.org/FieldTheory.

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

[1.4] N. Bleistein and R. A. Handelsman, *Asymptotic Expansions of Integrals* (Dover, New York, 1986).

[1.5] P. Cvitanović, "Chaotic field theory: A sketch," *Physica* **A 288**, 61 (2000);

[1.6] www.classicgaming.com/pac-man/home.html

[1.7] Read section 2.F of ref. [2].

[1.8] Read chapter 5 of ref. [2], pp. 61-64 up to eq. (5.6), and do the exercise 5.A.1. (reproduced as the exercise **??** here).

[1.9] R.B. Dingle, *Asymptotic Expansions: their Derivation and Interpretation* (Academic Press, London, 1973).

[1.10] P. Cvitanović, "Asymptotic estimates and gauge invariance", *Nucl. Phys.* **B127**, 176 (1977).

[1.11] P. Cvitanović, *Group Theory - Birdtracks, Lie's, and Exceptional Groups*, (Princeton Univ. Press, 2008); birtracks.eu.

Exercises

1.1. **Free-field theory combinatorics.** Check that there indeed are no combinatorial prefactors in the expansion (2.31).

1.2. **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 (2.23) for $g = 0.1$, $g = 0.02$, $g = 0.01$. The prettiest plot makes it into these notes as figure 2.2!

1.3. **Complex Gaussian integrals.** F
exercise 3.B.1 of ref. [2].

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

1.5. **Convexity of exponentials.** Pr
(2.25). Matthias Eschrig suggest th
proof be offered, applicable to any m
ing sequence with alternating signs.

1.6. **Wick expansion for ϕ^4 theories.** D
the combinatorial signs.

1.7. **Wick expansions.** Read sect. 3
3.C.2 of ref. [2].

Chapter 2

Path integrals

The path integral (3.35) 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 2.1 (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 $S[q]$ configurations q^c are determined by the zero-slope, saddle-point condition

$$\frac{d}{d\phi_\ell} S[q^c] + J_\ell = 0 \,. \tag{2.1}$$

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 (3.35) is given by the extremal configuration alone

$$\begin{aligned} Z[J] &= e^{W[J]} \to \sum_c e^{W_c[J]} = e^{W_c[J] + \ln n_c} \\ W_c[J] &= S[q^c] + q^c \cdot J \,. \end{aligned} \tag{2.2}$$

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

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

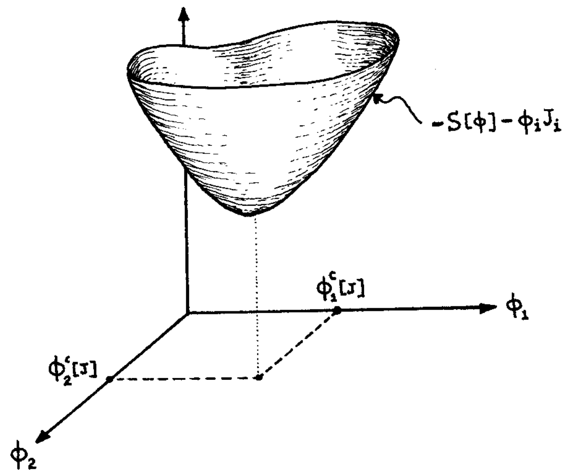


Figure 2.1: In the classical $\hbar \to 0$ limit (or the low temperature $T = 1/\beta$ limit) the path integral (2.8) is dominated by the minima of the integrand's exponent. The location ϕ^c of a minimum is determined by the extremum condition $\partial_\ell S[\phi^c] + J_\ell = 0$.

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 $S_I[q]$

$$\begin{aligned} S_0[q] &= -\sum_\ell q_\ell \left(M^{-1}\right)_{\ell,\ell'} q_\ell \,, \\ S_I[q] &= -(\cdots)_{\ell,\ell',\ell''} q_\ell q_{\ell'} q_{\ell''} + \cdots \,. \end{aligned} \tag{2.3}$$

Rewrite the partition sum (3.35) as

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

As the expectation value of any analytic function

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

can be recast in terms of derivatives with respect to J

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

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

exercise 1.3

$$\begin{aligned} e^{W[J]} &= e^{W_c[J]} e^{S_I[\frac{d}{dJ}]} \int [dq]\, e^{-\frac{1}{2} q^T \cdot M^{-1} \cdot q + q \cdot J} \Big|_{J=0} \\ &= |\det M|^{\frac{1}{2}}\, e^{W_c[J]} e^{S_I[\frac{d}{dJ}]}\, e^{\frac{1}{2} J^T \cdot M \cdot J} \Big|_{J=0} \,. \end{aligned} \tag{2.4}$$

M is invertible only if the minima in figure 2.1 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 [9]. 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 (2.4).

exercise 4.4

Expanding the exponentials and evaluating the $\frac{d}{dJ}$ derivatives in (2.4) 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 2.1 by a parabola, i.e., keeping only the quadratic terms in the Taylor expansion (2.3).

2.1 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

$$
\mathcal{H}_L[\phi] = \frac{r}{2}\phi_\ell\phi_\ell + \frac{c}{2}\partial_\mu\phi_\ell\partial_\mu\phi_\ell + u\sum_{\ell=1}^{N^d}\phi_\ell^4 \tag{2.5}
$$

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 (2.5) is replaced by

$$
\begin{aligned}
\mathcal{H}[\phi] &= \frac{1}{2}\partial_\mu\phi_\ell\partial_\mu\phi_\ell + \frac{m_0^2}{2}\phi_\ell\phi_\ell + \frac{g_0}{4!}\sum_\ell \phi_\ell^4 \\
m_0^2 &= \frac{r}{c}, \qquad g_0 = 4!\frac{u}{c^2} .
\end{aligned} \tag{2.6}
$$

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

$$
\begin{aligned}
S[\phi] &= -\frac{1}{2}(M^{-1})_{\ell\ell'}\phi_\ell\phi_{\ell'} + S_I[\phi], \\
S_I[\phi] &= \frac{1}{3!}\gamma_{\ell_1\ell_2\ell_3}\ \phi_{\ell_1}\phi_{\ell_2}\phi_{\ell_3} + \frac{1}{4!}\gamma_{\ell_1\ell_2\ell_3\ell_4}\ \phi_{\ell_1}\phi_{\ell_2}\phi_{\ell_3}\phi_{\ell_4} + \cdots .
\end{aligned} \tag{2.7}
$$

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

$$
\begin{aligned}
Z[J] &= e^{W[J]} = \int [d\phi] e^{S[\phi]+\phi\cdot J} \qquad (2.8)\\
&= Z[0]\left(1 + \sum_{n=1}^{\infty}\sum_{\ell_1\ell_2\cdots\ell_n} G_{\ell_1\ell_2\cdots\ell_n}\frac{J_{\ell_1}J_{\ell_2}\ldots J_{\ell_n}}{n!}\right), \\
G_{\ell_1\ell_2\cdots\ell_n} &= \langle\phi_{\ell_1}\phi_{\ell_2}\ldots\phi_{\ell_n}\rangle = \frac{1}{Z[0]}\frac{d}{dJ_{\ell_1}}\cdots\frac{d}{dJ_{\ell_n}}Z[J]\bigg|_{J=0} . \qquad (2.9)
\end{aligned}
$$

The "bare mass" m_0 and the "bare coupling" g_0 in (2.6) 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.

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,"

$$S[\phi] = -\frac{M^2}{2}\phi^T \cdot \phi - \frac{C}{2}\left[\left(\sigma_\mu - \mathbf{1}\right)\phi\right]^T \cdot \left(\sigma_\mu - \mathbf{1}\right)\phi + S_I[\phi] . \tag{2.10}$$

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 (1.38).

Consider the action

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

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

$$S[\sigma\phi] = S[\phi] = -\frac{1}{2}\phi^T \cdot M^{-1} \cdot \phi - \frac{\beta g_0}{4!}\sum_{\ell=1}^{N^d}\phi_\ell^4 . \tag{2.11}$$

2.2 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

$$I = \int_{-\infty}^{\infty} dx\, e^{-t\Phi(x)} \tag{2.12}$$

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,

$$I \approx \sum_{x^*} \sqrt{2\pi/t\Phi''(x^*)}\, e^{-t\Phi(x^*)} . \tag{2.13}$$

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

exercise 1.3

$$\int [dx] e^{-\frac{1}{2}x^T \cdot M^{-1} \cdot x + x \cdot J} = (\det M)^{\frac{1}{2}} \, e^{\frac{1}{2}J^T \cdot M \cdot J} \,, \qquad (2.14)$$

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

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

The stationary phase estimate of (2.12) is

exercise ??

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

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 (2.14) 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 (4.4) on Airy integral).

The "path integral" (2.8) 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 2.1 (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 $S[\phi]$ configurations ϕ^c are determined by the zero-slope, saddle-point condition

$$\frac{d}{d\phi_\ell} S[\phi^c] + J_\ell = 0 \,. \qquad (2.15)$$

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 (2.8) is given by the extremal configuration alone

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

$$W_c[J] = S[\phi^c] + \phi^c \cdot J \,. \qquad (2.16)$$

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 c-th 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 $S_I[\phi]$

$$\begin{aligned} S_0[\phi] &= -\sum_\ell \phi_\ell \left(\frac{\beta r}{2c} + 12\frac{\beta u}{c^2}({\phi^c}_\ell)^2\right)\phi_\ell + \frac{\beta}{2}\sum_{\ell,\ell'}\phi_\ell \Delta_{\ell\ell'}\phi_{\ell'}\,, \\ S_I[\phi] &= -\frac{\beta u}{c^2}\sum_{\ell=1}^{N^d}\phi_\ell^4\,. \end{aligned} \tag{2.17}$$

Spatially nonuniform ${\phi^c}_\ell$ are conceivable. The *mean field theory* assumption is that the translational invariance of the lattice is not broken, and ${\phi^c}_\ell$ is independent of the lattice point, ${\phi^c}_\ell \to \phi^c$. In the ϕ^4 theory considered here, it follows from (2.15) 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 configuration with the same $S[\phi^c]$, and in the thermodynamic limit we can neglect the "mean field entropy" $\ln n_c$ in (2.16) when computing free energy density per site [3],

$$-\beta f[J] = \lim_{N\to\infty} W[J]/N^d\,. \tag{2.18}$$

We collect the matrix of bilinear ϕ coefficients in

$$(M^{-1})_{\ell\ell'} = \beta m_0'^2\delta_{\ell\ell'} - \beta c\Delta_{\ell\ell'}\,, \qquad m_0'^2 = m_0^2 + 12u(\phi^c)^2 \tag{2.19}$$

in order to be able to rewrite the partition sum (2.8) as

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

As the expectation value of any analytic function

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

can be recast in terms of derivatives with respect to J

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

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

exercise 1.3

$$\begin{aligned} e^{W[J]} &= e^{W_c[J]} e^{S_I[\frac{d}{dJ}]}\int [d\phi] e^{-\frac{1}{2}\phi^T\cdot M^{-1}\cdot\phi + \phi\cdot J}\Big|_{J=0} \\ &= |\det M|^{\frac{1}{2}}\, e^{W_c[J]} e^{S_I[\frac{d}{dJ}]}\, e^{\frac{1}{2}J^T\cdot M\cdot J}\Big|_{J=0}\,. \end{aligned} \tag{2.20}$$

M is invertible only if the minima in figure 2.1 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 [9]. 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 (2.20).

As we shall show in sect. 2.6, expanding the exponentials and evaluating the $\frac{d}{dJ}$ derivatives in (2.20) 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 2.1 by a parabola, i.e., keeping only the quadratic terms in the Taylor expansion (2.17). For a single minimum the "free energy" is in this approximation

$$W[J]_{\text{1-loop}} = W_c[J] + \frac{1}{2}\text{tr} \ln M , \tag{2.21}$$

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.

exercise 1.4

2.3 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 $[1\times 1]$ 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

$$Z[J] = \int \frac{d\phi}{\sqrt{2\pi}} e^{-\phi^2/2 - g\phi^4/4 + \phi J} . \tag{2.22}$$

Substituting M as defined by (2.19) 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 (2.20) 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

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

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 (2.31) 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:

$$\begin{aligned} Z[0] &= \sum_n Z_n g^n , \\ Z_n &= \frac{(-1)^n}{n!4^n} \int \frac{d\phi}{\sqrt{2\pi}} \phi^{4n} e^{-\phi^2/2} = \frac{(-1)^n}{16n!}\frac{(4n)!}{(2n)!} . \end{aligned} \tag{2.23}$$

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

$$g^n Z_n \approx \frac{1}{\sqrt{n\pi}} \left(\frac{4gn}{e}\right)^n . \tag{2.24}$$

exercise 1.2

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 (2.23). 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.

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 [9]. Consider the residual error after inclusion of the first n perturbative corrections:

$$\begin{aligned} R_n &= \left| Z(g) - \sum_{m=0}^{n} g^m Z_m \right| \\ &= \int \frac{d\phi}{\sqrt{2\pi}} e^{-\phi^2/2} \left| e^{-g\phi^4/4} - \sum_{m=0}^{n} \frac{1}{m!} \left(-\frac{g}{4}\right)^m \phi^{4m} \right| \\ &\leq \int \frac{d\phi}{\sqrt{2\pi}} e^{-\phi^2/2} \frac{1}{(n+1)!} \left(\frac{g\phi^4}{4}\right)^{n+1} = g^{n+1} \left|Z_{n+1}\right| . \end{aligned} \tag{2.25}$$

exercise 1.5

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 (2.24) the minimum is reached at $4g\, n_{min} \approx 1$, with the minimum error

$$g^n Z_n\Big|_{min} \approx \sqrt{\frac{4g}{\pi}}\, e^{-1/4g}. \tag{2.26}$$

As illustrated by the figure 2.2, 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 that humanity has been able to perform so far stop at $n \leq 5$.

2.4 Free propagation

In many field theory textbooks much time is spent on “non-interacting fields”, “free propagation”, etc... As a matter of fact, papers which attempt to “derive” quantum mechanics from deeper principles most 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.

2.5 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

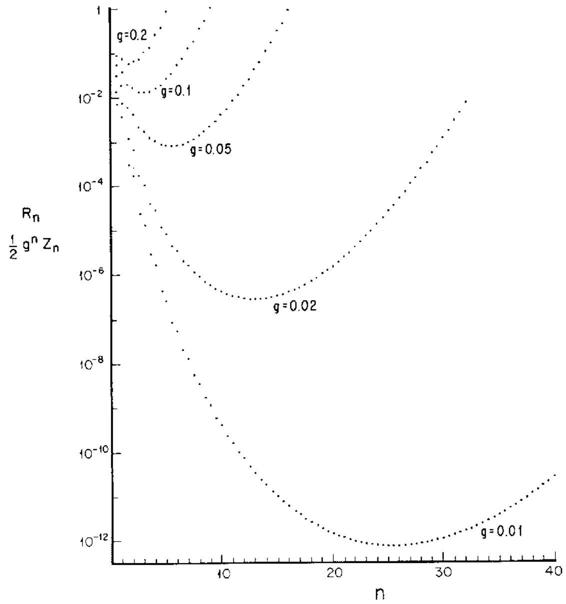


Figure 2.2: Plot of the saddle-point estimate of Z_n vs. the exact result (2.23) for $g = 0.1$, $g = 0.02$, $g = 0.01$.

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

$$\begin{aligned} Z_0[J] = e^{W_0[J]} &= \int [d\phi] e^{-\frac{1}{2}\phi^T \cdot M^{-1} \cdot \phi + \phi \cdot J} = |\det M|^{\frac{1}{2}} \, e^{\frac{1}{2} J^T \cdot M \cdot J} \\ W_0[J] &= \frac{1}{2} J^T \cdot M \cdot J + \frac{1}{2} \mathrm{tr} \ln M \,. \end{aligned} \qquad (2.27)$$

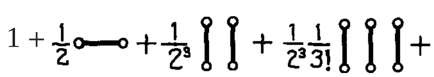
The full n-point correlation functions (2.9) vanish for n odd, and for n even they are given by products of distinct combinations of 2-point correlations

$$\begin{aligned} G_{\ell\ell'} &= (M)_{\ell\ell'} \\ G_{\ell_1\ell_2\ell_3\ell_4} &= (M)_{\ell_1\ell_2}(M)_{\ell_3\ell_4} + (M)_{\ell_1\ell_3}(M)_{\ell_2\ell_4} + (M)_{\ell_1\ell_4}(M)_{\ell_2\ell_3} \\ G_{\ell_1\ell_2\cdots\ell_n} &= (M)_{\ell_1\ell_2} \cdots (M)_{\ell_{n-1}\ell_n} + (M)_{\ell_1\ell_3} \cdots (M)_{\ell_{n-1}\ell_n} + \cdots \end{aligned} \qquad (2.28)$$

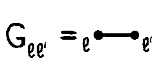
Keeping track of all these dummy indices (and especially when they turn into a zoo of of continuous coordinates and discrete indices) is a pain, and it is much easier to visualize this diagrammatically. Defining the propagator as a line connecting 2 lattice sites, and the probe J_ℓ as a source/sink from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

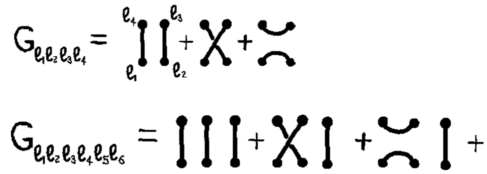
$(M)_{\ell_1\ell_2} = \ell_1$ $\ell_2\,,\qquad J_\ell =$  $\ell\,,$ (2.29)

we expand the free-field theory partition function (2.27) as a Taylor series in $J^T \cdot M^{-1} \cdot J$

$\dfrac{Z_0[J]}{Z_0[0]} =$  $+ \cdots \,.$ (2.30)

In the diagrammatic notation the non-vanishing n-point correlations (2.28) are drawn as





$$+ \text{(11 terms)}\,. \tag{2.31}$$

exercise 1.1

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.

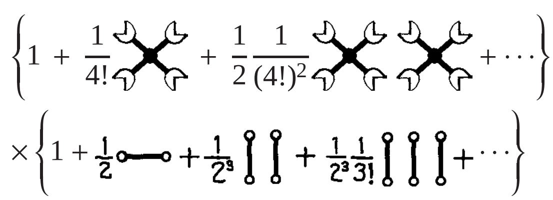
2.6 Feynman diagrams

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 [5], 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.

2.6.1 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 (2.20)

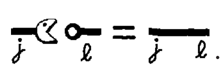
$$e^{S_I[\frac{d}{dJ}]}\, e^{\frac{1}{2} J^T \cdot M \cdot J} \quad = $$



$$\tag{2.32}$$

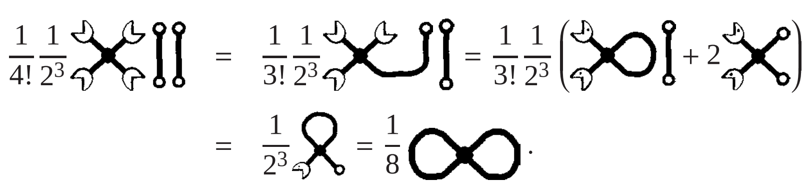
Here we have indicated $\frac{d}{dJ}$ as a pac-man [6] that eats J, leaving a delta function in its wake

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



$$\tag{2.33}$$

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 $\frac{1}{2}\left(\frac{1}{2} J^T \cdot M \cdot J\right)^2$ term, the next pac-man has three J's to bite into in two distinct ways, and so forth:



$$\tag{2.34}$$

In the hum-drum field theory textbooks this process of tying together vertices by propagators is called the *Wick expansion*. Professionals have smarter ways of

exercise 1.7

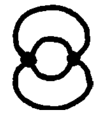
generating Feynman diagrams [2], but this will do for the problem at hand.

It is easy enough to prove this to all orders [7], but to this order you can simply check by expanding the exponential (2.8) that the free energy $W[J]$ perturbative corrections are the connected, diagrams with $J = 0$

exercise 1.6

$$W[0] = S[\phi^c] + \frac{1}{2}\mathrm{tr}\,\ln M + \frac{1}{8}$$

$$+\frac{1}{16}$$

$$+\frac{1}{48}$$

$$. \qquad (2.35)$$

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 M, and learn how to evaluate diagrammatic perturbative corrections.

Commentary

Remark 2.1 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 [9]. 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 $|\det M|^{\frac{1}{2}}$ explicit dependence on the momentum $k^{\frac{1}{4}}$. 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 [10].
- 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 $1/N$.

Chapter 3

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:

$$i\hbar\frac{\partial}{\partial t}\psi(t) = \hat{H}\psi(t)\,. \tag{3.1}$$

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

As the Schrödinger equation (3.1) 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

$$\mathbf{1} = \int dq^D\,|q\rangle\langle q| \tag{3.2}$$

we have

$$\psi(q,t) = \langle q|\psi(t)\rangle = \int dq'\,\langle q|e^{-\frac{i}{\hbar}\hat{H}t}|q'\rangle\langle q'|\psi(0)\rangle\,, \qquad t \geq 0\,. \tag{3.3}$$

In sect. 3.1 we will solve the problem and give the explicit formula (3.9) 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. 3.4 we shall derive Feynman's path integral formula for $K(q,q',t) = \langle q|e^{-\frac{i}{\hbar}\hat{H}t}|q'\rangle$.

3.1 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 (3.1)

$$i\hbar\frac{\partial}{\partial t}\psi(q,t) = \hat{H}(q,\frac{\hbar}{i}\frac{\partial}{\partial q})\psi(q,t), \tag{3.4}$$

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

$$H(q,p) = T(p) + V(q)\,, \qquad T(p) = \frac{p^2}{2m}\,, \tag{3.5}$$

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

$$\hat{H}\psi(q) = E\psi(q)\,, \tag{3.6}$$

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

$$\int dq^D\,\phi_n^*(q)\phi_m(q) = \int dq^D\,\langle n|q\rangle\langle q|m\rangle = \delta_{nm} \tag{3.7}$$

and complete

$$\sum_n \phi_n(q)\phi_n^*(q') = \delta(q-q')\,, \qquad \sum_n |n\rangle\langle n| = \mathbf{1} \tag{3.8}$$

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

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

The evolution of the wave function is then given by

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

Figure 3.1: 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''.

We can write this as

$$\begin{aligned} \psi(q,t) &= \int dq'^D K(q,q',t)\psi(q',0), \\ K(q,q',t) &= \sum_n \phi_n(q)\, e^{-iE_n t/\hbar} \phi_n^*(q') \\ &= \langle q|e^{-\frac{i}{\hbar}\hat{H}t}|q'\rangle \;=\; \sum_n \langle q|n\rangle e^{-iE_n t/\hbar} \langle n|q'\rangle\,, \end{aligned} \tag{3.9}$$

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

$$K(q,q',t_1+t_2) = \int dq''\, K(q,q'',t_2)K(q'',q',t_1) \tag{3.10}$$

forward in time, hence the name "propagator", see figure 3.1. 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

$$i\hbar\frac{\partial}{\partial t}K(q,q',t) = \hat{H}(q,\frac{i}{\hbar}\frac{\partial}{\partial q})K(q,q',t)\,. \tag{3.11}$$

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

$$\lim_{t\to 0_+} K(q,q',t) = \delta(q-q')\,. \tag{3.12}$$

This follows from the completeness relation (3.8).

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/Fourier transform, the energy dependent Green's function

$$G(q, q', E + i\epsilon) = \frac{1}{i\hbar} \int_0^\infty dt\, e^{\frac{i}{\hbar}Et - \frac{\epsilon}{\hbar}t} K(q, q', t) = \sum_n \frac{\phi_n(q)\phi_n^*(q')}{E - E_n + i\epsilon}\,. \qquad (3.13)$$

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 3.1 as a "multi-slit" experiment, with an infinitesimal "slit" placed at every q' point. The Feynman path integral follows from two observations:

1. Sect. 3.3: For short time the propagator can be expressed in terms of classical functions (Dirac).

2. Sect. 3.4: The group property (3.10) enables us to represent finite time evolution as a product of many short time evolution steps (Feynman).

3.2 Matrix-valued functions

How are we to think of the quantum operator

$$\hat{H} = \hat{T} + \hat{V}\,, \qquad \hat{T} = \hat{p}^2/2m\,, \qquad \hat{V} = V(\hat{q})\,, \qquad (3.14)$$

corresponding to the classical Hamiltonian (3.5)?

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, (3.9) 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

$$A'(x) = \frac{dA(x)}{dx}\,, \qquad A'_{ij}(x) = \frac{d}{dx}A_{ij}(x)\,. \qquad (3.15)$$

Derivatives of products of matrices are evaluated by the chain rule

$$\frac{d}{dx}(A\mathbf{B}) = \frac{dA}{dx}\mathbf{B} + A\frac{d\mathbf{B}}{dx}\,. \qquad (3.16)$$

A matrix and its derivative matrix in general do not commute

$$\frac{d}{dx}A^2 = \frac{dA}{dx}A + A\frac{dA}{dx}\,. \qquad (3.17)$$

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

$$\frac{d}{dx}A^{-1} = -\frac{1}{A}\frac{dA}{dx}\frac{1}{A}\,. \qquad (3.18)$$

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:

$$e^A = \sum_{k=0}^{\infty} \frac{1}{k!} A^k , \qquad A^0 = \mathbf{1} \tag{3.19}$$

$$= \lim_{N\to\infty} \left(\mathbf{1} + \frac{1}{N} A \right)^N \tag{3.20}$$

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 (3.20). 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

$$\ln(1 - B) = - \sum_{k=0}^{\infty} \frac{B^k}{k!} . \tag{3.21}$$

Consider now the determinant

$$\det e^A = \lim_{N\to\infty} (\det (\mathbf{1} + A/N))^N .$$

To the leading order in $1/N$

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

hence

$$\det e^A = \lim_{N\to\infty} \left(1 + \frac{1}{N} \mathrm{tr}\, A + O(N^{-2})\right)^N = e^{\mathrm{tr}\, A} \tag{3.22}$$

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

$$\ln \det M = \mathrm{tr}\, \ln M . \tag{3.23}$$

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 BakerCampbellHausdorff commutator expansion

$$e^{t\mathbf{A}} \mathbf{B} e^{-t\mathbf{A}} = \mathbf{B} + t[\mathbf{A}, \mathbf{B}] + \frac{t^2}{2} [\mathbf{A}, [\mathbf{A}, \mathbf{B}]] + \frac{t^3}{3!} [\mathbf{A}, [\mathbf{A}, [\mathbf{A}, \mathbf{B}]]] + \cdots \tag{3.24}$$

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

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

Expanding $\exp(\mathbf{A}+\mathbf{B})$, $\exp \mathbf{A}$, $\exp \mathbf{B}$ to first few orders using (3.19) yields

$$e^{(\mathbf{A}+\mathbf{B})/N} = e^{\mathbf{A}/N}e^{\mathbf{B}/N} - \frac{1}{2N^2}[\mathbf{A},\mathbf{B}] + O(N^{-3}) , \tag{3.25}$$

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

$$e^{\mathbf{A}} = \lim_{N\to\infty}\left(e^{\mathbf{B}/N}e^{\mathbf{C}/N}\right)^N . \tag{3.26}$$

3.3 Short time propagation

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

$$K(q,q',\Delta t) = \langle q|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|q'\rangle = \langle q|e^{-\hat{T}\lambda}e^{-\hat{V}\lambda}|q'\rangle + O(\Delta t^2) . \tag{3.27}$$

where $\lambda = \frac{i}{\hbar}\Delta t$. The error estimate follows from (3.25). 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

$$\mathbf{1} = \int dp^D\,|p\rangle\langle p| , \qquad \langle p|q\rangle = (2\pi\hbar)^{-D/2}e^{-\frac{i}{\hbar}p\cdot q} , \tag{3.28}$$

and evaluate the Gaussian integral

$$\begin{aligned}\langle q|e^{-\lambda\hat{T}}|q'\rangle &= \int dp^D\,\langle q|e^{-\hat{T}\lambda}|p\rangle\langle p|q'\rangle = \int \frac{dp^D}{(2\pi\hbar)^{D/2}}e^{-\lambda p^2/2m}e^{\frac{i}{\hbar}p\cdot(q-q')} \\ &= \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{D}{2}} e^{\frac{i}{\hbar}\frac{m}{2\Delta t}(q-q')^2} .\end{aligned} \tag{3.29}$$

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

$$K(q,q',\Delta t) = \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{D/2} e^{\frac{i}{\hbar}\Delta t\,L(q,\dot{q})} + O(\Delta t^2) , \tag{3.30}$$

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

$$L(q,\dot{q}) = \frac{m\dot{q}^2}{2} - V(q) . \tag{3.31}$$

3.4 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 (3.26) we have

$$e^{-\frac{i}{\hbar}\hat{H}t} = \lim_{N\to\infty}\left(e^{-\frac{i}{\hbar}\hat{T}\Delta t}e^{-\frac{i}{\hbar}\hat{V}\Delta t}\right)^N , \qquad \Delta t = t/N \tag{3.32}$$

Turn this into matrix multiplication by inserting the configuration representation completeness relations (3.2)

$$\begin{aligned} K(q,q',t) &= \langle q|e^{-\frac{i}{\hbar}\hat{H}t}|q'\rangle \qquad (3.33)\\ &= \int dq_1^D \cdots dq_{N-1}^D \langle q|e^{-\hat{H}\lambda}|q_{N-1}\rangle \cdots \langle q_1|e^{-\hat{H}\lambda}|q'\rangle \\ &= \lim_{N\to\infty}\int dq_1^D \cdots dq_{N-1}^D \langle q'|e^{-\hat{T}\lambda}e^{-\hat{V}\lambda}|q_{N-1}\rangle \cdots \langle q_1|e^{-\hat{T}\lambda}e^{-\hat{V}\lambda}|q\rangle \,. \end{aligned}$$

The next step relies on convolution of two Gaussians being a Gaussian. Substituting (3.30) we obtain that the total phase shift is given by the *Hamilton's principal function*, the integral of (3.31) evaluated along the given path p from $q' = q(0)$ to $q = q(t)$:

$$\begin{aligned} R[q] &= \lim_{N\to\infty}\sum_{j=0}^{N-1}\Delta t\left(\frac{m}{2}\left(\frac{q_{j+1}-q_j}{\Delta t}\right)^2 - V(q_j)\right), \qquad q_0 = q' \\ &= \int d\tau\, L(q(\tau),\dot{q}(\tau))\,, \end{aligned} \tag{3.34}$$

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

$$\begin{aligned} K(q,q',t) &= \lim_{N\to\infty}\int [dq]\, e^{\frac{i}{\hbar}R[q]} \qquad (3.35)\\ [dq] &= \prod_{j=1}^{N-1}\frac{dq_j^D}{(2\pi i\hbar\Delta t/m)^{D/2}}\,. \end{aligned}$$

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 3.1. The usual, more compact notation is

$$\begin{aligned} K(q,q',t) &= \int \mathcal{D}q\, e^{\frac{i}{\hbar}R[q]}\,, \qquad \text{or, more picturesquely} \\ &= C\sum_p e^{\frac{i}{\hbar}R[q_p]}\,, \qquad q' = q_p(0),\ q = q_p(t)\,, \end{aligned} \tag{3.36}$$

where $\int \mathcal{D}q$ is shorthand notation for the $N \to \infty$ limit in (3.35),

$$\int \mathcal{D}q = \lim_{N\to\infty}\int [dq]\,, \tag{3.37}$$

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

Chapter 4

WKB quantization

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

$$\psi = Ae^{\frac{i}{\hbar}pq} \tag{4.1}$$

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 classical 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 - classical 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 classical flow that plays no role in classical mechanics.

4.1 WKB ansatz

Consider a time-independent Schrödinger equation in 1 spatial dimension:

$$-\frac{\hbar^2}{2m}\psi''(q) + V(q)\psi(q) = E\psi(q)\,, \tag{4.2}$$

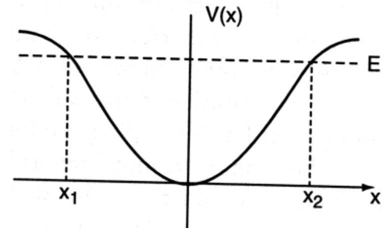


Figure 4.1: A 1-dimensional potential, location of the two turning points at fixed energy E.

with potential $V(q)$ growing sufficiently fast as $q \to \pm\infty$ so that the classical particle motion is confined for any E. Define the local momentum $p(q)$ and the local wavenumber $k(q)$ by

$$p(q) = \pm\sqrt{2m(E - V(q))}, \qquad p(q) = \hbar k(q)\,. \tag{4.3}$$

The variable wavenumber form of the Schrödinger equation

$$\psi'' + k^2(q)\psi = 0 \tag{4.4}$$

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:

$$(S')^2 = p^2 + \hbar^2\frac{A''}{A} \tag{4.5}$$

$$S''A + 2S'A' = \frac{1}{A}\frac{d}{dq}(S'A^2) = 0\,. \tag{4.6}$$

The Wentzel-Kramers-Brillouin *(WKB)* or *semiclassical* approximation consists of dropping the $\hbar^2$ term in (4.5). 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 (4.5) we obtain the phase increment of a wave function initially at q, at energy E

$$S(q, q', E) = \int_{q'}^{q} dq''\, p(q'')\,. \tag{4.7}$$

This integral over a particle trajectory of constant energy, called the *action*, will play a key role in all that follows. The integration of (4.6) is even easier

$$A(q) = \frac{C}{|p(q)|^{\frac{1}{2}}}, \qquad C = |p(q')|^{\frac{1}{2}}\psi(q')\,, \tag{4.8}$$

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

$$\psi_{sc}(q, q', E) = \frac{C}{|p(q)|^{\frac{1}{2}}} e^{\frac{i}{\hbar}S(q,q',E)}\,. \tag{4.9}$$

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

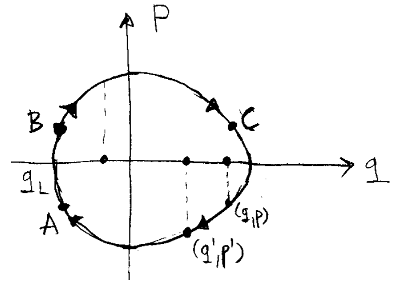


Figure 4.2: A 1-dof phase space trajectory of a particle moving in a bound potential.

The WKB ansatz generalizes the free motion wave function (4.1), 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 4.1, where all energy is potential, and

$$p(q) \to 0 \quad \text{as} \quad q \to q_0\,, \tag{4.10}$$

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 4.1), 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 4.2), 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

$$\widetilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}}\int dq\, e^{-\frac{i}{\hbar}qp}\psi(q)\,, \tag{4.11}$$

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

$$\psi(q) = \frac{1}{\sqrt{2\pi\hbar}}\int dp\, e^{\frac{i}{\hbar}qp}\,\widetilde{\psi}(p)\,, \tag{4.12}$$

and so on.

The only rub is that one usually cannot evaluate these transforms exactly. But, as the WKB wave function (4.9) 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.

4.2 Method of stationary phase

All "semiclassical" approximations are based on saddle point evaluations of integrals of the type

$$I = \int dx\, A(x)\, e^{is\Phi(x)}\,, \qquad x, \Phi(x) \in \mathbb{R}\,, \tag{4.13}$$

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,

$$I = \int dx\, A(x)\, e^{is(\Phi(x_0)+\frac{1}{2}\Phi''(x_0)\delta x^2+\ldots)} . \tag{4.14}$$

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

$$I \approx A(x_0)\, e^{is\Phi(x_0)} \int dx\, e^{\frac{1}{2}is\Phi''(x_0)(x-x_0)^2} . \tag{4.15}$$

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*

exercise 4.1

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{-\frac{x^2}{2ia}} = \sqrt{ia} = |a|^{1/2}\, e^{i\frac{\pi}{4}\frac{a}{|a|}} \tag{4.16}$$

we obtain

$$I \approx A(x_0) \left| \frac{2\pi}{s\Phi''(x_0)} \right|^{1/2} e^{is\Phi(x_0) \pm i\frac{\pi}{4}} , \tag{4.17}$$

where $\pm$ corresponds to the positive/negative sign of $s\Phi''(x_0)$.

4.3 WKB quantization

We can now evaluate the Fourier transforms (4.11), (4.12) to the same order in $\hbar$ as the WKB wave function using the stationary phase method,

$$\begin{aligned} \widetilde{\psi}_{sc}(p) &= \frac{C}{\sqrt{2\pi\hbar}} \int \frac{dq}{|p(q)|^{\frac{1}{2}}}\, e^{\frac{i}{\hbar}(S(q)-qp)} \\ &\approx \frac{C}{\sqrt{2\pi\hbar}} \frac{e^{\frac{i}{\hbar}(S(q^*)-q^*p)}}{|p(q^*)|^{\frac{1}{2}}} \int dq\, e^{\frac{i}{2\hbar}S''(q^*)(q-q^*)^2} , \end{aligned} \tag{4.18}$$

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 (4.16)

$$\widetilde{\psi}_{sc}(p) = \frac{C}{|p(q^*)p'(q^*)|^{\frac{1}{2}}} e^{\frac{i}{\hbar}[S(q^*)-q^*p]+\frac{i\pi}{4}\mathrm{sgn}[S''(q^*)]} . \tag{4.19}$$

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

$$\tilde{S}(p) = S(q(p)) - q(p)p$$

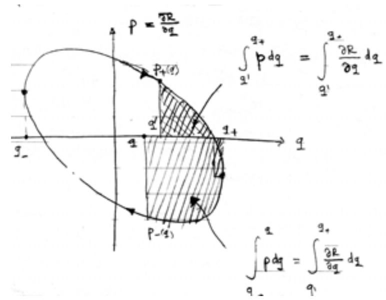


Figure 4.3: $S_p(E)$, the action of a periodic orbit p at energy E, equals the area in the phase space traced out by the 1-dof trajectory.

which can be used to expresses everything in terms of the p variable,

$$q^* = q(p), \quad \frac{d}{dq}q = 1 = \frac{dp}{dq}\frac{dq(p)}{dp} = q'(p)p'(q^*) . \tag{4.20}$$

As the classical trajectory crosses q_L, the weight in (4.19),

$$\frac{d}{dq}p^2(q_L) = 2p(q_L)p'(q_L) = -2mV'(q) , \tag{4.21}$$

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 (4.19) is $-\frac{\pi}{4}$. To go back from the p to the q representation, just turn figure 4.2 quarter-turn anticlockwise. Everything is the same if you replace $(q, p) \to (-p, q)$; so, without much ado we get the semiclassical wave function at the point (q_B, p_B),

$$\psi_{sc}(q) = \frac{e^{\frac{i}{\hbar}(\tilde{S}(p^*)+qp^*)-\frac{i\pi}{4}}}{|q^*(p^*)|^{\frac{1}{2}}}\widetilde{\psi}_{sc}(p^*) = \frac{C}{|p(q)|^{\frac{1}{2}}}e^{\frac{i}{\hbar}S(q)-\frac{i\pi}{2}} . \tag{4.22}$$

The extra $|p'(q^*)|^{1/2}$ weight in (4.19) is cancelled by the $|q'(p^*)|^{1/2}$ term, by the Legendre relation (4.20).

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 4.2 by 180^o, and flipping coordinates $(q, p) \to (-q, -p)$. While a turning point is not an invariant concept (for a sufficiently short trajectory segment, it can be undone by a 45^o 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 (4.8), 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,

$$\frac{1}{\hbar}\oint p(q)dq = 2\pi\left(n + \frac{m}{4}\right) , \tag{4.23}$$

where m is the number of turning points along the trajectory - for this 1-dof problem, $m = 2$.

The action integral in (4.23) is the area (see figure 4.3) enclosed by the classical phase space loop of figure 4.2, 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 classical quantities, the periodic orbit action S, and the topological index m.

4.3.1 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 4.2 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

$$E_n = \hbar\omega(n + 1/2) \tag{4.24}$$

turns out to be the *exact* harmonic oscillator spectrum. The stationary phase condition (4.18) 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 (4.5) as a short wavelength approximation.

4.4 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 (4.16), 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 (4.14) fails whenever $\Phi''(x) = 0$, or, in our the WKB ansatz (4.18), whenever the momentum $p'(q) = S''(q)$ vanishes. In that case we have to go beyond the quadratic approximation (4.15) to the first nonvanishing term in the Taylor expansion of the exponent. If $\Phi'''(x_0) \neq 0$, then

$$I \approx A(x_0)e^{is\Phi(x_0)} \int_{-\infty}^{\infty} dx\, e^{is\Phi'''(x_0)\frac{(x-x_0)^3}{6}} . \tag{4.25}$$

Airy functions can be represented by integrals of the form

$$Ai(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dy\, e^{i(xy - \frac{y^3}{3})} . \tag{4.26}$$

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

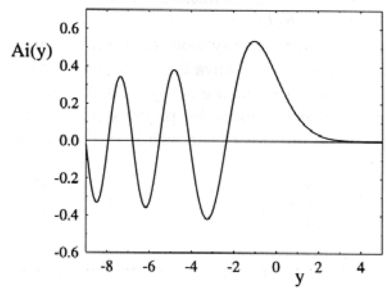


Figure 4.4: Airy function $Ai(q)$.

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 $V'(q_0) \to z$ after appropriate rescalings),

$$\psi'' = z\psi , \qquad (4.27)$$

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 (4.4)) 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 4.4. 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 classical 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 classical trajectory. While in the q-representation the WKB ansatz at a turning point is singular, along the p direction the classical 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 classical 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 classical 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 semiclassical 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 classical 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 4.1 Airy function. The stationary phase approximation is all that is needed for the semiclassical approximation, with the proviso that D in (**??**) has no zero eigenvalues. The zero eigenvalue case would require going beyond the Gaussian saddle-point approximation, which typically leads to approximations of the integrals in terms of Airy functions [9].

exercise 4.4

Remark 4.2 Bohr-Sommerfeld quantization. Bohr-Sommerfeld quantization condition was the key result of the old quantum theory, in which the electron trajectories were purely classical. 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 [**?**] added the topological indices.

Exercises

4.1. **WKB ansatz.** Try to show that no other ansatz other than (**??**) gives a meaningful definition of the momentum in the $\hbar \to 0$ limit.

4.2. **Fresnel integral.** Derive the Fresnel integral

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, e^{-\frac{x^2}{2ia}} = \sqrt{ia} = |a|^{1/2} e^{i\frac{\pi}{4}\frac{a}{|a|}} .$$

4.3. **Sterling formula for $n!$.** Compute an approximate value of $n!$ for large n using the stationary phase approximation. Hint: $n! = \int_0^\infty dt\, t^n e^{-t}$.

4.4. **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

$$Ai(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} dy\, e^{i(xy-\frac{y^3}{3})} . \tag{4.28}$$

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.

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Appendix A

Group theory

A.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.

A.1.1 Projection operators

For $\mathbf{M}$ a hermitian matrix, there exists a diagonalizing unitary matrix $\mathbf{C}$ such that

$$\mathbf{CMC}^\dagger = \left(\begin{array}{c|c|c} \begin{array}{ccc} \lambda_1 & \dots & 0 \\ & \ddots & \\ 0 & \dots & \lambda_1 \end{array} & 0 & 0 \\ \hline 0 & \begin{array}{cccc} \lambda_2 & 0 & \dots & 0 \\ 0 & \lambda_2 & & \\ \vdots & & \ddots & \vdots \\ 0 & & \dots & \lambda_2 \end{array} & 0 \\ \hline 0 & 0 & \begin{array}{cc} \lambda_3 & \dots \\ \vdots & \ddots \end{array} \end{array}\right) . \tag{A.1}$$

Here $\lambda_i \neq \lambda_j$ are the r distinct roots of the minimal *characteristic* (or *secular*) polynomial

$$\prod_{i=1}^{r} (\mathbf{M} - \lambda_i \mathbf{1}) = 0 \,. \tag{A.2}$$

In the matrix $\mathbf{C}(\mathbf{M}-\lambda_2\mathbf{1})\mathbf{C}^\dagger$ the eigenvalues corresponding to λ_2 are replaced by zeroes:

$$\left(\begin{array}{cc|ccc|ccc}
\lambda_1-\lambda_2 & & & & & & & \\
 & \lambda_1-\lambda_2 & & & & & & \\
\hline
 & & 0 & & & & & \\
 & & & \ddots & & & & \\
 & & & & 0 & & & \\
\hline
 & & & & & \lambda_3-\lambda_2 & & \\
 & & & & & & \lambda_3-\lambda_2 & \\
 & & & & & & & \ddots
\end{array}\right),$$

and so on, so the product over all factors $(\mathbf{M}-\lambda_2\mathbf{1})(\mathbf{M}-\lambda_3\mathbf{1})\ldots$, with exception of the $(\mathbf{M}-\lambda_1\mathbf{1})$ factor, has nonzero entries only in the subspace associated with λ_1:

$$\mathbf{C}\prod_{j\neq 1}(\mathbf{M}-\lambda_j\mathbf{1})\mathbf{C}^\dagger=\prod_{j\neq 1}(\lambda_1-\lambda_j)\left(\begin{array}{ccc|cccc}
1 & 0 & 0 & & & & \\
0 & 1 & 0 & & 0 & & \\
0 & 0 & 1 & & & & \\
\hline
 & & & 0 & & & \\
 & 0 & & & 0 & & \\
 & & & & & 0 & \\
 & & & & & & \ddots
\end{array}\right).$$

Thus we can associate with each distinct root λ_i a *projection operator* $\mathbf{P}_i$,

$$\mathbf{P}_i=\prod_{j\neq i}\frac{\mathbf{M}-\lambda_j\mathbf{1}}{\lambda_i-\lambda_j}, \tag{A.3}$$

which acts as identity on the ith subspace, and zero elsewhere. For example, the projection operator onto the λ_1 subspace is

$$\mathbf{P}_1=\mathbf{C}^\dagger\left(\begin{array}{ccc|cccc}
1 & & & & & & \\
 & \ddots & & & & & \\
 & & 1 & & & & \\
\hline
 & & & 0 & & & \\
 & & & & 0 & & \\
 & & & & & \ddots & \\
 & & & & & & 0
\end{array}\right)\mathbf{C}. \tag{A.4}$$

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 $\mathbf{M}$ we find convenient, the algebraic relations they satisfy, and orthonormality and completeness of $\mathbf{P}_i$: The matrices $\mathbf{P}_i$ are *orthogonal*

$$\mathbf{P}_i\mathbf{P}_j=\delta_{ij}\mathbf{P}_j, \qquad (\text{no sum on } j), \tag{A.5}$$

and satisfy the *completeness relation*

$$\sum_{i=1}^{r}\mathbf{P}_i=\mathbf{1}. \tag{A.6}$$

As $\mathrm{tr}\,(\mathbf{C}\mathbf{P}_i\mathbf{C}^\dagger) = \mathrm{tr}\,\mathbf{P}_i$, the dimension of the ith subspace is given by

$$d_i = \mathrm{tr}\,\mathbf{P}_i \,. \tag{A.7}$$

It follows from the characteristic equation (A.2) and the form of the projection operator (A.3) that λ_i is the eigenvalue of $\mathbf{M}$ on $\mathbf{P}_i$ subspace:

$$\mathbf{M}\mathbf{P}_i = \lambda_i \mathbf{P}_i \,, \qquad (\text{no sum on } i) \,. \tag{A.8}$$

Hence, any matrix polynomial $f(\mathbf{M})$ takes the scalar value $f(\lambda_i)$ on the $\mathbf{P}_i$ subspace

$$f(\mathbf{M})\mathbf{P}_i = f(\lambda_i)\mathbf{P}_i \,. \tag{A.9}$$

This, of course, is the reason why one wants to work with irreducible reps: they reduce matrices and "operators" to pure numbers.

A.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:

$$[\mathbf{M}_1, \mathbf{M}_2] = 0 \,, \tag{A.10}$$

or, equivalently, if projection operators $\mathbf{P}_j$ constructed from $\mathbf{M}_2$ commute with projection operators $\mathbf{P}_i$ constructed from $\mathbf{M}_1$,

$$\mathbf{P}_i \mathbf{P}_j = \mathbf{P}_j \mathbf{P}_i \,. \tag{A.11}$$

Usually the simplest choices of independent invariant matrices do not commute. In that case, the projection operators $\mathbf{P}_i$ constructed from $\mathbf{M}_1$ can be used to project commuting pieces of $\mathbf{M}_2$:

$$\mathbf{M}_2^{(i)} = \mathbf{P}_i \mathbf{M}_2 \mathbf{P}_i \,, \qquad (\text{no sum on } i) \,.$$

That $\mathbf{M}_2^{(i)}$ commutes with $\mathbf{M}_1$ follows from the orthogonality of $\mathbf{P}_i$:

$$[\mathbf{M}_2^{(i)}, \mathbf{M}_1] = \sum_j \lambda_j [\mathbf{M}_2^{(i)}, \mathbf{P}_j] = 0 \,. \tag{A.12}$$

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 (A.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.

According to (**??**), an invariant matrix $\mathbf{M}$ commutes with group transformations $[G, \mathbf{M}] = 0$. Projection operators (A.3) constructed from $\mathbf{M}$ are polynomials in $\mathbf{M}$, so they also commute with all $g \in \mathcal{G}$:

$$[G, \mathbf{P}_i] = 0 \tag{A.13}$$

Hence, a $[d\times d]$ matrix rep can be written as a direct sum of $[d_i\times d_i]$ matrix reps:

$$G = \mathbf{1}G\mathbf{1} = \sum_{i,j} \mathbf{P}_i G \mathbf{P}_j = \sum_i \mathbf{P}_i G \mathbf{P}_i = \sum_i G_i\,. \tag{A.14}$$

In the diagonalized rep (A.4), the matrix $\mathbf{g}$ has a block diagonal form:

$$\mathbf{C}\mathbf{g}\mathbf{C}^\dagger = \begin{bmatrix} \mathbf{g}_1 & 0 & 0 \\ 0 & \mathbf{g}_2 & 0 \\ 0 & 0 & \ddots \end{bmatrix}, \qquad \mathbf{g} = \sum_i \mathbf{C}^i \mathbf{g}_i \mathbf{C}_i\,. \tag{A.15}$$

The rep $\mathbf{g}_i$ acts only on the d_i-dimensional subspace V_i consisting of vectors $\mathbf{P}_i q$, $q \in V$. 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:

$$V \overset{\mathbf{M}}{\rightarrow} V_1 \oplus V_2 \oplus \ldots \oplus V_r\,. \tag{A.16}$$

References

[A.1] P. Cvitanović, *Group Theory*, ChaosBook.org/GroupTheory (Princeton University Press, Princeton, NJ, 2006).

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