QUANTUM FIELD THEORY a cyclist tour

lecture notes - Spring 2005 Predrag Cvitanović



Incomplete and unassuming notes for the Georgia Tech graduate quantum field theory course (PHYS-7147 - Spring 2005), version 3.3, Feb 14 2005.

What reviewers say. \cdots N. Bohr - "The most important work since that Schrödinger killed the cat." \cdots R.P. Feynman - "Great doorstop!"

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Chapter 1

Path integral formulation of Quantum Mechanics

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

Have: the Schrödinger equation, that is the (infinitesimal time) evolution law for any quantum wavefunction:

$$i\hbar\frac{\partial}{\partial t}\psi(t) = \hat{H}\psi(t). \qquad (1.1)$$

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

As the Schrödinger equation (1.1) is a linear equation, the solution can be written down immediately:

$$\psi(t) = e^{-\frac{i}{\hbar}Ht}\psi(0), \qquad t \ge 0.$$

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 completness relation

$$\mathbf{1} = \int dq^D \, |q\rangle\langle q| \tag{1.2}$$

we have

$$\psi(q,t) = \langle q|\psi(t)\rangle = \int dq' \langle q|e^{-\frac{i}{\hbar}\hat{H}t}|q'\rangle\langle q'|\psi(0)\rangle, \qquad t \ge 0.$$
(1.3)

In sect. 1.1 we will solve the problem and give the explicit formula (1.9) for the propagator. However, this solution is useless - it requires knowing all quantum eigenfunctions, that is it is a solution which we can implement provided that we have already solved the quantum problem. In sect. 1.4 we shall derive Feynman's path integral formula for $K(q,q',t) = \langle q | e^{-\frac{i}{\hbar}\hat{H}t} | q' \rangle$.

1.1 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 (1.1)

$$i\hbar\frac{\partial}{\partial t}\psi(q,t) = \hat{H}(q,\frac{\hbar}{i}\frac{\partial}{\partial q})\psi(q,t), \qquad (1.4)$$

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

$$H(q,p) = T(p) + V(q), \qquad T(p) = \frac{p^2}{2m},$$
(1.5)

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

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

of the time independent Schrödinger equation

$$\ddot{H}\psi(q) = E\psi(q), \qquad (1.6)$$

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

$$\int dq^D \phi_n^*(q) \phi_m(q) = \int dq^D \langle n|q \rangle \langle q|m \rangle = \delta_{nm}$$
(1.7)

and complete

$$\sum_{n} \phi_n(q) \phi_n^*(q') = \delta(q - q'), \qquad \sum_{n} |n\rangle \langle n| = \mathbf{1}$$
(1.8)

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 1.1: Propagation from q' to q in time t = t' + t'' receives contributions from all paths from q' to q'' for time t' followed by propagation from q'' to q in time t''.

We can write this as

$$\psi(q,t) = \int dq'^{D} K(q,q',t) \psi(q',0),$$

$$K(q,q',t) = \sum_{n} \phi_{n}(q) e^{-iE_{n}t/\hbar} \phi_{n}^{*}(q')$$

$$= \langle q|e^{-\frac{i}{\hbar}\hat{H}t}|q'\rangle = \sum_{n} \langle q|n\rangle e^{-iE_{n}t/\hbar} \langle n|q'\rangle, \qquad (1.9)$$

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

$$K(q,q',t_1+t_2) = \int dq'' K(q,q'',t_2) K(q'',q',t_1)$$
(1.10)

forward in time, hence the name "propagator", see figure 1.1. In nonrelativistic 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

$$i\hbar\frac{\partial}{\partial t}K(q,q',t) = \hat{H}(q,\frac{i}{\hbar}\frac{\partial}{\partial q})K(q,q',t).$$
(1.11)

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

$$\lim_{t \to 0_+} K(q, q', t) = \delta(q - q').$$
(1.12)

This follows from the completeness relation (1.8).

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

$$G(q,q',E+i\epsilon) = \frac{1}{i\hbar} \int_0^\infty dt \, e^{\frac{i}{\hbar}Et - \frac{\epsilon}{\hbar}t} K(q,q',t) = \sum_n \frac{\phi_n(q)\phi_n^*(q')}{E - E_n + i\epsilon} \,.(1.13)$$

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Here ϵ is a small positive number, ensuring that the propagation is forward in time (and the very existence of the integral).

This completes our lightning review of quantum mechanics.

Feynman arrived to his formulation of quantum mechanics by thinking of figure 1.1 as a "multi-slit" experiment, with an infinitesimal "slit" placed at every q' point. The Feynman path integral follows from two observations:

- 1. For short time the propagator can be expressed in terms of classical functions (Dirac).
- 2. The group property (1.10) enables us to represent finite time evolution as a product of many short time evolution steps (Feynman).

1.2 Matrix-valued functions

How are we to think of the quantum operator

$$\hat{H} = \hat{T} + \hat{V}, \qquad \hat{T} = \hat{p}^2/2m, \qquad \hat{V} = V(\hat{q}), \qquad (1.14)$$

corresponding to the classical Hamiltonian (1.5)?

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, (1.9) 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

$$A'(x) = \frac{dA(x)}{dx}, \qquad A'_{ij}(x) = \frac{d}{dx}A_{ij}(x).$$
(1.15)

Derivatives of products of matrices are evaluated by the chain rule

$$\frac{d}{dx}(A\mathbf{B}) = \frac{dA}{dx}\mathbf{B} + A\frac{d\mathbf{B}}{dx}.$$
(1.16)

A matrix and its derivative matrix in general do not commute

$$\frac{d}{dx}A^2 = \frac{dA}{dx}A + A\frac{dA}{dx}.$$
(1.17)

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

$$\frac{d}{dx}A^{-1} = -\frac{1}{A}\frac{dA}{dx}\frac{1}{A}.$$
(1.18)

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:

$$e^{A} = \sum_{k=0}^{\infty} \frac{1}{k!} A^{k}, \qquad A^{0} = \mathbf{1}$$
 (1.19)

$$= \lim_{N \to \infty} \left(\mathbf{1} + \frac{1}{N} A \right)^N \tag{1.20}$$

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 (1.20). 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.

As a simple application, we use the two definitions Consider now the determinant

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

To the leading order in 1/N

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

hence

$$\det e^{A} = \lim_{N \to \infty} \left(1 + \frac{1}{N} \operatorname{tr} A + O(N^{-2}) \right)^{N} = e^{\operatorname{tr} A}$$
(1.21)

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 commutator expansion

$$e^{t\mathbf{A}}\mathbf{B}e^{-t\mathbf{A}} = \mathbf{B} + t[\mathbf{A}, \mathbf{B}] + \frac{t^2}{2}[\mathbf{A}, [\mathbf{A}, \mathbf{B}]] + \frac{t^3}{3!}[\mathbf{A}, [\mathbf{A}, [\mathbf{A}, \mathbf{B}]]] + \cdots (1.22)$$

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 (1.19) yields

$$e^{(\mathbf{A}+\mathbf{B})/N} = e^{\mathbf{A}/N}e^{\mathbf{B}/N} - \frac{1}{2N^2}[\mathbf{A},\mathbf{B}] + O(N^{-3}),$$
 (1.23)

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

$$e^{\mathbf{A}} = \lim_{N \to \infty} \left(e^{\mathbf{B}/N} e^{\mathbf{C}/N} \right)^N \,. \tag{1.24}$$

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1.3 Short time propagation

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

$$K(q,q',\Delta t) = \langle q|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|q'\rangle = \langle q|e^{-\hat{T}\lambda}e^{-\hat{V}\lambda}|q'\rangle + O(\Delta t^2).$$
(1.25)

where $\lambda = \frac{i}{\hbar}\Delta t$. The error estimate follows from (1.23). 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

$$\mathbf{1} = \int dp^D |p\rangle \langle p|, \qquad \langle p|q\rangle = (2\pi\hbar)^{-D/2} e^{-\frac{i}{\hbar}p \cdot q}$$
(1.26)

$$\begin{aligned} \langle q|e^{-\lambda\hat{T}}|q'\rangle &= \int dp^D \,\langle q|e^{-\hat{T}\lambda}|p\rangle \langle p|q'\rangle = \int \frac{dp^D}{(2\pi\hbar)^{\frac{D}{2}}} e^{-\lambda p^2/2m} e^{\frac{i}{\hbar}p\cdot(q-q')} \\ &= \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{D}{2}} e^{\frac{i}{\hbar}\frac{1}{2}m(\frac{q-q'}{\Delta t})^2\Delta t} \,. \end{aligned}$$
(1.27)

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

$$K(q,q',\Delta t) = \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{D/2} e^{\frac{i}{\hbar}\Delta t L(q,\dot{q})} + O(\Delta t^2), \qquad (1.28)$$

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

$$L(q, \dot{q}) = \frac{m\dot{q}^2}{2} - V(q).$$
(1.29)

1.4 Path integral

Now we turn expressing 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 (1.24) we have

$$e^{-\frac{i}{\hbar}\hat{H}t} = \lim_{N \to \infty} \left(e^{-\frac{i}{\hbar}\hat{T}\Delta t} e^{-\frac{i}{\hbar}\hat{V}\Delta t} \right)^N, \qquad \Delta t = t/N \tag{1.30}$$

Turn this into matrix multiplication by inserting the configuration representation completness relations (1.2)

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

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

$$= \lim_{N \to \infty} \int dq_1^D \cdots dq_{N-1}^D \langle q' | e^{-\hat{T}\lambda} e^{-\hat{V}\lambda} | q_{N-1} \rangle \cdots \langle q_1 | e^{-\hat{T}\lambda} e^{-\hat{V}\lambda} | q \rangle.$$
(1.31)



Figure 1.2: Path integral receives contributions from all paths propagating forward from q' to q_j to q_{j+1} , j = 1, 2, ..., N-1, ending in q in total time t.

Substituting (1.28) we obtain that the total phase shift is given by the Hamilton's principal function, the integral of (1.29) evaluated along the given path p from q' = q(0) to q = q(t):

$$R[q] = \lim_{N \to \infty} \sum_{j=0}^{N-1} \Delta t \left(\frac{m}{2} \left(\frac{q_{j+1} - q_j}{\Delta t} \right)^2 - V(q_j) \right), \qquad q_0 = q'$$
$$= \int d\tau L(q(\tau), \dot{q}(\tau)), \qquad (1.32)$$

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

$$K(q,q',t) = \lim_{N \to \infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{DN/2} \int dq_1^D \cdots dq_{N-1}^D e^{\frac{i}{\hbar}R[q]}.$$
 (1.33)

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 1.2. The usual, more compact notation is

$$K(q,q',t) = \int \mathcal{D}q \, e^{\frac{i}{\hbar}R[q]}, \quad or, \text{ more pictoresquely} \\ = C \sum_{p} e^{\frac{i}{\hbar}R[q_{p}]}, \quad q' = q_{p}(0), q = q_{p}(t), \quad (1.34)$$

where $\int \mathcal{D}q$ is shorthand notation for the $N \to \infty$ limit in (1.33),

$$\int \mathcal{D}q = \lim_{N \to \infty} \int [dq], \qquad [dq] = \prod_{j=1}^{N-1} \frac{dq_j^D}{\left(2\pi i\hbar\Delta t/m\right)^{D/2}} \tag{1.35}$$

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 perils of path integrals:

- $N \to \infty$ continuum limit
 - fraught with perils sides of the road are littered with corpses of the careless

1.5 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.

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Chapter 2

WKB quantization

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

$$\psi = A e^{\frac{i}{\hbar} pq} \tag{2.1}$$

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 suprisingly 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.

2.1 WKB ansatz

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

$$-\frac{\hbar^2}{2m}\psi''(q) + V(q)\psi(q) = E\psi(q), \qquad (2.2)$$



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

$$p(q) = \pm \sqrt{2m(E - V(q))}, \quad p(q) = \hbar k(q).$$
 (2.3)

The variable wavenumber form of the Schrödinger equation

$$\psi'' + k^2(q)\psi = 0 \tag{2.4}$$

suggests 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:

$$(S')^2 = p^2 + \hbar^2 \frac{A''}{A}$$
(2.5)

$$S''A + 2S'A' = \frac{1}{A} \frac{d}{dq} (S'A^2) = 0.$$
(2.6)

The Wentzel-Kramers-Brillouin (WKB) or semiclassical approximation consists of dropping the \hbar^2 term in (2.5). 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 (2.5) we obtain the phase increment of a wave function initially at q, at energy E

$$S(q,q',E) = \int_{q'}^{q} dq'' p(q'') \,. \tag{2.7}$$

This integral over a particle trajectory of constant energy. called the action. will play a key role in all that follows. The integration of (2.6) is even easier

$$A(q) = \frac{C}{|p(q)|^{\frac{1}{2}}}, \qquad C = |p(q')|^{\frac{1}{2}}\psi(q'), \qquad (2.8)$$

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

$$\psi_{sc}(q,q',E) = \frac{C}{|p(q)|^{\frac{1}{2}}} e^{\frac{i}{\hbar}S(q,q',E)} .$$
(2.9)

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

E.



Figure 2.2: A 1-dof phase space trajectory of a particle moving in a bound potential.

The WKB ansatz generalizes the free motion wave function (2.1), 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 $\frac{1}{\hbar}qp$ 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 2.1, where all energy is potential, and

$$p(q) \to 0 \quad as \quad q \to q_0 \,, \tag{2.10}$$

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 2.1), 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, 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's idea was to proceed from the initial point (q', p') to a point (q_A, p_A) preceeding the turning point in the $\psi(q)$ representation, then switch to the momentum representation

$$\widetilde{\psi}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int dq \, e^{-\frac{i}{\hbar}qp} \psi(q) \,, \tag{2.11}$$

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

$$\psi(q) = \frac{1}{\sqrt{2\pi\hbar}} \int dp \, e^{\frac{i}{\hbar}qp} \,\widetilde{\psi}(p) \,, \tag{2.12}$$

and so on.

The only rub is that one usually cannot evaluate these transforms exactly. But, as the WKB wave function (2.9) is approximate anyway, it suffices to estimate these transforms to leading order in \hbar accuracy. This is accomplished by the method of stationary phase.

2.2 Method of stationary phase

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

$$I = \int dx A(x) e^{is\Phi(x)}, \qquad x, \Phi(x) \in \mathbb{R}, \qquad (2.13)$$

where s is assumed to be a large, real parameter, and $\Phi(x)$ is a real-valued function. In our applications $s = 1/\hbar$ will always be assumed large.

For large s, the phase oscillates rapidly and "averages to zero" everywhere except at the extremal points $\Phi'(x_0) = 0$. The method of approximating an integral by its values at extremal points is called the method of stationary phase. Consider first the case of a 1-dimensional integral, and expand $\Phi(x_0 + \delta x)$ around x_0 to second order in δx ,

$$I = \int dx \, A(x) \, e^{is(\Phi(x_0) + \frac{1}{2}\Phi''(x_0)\delta x^2 + \dots)} \,. \tag{2.14}$$

Assume (for time being) that $\Phi''(x_0) \neq 0$, with either sign, $\operatorname{sgn}[\Phi''] = \Phi''/|\Phi''| = \pm 1$. 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

$$I \approx A(x_0) e^{is\Phi(x_0)} \int dx \, e^{\frac{1}{2}is\Phi''(x_0)(x-x_0)^2} \,. \tag{2.15}$$

Using the Fresnel integral formula

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx \, e^{-\frac{x^2}{2ia}} = \sqrt{ia} = |a|^{1/2} \, e^{i\frac{\pi}{4}\frac{a}{|a|}} \tag{2.16}$$

we obtain

$$I \approx A(x_0) \left| \frac{2\pi}{s\Phi''(x_0)} \right|^{1/2} e^{is\Phi(x_0)\pm i\frac{\pi}{4}}, \qquad (2.17)$$

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

2.3 WKB quantization

We can now evaluate the Fourier transforms (2.11), (2.12) to the same order in \hbar as the WKB wave function using the stationary phase method,

$$\widetilde{\psi}_{sc}(p) = \frac{C}{\sqrt{2\pi\hbar}} \int \frac{dq}{|p(q)|^{\frac{1}{2}}} e^{\frac{i}{\hbar}(S(q)-qp)} \\ \approx \frac{C}{\sqrt{2\pi\hbar}} \frac{e^{\frac{i}{\hbar}(S(q^*)-q^*p)}}{|p(q^*)|^{\frac{1}{2}}} \int dq \, e^{\frac{i}{2\hbar}S''(q^*)(q-q^*)^2}, \qquad (2.18)$$

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 (2.16)

$$\widetilde{\psi}_{sc}(p) = \frac{C}{|p(q^*)p'(q^*)|^{\frac{1}{2}}} e^{\frac{i}{\hbar}[S(q^*) - q^*p] + \frac{i\pi}{4} \operatorname{sgn}[S''(q^*)]}.$$
(2.19)

As we continue from (q_A, p_A) to (q_B, p_B) , nothing problematic occurrs - $p(q^*)$ 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 2.3: $S_p(E)$, 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,

$$q^* = q(p), \quad \frac{d}{dq}q = 1 = \frac{dp}{dq}\frac{dq(p)}{dp} = q'(p)p'(q^*).$$
 (2.20)

As the classical trajectory crosses q_L , the weight in (2.19),

$$\frac{d}{dq}p^2(q_L) = 2p(q_L)p'(q_L) = -2mV'(q), \qquad (2.21)$$

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 (2.19) is $-\frac{\pi}{4}$. To go back from the p to the q representation, just turn figure 2.2 90° anticlockwise. Everything is the same if you replace $(q, p) \rightarrow (-p, q)$; so, without much ado we get the semiclassical wave function at the point (q_B, p_B) ,

$$\psi_{sc}(q) = \frac{e^{\frac{i}{\hbar}(\tilde{S}(p^*) + qp^*) - \frac{i\pi}{4}}}{|q^*(p^*)|^{\frac{1}{2}}} \,\widetilde{\psi}_{sc}(p^*) = \frac{C}{|p(q)|^{\frac{1}{2}}} e^{\frac{i}{\hbar}S(q) - \frac{i\pi}{2}} \,. \tag{2.22}$$

The extra $|p'(q^*)|^{1/2}$ weight in (2.19) is cancelled by the $|q'(p^*)|^{1/2}$ term, by the Legendre relation (2.20).

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 2.2 by 180°, and flipping coordinates $(q, p) \rightarrow (-q, -p)$. While a turning point is not an invariant concept (for a sufficiently short trajectory segment, it can be undone by a 45° turn), for a complete period (q, p) = (q', p') the total phase slip is always $-2 \cdot \pi/2$, as a loop always has m = 2 turning points.

The WKB quantization condition follows by demanding that the wave function computed after a complete period be single-valued. With the normalization (2.8), 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 ,

$$\frac{1}{\hbar} \oint p(q)dq = 2\pi \left(n + \frac{m}{4}\right), \qquad (2.23)$$

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

The action integral in (2.23) is the area (see figure 2.3) enclosed by the classical phase space loop of figure 2.2, and the quantization condition says



Figure 2.4: Airy function Ai(q).

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.

2.3.1 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 2.2 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

$$E_n = \hbar\omega(n+1/2) \tag{2.24}$$

turns out to be the exact harmonic oscillator spectrum. The stationary phase condition (2.18) 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 (2.5) as a short wavelength approximation.

2.4 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 (2.16), 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 (2.14) fails whenever $\Phi''(x) = 0$, or, in our the WKB ansatz (2.18), whenever the momentum p'(q) = S''(q)vanishes. In that case we have to go beyond the quadratic approximation (2.15) to the first nonvanishing term in the Taylor expansion of the exponent. If $\Phi'''(x_0) \neq 0$, then

$$I \approx A(x_0) e^{is\Phi(x_0)} \int_{-\infty}^{\infty} dx \, e^{is\Phi'''(x_0)\frac{(x-x_0)^3}{6}} \,.$$
(2.25)

Airy functions can be represented by integrals of the form

$$Ai(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dy \, e^{i(xy - \frac{y^3}{3})} \,. \tag{2.26}$$

Derivations of the WKB quantization condition given in standard quantum mechanics textbooks rely on expanding the potential close to the turning point

$$V(q) = V(q_0) + (q - q_0)V'(q_0) + \cdots,$$

solving the Airy equation

$$\psi'' = q\psi, \qquad (2.27)$$

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 and learning about their asymptotics - a challenge that we will have to eventually overcome, in order to incorporate diffraction phenomena into semiclassical quantization.

- 2) what does the wave function look like?
- 3) generically useful when Gaussian approximations fail

The physical origin of the topological phase is illustrated by the shape of the Airy function, figure 2.4. For a potential with a finite slope V'(q)the wave function pentrates into the forbidden region, and accomodates a bit more of a stationary wavelength then what one would expect from the classical trajectory alone. For infinite walls (that is, 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 $-\pi/2$.

Commentary

Remark 2.1 <u>Airy function.</u> 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 [3.4].

Remark 2.2 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.

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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 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 inbetween 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.

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Exercises

Exercise 2.1 **WKB ansatz.** Try to show that no other ansatz other than (??) gives a meaningful definition of the momentum in the $\hbar \rightarrow 0$ limit. **Exercise** 2.2 **Freshel integral**.

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

Exercise ${}^{t}2'3^{-\infty}$ Sterling formula for n!. Compute an approximate value of n! for large n using the stationary phase approximation. Hint: n $if t t^n e^{-t}$. **Exercise** 2.4 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

$$Ai(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dy \, e^{i(xy - \frac{y^3}{3})} \,. \tag{2.28}$$

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.

Chapter 3

Lattice field theory

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Field theory is developed at not quite the pedestrian level, perhaps a cyclist level. We do it all on a finite lattice, without any functional integrals voodoo; all we have to know is how to manipulate finite dimensional vectors and matrices. More of such stuff can be found in ref. [3.2].

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. [3.1], or any other decent introduction to critical phenomena.

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

$$I = \int_{-\infty}^{\infty} dx \, e^{-t\Phi(x)} \tag{3.1}$$

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,

$$I \approx \sum_{x^*} \sqrt{2\pi/t \Phi''(x^*)} e^{-t\Phi(x^*)}.$$
(3.2)

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

$$\int [dx] e^{-\frac{1}{2}x^T \cdot M^{-1} \cdot x + x \cdot J} = (\det M)^{\frac{1}{2}} e^{\frac{1}{2}J^T \cdot M \cdot J}, \qquad (3.3)$$
$$[dx] = \frac{dx_1}{\sqrt{2\pi}} \frac{dx_2}{\sqrt{2\pi}} \cdots \frac{dx_D}{\sqrt{2\pi}},$$

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

The stationary phase estimate of (3.1) is

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

where x^* are the stationary phase points

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

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

These integrals is all that is needed for the semiclassical approximation, with the proviso that M^{-1} in (3.3) has no zero eigenvalues.

3.1 Saddle-point expansions are asymptotic

The first trial ground for testing our hunches about field theory is the zerodimensional 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 $\phi^2 \rightarrow M\phi^2$, $\sqrt{M}J \rightarrow J$, 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

$$Z[J] = \int \frac{d\phi}{\sqrt{2\pi}} e^{-\phi^2/2 - g\phi^4/4 + \phi J} \,. \tag{3.4}$$

Substituting M as defined by (3.22) 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, $r + 12u(\phi^c)^2 \rightarrow 0$, the perturbation theory

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fails us badly, and that is one of the reasons why we need the renormalization theory.

The idea of the saddle-point expansion (3.23) 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

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

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 (3.29) 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:

$$Z[0] = \sum_{n} Z_{n} g^{n},$$

$$Z_{n} = \frac{(-1)^{n}}{n! 4^{n}} \int \frac{d\phi}{\sqrt{2\pi}} \phi^{4n} e^{-\phi^{2}/2} = \frac{(-1)^{n}}{16n!} \frac{(4n)!}{(2n)!}.$$
(3.5)

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

$$g^n Z_n \approx \frac{1}{\sqrt{n\pi}} \left(\frac{4gn}{e}\right)^n$$
 (3.6)

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! page 42 Why? Consider again (3.5). 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 [3.9]. Consider the residual error after inclusion of the first n perturbative corrections:

$$R_{n} = \left| Z(g) - \sum_{m=0}^{n} g^{m} Z_{m} \right|$$

$$= \int \frac{d\phi}{\sqrt{2\pi}} e^{-\phi^{2}/2} \left| e^{-g\phi^{4}/4} - \sum_{m=0}^{n} \frac{1}{m!} \left(-\frac{g}{4} \right)^{m} \phi^{4m} \right|$$

$$\leq \int \frac{d\phi}{\sqrt{2\pi}} e^{-\phi^{2}/2} \frac{1}{(n+1)!} \left(\frac{g\phi^{4}}{4} \right)^{n+1} = g^{n+1} |Z_{n+1}| . \quad (3.7)$$

The inequality follows from the convexity of exponentials, a generalization of the inequality $e^x \ge 1+x$. The error decreases as long as $g^n |Z_n|$ decreases. From (3.6) the minimum is reached at $4g n_{min} \approx 1$, with the minimum error

$$g^n Z_n|_{min} \approx \sqrt{\frac{4g}{\pi}} e^{-1/4g}.$$
(3.8)

As illustrated by the figure 3.1, 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 $n_{min} \approx 1/\alpha \approx 137$

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3.5

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Figure 3.1: Plot of the saddle-point estimate of Z_n vs. the exact result (3.5) for g = 0.1, g = 0.02, g = 0.01.

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 $n \leq 5$.

Commentary

Remark 3.1 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 [3.4]. In case at hand, the phase transition $\phi^c = 0 \rightarrow \pm \phi^c \neq 0$ 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 [3.10].

• 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.

3.2 Path integrals

The path integral (1.33) 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 3.2 (in order to be able to draw this on a piece of paper, we have supressed 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

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

$$(3.9)$$

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 (1.33) is given by the extremal configuration alone

$$Z[J] = e^{W[J]} \to \sum_{c} e^{W_{c}[J]} = e^{W_{c}[J] + \ln n_{c}}$$
$$W_{c}[J] = S[q^{c}] + q^{c} \cdot J . \qquad (3.10)$$

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

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

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

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

term $S_I[q]$

$$S_{0}[q] = -\sum_{\ell} q_{\ell} (M^{-1})_{\ell,\ell'} q_{\ell} ,$$

$$S_{I}[q] = -(\cdots)_{\ell,\ell',\ell''} q_{\ell} q_{\ell'} q_{\ell''} + \cdots .$$
(3.11)

Rewrite the partition sum (1.33) 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

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

can be recast in terms of derivatives with respect to J

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

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

$$e^{W[J]} = e^{W_c[J]} e^{S_I[\frac{d}{dJ}]} \int [dq] e^{-\frac{1}{2}q^T \cdot M^{-1} \cdot q + q \cdot J} \Big|_{J=0}$$

= $\left| \det M \right|^{\frac{1}{2}} e^{W_c[J]} e^{S_I[\frac{d}{dJ}]} e^{\frac{1}{2}J^T \cdot M \cdot J} \Big|_{J=0}.$ (3.12)

M is invertible only if the minima in figure 3.2 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 [3.4]. 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 (3.12).

Expanding the exponentials and evaluating the $\frac{d}{dJ}$ derivatives in (3.12) 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 3.2 by a parabola, that is, keeping only the quadratic terms in the Taylor expansion (3.11).

3.3 Field theory - setting up the notation

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

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

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

$$\mathcal{H}_L[\phi] = \frac{r}{2} \phi_\ell \phi_\ell + \frac{c}{2} \partial_\mu \phi_\ell \partial_\mu \phi_\ell + u \sum_{\ell=1}^{N^a} \phi_\ell^4 \,. \tag{3.13}$$

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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 $h \to c^{1/2}h$, $\phi \to c^{-1/2}\phi$, and the \mathcal{H}_L in (3.13) is replaced by

$$\mathcal{H}[\phi] = \frac{1}{2} \partial_{\mu} \phi_{\ell} \partial_{\mu} \phi_{\ell} + \frac{m_0^2}{2} \phi_{\ell} \phi_{\ell} + \frac{g_0}{4!} \sum_{\ell} \phi_{\ell}^4$$
$$m_0^2 = \frac{r}{c}, \qquad g_0 = 4! \frac{u}{c^2}.$$
(3.14)

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

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

The actions we learn to handle here are of form

$$S[\phi] = -\frac{1}{2} (M^{-1})_{\ell\ell'} \phi_{\ell} \phi_{\ell'} + S_I[\phi] ,$$

$$S_I[\phi] = \frac{1}{3!} \gamma_{\ell_1 \ell_2 \ell_3} \phi_{\ell_1} \phi_{\ell_2} \phi_{\ell_3} + \frac{1}{4!} \gamma_{\ell_1 \ell_2 \ell_3 \ell_4} \phi_{\ell_1} \phi_{\ell_2} \phi_{\ell_3} \phi_{\ell_4} + \cdots . (3.15)$$

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

$$Z[J] = e^{W[J]} = \int [d\phi] e^{S[\phi] + \phi \cdot J}$$
(3.16)
$$= Z[0] \left(1 + \sum_{n=1}^{\infty} \sum_{\ell_1 \ell_2 \cdots \ell_n} G_{\ell_1 \ell_2 \cdots \ell_n} \frac{J_{\ell_1} J_{\ell_2} \dots J_{\ell_n}}{n!} \right),$$
$$G_{\ell_1 \ell_2 \cdots \ell_n} = \langle \phi_{\ell_1} \phi_{\ell_2} \dots \phi_{\ell_n} \rangle = \frac{1}{Z[0]} \frac{d}{dJ_{\ell_1}} \dots \frac{d}{dJ_{\ell_n}} Z[J] \Big|_{J=0}.$$
(3.17)

The "bare mass" m_0 and the "bare coupling" g_0 in (3.14) 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.

3.4 Saddle-point expansions

The "path integral" (3.16) 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 3.3 (in order to be able to draw this on a piece of paper, we have suppressed a large number of ϕ_{ℓ} coordinates).

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Figure 3.3: For the low temperature $T = 1/\beta$ the path integral (3.16) is dominated by the minima of the integrand's exponent. The location ϕ^c of a minimum is determined by the extremum condition $\partial_\ell S[\phi^c] + J_\ell = 0$.

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

$$\frac{d}{d\phi_{\ell}}S[\phi^{c}] + J_{\ell} = 0.$$
(3.18)

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 (3.16) is given by the extremal configuration alone

$$Z[J] = e^{W[J]} \to \sum_{c} e^{W_{c}[J]} = e^{W_{c}[J] + \ln n_{c}}$$
$$W_{c}[J] = S[\phi^{c}] + \phi^{c} \cdot J .$$
(3.19)

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 $S_I[\phi]$

$$S_{0}[\phi] = -\sum_{\ell} \phi_{\ell} \left(\frac{\beta r}{2c} + 12 \frac{\beta u}{c^{2}} (\phi^{c}_{\ell})^{2} \right) \phi_{\ell} + \frac{\beta}{2} \sum_{\ell,\ell'} \phi_{\ell} \Delta_{\ell\ell'} \phi_{\ell'} ,$$

$$S_{I}[\phi] = -\frac{\beta u}{c^{2}} \sum_{\ell=1}^{N^{d}} \phi_{\ell}^{4} . \qquad (3.20)$$

3.4. SADDLE-POINT EXPANSIONS

Spatially nonuniform ϕ_{ℓ}^{c} are conceivable. The mean field theory assumption is that the translational invariance of the lattice is not broken, and ϕ_{ℓ}^{c} is independent of the lattice point, $\phi_{\ell}^{c} \rightarrow \phi^{c}$. In the ϕ^{4} theory considered here, it follows from (3.18) 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 (3.19) when computing free energy density per site [3.3],

$$-\beta f[J] = \lim_{N \to \infty} W[J]/N^d.$$
(3.21)

We collect the matrix of bilinear ϕ coefficients in

$$(M^{-1})_{\ell\ell'} = \beta m_0^{\prime 2} \delta_{\ell\ell'} - \beta c \Delta_{\ell\ell'}, \qquad m_0^{\prime 2} = m_0^2 + 12u(\phi^c)^2 \tag{3.22}$$

in order to be able to rewrite the partition sum (3.16) 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

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

can be recast in terms of derivatives with respect to J

$$\int [d\phi]g(\phi)e^{-\frac{1}{2}\phi^T \cdot M^{-1} \cdot \phi} = g(\frac{d}{dJ}) \int [d\phi]e^{-\frac{1}{2}\phi^T \cdot M^{-1} \cdot \phi + \phi \cdot J} \bigg|_{J=0}$$

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

$$e^{W[J]} = e^{W_c[J]} e^{S_I[\frac{d}{dJ}]} \int [d\phi] e^{-\frac{1}{2}\phi^T \cdot M^{-1} \cdot \phi + \phi \cdot J} \Big|_{J=0}$$

= $\left| \det M \right|^{\frac{1}{2}} e^{W_c[J]} e^{S_I[\frac{d}{dJ}]} e^{\frac{1}{2}J^T \cdot M \cdot J} \Big|_{J=0}$. (3.23)

M is invertible only if the minima in figure 3.3 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 [3.4]. 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 (3.23).

As we shall show in sect. 3.6, expanding the exponentials and evaluating the $\frac{d}{dJ}$ derivatives in (3.23) 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 3.3 by a parabola, that is, keeping only the quadratic terms in the Taylor expansion (3.20). For a single minimum the "free energy" is in this approximation

$$W[J]_{1-loop} = W_c[J] + \frac{1}{2} \operatorname{tr} \ln M,$$
 (3.24)

where we have used the matrix identity $\ln \det M = \operatorname{tr} \ln M$, 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.



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3.5 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 glimpse of the theory by starting with no interactions, $S_I[\phi] = 0$. The free-field partition function (which sometimes ekes living under the name "Gaussian model") is

$$Z_{0}[J] = e^{W_{0}[J]} = \int [d\phi] e^{-\frac{1}{2}\phi^{T} \cdot M^{-1} \cdot \phi + \phi \cdot J} = |\det M|^{\frac{1}{2}} e^{\frac{1}{2}J^{T} \cdot M \cdot J}$$
$$W_{0}[J] = \frac{1}{2}J^{T} \cdot M \cdot J + \frac{1}{2} \operatorname{tr} \ln M.$$
(3.25)

The full n-point correlation functions (3.17) vanish for n odd, and for n even they are given by products of distinct combinations of 2-point correlations

$$G_{\ell\ell'} = (M)_{\ell\ell'}$$

$$G_{\ell_1\ell_2\ell_3\ell_4} = (M)_{\ell_1\ell_2}(M)_{\ell_3\ell_4} + (M)_{\ell_1\ell_3}(M)_{\ell_2\ell_4} + (M)_{\ell_1\ell_4}(M)_{\ell_2\ell_3}$$

$$G_{\ell_1\ell_2\cdots\ell_n} = (M)_{\ell_1\ell_2}\cdots(M)_{\ell_{n-1}\ell_n} + (M)_{\ell_1\ell_3}\cdots(M)_{\ell_{n-1}\ell_n} + (3.26)$$

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

$$(M)_{\ell_1\ell_2} = \ell_1 \bullet \bullet \bullet_{\ell_2}, \qquad J_\ell = \bullet \bullet_\ell, \qquad (3.27)$$

we expand the free-field theory partition function (3.25) as a Taylor series in $J^T \cdot M^{-1} \cdot J$

$$\frac{Z_0[J]}{Z_0[0]} = 1 + \frac{1}{2} \mathbf{c} - \mathbf{c} + \frac{1}{2^3} \mathbf{\hat{j}} \mathbf{\hat{j}} + \frac{1}{2^3} \frac{1}{3!} \mathbf{\hat{j}} \mathbf{\hat{j}} \mathbf{\hat{j}} + \cdots$$
(3.28)

In the diagrammatic notation the non-vanishing n-point correlations (3.26) are drawn as

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.

3.6 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 [3.5], as both the number of Feynman diagrams and the difficulty of their evaluation explodes combinatorially, but as 99% of physicists stop at a 1-loop correction, for the purpose at hand this is a perfectly sensible way to proceed.

3.6.1 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 (3.23)

$$e^{S_{I}\left[\frac{d}{dJ}\right]}e^{\frac{1}{2}J^{T}\cdot M\cdot J} = \left\{1 + \frac{1}{4!} + \frac{1}{2!} + \frac$$

Here we have indicated $\frac{d}{dJ}$ as a pac-man [3.6] that eats J, leaving a delta function in its wake

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

$$\frac{d}{dJ_j} \mathcal{I}_\ell = \frac{1}{j - \ell}.$$
(3.31)

For example, the rightmost pac-man in the $\sum_{\ell} \left(\frac{d}{dJ}_{\ell}\right)^4$ interaction term quartic in derivative has four ways of munching $\left(\frac{d}{dJ}_{\ell}\right)^4$ 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:

$$\frac{1}{4!} \frac{1}{2^3} \sqrt[6]{2^3} \left(\frac{1}{3!} \frac{1}{2^3} \sqrt[6]{2^3} \right)^{-1} = \frac{1}{3!} \frac{1}{2^3} \left(\sqrt[6]{2^3} \sqrt[6]{2^3} + 2\sqrt[6]{2^3} \right)^{-1} = \frac{1}{2^3} \sqrt[6]{2^3} = \frac{1}{8} \sqrt[6]{2^3} .$$
(3.32)

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 generating Feynman diagrams [3.2], but this will do for the problem at hand.

It is easy enough to prove this to all orders [3.7], but to this order you can simply check by expanding the exponential (3.16) that the free energy W[J] perturbative corrections are the connected, diagrams with J = 0

$$W[0] = S[\phi^{c}] + \frac{1}{2} \operatorname{tr} \ln M + \frac{1}{8} \bigcirc \bigcirc + \frac{1}{16} \bigcirc \bigcirc + \frac{1}{48} \bigcirc \bigcirc \stackrel{\text{page 42}}{(3.33)}$$

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.

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3.6

3.7 Propagator in the space representation

In order to describe the spatial variation in (3.14) we need to define a lattice derivative.

3.7.1 Lattice derivatives

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

$$\phi_{\ell} = \phi(x), \qquad x = a\ell = lattice \ point, \quad \ell \in \mathbf{Z}^a, \qquad (3.34)$$

where a is the lattice spacing and there are N^d points in all. A vector ϕ specifies a lattice configuration. Assume the lattice is hyper-cubic, and let $\hat{n}_{\mu} \in \{\hat{n}_1, \hat{n}_2, \dots, \hat{n}_d\}$ be the unit lattice cell vectors pointing along the d positive directions, $|\hat{n}_{\mu}| = 1$. The lattice partial derivative is then

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

Anything else with the correct $a \rightarrow 0$ limit would do, but this is the simplest choice. We can rewrite the derivative as a linear operator, by introducing the hopping operator (or "shift", or "step") in the direction μ

$$\left(\mathbf{h}_{\mu}\right)_{\ell j} = \delta_{\ell + \hat{n}_{\mu}, j} \,. \tag{3.35}$$

As **h** will play a central role in what follows, it pays to understand what it does, so we write it out for the 1-dimensional case in its full $[N \times N]$ matrix glory:

$$\mathbf{h} = \begin{pmatrix} 0 & 1 & & & \\ & 0 & 1 & & \\ & & 0 & 1 & & \\ & & & \ddots & \\ & & & & 0 & 1 \\ 1 & & & & & 0 \end{pmatrix} .$$
(3.36)

We will assume throughout that the lattice is periodic in each \hat{n}_{μ} direction; this is the easiest boundary condition to work with if we are interested in large lattices where surface effects are negligible. We will (perhaps) briefly discuss other boundary conditions in sect. ??.

Applied on the lattice configuration $\phi = (\phi_1, \phi_2, \dots, \phi_N)$, the hopping operator shifts the lattice by one site, $\mathbf{h}\phi = (\phi_2, \phi_3, \dots, \phi_N, \phi_1)$. Its transpose shifts the entries the other way, so the transpose is also the inverse

$$\mathbf{h}^{-1} = \mathbf{h}^T \,. \tag{3.37}$$

The lattice derivative can now be written as a multiplication by a matrix:

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

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

$$\partial = \frac{1}{a} \begin{pmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & -1 & 1 & & \\ & & & -1 & 1 & \\ & & & & \ddots & \\ & & & & & 1 \\ 1 & & & & & -1 \end{pmatrix} .$$
(3.38)

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" you say "it is just a matrix, no big deal, I know what a matrix is". OK?

3.7.2 Lattice Laplacian

In order to get rid of some of the lattice indices in (3.15) it is convenient to employ vector notation for the terms bilinear in ϕ , and keep the rest lumped into "interaction",

$$S[\phi] = -\frac{\beta m_0^2}{2} \phi^T \cdot \phi - \frac{\beta}{2a^2} \left[(\mathbf{h}_{\mu} - \mathbf{1}) \phi \right]^T \cdot (\mathbf{h}_{\mu} - \mathbf{1}) \phi + S_I[\phi]. \quad (3.39)$$

In the Landau case (3.14) 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 (3.67).

In the continuum integration by parts moves ∂_{μ} around; on a lattice this amounts to a matrix transposition

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

If you are wandering where the "integration by parts" minus sign is, it is there in discrete case at well. It comes from the identity $\partial^T = -\mathbf{h}^{-1}\partial$. The combination $\Delta = \mathbf{h}^{-1}\partial^2$

$$\Delta = -\frac{1}{a^2} \sum_{\mu=1}^{d} (\mathbf{h}_{\mu}^{-1} - \mathbf{1}) (\mathbf{h}_{\mu} - \mathbf{1}) = -\frac{2}{a^2} \sum_{\mu=1}^{d} \left(\mathbf{1} - \frac{1}{2} (\mathbf{h}_{\mu}^{-1} + \mathbf{h}_{\mu}) \right) (3.40)$$

is the lattice Laplacian. We shall show in sect. 3.9 that this Laplacian has the correct continuum limit. It is the simplest spatial derivative allowed for $x \rightarrow -x$ symmetric actions. In the 1-dimensional case the $[N \times N]$ matrix representation of the lattice Laplacian is:

$$\Delta = \frac{1}{a^2} \begin{pmatrix} -2 & 1 & & & 1\\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & & \\ & & 1 & \ddots & \\ & & & 1 & \ddots & \\ 1 & & & & 1 & -2 \end{pmatrix} .$$
(3.41)

The lattice Laplacian measures the second variation of a field ϕ_{ℓ} across three neighboring sites. 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, $\phi_{\ell} = \phi(\ell)$, where $\phi(\ell)$ is defined by the value of the continuum function $\phi(x) = x^2$ at the lattice point ℓ .

3.7.3 Inverting the Laplacian

Evaluation of perturbative corrections in (3.23) requires that we come to grips with the "free" or "bare" propagator M. While the inverse propagator M^{-1} is a simple one-step difference operator (3.22), its inverse is a messier object. A way to compute is to start expanding M as a power series in the Laplacian

$$\beta M = \frac{1}{m_0^{\prime 2} \mathbf{1} - \Delta} = \frac{1}{m_0^{\prime 2}} \sum_{k=0}^{\infty} \left(\frac{c}{m_0^{\prime 2}}\right)^k \Delta^m.$$
(3.42)

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

$$\Delta^{2} = \frac{1}{a^{4}} \begin{pmatrix} 6 & -4 & 1 & 1 & -4 \\ -4 & 6 & -4 & & & \\ 1 & -4 & 6 & -4 & 1 & & \\ & & -4 & & \ddots & & \\ & & & & & -4 \\ -4 & 1 & & & 1 & -4 & 6 \end{pmatrix} .$$
(3.43)

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 operator, connecting every lattice site to any other lattice site [3.8].

This matrix 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. 3.8.

3.7.4 Why is propagator called "propagator"?

In statistical mechanics, M is the (bare) 2-point correlation. In quantum field theory, it is called a propagator. Why?

Until now the collective indices have stood for all particle labels; spacetime location, spin, field type and so on. 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?

Our formulation is inevitably phenomenological: we have no idea what the structure of our space on distances much shorter than inter-atomic 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 hops from one space-time cell to another space-time 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 particle physics we have no indication of having reached the distance scales in which any new space-time structure is being sensed: hence for us this hopping probability has no direct physical significance. It is simply a phenomenological parameter: in the continuum limit it will be replaced by the mass of the particle.

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skip the rest of this section, unfinished

We assume for the time being that the state of a particle is specified by its space-time position, and that it has no further labels (such as spin or color): $a = (x1, x \ d)$. 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



with all possible paths connecting the two cells:

$$A_{\cdot\cdot} = sIh^L N_{ij}(L) \tag{3.44}$$

 $N_{ij}(L)$ is the number of all paths of length L connecting lattice sites i and j. Define a stepping matrix

$$(S^{\mu})ij = 6_{i+n_{\mu},j}.$$
(3.45)

If a particle is introduced into the *i*-th cell by a source

$$J_k = \delta'_{ik}$$

the stepping matrix moves it into a neighboring cell:

 $(S^{\mu}J)_k = 6i + n, ki + n$

The operator

$$d(h \cdot S)ij = \sum_{\mu} it_{\mu}[(S^{\mu})ij + (S^{\mu})jil\mu = 1 h\mu = (h, h, \dots, h), h)$$
(3.46)

generates all paths of length 1 with probability h:

 $(h \cdot S)J = hi - thcell$

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

 \mathcal{Z}

(has) $21 = h^2$

I and so on. Note that the k-th component of the vector $(h \cdot S)^L J$ counts the number of paths of length L connecting the i-th and the k-th spacetime cells. The total probability that the particle stops in the k-th cell is given by

s ZNS?J.

I ki a

(5.4)

The value of the field at a space-time point it measures the probability of observing the particle introduced into the system by the source J. The Euclidean free scalar particle propagator (5.1) is given by

 $A \ s \ (5.5)$

$$ij = OAK$$

or, in the continuum limit do by

$$dik \cdot (x-y)A(X,Y)dkeI - +m^2(2\pi)dk^2$$

Interpreting ϕ as a field is consistent with the previous definition of a free field, equations (2.22) and (2.25).

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3.8 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 $\phi \to \mathbf{h}\phi$ translation on the action (3.20)

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

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

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

If a function (in this case, the action $S[\phi]$) defined on a vector space (in this case, the configuration ϕ) commutes with a linear operator \mathbf{h} , then the eigenvalues of \mathbf{h} can be used to decompose the ϕ vector space into invariant subspaces. For a hyper-cubic lattice the translations in different directions commute, $\mathbf{h}_{\mu}\mathbf{h}_{\nu} = \mathbf{h}_{\nu}\mathbf{h}_{\mu}$, so it is sufficient to understand the spectrum of the 1-dimensional shift operator (3.36). To develop a feeling for how this reduction to invariant subspaces works in practice, let us continue in the humble spirit of sect. 3.1, by expanding the scope of our deliberations to a lattice consisting of 2 points.

3.8.1 A 2-point lattice diagonalized

The action of the shift operator **h** (3.36) on a 2-point lattice $\phi = (\phi_1, \phi_2)$ is to permute the two lattice sites

$$\mathbf{h} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \,.$$

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

$$(\mathbf{h}+1)(\mathbf{h}-1)=0\,,$$

with eigenvalues $\lambda = 1, \lambda_2 = -1$. Construct now the symmetrization, antisymmetrization projection operators

$$P_1 = \frac{\mathbf{h} - \lambda_2 \mathbf{1}}{\lambda_1 - \lambda_2} = \frac{\mathbf{h} - (-\mathbf{1})}{1 - (-1)} = \frac{1}{2} (\mathbf{1} + \mathbf{h}) = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$
(3.48)

$$P_2 = \frac{\mathbf{h} - \mathbf{1}}{-1 - 1} = \frac{1}{2}(\mathbf{1} - \mathbf{h}) = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$
(3.49)

Noting that $P_1 + P_2 = \mathbf{1}$, we can project the lattice configuration ϕ onto the two eigenvectors of \mathbf{h} :

$$\phi = \mathbf{1}\phi = P_1 \cdot \phi + P_2 \cdot \phi,$$

$$\begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = \frac{(\phi_1 + \phi_2)}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{(\phi_1 - \phi_2)}{\sqrt{2}} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$
(3.50)

As $P_1P_2 = 0$, the symmetric and the antisymmetric configurations transform separately under any linear transformation constructed from **h** and its powers.

In this way the characteristic equation $\mathbf{h}^2 = \mathbf{1}$ enables us to reduce the 2-dimensional lattice configuration to two 1-dimensional ones, on which the value of the shift operator \mathbf{h} is $\lambda = 1, -1$, and the eigenvectors are $\frac{1}{\sqrt{2}}(1, 1)$, $\frac{1}{\sqrt{2}}(1, -1)$. We have inserted $\sqrt{2}$ factors only for convenience, in order that the eigenvectors be normalized unit vectors.

3.8.2 Discrete Fourier transforms

Now let us generalize this reduction to a 1-dimensional periodic lattice with N sites.

Each application of **h** translates the lattice one step; in N steps the lattice is back in the original configuration $\Phi_5 \bullet \Phi_2 \bullet \Phi_3 \bullet \Phi_2$

$$\mathbf{h}^N = \mathbf{1} \qquad \qquad \mathbf{h}^N = \mathbf{1}$$

so the eigenvalues of \mathbf{h} are the N distinct N-th roots of unity

$$\mathbf{h}^{N} - \mathbf{1} = \prod_{k=0}^{N-1} (\mathbf{h} - \omega^{k} \mathbf{1}) = 0, \qquad \omega = e^{i\frac{2\pi}{N}}.$$
 (3.51)

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

$$P_k = \prod_{j \neq k} \frac{\mathbf{h} - \lambda_j \mathbf{1}}{\lambda_k - \lambda_j} \,. \tag{3.52}$$

A factor $(\mathbf{h} - \lambda_j \mathbf{1})$ 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 eigendirection 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

$$\sum_{k} P_k = \mathbf{1} \tag{3.53}$$

and orthonormal

$$P_k P_j = \delta_{kj} P_k \qquad (no \ sum \ on \ k) \,. \tag{3.54}$$

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 [3.11]. 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

$$\mathbf{h}\,\varphi_k \qquad = \quad \omega^k \varphi_k \tag{3.55}$$

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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 unit vectors

$$\varphi_{k}^{\dagger} \cdot \varphi_{k} = \frac{1}{N} \sum_{k=0}^{N-1} 1 = 1 , \quad (no \ sum \ on \ k)$$

$$\varphi_{k}^{\dagger} = \frac{1}{\sqrt{N}} \left(1, \omega^{-k}, \omega^{-2k}, \cdots, \omega^{-(N-1)k} \right) . \quad (3.56)$$

The eigenvectors are orthonormal

$$\varphi_k^{\dagger} \cdot \varphi_j = \delta_{kj} \,, \tag{3.57}$$

as the explicit evaluation of $\varphi_k^{\dagger} \cdot \varphi_j y_i$ $\omega_k^{\dagger} \psi_j^{\ast} w_k^{\ast}$: delta function for a periodic lattice

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 $k = j \pmod{N}$, in which case each term in the sum equals 1.

The projection operators can be expressed in terms of the eigenvectors (3.55), (3.56) as

$$(P_k)_{\ell\ell'} = (\varphi_k)_{\ell} (\varphi_k^{\dagger})_{\ell'} = \frac{1}{N} e^{i\frac{2\pi}{N}(\ell-\ell')k} , \qquad (no \ sum \ on \ k) .$$
 (3.59)

The completeness (3.53) follows from (3.58), and the orthonormality (3.54) from (3.57).

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

$$(P_k \cdot \phi)_{\ell} = \tilde{\phi}_k (\varphi_k)_{\ell} , \qquad (no \ sum \ on \ k)$$

$$\tilde{\phi}_k = \varphi_k^{\dagger} \cdot \phi = \frac{1}{\sqrt{N}} \sum_{\ell=0}^{N-1} e^{-i\frac{2\pi}{N}k\ell} \phi_{\ell} \qquad (3.60)$$

We recognize ϕ_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).

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

.

$$\tilde{M}_{kk'} = (\varphi_k^{\dagger} \cdot \mathbf{M} \cdot \varphi_{k'}) \tag{3.61}$$

is the Fourier space representation of M. No need to stop here - the terms in the action (3.15) that couple 3, 4, \cdots fields also have the Fourier space representations

$$\begin{aligned} \gamma_{\ell_1\ell_2\cdots\ell_n} \phi_{\ell_1}\phi_{\ell_2}\cdots\phi_{\ell_n} &= \tilde{\gamma}_{k_1k_2\cdots k_n} \tilde{\phi}_{k_1}\tilde{\phi}_{k_2}\cdots\tilde{\phi}_{k_n}, \\ \tilde{\gamma}_{k_1k_2\cdots k_n} &= \gamma_{\ell_1\ell_2\cdots\ell_n}(\varphi_{k_1})_{\ell_1}(\varphi_{k_2})_{\ell_2}\cdots(\varphi_{k_n})_{\ell_n} \\ &= \frac{1}{N^{n/2}}\sum_{\ell_1\cdots\ell_n}\gamma_{\ell_1\ell_2\cdots\ell_n} e^{-i\frac{2\pi}{N}(k_1\ell_1+\cdots+k_n\ell_n)} \hat{\beta}.62) \end{aligned}$$

According to (3.57) the matrix $U_{k\ell} = (\varphi_k)_{\ell} = \frac{1}{\sqrt{N}} e^{i\frac{2\pi}{N}k\ell}$ is a unitary matrix, and 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 (3.16) 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 **M** is the trace in either representation

$$\operatorname{tr} \mathbf{M} = \sum_{\ell} M_{\ell\ell} = \sum_{kk'} \sum_{\ell} (P_k \mathbf{M} P_{k'})_{\ell\ell}$$
$$= \sum_{kk'} \sum_{\ell} (\varphi_k)_{\ell} (\varphi_k^{\dagger} \cdot \mathbf{M} \cdot \varphi_{k'}) (\varphi_{k'}^{\dagger})_{\ell} = \sum_{kk'} \delta_{kk'} \tilde{M}_{kk'} = \operatorname{tr} \tilde{\mathbf{N}} \mathbf{I}.63)$$

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

3.8.3 Lattice Laplacian diagonalized

Now use the eigenvalue equation (3.55) to convert **h** matrices into scalars. If **M** commutes with **h**, then $(\varphi_k^{\dagger} \cdot \mathbf{M} \cdot \varphi_{k'}) = \tilde{M}_k \delta_{kk'}$, and the matrix **M** acts as a multiplication by the scalar M_k on the k-th subspace. For example, for the 1-dimensional version of the lattice Laplacian (3.40) the projection on the k-th subspace is

$$\begin{aligned} (\varphi_k^{\dagger} \cdot \Delta \cdot \varphi_{k'}) &= \frac{2}{a^2} \left(\frac{1}{2} (\omega^{-k} + \omega^k) - 1 \right) (\varphi_k^{\dagger} \cdot \varphi_{k'}) \\ &= \frac{2}{a^2} \left(\cos \left(\frac{2\pi}{N} k \right) - 1 \right) \delta_{kk'} \end{aligned}$$
(3.64)

In the k-th subspace the bare propagator (3.42) is simply a number, and, in contrast to the mess generated by (3.42), there is nothing to inverting M^{-1} :

$$(\varphi_{\mathbf{k}}^{\dagger} \cdot M \cdot \varphi_{\mathbf{k}'}) = (\tilde{G}_0)_{\mathbf{k}} \delta_{\mathbf{k}\mathbf{k}'} = \frac{1}{\beta} \frac{\delta_{\mathbf{k}\mathbf{k}'}}{m_0'^2 - \frac{2}{a^2} \sum_{\mu=1}^d \left(\cos\left(\frac{2\pi}{N}k_{\mu}\right) - 1\right)}, (3.65)$$

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

Going back to the partition function (3.23) 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 $(\tilde{G}_0)_k$

$$J^T \cdot M \cdot J = \sum_{k,k'} (J^T \cdot \varphi_k) (\varphi_k^{\dagger} \cdot M \cdot \varphi_{k'}) (\varphi_{k'}^{\dagger} \cdot J) = \sum_k \tilde{J}_k^{\dagger} (\tilde{G}_0)_k \tilde{J}_k . (3.66)$$

What's the price? The interaction term $S_I[\phi]$ (which in (3.23) was local in the configuration space) now has a more challenging k dependence in the Fourier transform version (3.62). For example, the locality of the quartic term leads to the 4-vertex momentum conservation in the Fourier space

$$S_{I}[\phi] = \frac{1}{4!} \gamma_{\ell_{1}\ell_{2}\ell_{3}\ell_{4}} \phi_{\ell_{1}}\phi_{\ell_{2}}\phi_{\ell_{3}}\phi_{\ell_{4}} = -\beta u \sum_{\ell=1}^{N^{d}} (\phi_{\ell})^{4} \Rightarrow$$
$$= -\beta u \frac{1}{N^{3d/2}} \sum_{\{\mathbf{k}_{i}\}}^{N} \delta_{0,\mathbf{k}_{1}+\mathbf{k}_{2}+\mathbf{k}_{3}+\mathbf{k}_{4}} \tilde{\phi}_{\mathbf{k}_{1}}\tilde{\phi}_{\mathbf{k}_{2}}\tilde{\phi}_{\mathbf{k}_{3}}\tilde{\phi}_{\mathbf{k}_{4}}.$$
(3.67)

3.9 Continuum field theory

3.10 Summary and outlook

We have formulated the standard field-theoretic perturbation theory. From here, any generalization and future direction is wide open.

Acknowledgement. I am indebted to Benny Lautrup both for my first introduction to a lattice field theory, and for the interpretation of the Fourier transform as the spectrum of the shift operator.

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- [3.7] Read section 2.F of ref. [3.2].
- [3.8] Read chapter 5 of ref. [3.2], pp. 61-64 up to eq. (5.6), and do the exercise 5.A.1. (reproduced as the exercise 3.8 here).

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Exercises

Exercise 3.1 Free-field theory combinatorics. Check that there indeed are **Exercise** 3.2 Refaiters in the provide series 29. 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 q; plot both your error and the the exact result (3.5) for g = 0.1, g = 0.02, g = 0.01. The prettiest plot makes it into these notes as Exercise 3.3 Complex Gaussian integrals. Read sect. 3.B, do exercise 3.B.1 Exercise [3.2] **Prove** $\ln \det = \operatorname{tr} \ln t$. (link here the $\ln \det = \operatorname{tr} \ln \operatorname{problem sets}$, $\mathbf{E}_{\mathbf{xercise}}^{lready}$ **Convexity of exponentials.** Prove the inequality (3.7). Matthias Eschrig suggest that a more general proof be offered, applicable to any monotone descreasing sequence with alternating signs. Exercise 3.6 Wick expansion for ϕ^{\pm} theories. Derive (3.33), check the combinatorial signs Exercise 3.7 Wick expansions. Read sect. 3.C and do exercise 3.C.2 of Exercise 3.8 Propagators in the configuration space. Define the finite difference operator by f(x + f(x - a)) $\partial f(x)$ 2 a where a is the lattice spacing. Show that

1 d h (So' + Sri 2d+a'3'

P if ji ,

where $\partial^2 = 911\partial 11$ is the finite difference Laplacian. Show that the Euclidean scalar lattice propagator (??) is given by

-1 ha' 2 ij s

The mass in the continuum propagator (5.6) is related to the hopping parameter by s

(5.9)

If the particle does not like hopping $(h \rightarrow O)$, the mass is infinite and there is no propagation. If the particle does not like stopping (s -0), the mass is zero and the particle zips all over the space. Diagonalize 32 by Fourier transforming and derive (5.6).

$\textbf{Appendix} \ A$

Group theory

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A.1 Invariant matrices and reducibility

The basic idea is simple; any hermitian (or, for real matrices, any symmetric) matrix can be brought to diagonal form. If this matrix is an invariant matrix, it decomposes the space into direct sums of lower-dimensional subspaces. This topic is developed at great length in ref. [A.1]. For the humble application at hand, even this appendix is an overkill, but it might give you a feeling for how the Fourier analysis fits into the general theory of invariance groups and their representations.

A.1.1 Definitions

Let V be the defining d-dimensional complex vector space, $\overline{V} = \{\overline{x} \mid \overline{x}^* \in V\}$ the conjugate space, and \mathcal{G} a group acting linearly on V. The action of $g \in \mathcal{G}$ on a vector $x \in V$ is given by a $[d \times d]$ matrix representation G

$$x'_{a} = G^{b}_{a} x_{b} \qquad a, b = 1, 2, \dots, d.$$
 (A.1)

The repeated indices are always summed over unless explicitly stated otherwise.

We distinguish the components of defining space vectors, resp. conjugate vectors, by lower, resp. upper indices

$$\begin{aligned}
x &= (x_1, x_2, \dots, x_n) , x \in V \\
\bar{x} &= (x^1, x^2, \dots, x^n) , \bar{x} \in \bar{V}.
\end{aligned}$$
(A.2)

The two spaces are related by complex conjugation, which is here indicating by raising the vector index:

$$x^a = (x_a)^*.$$

The action of $g\in \mathcal{G}$ on a vector $\bar{q}\in \bar{V}$ is given by the conjugate representation G^{\dagger}

$$x'^{a} = x^{b} (G^{\dagger})^{a}_{b}, \qquad (G^{\dagger})^{a}_{b} \equiv (G^{b}_{a})^{*}$$
 (A.3)

A.1.2 Projection operators

A matrix is hermitian if its elements satisfy

$$(M^{\dagger})^a_b = M^a_b \,. \tag{A.4}$$

For M a hermitian matrix, there exists a diagonalizing unitary matrix C:

$$CMC^{\dagger} = \begin{pmatrix} \begin{array}{cccc} \lambda_{1} & 0 \\ 0 & \lambda_{1} \\ \end{array} & \begin{array}{c} 0 & & 0 \\ \lambda_{2} & 0 & & \\ 0 & \lambda_{2} & & \\ \vdots & \ddots & \vdots \\ 0 & & \ddots & \lambda_{2} \\ \end{array} & \begin{array}{c} \lambda_{3} & \dots \\ \vdots & \ddots \end{array} \end{pmatrix}, \ \lambda_{i} \neq \lambda_{j} . (A.5)$$

Here λ_i are the r distinct roots of the minimal characteristic polynomial

$$\prod_{i=1}^{r} (M - \lambda_i \mathbf{1}) = 0.$$
(A.6)

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

$$C(M - \lambda_2 \mathbf{1})C^{\dagger} = \begin{pmatrix} \lambda_1 - \lambda_2 & & & \\ & \lambda_1 - \lambda_2 & & \\ & & 0 & & \\ & & & 0 & \\ & & & & \ddots & \\ & & & & & 0 & \\ & & & & & \lambda_3 - \lambda_2 & \\ & & & & & & \lambda_3 - \lambda_2 & \\ & & & & & & \ddots & \end{pmatrix}$$

so the product over all factors $(M - \lambda_1 \mathbf{1})(M - \lambda_3 \mathbf{1})\dots$ with exception of the $(M - \lambda_2 \mathbf{1})$ factor has non-zero entries only in the subspace associated with λ_1 :

In this way we can associate with each distinct root λ_i a projection operator P_i

$$P_i = \prod_{j \neq i} \frac{M - \lambda_j \mathbf{1}}{\lambda_i - \lambda_j}, \qquad (A.7)$$

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which is identity on the *i*th subspace, and zero elsewhere. For example, the projection operator onto the λ_1 subspace is

It follows from the characteristic equation (A.6) that λ_i is the eigenvalue of M on P_i subspace:

$$MP_i = \lambda_i P_i , \qquad (no \ sum \ on \ i),$$
(A.9)

and that any matrix polynomial f(M) takes scalar value $f(\lambda_i)$ on the P_i subspace

$$f(M)P_i = f(\lambda_i)P_i.$$
(A.10)

The matrices P_i are orthonormal

$$P_i P_j = \delta_{ij} P_j , \qquad (no \ sum \ on \ j) , \qquad (A.11)$$

and satisfy a completeness relation

$$\sum_{i=1}^{r} P_i = \mathbf{1}.$$
(A.12)

As tr (CP_iC^+) = tr P_i , the dimension of the *i*-th subspace is given by

$$d_i = \operatorname{tr} P_i \,. \tag{A.13}$$

A.1.3 Decomposition of representations

A matrix M is invariant if it commutes with all group transformations [G, M] = 0. Projection operators (A.7) constructed from M are polynomials in M, so they also commute with all $g \in \mathcal{G}$:

$$[G, P_i] = 0, \tag{A.14}$$

(remember that P_i are $[d \times d]$ matrices). Hence a $[d \times d]$ matrix representation can be written as a direct sum of $[d_i \times d_i]$ matrix representations

$$G = \mathbf{1}G\mathbf{1} = \sum_{i,j} P_i G P_j = \sum_i P_i G P_i = \sum_i G_i.$$
(A.15)

In the diagonalized representation (A.8), the matrix G has a block diagonal form:

$$CGC^{\dagger} = \begin{bmatrix} G_1 & 0 & 0 \\ 0 & G_2 & 0 \\ 0 & 0 & \ddots \end{bmatrix} , \qquad G = \sum_i C^i G_i C_i .$$
 (A.16)

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 \diamond

Representation G_i acts only on the d_i dimensional subspace V_i consisting of vectors P_iq , $q \in \tilde{V}$. In this way an invariant $[d \times d]$ hermitian matrix M with r distinct eigenvalues induces a decomposition of a d-dimensional vector space \tilde{V} into a direct sum of d_i -dimensional vector subspaces V_i

$$\tilde{V} \stackrel{M}{\longrightarrow} V_1 \oplus V_2 \oplus \ldots \oplus V_r \,. \tag{A.17}$$

On the one-dimensional spaces the group acts trivially, G = 1.

If a projection operator projects onto a zero-dimensional subspace, it must vanish identically

$$d_i = 0 \implies P_i = 0. \tag{A.18}$$

This follows from (A.8); d_i is the number of 1's on the diagonal on the right-hand side. The general form of P_i is

$$P_i = \sum_{k=1}^r c_k M_k \tag{A.19}$$

where M_k are the invariant matrices used in construction of the projector operators, and c_k are numerical coefficients. Vanishing of P_i therefore implies linear dependence among invariant matrices M_k .

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