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Quantum Field Theory and Critical Phenomena

FIFTH EDITION

JEAN ZINN-JUSTIN



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JEAN ZINN-JUSTIN

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Introduced as a quantum extension of Maxwell's classical theory, quantum electrodynamics (QED) has been the first example of a local quantum field theory (QFT). Eventually, QFT has become the framework for the discussion of all fundamental interactions at the microscopic scale except, possibly, gravity. More surprisingly, it has also provided a framework for the understanding of second order phase transitions in statistical mechanics. In fact, as hopefully this work will illustrate, QFT is the natural framework for the discussion of most systems involving an infinite number of degrees of freedom with local couplings. These systems range from cold Bose gases at the condensation temperature (about ten nanokelvin) to conventional phase transitions (from a few degrees to several hundred) and high energy particle physics up to TeVs, altogether more than *twenty orders of magnitude* in the energy scale.

Therefore, although excellent textbooks about QFT had already been published, I thought, many years ago, that it might not be completely worthless to present a work in which the strong formal relations between particle physics and the theory of critical phenomena are systematically emphasized. This option explains some of the choices made in the presentation. A formulation in terms of field integrals is adopted to study the properties of QFT. Less important, perhaps, in general the space–time metric is chosen Euclidean, as is natural for statistical mechanics, and in particle physics often convenient for perturbative calculations, and necessary for numerical simulations. The language of particle physics. Renormalization and renormalization group (RG) properties are systematically discussed, whereas limited space is devoted to scattering theory. Only formal aspects of QED are considered, since excellent textbooks cover this subject extensively.

For what follows, note that, in a deep quantum relativistic context, one can set $\hbar = c = 1$, and energies are then proportional to momenta and masses, and inverse of distances.

In QFT, the basic analytic tool to calculate physical quantities is an expansion in powers of the interactions. The initial (or bare) Lagrangian of QED generates an expansion in terms of the *bare fine-structure constant* $\alpha_0 = e_0^2/4\pi\hbar c$. In a straightforward perturbative calculation, one discovers that all physical quantities are infinite, the *locality* of QED generating *short-distance singularities* (one speaks about ultraviolet (UV) divergences).

This situation has to be contrasted with what happens in classical or non-relativistic quantum mechanics (QM); there, the replacement of macroscopic by point-like objects leads, in general, to no mathematical inconsistencies, and is often a very good approximation: the absence of this property would indeed have made progress in physics quite difficult. To summarize: in the latter theories, *phenomena at very different scales, to a good approximation, decouple.* Most surprisingly, this is no longer the case in QFT.

In QED, a remedy to the infinity problem was found empirically: one first *regularizes* QED (*i.e.* one renders the perturbative expansion finite) by artificially modifying the theory at short distance, or equivalently at large momentum, at a scale characterized by

a large momentum cut-off Λ (in general, introducing non-physical short-distance properties). Inspired by methods of condensed matter physics, one then re-expresses all physical quantities in terms of the measured fine structure constant and the physical masses of particles, in place of the original (bare) parameters of the Lagrangian. After this change of parametrization, the cut-off is removed, and somewhat miraculously, order by order in perturbation theory, all other physical quantities have a finite limit. Moreover, the limit is independent of the precise form of the regularization. This strange method, called *renormalization*, did soon find an experimental confirmation: it led to predictions agreeing with increasingly impressive precision with experiments.

Therefore, it became then natural to search for other *renormalizable* QFTs, to describe all interactions. This led to another major achievement: a renormalizable QFT for all three, strong, weak, and electromagnetic interactions. The so-called Standard Model (SM), whose formal structure was proposed more than forty years ago, completely describes physics at the microscopic scale, and has been comforted in 2012, in a spectacular way, by the discovery, at the Large Hadron Collider of the European Center for Nuclear Research (CERN), of the last missing particle of the model, the Higgs scalar boson.

The impressive success of a strategy based on looking for renormalizable QFTs, that led to the SM, then slowly promoted *renormalizability* as a kind of additional law of nature. In particular, once the SM of weak, electromagnetic and strong interactions was established, much effort was devoted to cast gravity in the same framework. Despite ingenious attempts, no renormalizable form of quantum gravity has been found yet.

In a massless renormalizable QFT, it is necessary to introduce a reference physical energy scale at which the physical coupling constants are defined. It was realized early on, first as a mathematical curiosity, that an RG could be associated with a change of the reference scale at constant physical properties. The RG describes how the physical (or effective) coupling constants vary with the reference scale.

Eventually, it was realized that this property could also be used to discuss the shortdistance properties of some physical processes. In asymptotically free QFTs (where the free QFT is an ultraviolet (UV) RG fixed point), these effective couplings become small at large-Euclidean momenta and, therefore, perturbation theory, improved by RG, can be used. In particle physics, the theory of strong interactions, based on SU(3) gauge symmetry, shares this property. Later, Weinberg argued that the existence of UV RG fixed points (like in non-Abelian gauge theories, or non-linear σ models), that is, the existence of limits for the effective short-distance couplings, was a necessary condition for the consistency of a QFT on all scales. However, most of the field theories proposed to describe strong, electromagnetic and weak interactions are not asymptotically free.

Of course, the existence of other non-trivial fixed points cannot be established in the framework of perturbation theory. However, many numerical simulations of field theories on the lattice, which make non-perturbative explorations possible, have failed to discover non-trivial fixed points. Therefore, presumably, the present SM, which describes so precisely particle physics at present scale, is not consistent on all scales, and has to be modified at shorter distance.

This also suggests that the property of renormalizability has a different origin.

Somewhat surprisingly, in statistical physics, QFT has also become an essential tool for the understanding of the critical behaviour of a large class of second-order phase transitions with short-range interactions. Near the critical temperature, cooperative phenomena generate a large scale, associated with the so-called *correlation length*. Moreover, the large-scale properties of the system become independent of most of the details of the microscopic dynamics. First attempts to explain these properties were based on

usual ideas: a description only involving macroscopic degrees of freedom adapted to the scale of the correlation length. Such a description naturally emerges in simple approximations like *mean-field theory*. It is consistent with the general probabilistic idea that averages over a large number of independent stochastic variables obey a Gaussian distribution. The corresponding general ideas were summarized in Landau's theory of critical phenomena. However, it slowly became clear that the predictions of such a theory were too universal, conflicting with numerical calculations of critical exponents, experimental data and exact results in two dimensions. These results supported the concept of a more restricted *universality*: broad classes of systems have indeed the same large distance properties, but, unlike in mean-field theory, these properties seemed to depend on a small number of qualitative features, like dimension of space, number of components of the order parameter, symmetries, and so on. Actually, an analysis of the leading corrections to mean-field or Gaussian approximations indeed reveals that, at least in low-space dimensions, the short distance never completely decouple, a most unusual situation.

To explain this remarkable phenomenon, that is, that large distance properties of second order phase transitions are, to a large extent, short-distance insensitive, although degrees of freedom on all scales remain coupled, Wilson, partially inspired by some prior attempts of Kadanoff, introduced the RG idea: starting from a microscopic Hamiltonian, one integrates out, recursively, the degrees of freedom corresponding to short-distance fluctuations, and generates a scale-dependent effective Hamiltonian. Universality then relies upon the existence of IR fixed points in Hamiltonian space. One of the spectacular implications is that the universal properties of a large class of critical phenomena can be accurately predicted by the same QFT methods that had been invented for particle physics. At leading order in the critical domain, the physics of the fixed-point Hamiltonian can be reproduced by renormalizable (or super-renormalizable) QFTs.

Predictions obtained from a RG analysis of simple field theories like the $(\phi^2)^2$ QFT have been successfully compared to experiments as well as numerical data from lattice models. The same QFT methods have been shown to describe vastly different physical systems at criticality, like ferromagnets, liquid-vapour, binary mixtures, superfluid helium and, even more surprisingly, statistical properties of polymers.

If QFT has led to an understanding of the concept of universality and made the calculation of many universal physical quantities possible, conversely, critical phenomena have shed a new light on the origin of renormalizable QFTs and of the renormalization process in particle physics.

Let us describe again, in general terms, the renormalization method. Starting from an initial Lagrangian, assumed to be *renormalizable*, expressed in terms of *bare parameters*, one generates an expansion in powers of the interactions. The *perturbative expansion* is then plagued by UV divergences. To render the perturbative expansion finite, one introduces a large-momentum cut-off Λ , which generates an artificial, and somewhat arbitrary short-distance structure, with non-physical properties. One then calculates quantities at the physical scale and *tunes the bare parameters* as functions of the cut-off, in such way that observables at the physical scale have a finite infinite Λ limit. Since the paradoxical conclusion that the Lagrangian in relativistic QFT is non-physical. The insistence for taking the infinite cut-off limit was motivated by the wish to construct a renormalized QFT physically consistent on all scales. Formalisms were developed (like the Bogoliubov–Parasiuk–Hepp–Zimmermann (BPHZ) formalism) to generate directly a renormalized perturbation theory, in which the Lagrangian was reduced to a device for generating Feynman rules. However, another interpretation of the bare QFT and

the renormalization procedure, directly inspired from the functional RG as applied to critical phenomena by Wilson, has gained strength over the years. At very short distance (the Planck scale ?), the familiar notion of local QFT loses its meaning. However, the necessary non-local effects, which render the more fundamental theory finite, are limited to this microscopic scale (the equivalent of the condition of short-range forces in statistical systems). Dynamical effects, of a nature which at present can only be guessed, generate at distances large compared to the microscopic scale (equivalently, at lower energies) physics associated with the appearance of very low mass particles (compared to the Planck mass, for example, all known particles are almost massless). At large distance, physics can be described by an *effective local QFT*, whose action is a linear combination of all local monomials consistent with symmetries, and other possible requirements. With increasing distance, at least in a mean-field like approximation, all interactions scale as dimensional analysis (or power counting) indicates. Eventually, non-renormalizable interactions become very small, dimensionless renormalizable interactions survive, and unprotected terms, with positive dimension, like mass terms, diverge.

Actually, this picture has to be corrected, because the UV divergences and the necessity of introducing a large-momentum cut-off (a substitute for the unknown microscopic physics) show that microscopic scale and the physical scale do not completely decouple. The flow of interactions has to be described by a RG that interpolates between the microscopic scale and the physical scale. Still, as we shall argue, the flow of renormalizable interactions is only logarithmic, while the other terms have a power-law behaviour. Thus, the mean-field analysis of the hierarchy of interactions remains qualitatively correct.

This scheme has the following consequences: it explains the emergence of renormalizable QFTs. The role of renormalization theory is to prove, order by order in perturbation theory, that physics at the physical scale is, to a large extent, but not completely, shortdistance insensitive (and thus insensitive to the precise cut-off implementation), but in a more subtle way as in classical physics. However, the initial (bare) parameters have to be considered as being given, and one has, therefore, to prove, beyond perturbation theory, that the change of parametrization, assumed in the renormalization theory, from bare to physical effective parameters, is possible. In particular, this leads to the triviality issue for IR-free theories (like QED): the physical charge decreases logarithmically with the cut-off and, therefore, the cut-off cannot be sent to infinity. The corresponding coupling constants are expected to be small (this is consistent with the small value of α). Moreover, most QFTs cannot be made consistent on all scales. The possibility of very small non-renormalizable interactions, since proportional to the inverse of the power of cut-off, has to be considered. General Relativity may be of this nature.

The origin of the Higgs boson, which is involved in most of the parameters of the SM, and the necessary *fine tuning* of its mass term in the Lagrangian, become essential physics issues. In contrast to critical phenomena in which a control parameter, like the temperature, can be adjusted to make the correlation length large, in particle physics the existence of small mass particles has to be explained by general properties of the unknown fundamental theory. This is the famous *hierarchy* problem. Spontaneous breaking of a continuous symmetry, gauge principle, and chiral invariance (but whose natural implementation seems to require additional space dimensions) are the known mechanisms which generate massless particles. Supersymmetry can be helpful to deal with scalar bosons. At present, the set of general conditions to be imposed on any fundamental theory, that is, in the language of critical phenomena the complete description of the universality class of particle physics has not been formulated. This is also a fundamental problem of the SM.

On the other hand, since the large distance physics is, to a large extent, short-distance insensitive, the real nature of the fundamental theory may remain, in the foreseeable future, elusive, in the same way as a precise knowledge of the critical exponents of the liquid-vapour phase transition gives limited information about real interactions in water.

This work, which does not claim to shed any light on these difficult problems, simply tries to describe particle physics and critical phenomena in statistical mechanics in a unified framework.

Chapters 1–7 deal with functional integrals, perturbation theory, functional methods and discuss general properties of scalar boson QFTs. Chapters 8–13 provide an introduction to renormalization theory with the simple example of the ϕ^4 QFT in four dimensions, and RG equations are derived. Composite operators and the short-distance expansion are discussed. Relativistic fermions are described. Renormalization properties of theories with symmetries are studied, and specific applications to particle physics are emphasized.

Chapters 14–19 are devoted to critical phenomena in macroscopic phase transitions: general properties, mean-field approximation, and mainly applications of QFT methods and RG, with the calculation of universal quantities, in particular, with Wilson–Fisher ε expansion, large N techniques and non-linear σ -model for O(N)-symmetric models.

With Chapters 20–26, we return to particle physics. Chapter 20 deals with spontaneous fermion mass generation. We then discuss gauge theories, Abelian and non-Abelian. In particular, Chapter 22 briefly describes the SM of particle physics. Chapter 26 introduces Becchi–Rouet–Stora–Tyutin (BRST) symmetry, the Zinn-Justin (ZJ) equation and the proof of the renormalizability of gauge theories. Chapter 27 contains a short introduction to supersymmetry. Chapter 28 gathers the few elements of classical and quantum gravity needed in the work.

In Chapters 29–31, we focus on two-dimensional field theories, of relevance both for particle and statistical physics. Chapter 29 is devoted to QFTs defined on homogeneous spaces, and Chapters 30 and 31 describe exactly-solvable two-dimensional QFTs.

Chapter 32 provides an introduction to finite-size effects, and Chapter 33 to finite temperature relativistic QFT. Chapters 34–36 deal with stochastic evolution equations, and their application to critical dynamics in phase transitions. Chapters 37–42 describe the role of instantons in QM and QFT, the application of instanton calculus to the analysis of large-order behaviour of perturbation theory, and the problem of summation of the perturbative expansion. In particular, Chapter 41 applies this information to the evaluation of critical exponents and several other universal quantities.

I am fully aware that this work is largely incomplete. My ignorance or lack of understanding of many important topics is of course mostly responsible for this weakness. A lack of space has also forced me to remove an introduction to large random matrices, and prevented me from adding some other topics. Anyway, I believe that a complete survey of QFT and its applications is beyond the scope of a single physicist.

This work incorporates notes for lectures delivered in numerous summer schools, most notably, Cargèse 1973, Bonn 1974, Karpacz 1975, Basko Polje 1976, and Les Houches 1982, as well as for graduate lectures in universities like Princeton, Louvain-la-Neuve, Berlin, Lausanne, Cambridge (Harvard), Ecole Normale Supérieure, Paris 7, and so on.

Conversely, since some relevant material that I have gathered over the years can no longer find a place in this work, some elements have been published in four reviews (in the form of Physics Reports) and in three companion volumes, Refs. [6, 64] and J. Zinn-Justin, *From random walks to random matrices* (Oxford Univ. Press 2019).

Finally, comments or corrections are most welcome, and can be sent to the email address: jean.zinn-justin@cea.fr.

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Some general references for the whole work

In addition to the works explicitly quoted in the text, a number of textbooks or reviews have been a direct source of inspiration:

S. Weinberg, *The Quantum Theory of Fields*, 2 volumes, (Cambridge Univ. Press 1995, 1996);

A.N. Vasiliev, Functional Methods in Quantum Field Theory and Statistical Physics, (St Petersburg 1976), English translation (Gordon and Breach, Amsterdam 1998);

L.D. Faddeev and A.A. Slavnov, *Gauge Fields: Introduction to Quantum Field Theory* (Benjamin, Reading, MA 1980);

T.D. Lee, *Particle Physics and Introduction to Field Theory* (Harwood Academic, New York 1981);

A.M. Polyakov, Gauge Fields and Strings (Harwood Academic, New York 1988);

J. Drouffe and C. Itzykson, *Théorie Statistique des Champs* (InterEditions 1989), English version: *Statistical Field Theory*, (Cambridge Univ. Press 1989);

Construction of field theories from a more rigorous point of view is discussed in

R.F. Streater and A.S. Wightman, *PCT*, Spin & Statistics and All That (Benjamin, New York 1964);

G. Glimm and A. Jaffe, *Quantum Physics: A Functional Integral Point of View* (Springer-Verlag, Berlin 1981).

Critical Phenomena, Random Systems, Gauge Theories, Proceedings of Les Houches Summer School 1984, K. Osterwalder and R. Stora eds. (Elsevier, Amsterdam 1986).

Contents

1 Gaussian integrals. Algebraic preliminaries		1
1.1 Gaussian integrals: Wick's theorem		1
1.2 Perturbative expansion. Connected contributions		3
1.3 The steepest descent method $\ldots \ldots \ldots$		4
1.4 Complex structures and Gaussian integrals		5
1.5 Grassmann algebras. Differential forms		6
1.6 Differentiation and integration in Grassmann algebras		8
1.7 Gaussian integrals with Grassmann variables		13
1.8 Legendre transformation	•	16
2 Euclidean path integrals and quantum mechanics (QM)		18
2.1 Markovian evolution and locality		19
2.2 Statistical operator: Path integral representation		20
2.3 Explicit evaluation of a path integral: The harmonic oscillator \ldots \ldots		24
2.4 Partition function: Classical and quantum statistical physics		25
2.5 Correlation functions. Generating functional		27
2.6 Harmonic oscillator. Correlation functions and Wick's theorem		30
2.7 Perturbed harmonic oscillator		33
2.8 Semi-classical expansion		35
A2 Additional remarks		38
A2.1 A useful relation between determinant and trace		38
A2.2 The two-point function: An integral representation		39
A2.3 Time-ordered products of operators		40
3 Quantum mechanics (QM): Path integrals in phase space		42
3.1 General Hamiltonians: Phase-space path integral		42
3.2 The harmonic oscillator. Perturbative expansion		45
3.3 Hamiltonians quadratic in momentum variables		47
3.4 The spectrum of the $O(2)$ -symmetric rigid rotator $\ldots \ldots \ldots \ldots \ldots$		51
3.5 The spectrum of the $O(N)$ -symmetric rigid rotator		52
A3 Quantization. Topological actions: Quantum spins, magnetic monopoles		56
A3.1 Symplectic form and quantization: General remarks		56
A3.2 Classical equations of motion and quantization		58
A3.3 Topological actions	•	60
4 Quantum statistical physics: Functional integration formalism		64
4.1 One-dimensional QM: Holomorphic representation		64
4.2 Holomorphic path integral		67

4.3 Several degrees of freedom. Boson interpretation	. 71
4.4 The Bose gas. Field integral representation	. 72
4.5 Fermion representation and complex Grassmann algebras $\hfill \hfill \hfil$. 80
4.6 Path integrals with fermions	. 83
4.7 The Fermi gas. Field integral representation	. 87
5 Quantum evolution: From particles to non-relativistic fields	. 90
5.1 Time evolution and scattering matrix in quantum mechanics (QM)	. 90
5.2 Path integral and S-matrix: Perturbation theory $\ldots \ldots \ldots \ldots$. 92
5.3 Path integral and S-matrix: Semi-classical expansions \ldots \ldots \ldots	. 95
5.4 S-matrix and holomorphic formalism $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$. 99
5.5 The Bose gas: Evolution operator $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$	102
5.6 Fermi gas: Evolution operator \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots	103
A5 Perturbation theory in the operator formalism	104
6 The neutral relativistic scalar field	105
6.1 The relativistic scalar field	105
6.2 Quantum evolution and the S-matrix	110
6.3 S-matrix and field asymptotic conditions	112
6.4 The non-relativistic limit: The ϕ^4 QFT	116
6.5 Quantum statistical physics	118
6.6 Källen–Lehmann representation and field renormalization	122
7 Perturbative quantum field theory (QFT): Algebraic methods	125
7.1 Generating functionals of correlation functions	126
7.2 Perturbative expansion. Wick's theorem and Fevnman diagrams	127
7.3 Connected correlation functions: Generating functional	129
7.4 The example of the ϕ^4 QFT	131
7.5 Algebraic properties of field integrals. Quantum field equations	133
7.6 Connected correlation functions. Cluster properties	139
7.7 Legendre transformation. Vertex functions	141
7.8 Momentum representation	144
7.9 Loop or semi-classical expansion	146
7.10 Vertex functions: One-line irreducibility	151
7.11 Statistical and quantum interpretation of the vertex functional	152
A7 Additional results and methods	155
A7.1 Generating functional at two loops	155
A7.2 The background field method	156
A7.3 Connected Feynman diagrams: Cluster properties	157
8 Ultraviolet divergences: Effective field theory (EFT)	160
8.1 Gaussian expectation values and divergences: The scalar field	161
8.2 Divergences of Feynman diagrams: Power counting	162
8.3 Classification of interactions in scalar quantum field theories	164
8.4 Momentum regularization	166
8.5 Example: The $\phi_{d=6}^3$ field theory at one-loop order	169
8.6 Operator insertions: Generating functionals, power counting	173
8.7 Lattice regularization. Classical statistical physics	175
8.8 Effective QFT. The fine-tuning problem	176
8.9 The emergence of renormalizable field theories	179
A8 Technical details	181

Co	nte	nts
00	1000	1000

A8.1 Schwinger's proper-time representation	181
A8.2 Regularization and one-loop divergences	181
A8.3 More general momentum regularizations	184
9 Introduction to renormalization theory and renormalization group (RG)	185
9.1 Power counting. Dimensional analysis	186
9.2 Regularization. Bare and renormalized QFT	187
9.3 One-loop divergences	191
9.4 Divergences beyond one-loop: Skeleton diagrams	194
9.5 Callan–Symanzik equations	196
9.6 Inductive proof of renormalizability	198
9.7 The $\langle \phi^2 \phi^2 \rangle$ vertex function	203
9.8 The renormalized action: General construction	204
9.9 The massless theory	204
9.10 Homogeneous RG equations: Massive QFT	208
9.11 EFT and RG	210
9.12 Solution of bare RG equations: The triviality issue	212
A9 Functional RG equations. Super-renormalizable QFTs. Normal order	214
A9.1 Large-momentum mode integration and functional RG equations	214
A9.2 The ϕ^4 QFT in three dimensions: Divergences	216
A9.3 Super-renormalizable scalar QFTs in two dimensions: Normal order	218
10 Dimensional continuation regularization minimal subtraction (MS)	
Renormalization group (RG) functions	220
10.1 Dimensional continuation and dimensional regularization	220
10.2 BG functions	220
10.3 The structure of renormalization constants	224
10.4 MS scheme	220
10.5 RG functions at two-loop order: The ϕ^4 OFT	230
10.6 Generalization to N -component fields	235
A10 Feynman parametrization	239
11 Ponormalization of local polynomials. Short distance expansion (SDE)	240
11 1 Renormalization of operator insertions	240
11.1 Renormalization of operator insertions	240
11.2 Quantum neu equations	240
11.5 Short-distance expansion of operator products	240
11.4 Large-momentum expansion of the SDE coefficients. C5 equations	255
11.5 SDE beyond leading ofder. General operator product	255
11.0 Eight-cone expansion of operator products	200
12 Relativistic fermions: Introduction	258
12.1 Massive Dirac fermions	258
12.2 Self-interacting massive fermions: Non-relativistic limit	263
12.3 Free Euclidean relativistic fermions	265
12.4 Partition function. Correlations	269
12.5 Generating functionals	270
12.6 Connection between spin and statistics	272
12.7 Divergences and momentum cut-off	274
12.8 Dimensional regularization	276
12.9 Lattice fermions and the doubling problem	276
A12 Euclidean fermions, spin group and γ matrices	280

xvii

A12.1 Spin group. Dirac γ matrices $\ldots \ldots \ldots$	280
A12.2 The example of dimension 4	288
A12.3 The Fierz transformation	289
A12.4 Traces of products of γ matrices $\ldots \ldots \ldots$	290
13 Symmetries, chiral symmetry breaking, and renormalization	292
13.1 Lie groups and algebras: Preliminaries	293
13.2 Linear global symmetries and WT identities	295
13.3 Linear symmetry breaking	298
13.4 Spontaneous symmetry breaking	301
13.5 Chiral symmetry breaking in strong interactions: Effective theory	304
13.6 The linear σ_{-model}	306
13.7 WT identities	310
13.7 W1 Identifies	212
A13 Currents and Noether's theorem	315
A12.1 Currents in elegsical field theory	917 917
A13.1 Currents in classical-neid theory	017 910
A13.2 The energy-momentum tensor	210
A13.5 Euclidean theory: Dilatation and conformal invariance	320
A13.4 QF1: Currents and correlation functions	322
A13.5 Energy-momentum tensor and QFT	323
14 Critical phenomena: General considerations. Mean-field theory (MFT)	324
14.1 The transfer matrix	325
14.2 The infinite transverse size limit: Ising-like systems	328
14.3 Continuous symmetries	331
14.4 Mean-field approximation	332
14.5 Universality within mean-field approximation	337
14.6 Beyond the mean-field approximation	342
14.7 Power counting and the role of dimension $4 \ldots \ldots \ldots \ldots \ldots \ldots$	345
14.8 Tricritical points	346
A14 Additional considerations	347
A14.1 High-temperature expansion	347
A14.2 Mean-field approximation: General formalism	348
A14.3 Mean-field expansion	351
A14.4 High-, low-temperature, and mean-field expansions	352
A14.5 Quenched averages	354
15 The renormalization group (RG) approach: The critical theory near	
four dimensions	357
15.1 RG: The general idea	358
15.2 The Gaussian fixed point	363
15.3 Critical behaviour: The effective ϕ^4 field theory	366
15.4 RG equations near four dimensions	368
15.5 Solution of the RG equations: The ε -expansion	370
15.6 Critical correlation functions with $\phi^2(x)$ insertions	372
15.7 The $O(N)$ -symmetric $(\phi^2)^2$ field theory	376
15.8 Statistical properties of long self-repelling chains	377
15.9 Liquid-vapour phase transition and ϕ^4 field theory	389
15.10 Superfluid transition	387
16 Critical domain. Universality a expansion	201
To Critical domain: Universality, ε -expansion	391

Conte	ents
-------	------

16.1 Strong scaling above T_c : The renormalized theory $\ldots \ldots \ldots \ldots \ldots$	392
16.2 Critical domain: Homogeneous RG equations	396
16.3 Scaling properties above T_c	396
16.4 Correlation functions with ϕ^2 insertions $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$	399
16.5 Scaling properties in a magnetic field and below T_c	400
16.6 The N-vector model \ldots	403
16.7 The general N -vector model $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$	405
16.8 Asymptotic expansion of the two-point function	410
16.9 Some universal quantities as ε expansions $\ldots \ldots \ldots \ldots \ldots \ldots \ldots$	412
16.10 Conformal bootstrap	420
17 Critical phenomena: Corrections to scaling behaviour	421
17.1 Corrections to scaling: Generic dimensions	421
17.2 Logarithmic corrections at the upper-critical dimension	423
17.3 Irrelevant operators and the question of universality	426
17.4 Corrections coming from irrelevant operators Improved action	428
17.5 Application: Uniaxial systems with strong dipolar forces	431
	101
18 $O(N)$ - symmetric vector models for N large	436
18.1 The large N action	436
18.2 Large N limit: Saddle point equations, critical domain	438
18.3 Renormalization group (RG) functions and leading corrections to scaling	445
18.4 Small-coupling constant, large-momentum expansions for $d < 4$	447
18.5 Dimension 4: Triviality issue for N large $\ldots \ldots \ldots \ldots \ldots \ldots \ldots$	448
18.6 The $(\phi^2)^2$ field theory and the non-linear σ -model for N large	449
18.7 The $1/N$ -expansion: An alternative field theory $\ldots \ldots \ldots \ldots \ldots$	453
18.8 Explicit calculations	455
19 The non-linear σ -model near two dimensions: Phase structure \ldots	458
19.1 The non-linear σ -model: Definition $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$	459
19.2 Perturbation theory. Power counting	461
19.3 IR divergences	463
19.4 UV regularization \ldots	464
19.5 WT identities and master equation	466
19.6 Renormalization	469
19.7 The renormalized action: Solution to the master equation	471
19.8 Renormalization of local functionals	474
19.9 A linear representation	475
19.10 $(\phi^2)^2$ field theory in the ordered phase and non-linear σ -model	476
19.11 Renormalization, RG equations	479
19.12 RG equations: Solutions (magnetic terminology)	480
19.13 Results beyond one-loop order	486
19.14 The dimension 2: Asymptotic freedom	488
20 Gross-Neveu-Yukawa and Gross-Neveu models	489
20 1 The GNV model: Spontaneous mass generation	403
20.2 RG equations near four dimensions	404
20.2 The GNV model in the large N limit	408
20.0 The civit model in the farge 1, million	501
20.5 The GN model	504
	504
21 Abelian gauge theories: The tramework of quantum electrodynamics (QED)	507

xix

21.1 The free massive vector field: Quantization				507
21.2 The Euclidean free action. The two-point function				509
21.3 Coupling to matter				512
21.4 The massless limit: Gauge invariance				514
21.5 Massless vector field, gauge invariance, and quantization				516
21.6 Equivalence with covariant quantization				519
21.7 Gauge symmetry and parallel transport				521
21.8 Perturbation theory: Regularization				522
21.9 WT identities and renormalization				526
21.10 Gauge dependence: The fermion two-point function				528
21.11 Renormalization and RG equations				531
21.12 One-loop β function and the triviality issue				532
21.13 The Abelian Landau–Ginzburg–Higgs model				535
21.14 The Landau–Ginzburg–Higgs model: WT identities				537
21.15 Spontaneous symmetry breaking: Decoupling gauge				538
21.16 Physical observables. Unitarity of the S-matrix				539
21.17 Stochastic quantization: The example of gauge theories				540
A21 Additional remarks				542
A21.1 Vacuum energy and Casimir effect				542
A21.2 Gauge dependence				545
A21.3 Divergences at one loop from Schwinger's representation				546
22 Non Abelian gauge theories: Introduction				E 10
22 Non-Ademan gauge incorres: Introduction	•••	·	• •	040 E 40
22.1 Geometric construction: Paranel transport	•••	·	• •	040 551
22.2 Gauge-invariant actions	•••	·	• •	551
22.3 Hamiltonian formalism. Quantization in the temporal gauge	•••	·	• •	551
22.4 Covariant gauges	•••	·	• •	504 557
22.5 Perturbation theory, regularization	•••	·	• •	557
A22 Massive Yang Mills fields	•••	•	• •	565
	•••	·	• •	909
23 The Standard Model (SM) of fundamental interactions			• •	567
23.1 Weak and electromagnetic interactions: Gauge and scalar fields	•	•	• •	568
23.2 Leptons: Minimal SM extension with Dirac neutrinos		•		570
23.3 Quarks and weak–electromagnetic interactions		•		573
23.4 QCD. RG equations and β function $\ldots \ldots \ldots \ldots \ldots \ldots$			• •	576
23.5 General RG β -function at one-loop order: Asymptotic freedom	•	•	• •	578
23.6 Axial current, chiral gauge theories, and anomalies		•	• •	582
23.7 Anomalies: Applications in particle physics		•	• •	591
24 Large-momentum behaviour in quantum field theory (QFT)				593
24.1 The $(\phi^2)^2$ Euclidean field theory: Large-momentum behaviour				593
24.2 General ϕ^4 -like field theories: d=4				598
24.3 Theories with scalar bosons and Dirac fermions				600
24.4 Gauge theories				602
24.5 Applications: The theory of strong interactions				604
25 Lattice gauge theories: Introduction				607
25 1 Cauge invariance on the lattice: Parallel transport	•	·	• •	607
25.1 Gauge invariance on the latence. I draffer transport	• •	•	• •	600
25.3 Wilson's loop and confinement	••	·	• •	611
20.0 whom 5 loop and commentent $\ldots \ldots \ldots \ldots \ldots \ldots$	• •	·	• •	011

C_{0}	nt	Pr	\mathbf{t}	c
$\cup \upsilon$	111	C1	$\iota\iota$	5

25.4 Mean-field approximation			617
A25 Gauge theory and confinement in two dimensions			621
26 Becchi–Rouet–Stora–Tvutin (BRST) symmetry. Gauge theories:			
Zinn-Justin equation (ZJ) and renormalization			623
26.1 ST identities: The origin			624
26.2 From ST symmetry to BRST symmetry			626
26.3 BRST symmetry: More general coordinates. Group structure			628
26.4 Stochastic equations			630
26.5 BRST symmetry Grassmann coordinates and gradient equations	•		632
26.6 Gauge theories: Notation and algebraic structure	•	• •	635
26.7 Gauge theories: Quantization	•	• •	636
26.8 WT identities and ZI equation	·	• •	639
26.9 Renormalization: General considerations	•	• •	641
26.10 The renormalized gauge action	·	• •	642
26.11 Gauge independence: Physical observables	•	• •	647
A26 BRST symmetry and 7 Leguation: Additional remarks	•	• •	649
A26 1 BRST symmetry and 71 equation	•	• •	640
A20.1 Dito1 Symmetry and 25 equation	·	• •	650
A20.2 Canonical invariance of the 25 equation	·	• •	651
A20.5 Elements of Ditor conomology	·	• •	654
A20.4 From DRST symmetry to supersymmetry	·	• •	004
27 Supersymmetric quantum field theory (QFT): Introduction	•		656
27.1 Scalar superfields in three dimensions	•		656
27.2 The $O(N)$ supersymmetric non-linear σ model $\ldots \ldots \ldots$	•		661
27.3 Supersymmetry in four dimensions	•		662
27.4 Vector superfields and gauge invariance	•		666
28 Elements of classical and quantum gravity			670
28.1 Manifolds. Change of coordinates. Tensors			671
28.2 Parallel transport: Connection, covariant derivative			673
28.3 Riemannian manifold. The metric tensor			677
28.4 The curvature (Riemann) tensor			678
28.5 Fermions, vielbein, spin connection			682
28.6 Classical GR. Equations of motion			684
28.7 Quantization in the temporal gauge: Pure gravity			687
28.8 Observational cosmology: A few comments			690
20 Conoralized non linear σ models in two dimensions			602
29 Generalized non-initial o-models in two dimensions	·	• •	602
29.1 Homogeneous spaces and Goldstone modes	·	• •	605
29.2 W1 Identities and renormalization in linear coordinates	·	• •	600
29.5 Renormalization in general coordinates. DRST symmetry	·	• •	702
29.4 Symmetric spaces: Demittion	·	• •	703
29.5 Classical field equations. Conservation laws	·	• •	704
29.0 GF 1: Perturbative expansion and KG	•	• •	700
29.7 Generalizations	·	• •	719
A29 nonogeneous spaces: A rew algebraic properties	·	• •	719
A29.1 Fure gauge. Maurer-Cartan equations	·	• •	113
A29.2 Interrit and curvature in nonnogeneous spaces	·	• •	114
A29.5 Explicit expressions for the metric	·	• •	715
A29.4 Symmetric spaces: Classification	•	• •	(1)

xxi

30 A few solvable two-dimensional quantum field theories (QFT)	721
30.1 The free massless scalar field	721
30.2 The free massless Dirac fermion	725
30.3 The gauge-invariant fermion determinant and the anomaly	728
30.4 The sG model	731
30.5 The Schwinger model	732
30.6 The massive Thirring model	736
30.7 A generalized Thirring model with two fermions	739
30.8 The $SU(N)$ Thirring model	742
$\Delta 30$ Two-dimensional models: Δ few additional results	745
A 30.1 Four-fermion current interactions: RG β -function	745
A30.2 The Schwinger model: The anomaly	745
A 30.2 Solitons in the sC model	740
	740
31 O(2) spin model and the Kosterlitz–Thouless's (KT) phase transition	747
31.1 The spin correlation functions at low temperature	748
31.2 Correlation functions in a field	749
31.3 The Coulomb gas in two dimensions $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$	750
31.4 $O(2)$ spin model and Coulomb gas $\ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots \ldots$	755
31.5 The critical two-point function in the $O(2)$ model $\ldots \ldots \ldots \ldots \ldots$	756
31.6 The generalized Thirring model	758
32 Finite-size effects in field theory. Scaling behaviour	760
32.1 BC in finite geometries	760
22.2 Momentum quantization	764
32.2 Momentum quantization $\dots \dots \dots$	766
22.5 The ϕ field theory in a periodic hypercube	700
32.4 The φ field theory. Cylindrical geometry	776
52.5 Finite size effects in the non-linear <i>o</i> -model	700
	102
A32.1 Perturbation theory in a mile volume	182
A32.2 Discrete symmetries and finite-size effects	783
33 Quantum field theory (QFT) at finite temperature: Equilibrium properties	786
33.1 Finite- (and high-) temperature field theory	786
33.2 The example of the $\phi_{1,d-1}^4$ field theory $\ldots \ldots \ldots \ldots \ldots \ldots \ldots$	790
33.3 High temperature and critical limits	796
33.4 The non-linear σ -model in the large N limit $\ldots \ldots \ldots \ldots \ldots$	799
33.5 The perturbative non-linear σ -model at finite temperature \ldots \ldots	804
33.6 The GN model in the large N expansion $\ldots \ldots \ldots \ldots \ldots \ldots \ldots$	810
33.7 Abelian gauge theories: The QED framework	817
33.8 Non-Abelian gauge theories	824
A33 Feynman diagrams at finite temperature	828
A33.1 One-loop calculations	828
A33.2 Group measure	830
	0.01
34 Stocnastic differential equations: Langevin, Fokker-Planck (FP) equations	831
34.1 The Langevin equation	831
34.2 Lime-dependent probability distribution and FP equation	833
34.3 Equilibrium distribution. Correlation functions	835
34.4 A special class: Dissipative Langevin equations	838
34.5 The linear Langevin equation	839

Contents

34.6 Path integral representation	842
34.7 BRST and supersymmetry	843
34.8 Gradient time-dependent force and Jarzynski's relation	846
34.9 More general Langevin equations. Motion in Riemannian manifolds	848
A34 Markov's stochastic processes: A few remarks	852
A34.1 Discrete spaces: Markov's processes, phase transitions	852
A34.2 Stochastic process with prescribed equilibrium distribution	855
A34.3 Stochastic processes and phase transitions	856
25 Langevin field equations. Drepartics and reportedization	957
25.1 Langevin and Fokker Dlanck (FP) equations	001 857
25.2 Time dependent correlation functions and equilibrium	001
25.2 Denormalization and DDCT symmetry	000 961
25.4 Discinctive Longevin equation and supersymmetry	001
25.5 Supersymmetry and equilibrium completion functions	004
25.5 Supersymmetry and equilibrium correlation functions	007
35.6 Stochastic quantization of two-dimensional chiral models	808 071
35.7 Langevin equation and Riemannian manifolds	8/1
A35 The random field Ising model: Supersymmetry	874
36 Critical dynamics and renormalization group (RG)	875
36.1 Dissipative equation: RG equations in dimension $d = 4 - \varepsilon$	876
36.2 Dissipative dynamics: RG equations in dimension $d = 2 + \varepsilon$	880
36.3 Conserved order parameter $\ldots \ldots \ldots$	882
36.4 Relaxational model with energy conservation $\ldots \ldots \ldots \ldots \ldots \ldots$	883
36.5 A non-relaxational model \ldots	886
36.6 Finite size effects and dynamics	888
A36 RG functions at two loops	894
A36.1 Supersymmetric perturbative calculations at two loops	894
37 Instantons in quantum mechanics (QM)	899
37.1 The quartic anharmonic oscillator for negative coupling	899
37.2 A toy model: A simple integral	901
37.3 QM: Instantons	902
37.4 Instanton contributions at leading order	904
37.5 General analytic potentials: Instanton contributions	908
37.6 Evaluation of the determinant: The shifting method	909
37.7 Zero temperature limit: The ground state	915
A37 Exact Jacobian. WKB method.	916
A37.1 The exact Jacobian	916
A37.2 The WKB method	917
	010
38 Wietastable vacua in quantum field theory (QFI) $\dots \dots \dots \dots \dots$	919
38.1 The ϕ^2 QF1 for negative coupling	920
38.2 General potentials: Instanton contributions	924
38.3 The ϕ^+ QFT in dimension 4	926
38.4 Instanton contributions at leading order	927
38.5 Coupling constant renormalization	931
38.6 The imaginary part of the <i>n</i> -point function $\dots \dots \dots$	932
38.7 Ine massive theory \ldots \ldots \ldots \ldots \ldots \ldots	933
38.8 Cosmology: The decay of the false vacuum	934
A30 Instantons: Additional remarks	936

A38.1 Virial theorem	•	•	•	•	. 936 037
A38.3 Instantons and BC equations	•	·	·	•	. 937 030
A38.4 Conformal invariance	•	•	•	•	. 935 . 940
39 Degenerate classical minima and instantons					. 942
39.1 The quartic double-well potential				•	. 942
39.2 The periodic cosine potential				•	. 945
39.3 Instantons and stochastic dynamics	•			•	. 948
39.4 Instantons in stable boson field theories: General remarks .	•			•	. 951
39.5 Instantons in $CP(N-1)$ models $\ldots \ldots \ldots \ldots \ldots$	•		•	•	. 953
39.6 Instantons in the $SU(2)$ gauge theory $\ldots \ldots \ldots \ldots$	·	•	•	•	. 956
A39 Trace formula for periodic potentials	•	·	•	•	. 959
40 Large order behaviour of perturbation theory	•		•	•	. 960
$40.1 \text{ QM} \qquad \dots \qquad $	·	·	·	•	. 960
40.2 Scalar field theories: The example of the ϕ^2 field theory	·	·	·	·	. 963
40.3 The $(\phi^2)^2$ field theory in dimension 4 and $4 - \varepsilon$	·	·	·	•	. 964
40.4 Field theories with termions	•	·	·	•	. 908
	•	·	•	•	. 914
41 Critical exponents and equation of state from series summation		·	•	•	. 975
41.1 Divergent series: Borel summation	·	·	·	•	. 975
41.2 Dorer transformation. Series summation $(d^2)^2$ field theory	·	·	·	•	. 970 080
41.5 Summation method: Practical implementation	•	·	•	•	. 500
41.5 Field theory estimates of critical exponents for the $O(N)$ model	•	·	•	·	. 985 985
41.6 Other three-dimensional theoretical estimates					. 986
41.7 Critical exponents from experiments					. 987
41.8 Amplitude ratios					. 989
A41 Some other summation methods					. 990
A41.1 Order-dependent mapping method (ODM)					. 990
A41.2 Linear differential approximants				•	. 991
42 Multi-instantons in quantum mechanics (QM)					. 992
42.1 The quartic double-well potential					. 993
42.2 The periodic cosine potential $\ldots \ldots \ldots \ldots \ldots \ldots \ldots$				•	. 1000
42.3 General potentials with degenerate minima	•			•	. 1004
42.4 The $O(\nu)$ -symmetric anharmonic oscillator	•		•	•	. 1007
42.5 Generalized Bohr–Sommerfeld quantization formula	•	•	•	•	. 1009
A42 Additional remarks	·	•	•	•	. 1011
A42.1 Multi-instantons: The determinant	·	•	·	•	. 1011
A42.2 The instanton interaction	•	·	·	•	. 1012
A42.3 A simple example of non-Borel summability	·	·	·	•	. 1014
A42.4 Multi-instantons and WKB approximation	•	·	·	•	. 1016
	·	·	·	•	. 1019 1041
	•	·	·	•	. 1041

1 Gaussian integrals. Algebraic preliminaries

Since our study of perturbative aspects of quantum mechanics and quantum field theory (QFT) is largely based on functional (path or field) integrals and functional techniques, topics that may not be necessarily familiar to all readers, we begin this physics textbook with a discussion of the algebraic properties of Gaussian measures and Gaussian expectation values for a finite number of variables. The important role of Gaussian measures is not unrelated to the central limit theorem of probabilities, although the interesting physics is generally hidden in essential deviations from Gaussian distributions.

We first recall a few algebraic identities about Gaussian expectation values, in particular, Wick's theorem. We emphasize the role of cumulants. We discuss the steepest descent method, which reduces certain type of integrals to series whose terms are given by Gaussian expectation values.

The discussion of boson systems (see Chapter 4) also requires defining integrals over some type of formally complex conjugate variables.

By contrast, to discuss fermion systems, one first needs Grassmann or exterior algebras, and the corresponding generalization of the notions of differentiation and integration.

Both for complex and Grassmann integrals, we calculate Gaussian integrals and Gaussian expectation values, and prove generalized Wick's theorems.

Finally, as a preparation for the coming chapters, we recall the notions of generating functions and Legendre transformations.

All algebraic identities are derived for a finite number of variables, but the coming chapters will show that the extension to infinite systems is simple.

Notation. In most of this work, for vectors and matrices, boldface will denote a matrix or a vector in its entirety, and the corresponding italics with indices will denote elements.

1.1 Gaussian integrals: Wick's theorem

In this section, we briefly review a few basic algebraic properties of Gaussian integrals.

We first consider an *n*-dimensional Gaussian integral over real variables x_i , i = 1, ..., n, of the form,

$$\mathcal{Z}(\mathbf{S}) = \int_{\mathbb{R}^n} \mathrm{d}^n x \, \mathrm{e}^{-S_2(\mathbf{x})},\tag{1.1}$$

where S_2 is the real positive quadratic form,

$$S_2(\mathbf{x}) \equiv \frac{1}{2} \sum_{i, j=1}^n x_i S_{ij} x_j$$
, with $S_{ij} = S_{ji}$, and $\mathbf{S} > 0$. (1.2)

Since the matrix **S** is strictly positive, it can be diagonalized by an orthogonal transformation matrix **O**, and has positive eigenvalues s_i . Changing variables, $x_i \mapsto x'_i$ with

$$\sum_{j} O_{ij} x_j = x'_i \,, \quad |\det \mathbf{O}| = 1 \,,$$

a transformation of Jacobian unity, we obtain a product of independent x'_i integrals.

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Each integral yields a factor $\sqrt{2\pi/s_i}$. The result thus involves the product of all eigenvalues, that is, the determinant. The result is

$$\mathcal{Z}(\mathbf{S}) = (2\pi)^{n/2} \,(\det \mathbf{S})^{-1/2} \,. \tag{1.3}$$

Moreover, since both the initial integral and the determinant are analytic functions of the coefficients of the matrix \mathbf{S} , the identity can be extended by analytic continuation to complex matrices (the global sign then requires some special care).

We now consider the more general integral

$$\mathcal{Z}(\mathbf{S}, \mathbf{b}) = \int \mathrm{d}^n x \, \mathrm{e}^{-S_2(\mathbf{x}) + \mathbf{b} \cdot \mathbf{x}}, \quad \text{where } \mathbf{b} \cdot \mathbf{x} \equiv \sum_{i=1}^n b_i x_i \,. \tag{1.4}$$

To calculate $\mathcal{Z}(\mathbf{S}, \mathbf{b})$, one first looks for the minimum of the quadratic form, given by

$$\frac{\partial}{\partial x_i} \left(S_2(\mathbf{x}) - \mathbf{b} \cdot \mathbf{x} \right) = 0 \quad \Rightarrow \quad \sum_j S_{ij} x_j = b_i$$

The solution is

$$x_i = \sum_j \Delta_{ij} b_j$$
, with $\Delta \mathbf{S} = \mathbf{1}$. (1.5)

One then changes variables $\mathbf{x} \mapsto \mathbf{y}$, setting

$$x_i = \sum_j \Delta_{ij} b_j + y_i \quad \Rightarrow \quad -S_2(\mathbf{x}) + \mathbf{b} \cdot \mathbf{x} = w_2(\mathbf{b}) - S_2(\mathbf{y}), \tag{1.6}$$

with

$$w_2(\mathbf{b}) = \frac{1}{2} \sum_{i,j=1}^n b_i \Delta_{ij} b_j \,. \tag{1.7}$$

The integral becomes

$$\mathcal{Z}(\mathbf{S}, \mathbf{b}) = e^{w_2(\mathbf{b})} \int d^n y \ e^{-S_2(\mathbf{y})} = (2\pi)^{n/2} \left(\det \mathbf{S}\right)^{-1/2} e^{w_2(\mathbf{b})}.$$
 (1.8)

Gaussian expectation values. We consider the Gaussian expectation values,

$$\langle x_{k_1} x_{k_2} \cdots x_{k_\ell} \rangle \equiv \mathcal{Z}^{-1}(\mathbf{S}, 0) \int \mathrm{d}^n x \, x_{k_1} x_{k_2} \cdots x_{k_\ell} \, \mathrm{e}^{-S_2(\mathbf{x})}, \tag{1.9}$$

in which the normalization is determined by the condition $\langle 1 \rangle = 1$.

From expression (1.4), one derives

$$\frac{\partial}{\partial b_k} \mathcal{Z}(\mathbf{S}, \mathbf{b}) = \int \mathrm{d}^n x \, x_k \, \mathrm{e}^{-S_2(\mathbf{x}) + \mathbf{b} \cdot \mathbf{x}} \,. \tag{1.10}$$

Repeated differentiation with respect to \mathbf{b} then leads to the identity

$$\langle x_{k_1} x_{k_2} \cdots x_{k_\ell} \rangle = (2\pi)^{-n/2} \left(\det \mathbf{S} \right)^{1/2} \left[\frac{\partial}{\partial b_{k_1}} \frac{\partial}{\partial b_{k_2}} \cdots \frac{\partial}{\partial b_{k_\ell}} \mathcal{Z}(\mathbf{S}, \mathbf{b}) \right] \Big|_{\mathbf{b}=0}$$

Replacing the integral $\mathcal{Z}(\mathbf{S}, \mathbf{b})$ by its explicit form (1.8), one obtains

$$\langle x_{k_1} \cdots x_{k_\ell} \rangle = \left\{ \frac{\partial}{\partial b_{k_1}} \cdots \frac{\partial}{\partial b_{k_\ell}} e^{w_2(\mathbf{b})} \right\} \Big|_{\mathbf{b}=0}.$$
 (1.11)

More generally, if F(x) is a power series in the variables x_i , then

$$\langle F(x) \rangle = \left[F(\partial/\partial b) e^{w_2(\mathbf{b})} \right] \Big|_{\mathbf{b}=0}$$
 (1.12)

Wick's theorem. Using the identity (1.11), one derives a first form of Wick's theorem. Each time $\partial/\partial b$ acts on the exponential in the right-hand side, it generates a factor b. A second differential operator has to act on the same factor, otherwise the corresponding contribution vanishes when one sets $\mathbf{b} = 0$. This leads to the following expression for the expectation value of the product $x_{k_1} \cdots x_{k_\ell}$ with the normalized Gaussian weight $e^{-S_2(\mathbf{x})}$: one considers all possible pairings of the indices k_1, \ldots, k_ℓ (ℓ must thus be even); to each pair k_p , k_q , one associates the element $\Delta_{k_pk_q}$ of the matrix $\boldsymbol{\Delta}$. Then,

$$\langle x_{k_1} \cdots x_{k_\ell} \rangle = \sum_{\substack{\text{all possible pairings} \\ P \text{ of } \{k_1, \dots, k_\ell\}}} \Delta_{k_{P_1} k_{P_2}} \cdots \Delta_{k_{P_{\ell-1}} k_{P_\ell}}, \qquad (1.13)$$

$$= \sum_{\substack{\text{all possible pairings} \\ P \text{ of } \{k_1, \dots, k_\ell\}}} \langle x_{k_{P_1}} x_{k_{P_2}} \rangle \cdots \langle x_{k_{P_{\ell-1}}} x_{k_{P_\ell}} \rangle .$$
(1.14)

Equations (1.13) and (1.14), which express Wick's theorem, generalize immediately to an infinite number of variables [1] and, therefore, are useful in statistical and quantum theories, in their functional integral formulation.

1.2 Perturbative expansion. Connected contributions

1.2.1 Perturbation theory

We consider the more general integral

$$\mathcal{Z}(\lambda) = \int \mathrm{d}^n x \, \exp\left(-S_2(\mathbf{x}) - \lambda V(x)\right),\tag{1.15}$$

in which $S_2(\mathbf{x})$ is the quadratic form (1.2), V(x) a polynomial in the variables x_i , and λ a parameter. To calculate the integral, we expand the integrand in powers of λ . Formally,

$$\mathcal{Z}(\lambda) = \sum_{k=0}^{\infty} \frac{(-\lambda)^k}{k!} \int \mathrm{d}^n x \, \mathrm{e}^{-S_2(\mathbf{x})} \, V^k(x).$$

The successive terms in the expansion are proportional to Gaussian expectation values of polynomials, which can be evaluated with the use of Wick's theorem (1.13):

$$\mathcal{Z}(\lambda) = \mathcal{Z}(0) \sum_{k=0}^{\infty} \frac{(-\lambda)^k}{k!} \left\langle V^k(x) \right\rangle, \qquad (1.16)$$

where $\langle \bullet \rangle$ means Gaussian expectation value. Since the function $e^{-\lambda V}$ has a power series expansion in x, we also obtain a formal expression of the integral by applying the identity (1.12) with $F = e^{-\lambda V}$ ($w_2(\mathbf{b})$ being defined in equation (1.7)):

$$\mathcal{Z}(\lambda) = \mathcal{Z}(0) \left\{ \exp\left[-\lambda V\left(\frac{\partial}{\partial b}\right)\right] e^{w_2(\mathbf{b})} \right\} \Big|_{\mathbf{b}=0} .$$
(1.17)

1.2.2 Connected contributions or cumulants

In the expansion (1.16), the coefficient of λ is $\langle V(x) \rangle$. At order λ^2 appears the expectation value $\langle V(x)V(x) \rangle$. Using Wick's theorem, we note that some contributions have a factorized form when pairings remain internal to each V(x) factor. Their sum is simply $\langle V(x) \rangle \langle V(x) \rangle$. We call *connected* the genuine remaining contributions and use the notation $\langle \bullet \rangle_c$:

$$\left\langle V^2(x) \right\rangle = \left(\left\langle V(x) \right\rangle_c \right)^2 + \left\langle V^2(x) \right\rangle_c$$

 $(\langle V(x) \rangle_c = \langle V(x) \rangle)$. The argument generalizes to higher orders. At order k, we find a set of disconnected contributions, corresponding to all possible decompositions of k into a sum of positive integers $k = k_1 + k_2 + \cdots + k_p$. The corresponding contribution

$$\langle V^{k_1}(x) \rangle_c \langle V^{k_2}(x) \rangle_c \cdots \langle V^{k_p}(x) \rangle_c,$$

has, when all k_i are different, a coefficient 1/k! from perturbation theory, multiplied by a combinatorial factor associated with all possible ways of gathering k objects into clusters of $k_1 + k_2 \cdots$,

$$\frac{(-\lambda)^k}{k!} \times \frac{k!}{k_1!k_2!\cdots k_p!} \left\langle V^{k_1}(x) \right\rangle_c \left\langle V^{k_2}(x) \right\rangle_c \cdots \left\langle V^{k_p}(x) \right\rangle_c \,.$$

Instead, if k_i appears m times in the decomposition, one finds the same contribution m! times and, therefore, one has to divide by m!. Summing all the contributions, one obtains

$$\mathcal{W}(\lambda) \equiv \ln \mathcal{Z}(\lambda) = \ln \mathcal{Z}(0) + \sum_{k=1}^{\infty} \frac{(-\lambda)^k}{k!} \left\langle V^k(x) \right\rangle_c \,. \tag{1.18}$$

The new function $\mathcal{W}(\lambda)$, which is the sum of all connected expectation values, plays an important role in statistical physics and QFT.

1.3 The steepest descent method

To evaluate contour integrals in the complex domain, one can sometimes use the steepest descent method, which reduces their evaluation to Gaussian integrals. We consider the integral

$$\mathcal{I}(\lambda) = \int_{\mathbb{R}^n} \mathrm{d}^n x \, \mathrm{e}^{-S(\mathbf{x})/\lambda},\tag{1.19}$$

where $S(\mathbf{x})$ is an analytic function of the variables x_i . In the limit $\lambda \to 0_+$, the integral is dominated by the saddle points \mathbf{x}^s solution of $(\nabla \equiv (\partial/\partial x_1, \ldots, \partial/\partial x_n))$,

$$\nabla S(\mathbf{x})|_{\mathbf{x}=\mathbf{x}^{\mathrm{s}}} = 0. \tag{1.20}$$

To calculate the contribution of a leading *saddle point* \mathbf{x}^{s} , one changes variables $\mathbf{x} \mapsto \mathbf{y}$, and sets

$$\mathbf{x} = \mathbf{x}^{s} + \mathbf{y}\sqrt{\lambda}$$
, and $S_{i_{1},\dots,i_{k}}^{(k)} = \frac{\partial^{k}S}{\partial x_{i_{1}}\cdots\partial x_{i_{k}}}\Big|_{\mathbf{x}=\mathbf{x}^{s}}$

One then expands $S(\mathbf{x})$ in powers of λ (and thus of \mathbf{y}):

$$S(\mathbf{x}) = S(\mathbf{x}^{s}) + \frac{\lambda}{2!} \sum_{i,j} S_{ij}^{(2)} y_{i} y_{j} + \sum_{k=3}^{\infty} \frac{\lambda^{k/2}}{k!} \sum_{i_{1},\dots,i_{k}} S_{i_{1},\dots,i_{k}}^{(k)} y_{i_{1}} \cdots y_{i_{k}}.$$
 (1.21)

4

$$\mathcal{I}(\lambda) = \lambda^{n/2} e^{-S(\mathbf{x}^{s})/\lambda} \int d^{n} y \exp\left[-\frac{1}{2} \sum_{i,j} S_{ij}^{(2)} y_{i} y_{j} - R(\mathbf{y})\right], \quad \text{with}$$
$$R(\mathbf{y}) = \sum_{k=3}^{\infty} \frac{\lambda^{k/2-1}}{k!} \sum_{i_{1},\dots,i_{k}} S_{i_{1},\dots,i_{k}}^{(k)} y_{i_{1}} \cdots y_{i_{k}}. \quad (1.22)$$

One then expands the integrand in powers of $\sqrt{\lambda}$. At the leading order, one obtains

$$\mathcal{I}(\lambda) \underset{\lambda \to 0}{\sim} (2\pi\lambda)^{n/2} \left(\det \mathbf{S}^{(2)} \right)^{-1/2} e^{-S(\mathbf{x}^{s})/\lambda} .$$
(1.23)

At higher orders, the calculation involves Gaussian expectation values of polynomials, which can be evaluated using Wick's theorem.

1.4 Complex structures and Gaussian integrals

We will now introduce a formalism useful to describe boson systems (see Section 4.1). We consider the set of 2n complex variables $\{z_i, \bar{z}_i\}$. The variables z_i and \bar{z}_i are two *independent variables*, only formally conjugate, which provide a complex parametrization of phase space, related to the real position q_i and conjugate momentum p_i by

$$z_i = -i(p_i + iq_i)/\sqrt{2}, \quad \bar{z}_i = i(p_i - iq_i)/\sqrt{2}.$$
 (1.24)

We consider the Gaussian integral,

$$\mathcal{Z}(\mathbf{S}) = \int \left(\prod_{i=1}^{n} \frac{\mathrm{d}z_i \mathrm{d}\bar{z}_i}{2i\pi}\right) \exp\left(-\sum_{i,j=1}^{n} \bar{z}_i S_{ij} z_j\right),\tag{1.25}$$

in which **S** is a complex matrix with non-vanishing determinant. It can be calculated by changing to the real variables (p_i, q_i) , defined by equation (1.24) (then, $dz_i d\bar{z}_i = i dp_i dq_i)$, or by a change of variables like $\sum_i S_{ij} z_j = z'_i$. One finds

$$\mathcal{Z}(\mathbf{S}) = \left(\det \mathbf{S}\right)^{-1}.$$
 (1.26)

The generic Gaussian integral is

$$\mathcal{Z}(\mathbf{S}; \mathbf{b}, \bar{\mathbf{b}}) = \int \left(\prod_{i=1}^{n} \frac{\mathrm{d}z_i \mathrm{d}\bar{z}_i}{2i\pi}\right) \exp\left(-\sum_{i,j=1}^{n} \bar{z}_i S_{ij} z_j + \sum_{i=1}^{n} \left(\bar{b}_i z_i + b_i \bar{z}_i\right)\right), \quad (1.27)$$

The calculation of the integral proceeds as in the real case. One defines the complex matrix $\mathbf{\Delta} = \mathbf{S}^{-1}$. The terms, linear in z_i and \bar{z}_i , can be eliminated by the change of variables $z_i \mapsto v_i$, $\bar{z}_i \mapsto \bar{v}_i$, with

$$z_i = v_i + \sum_j \Delta_{ij} b_j , \qquad \bar{z}_i = \bar{v}_i + \sum_j \bar{b}_j \Delta_{ji} . \qquad (1.28)$$

The result is

$$\mathcal{Z}(\mathbf{S}; \mathbf{b}, \bar{\mathbf{b}}) = (\det \mathbf{S})^{-1} \exp\left(\sum_{i,j=1}^{n} \bar{b}_i \Delta_{ij} b_j\right).$$
(1.29)

Wick's theorem. We consider expectations of polynomials in z, \bar{z} with the normalized weight $\exp(-\sum_{i,j} \bar{z}_i S_{ij} z_j)/\mathcal{Z}(\mathbf{S})$. They can be generated by differentiating the expression (1.29) with respect to b_i and \bar{b}_j , and then setting $\mathbf{b} = \bar{\mathbf{b}} = 0$.

Each derivative with respect to b has to be paired with a derivative with respect to \bar{b} , otherwise the contribution vanishes for $\mathbf{b} = \bar{\mathbf{b}} = 0$. Only monomials with an equal number of factors z and \bar{z} have a non-vanishing expectation value. Eventually, one derives Wick's theorem for complex integrals in the form

$$\langle z_{i_1} \bar{z}_{j_1} \cdots z_{i_\ell} \bar{z}_{j_\ell} \rangle = \sum_{\substack{\text{all permutations} \\ P \text{ of } \{j_1, \dots, j_\ell\}}} \Delta_{i_1 j_{P_1}} \Delta_{i_2 j_{P_2}} \cdots \Delta_{i_\ell j_{P_\ell}}$$

$$= \sum_{\substack{\text{all permutations} \\ P \text{ of } \{j_1, \dots, j_\ell\}}} \langle z_{i_1} \bar{z}_{j_{P_1}} \rangle \langle z_{i_2} \bar{z}_{j_{P_2}} \rangle \cdots \langle z_{i_\ell} \bar{z}_{j_{P_\ell}} \rangle.$$

$$(1.30)$$

Conjugation. We define a conjugation, analogous to complex conjugation, by the transformation that acts as complex conjugation on complex numbers and exchanges z_i and \bar{z}_i . For example,

$$\sum_{i,j} \bar{z}_i S_{ij} z_j \mapsto \sum_{i,j} z_i S_{ij}^* \bar{z}_j \,.$$

We call a function of the $2n \ z, \overline{z}$ variables formally real if it is invariant under such a conjugation. For example,

$$\sum_{i,j} \bar{z}_i S_{ij} z_j = \sum_{i,j} z_i S_{ij}^* \bar{z}_j = \sum_{i,j} \bar{z}_i S_{ji}^* z_j \,,$$

and, thus, the matrix **S** is Hermitian. One then verifies that every formally real function integrated over a conjugated pair z, \bar{z} , again yields a formally real function.

1.5 Grassmann algebras. Differential forms

Theories involving fermions require a parallel formalism (Section 4.5). Since fermion wave functions or field correlation functions are antisymmetric with respect to the exchange of two arguments, the construction of generating functionals requires the introduction of anticommuting classical functions, and thus Grassmann variables [2].

Grassmann algebra. A Grassmann (or exterior) algebra \mathfrak{A} over \mathbb{R} or \mathbb{C} (real or complex) is an associative algebra constructed from a unit 1 and a set of generators θ_i with anticommuting products:

$$\theta_i \theta_j + \theta_j \theta_i = 0, \qquad \forall i, j.$$
(1.31)

As a consequence:

(i) if the number n of generators is finite, the elements of the algebra form a vector space of finite dimension 2^n over \mathbb{R} or \mathbb{C} . All elements can be written as linear combinations of the elements A_{ν} , $\nu = 1, \ldots, 2^n$ of the form

$$A_{\nu} \in \{1 \text{ and } \{\theta_{i_1}\theta_{i_2}\cdots\theta_{i_p}\}, \text{ with } i_1 < i_2 < \cdots < i_p, \ 1 \le p \le n\}.$$
(1.32)

(ii) \mathfrak{A} is a graded algebra: to each monomial $\theta_{i_1}\theta_{i_2}\cdots\theta_{i_p}$, one can associate an integer p that counts the number of generators in a product. In particular, if A_p and A_q are two monomials of degree p and q, respectively, then

$$A_p A_q = (-1)^{pq} A_q A_p \,.$$

(iii) Elements of \mathfrak{A} are invertible if, and only if the term of degree 0 in the expansion on the basis (1.32) does not vanish.

103

7

For example, the element $1 + \theta$ is invertible and its inverse is $1 - \theta$, but θ is not invertible. The inverse can be calculated by expanding in a formal power series starting from the inverse of the term of degree 0.

(vi) All elements in a Grassmann algebra, considered as functions of a generator θ_i , are first degree polynomials, that is, affine functions.

Grassmannian parity. In the algebra \mathfrak{A} , a simple automorphism P can be defined:

$$P(\theta_i) = -\theta_i \implies P^2 = \mathbf{1}.$$
(1.33)

Then, on a monomial of degree p, P acts like

$$P\left(\theta_{i_1}\cdots\theta_{i_p}\right) = (-1)^p \theta_{i_1}\cdots\theta_{i_p} \,. \tag{1.34}$$

The reflection P divides the algebra ${\mathfrak A}$ in two eigenspaces ${\mathfrak A}^\pm$ containing the even or odd elements

$$P\left(\mathfrak{A}^{\pm}\right) = \pm \mathfrak{A}^{\pm}$$

In particular, \mathfrak{A}^+ is a subalgebra, the subalgebra of commuting elements.

1.5.1 Differential forms

Notation. In this section, we use the convention of summation over *repeated upper and lower* indices.

Grassmann algebras can be used to represent explicitly differential forms (see also Section 28.1.3). The language of differential forms will not often be used in this work. However, it is interesting to recall one concept, the exterior derivative of forms whose generalization appears in the context of BRST symmetry (see Section 26.2). We consider totally antisymmetric tensors $\Omega_{\mu_1,\ldots,\mu_l}(x)$, which are functions of *n* commuting variables x^{μ} . Associating *n* Grassmann generators θ^{μ} with the variables x^{μ} , we can write the corresponding *l*-form

$$\Omega = \Omega_{\mu_1,\dots,\mu_l}(x)\theta^{\mu_1}\cdots\theta^{\mu_l}, \qquad (1.35)$$

where $l \leq n$, otherwise, the form vanishes.

One defines the differential operator d acting on forms by

$$\mathbf{d} \equiv \theta^{\mu} \frac{\partial}{\partial x^{\mu}} \,. \tag{1.36}$$

We note that if Ω is an *l*-form, $d\Omega$ is an (l + 1)-form (see Chapter 28 for details). One immediately notes that the square of d vanishes:

$$d^{2} = \theta^{\mu} \frac{\partial}{\partial x^{\mu}} \theta^{\nu} \frac{\partial}{\partial x^{\nu}} = 0, \qquad (1.37)$$

because the product $\theta^{\mu}\theta^{\nu}$ is antisymmetric in $\mu \leftrightarrow \nu$.

It is a cohomology operator. A form Ω that satisfies $d\Omega = 0$ is called *closed* and a form Ω that can be written as $\Omega = d\Omega'$ is called *exact*. The property (1.37) implies that any exact form is closed.

Note that, in the case of differential forms, one often writes the generators of the exterior algebra dx^{μ} instead of θ^{μ} , and then uses the wedge notation \wedge for the product to indicate that it is antisymmetric.

1.6 Differentiation and integration in Grassmann algebras

To be able to construct parallel formalisms for bosons and fermions based on functional integrals, it is necessary to define differentiation and integration in Grassmann algebras.

1.6.1 Differentiation in Grassmann algebras

A straightforward generalization of the usual rules of differentiation is inconsistent, due to the non-commutative character of the algebra. A suitable definition is obtained in the following way: considered as functions of a specific generator θ_i , all elements A of \mathfrak{A} can be written as

$$A = A_1 + \theta_i A_2$$

after some commutations, where A_1 and A_2 do not depend on θ_i . Then, one defines

$$\frac{\partial A}{\partial \theta_i} = A_2 \,. \tag{1.38}$$

Note that the differential operator $\partial/\partial \theta_i$ shares one property of the form differentiation (equation (1.37)): its square vanishes, $(\partial/\partial \theta_i)^2 = 0$.

Left and right differentiation. Equation (1.38) defines a left differentiation in the sense that the action of $\partial/\partial \theta_i$ consists in bringing θ_i on the left in a monomial and suppressing it. Similarly, a right differentiation could have been defined by commuting θ_i to the right.

Chain rule. One verifies that the chain rule applies to Grassmann differentiation. If $\sigma(\theta)$ belongs to \mathfrak{A}^- and $x(\theta)$ belongs to \mathfrak{A}^+ , one finds

$$\frac{\partial}{\partial \theta} f(\sigma, x) = \frac{\partial \sigma}{\partial \theta} \frac{\partial f}{\partial \sigma} + \frac{\partial x}{\partial \theta} \frac{\partial f}{\partial x}.$$
(1.39)

For the second term in the right-hand side, the order between factors matters.

Formal construction. One can verify that any Grassmann differential operator D (also called anti-derivation) acting on \mathfrak{A} and defined as in equation (1.38), satisfies the two algebraic formal rules:

(i) It is a linear mapping of \mathfrak{A} , considered as a vector space, into itself:

$$D(\lambda_1 A_1 + \lambda_2 A_2) = \lambda_1 D(A_1) + \lambda_2 D(A_2), \text{ for } \lambda_1, \lambda_2 \in \mathbb{R} \text{ or } \mathbb{C}.$$
(1.40)

(ii) By contrast with Leibniz's rule, it satisfies the condition

$$D(A_1A_2) = P(A_1) D(A_2) + D(A_1)A_2.$$
 (1.41)

The unusual form of equation (1.41) compared to the differentiation rule for commuting variables is required if one wants D to anticommute with P:

$$DP + PD = 0, \qquad (1.42)$$

which means that the image of \mathfrak{A}^{\pm} by D belongs to \mathfrak{A}^{\mp} .

Note that if A belongs to \mathfrak{A}^+ and F(x) is an ordinary function of real or complex variables, then,

$$D[F(A)] = D(A)F'(A), \text{ for } A \in \mathfrak{A}^+.$$
(1.43)

Finally, note that the form differentiation (1.36) shares all these properties, but acts on different variables.

Anticommutation relations. A short calculation shows that if D and D' are two operators satisfying conditions (1.40) and (1.41), then the anticommutator

$$\Delta = DD' + D'D \tag{1.44}$$

is a usual differential operator:

$$\Delta (\lambda_1 A_1 + \lambda_2 A_2) = \lambda_1 \Delta (A_1) + \lambda_2 \Delta (A_2),$$

$$\Delta (A_1 A_2) = \Delta (A_1) A_2 + A_1 \Delta (A_2).$$
(1.45)

Furthermore,

$$\Delta P = P\Delta. \tag{1.46}$$

These properties, which are the consequence of the addition of relation (1.42) to the definitions (1.40) and (1.41), makes it possible to extend the notion of Lie algebra, and are directly relevant to the discussion of *supersymmetries* (see Section 27.1).

1.6.2 A basis of differential operators

Since a differential operator satisfies conditions (1.40) and (1.41), it is completely defined by its action on the generators θ_i . In addition, any differential operator left-multiplied by an element of \mathfrak{A}^+ still satisfies conditions (1.40) and (1.41). We conclude that any differential operator can be expanded on a basis of operators $\partial/\partial\theta_i$ defined by

$$\frac{\partial}{\partial \theta_i} \theta_j = \delta_{ij} \tag{1.47}$$

with left coefficients in \mathfrak{A}^+ . It is simple to verify that the differential operators $\partial/\partial\theta_i$ coincide with the operators defined by equation (1.38). The nilpotent differential operators $\partial/\partial\theta_i$, together with the generators θ_i considered as operators acting on \mathfrak{A} by left-multiplication, satisfy the *anticommutation relations* (identical to the relations between fermion creation and annihilation operators)

$$\theta_i \theta_j + \theta_j \theta_i = 0, \quad \frac{\partial}{\partial \theta_i} \frac{\partial}{\partial \theta_j} + \frac{\partial}{\partial \theta_j} \frac{\partial}{\partial \theta_i} = 0, \quad \theta_i \frac{\partial}{\partial \theta_j} + \frac{\partial}{\partial \theta_j} \theta_i = \delta_{ij}.$$
(1.48)

Note the symmetry between the operators θ_i and $\partial/\partial \theta_i$.

The algebra of operators can be identified by introducing the linear combinations

$$\mathbf{D}_i^{\pm} = \frac{\partial}{\partial \theta_i} \pm \theta_i \,,$$

which satisfy

$$\{ D_i^{\pm}, D_j^{\pm} \} = \pm 2\delta_{ij}, \quad \{ D_i^+, D_j^- \} = 0.$$
 (1.49)

This shows that the operator algebra is the direct sum of two *Clifford algebras*.

1.6.3 Integration in Grassmann algebras

It is also convenient to define integration over Grassmann variables, for which the integral symbol notation is used, although integration and differentiation are identical operations,

$$\int \mathrm{d}\theta_i A \equiv \frac{\partial}{\partial \theta_i} A, \quad \forall A \in \mathfrak{A} \,. \tag{1.50}$$

The integral or derivative symbols are used depending on the context.

General properties. We will now show that this operation satisfies the formal properties we expect from a *definite* integral. Quite generally, we associate an operator I to a given differential operator D, which has the following defining properties: it is a linear operator acting on \mathfrak{A} , that is,

$$I(\lambda_1 A_1 + \lambda_2 A_2) = \lambda_1 I(A_1) + \lambda_2 I(A_2), \qquad (1.51)$$

and satisfies the three properties,

$$ID = 0, \qquad (1.52)$$

$$\mathsf{DI} = 0, \tag{1.53}$$

and

$$D(A) = 0 \Longrightarrow I(BA) = I(B)A.$$
(1.54)

In addition, it changes the grading in the same way as a differential operator:

 $\mathbf{PI} + \mathbf{IP} = 0.$

Let us explain the conditions (1.52-1.54): condition (1.52) expresses that, in the absence of boundary terms, the integral of a total derivative vanishes; condition (1.53) expresses that if we integrate over a variable, the result no longer depends on this variable. Finally, condition (1.54) implies that a factor whose derivative vanishes can be taken out of the integral.

In the case of Grassmann algebras, if $D^2 = 0$, D itself satisfies all conditions. The differential operators $\partial/\partial \theta_i$ indeed have a vanishing square.

1.6.4 Change of variables in a Grassmann integral We consider the integral

$$\int \mathrm{d}\theta \, f(\theta),\tag{1.55}$$

and perform the (necessarily) affine change of variables:

$$\theta = a\theta' + b, \qquad (1.56)$$

in which parity conservation implies that $a \in \mathfrak{A}^+$ and $b \in \mathfrak{A}^-$. The element *a* must be invertible, that is, its term of degree zero in the Grassmann variables must be different from zero. Then, using definition (1.50), one finds

$$\int d\theta f(\theta) = a^{-1} \int d\theta' f(\theta' a + b) = \int d\theta' \left(\frac{\partial \theta}{\partial \theta'}\right)^{-1} f(\theta(\theta')), \qquad (1.57)$$

where the latter form is independent of the specific parametrization (1.56). We have derived a very important property of Grassmann integrals: the *Jacobian* is a^{-1} , while in the case of commuting variables it is a.

Generalization. More generally, a change of variables

$$\theta_i = \theta_i(\theta'), \quad \theta_i, \theta'_i \in \mathfrak{A}^-,$$

for which the matrix $\partial \theta_i / \partial \theta'_j$ has an invertible part of degree zero, leads to a Jacobian that is the *inverse* of the determinant of $\partial \theta_i / \partial \theta'_j$:

$$\mathrm{d}\theta_1 \cdots \mathrm{d}\theta_n = \mathrm{d}\theta_1' \cdots \mathrm{d}\theta_n' J(\theta'), \qquad (1.58)$$

with

$$J = \det \frac{\partial \theta'_i}{\partial \theta_j} = \left(\det \frac{\partial \theta_i}{\partial \theta'_j} \right)^{-1}.$$
 (1.59)

The determinant is defined because all elements of the matrix $\partial \theta_i / \partial \theta'_i$ belong to \mathfrak{A}^+ .

The result can be derived by changing variables one at a time and using equation (1.57) repeatedly: $\theta_1 \mapsto \theta'_1$, then $\theta_2 \mapsto \theta'_2$, until, finally, $\theta_n \mapsto \theta'_n$. One obtains

$$J = \left. \frac{\partial \theta_1'}{\partial \theta_1} \right|_{\theta_2, \dots, \theta_n} \left. \frac{\partial \theta_2'}{\partial \theta_2} \right|_{\theta_1', \theta_3, \dots, \theta_n} \cdots \left. \frac{\partial \theta_{n-1}'}{\partial \theta_{n-1}} \right|_{\theta_1', \dots, \theta_{n-2}', \theta_n} \left. \frac{\partial \theta_n'}{\partial \theta_n} \right|_{\theta_1', \dots, \theta_{n-1}'}$$

One recognizes one form of the Jacobian for complex variables, but for the change of variables $\theta'_i \mapsto \theta_i$. Indeed, if we introduce the matrices

$$M_{ij}^{(p)} = \frac{\partial \theta_i'}{\partial \theta_j}, \ i, j \le p \le n \,,$$

using the chain rule (1.39), it is possible to verify the recursion relation

$$\frac{\partial \theta'_n}{\partial \theta_n}\Big|_{\theta'_1,\dots,\theta'_{n-1}} = \left.\frac{\partial \theta'_n}{\partial \theta_n}\right|_{\theta_1,\dots,\theta_{n-1}} - \sum_{i,j< n} \frac{\partial \theta'_n}{\partial \theta_i} \left[M^{n-1}\right]_{ij}^{-1} \frac{\partial \theta'_j}{\partial \theta_n} = \det M^{(n)} [M^{(n-1)}]^{-1}$$

The expression (1.59) follows.

Example. A straightforward verification of equation (1.58) is provided by the following example:

$$1 = \int \mathrm{d}\theta_1 \cdots \mathrm{d}\theta_n \,\theta_n \cdots \theta_1 \,.$$

After the linear change of variables $\theta \mapsto \theta'$,

$$\theta_i = \sum_j M_{ij} \theta'_j \,,$$

the result relies upon the identity

$$\theta_n \cdots \theta_1 = \theta'_n \cdots \theta'_1 \det \mathbf{M}.$$

1.6.5 Mixed change of variables

One can meet integrals involving both commuting and anticommuting variables (bosons and fermions). Calculations may then involve mixed changes of variables.

Denoting by θ , θ' and x, x', the anticommuting and commuting variables, respectively, we set (respecting parity):

$$x_a = x_a(x', \theta') \in \mathfrak{A}_+(\theta'), \qquad \theta_i = \theta_i(x', \theta') \in \mathfrak{A}_-(\theta').$$
(1.60)

We introduce the matrix **M** of partial derivatives,

$$\mathbf{M} = \begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{pmatrix},$$

with

$$\mathbf{A}_{ab} = \frac{\partial x_a}{\partial x'_b}, \quad \mathbf{B}_{ai} = \frac{\partial x_a}{\partial \theta'_i}, \quad \mathbf{C}_{ia} = -\frac{\partial \theta_i}{\partial x'_a}, \quad \mathbf{D}_{ij} = \frac{\partial \theta_i}{\partial \theta'_j}.$$

It is convenient to change variables in two steps:
(i) One first passes from (θ, x) to (θ, x') . This step generates the Jacobian

$$J_1 = \det \left. \frac{\partial x_a}{\partial x'_b} \right|_{\theta} = \det \left(\mathbf{A} - \mathbf{B} \mathbf{D}^{-1} \mathbf{C} \right).$$
(1.61)

(ii) One then goes from (θ, x') to (θ', x') . The second step just gives, as explained previously, the Jacobian

$$J_2 = (\det \mathbf{D})^{-1} . (1.62)$$

The complete Jacobian J, also called the *Berezinian* of the matrix of partial derivatives, is thus

$$J \equiv \frac{D(x,\theta)}{D(x',\theta')} = J_1 J_2 = \operatorname{Ber} \mathbf{M} \equiv \det \left(\mathbf{A} - \mathbf{B} \mathbf{D}^{-1} \mathbf{C} \right) \left(\det \mathbf{D} \right)^{-1}.$$
 (1.63)

For the Jacobian to be non-singular, the matrices **A** and **D** must be invertible (and, therefore, their contributions of degree 0 in θ' also).

Trace of mixed matrices. In the case of the integration over ordinary commuting variables, if one performs a change of variables infinitesimally close to the identity,

$$x_a = x'_a + \varepsilon f_a(x'),$$

from the general identity $\ln \det = \operatorname{tr} \ln$ (see Section A2.1), one infers that the Jacobian, expanded at first order in ε , becomes (one can also use the result (1.69) and Wick's theorem (1.78))

$$J = \det \frac{\partial x_a}{\partial x'_b} = 1 + \varepsilon \operatorname{tr} \frac{\partial f_a}{\partial x'_b} + O\left(\varepsilon^2\right) = 1 + \varepsilon \sum_a \frac{\partial f_a}{\partial x'_a} + O\left(\varepsilon^2\right).$$

In the mixed case,

$$x_a = x'_a + \varepsilon f_a(x', \theta'), \qquad \theta_i = \theta'_i + \varepsilon \varphi_i(x', \theta'), \tag{1.64}$$

we use the identity (1.63). We set

$$\mathbf{M} = 1 + \varepsilon \mathbf{M}_1 + O(\varepsilon^2), \quad \mathbf{M}_1 = \begin{pmatrix} \mathbf{A}_1 & \mathbf{B}_1 \\ \mathbf{C}_1 & \mathbf{D}_1 \end{pmatrix},$$

and obtain

$$J = 1 + \varepsilon \left(\operatorname{tr} \mathbf{A}_1 - \operatorname{tr} \mathbf{D}_1 \right) + O\left(\varepsilon^2\right), \quad \operatorname{tr} \mathbf{A}_1 - \operatorname{tr} \mathbf{D}_1 = \sum_a \frac{\partial f_a}{\partial x_a} - \sum_i \frac{\partial \varphi_i}{\partial \theta_i}.$$
(1.65)

Therefore, to maintain the connection between Jacobian and trace, one is led to define the supertrace of a mixed matrix, for which the notation Str will be used, as the difference of traces

$$\operatorname{Str} \mathbf{M}_1 = \operatorname{tr} \mathbf{A}_1 - \operatorname{tr} \mathbf{D}_1 \,. \tag{1.66}$$

It is simple to verify that the supertrace, like the usual trace, has a cyclic property,

$$\operatorname{Str} \mathbf{M}_1 \mathbf{M}_2 = \operatorname{Str} \mathbf{M}_2 \mathbf{M}_1.$$

1.7 Gaussian integrals with Grassmann variables

We consider now a Grassmann algebra \mathfrak{B} in which the generators are separated into two conjugated sets. We denote by θ_i and $\overline{\theta}_i$, $i = 1, \ldots, n$, the corresponding generators.

Complex conjugation. In many situations, a complex conjugation can be defined, which exchanges θ_i and $\bar{\theta}_i$. It has the properties of the Hermitian conjugation of operators: it acts by complex conjugation on complex numbers and

$$\theta_i^{\dagger} = \bar{\theta}_i, \quad \bar{\theta}_i^{\dagger} = \theta_i, \quad (A_1 A_2)^{\dagger} = A_2^{\dagger} A_1^{\dagger}, \quad \forall A_1, A_2 \in \mathfrak{B}.$$

$$(1.67)$$

An invariant quantity, like the integration measure $d\theta_i d\bar{\theta}_i$, is called *formally real*. It is possible to verify that if, in an integral, the integrand is formally real and one integrates over a pair of conjugated variables θ_i and $\bar{\theta}_i$, the result is still formally real.

The Gaussian integral. We calculate Gaussian integrals with, again, the motivation: a reduction of more general integrals to a finite or formal infinite sum of Gaussian integrals. We first consider the integral

$$\mathcal{Z}(\mathbf{S}) = \int \mathrm{d}\theta_1 \mathrm{d}\bar{\theta}_1 \mathrm{d}\theta_2 \mathrm{d}\bar{\theta}_2 \cdots \mathrm{d}\theta_n \mathrm{d}\bar{\theta}_n \exp\bigg(\sum_{i,j=1}^n \bar{\theta}_i S_{ij} \theta_j\bigg),\tag{1.68}$$

with S_{ij} complex. The quadratic form and, thus, the integrand is formally real if

$$\sum_{i,j=1}^{\nu} \left(\bar{\theta}_i S_{ij} \theta_j \right)^{\dagger} = \sum_{i,j=1}^{\nu} \bar{\theta}_j S_{ij}^* \theta_i = \sum_{i,j=1}^{\nu} \bar{\theta}_i S_{ij}^{\dagger} \theta_j \,,$$

that is, if the matrix \mathbf{S} is Hermitian.

According to the rules of Grassmann integration, the result is simply the coefficient of the product $\bar{\theta}_n \theta_n \cdots \bar{\theta}_1 \theta_1$ in the expansion of the integrand. The integrand can be rewritten as

$$\exp\left(\sum_{i,j=1}^{n} \bar{\theta}_i S_{ij} \theta_j\right) = \prod_{i=1}^{n} \exp\left(\bar{\theta}_i \sum_{j=1}^{n} S_{ij} \theta_j\right) = \prod_{i=1}^{n} \left(1 + \bar{\theta}_i \sum_{j=1}^{n} S_{ij} \theta_j\right).$$

In each factor, only the term proportional to $\bar{\theta}$ contributes to the integral. In the expansion of the product, the terms that give non-zero contributions to the integral thus are of the form

$$\sum_{\substack{\text{permutations}\\\{j_1,\ldots,j_n\}}} S_{nj_n} S_{n-1j_{n-1}} \cdots S_{1j_1} \bar{\theta}_n \theta_{j_n} \cdots \bar{\theta}_1 \theta_{j_1}.$$

A commutation of the generators to put them in the standard order $\bar{\theta}_n \theta_n \cdots \bar{\theta}_1 \theta_1$, generates a sign, which is the signature of the permutation. One then recognizes the coefficient as the determinant of S_{ij} . Thus,

$$\mathcal{Z}(\mathbf{S}) = \det \mathbf{S} \,. \tag{1.69}$$

The result is the inverse of the one obtained with complex commuting variables. In perturbative expansions, this leads to a sign $(-1)^L$ in front of the Feynman diagrams with L fermion loops.

For det $\mathbf{S} \neq 0$, a simpler calculation relies on the change of variables $\theta_i \mapsto \theta'_i$,

$$\sum_{j} S_{ij} \theta_j = \theta'_i \,. \tag{1.70}$$

Then, using the relations (1.58) and (1.59) for the Jacobian, one finds

$$\mathcal{Z}(\mathbf{S}) = \det \mathbf{S} \int d\theta'_1 d\bar{\theta}_1 \cdots d\theta'_n d\bar{\theta}_n \exp\left(\sum_{i=1}^n \bar{\theta}_i \theta'_i\right)$$
$$= \det \mathbf{S} \int \prod_{i=1}^n d\theta'_i d\bar{\theta}_i \left(1 + \bar{\theta}_i \theta'_i\right) = \det \mathbf{S}.$$

1.7.1 General Gaussian integrals

We introduce two other sets of Grassmann generators $\{\eta_i\}$ and $\{\bar{\eta}_i\}$, $i = 1, \ldots, n$, and consider the larger Grassmann algebra \mathfrak{C} generated by the set of the 4n generators $\{\theta_i, \bar{\theta}_i, \eta_i, \bar{\eta}_i\}$. Following the strategy of Section 1.1, we first calculate the integral

$$\mathcal{Z}_{\mathrm{G}}(\eta,\bar{\eta}) = \int \prod_{i} \mathrm{d}\theta_{i} \mathrm{d}\bar{\theta}_{i} \exp\bigg[\sum_{i,j=1}^{n} S_{ij}\bar{\theta}_{i}\theta_{j} + \sum_{i=1}^{n} \left(\bar{\eta}_{i}\theta_{i} + \bar{\theta}_{i}\eta_{i}\right)\bigg],\tag{1.71}$$

in which the integrand is an element of \mathfrak{C} , and S_{ij} is a complex matrix with det $\mathbf{S} \neq 0$.

Again we define $\Delta = \mathbf{S}^{-1}$. The calculation, as before, relies on a change of variables $\theta \mapsto \theta', \ \bar{\theta} \mapsto \bar{\theta}'$, with

$$\theta_i = \theta'_i - \sum_j \Delta_{ij} \eta_j, \quad \bar{\theta}_i = \bar{\theta}'_i - \sum_j \bar{\eta}_j \Delta_{ji},$$

and leads to the result

$$\mathcal{Z}_{\mathrm{G}}(\eta,\bar{\eta}) = \det \mathbf{S} \exp\left(-\sum_{i,j=1}^{n} \bar{\eta}_{i} \Delta_{ij} \eta_{j}\right).$$
(1.72)

Using the notation $\langle \bullet \rangle$ for expectation values with respect to the Gaussian weight of equation (1.71), with our definition of \mathcal{Z}_{G} , one finds (note the sign in equation (1.74)),

$$\frac{\partial}{\partial \bar{\eta}_i} \mathcal{Z}_{\mathcal{G}} = \det \mathbf{S} \left\langle \theta_i \right\rangle, \tag{1.73}$$

$$\frac{\partial}{\partial \eta_i} \mathcal{Z}_{\mathcal{G}} = \det \mathbf{S} \left\langle -\bar{\theta}_i \right\rangle. \tag{1.74}$$

Wick's theorem for Grassmann integrals. Gaussian expectation values are defined by

$$\langle \bar{\theta}_{i_1} \theta_{j_1} \bar{\theta}_{i_2} \theta_{j_2} \cdots \bar{\theta}_{i_n} \theta_{j_n} \rangle$$

$$= \frac{1}{\det \mathbf{S}} \int \left(\prod_i \mathrm{d}\theta_i \mathrm{d}\bar{\theta}_i \right) \bar{\theta}_{i_1} \theta_{j_1} \cdots \bar{\theta}_{i_n} \theta_{j_n} \exp\left(\sum_{i,j=1}^n \bar{\theta}_i S_{ij} \theta_j\right),$$
(1.75)

From equations (1.73) and (1.74), it follows that

$$\det \mathbf{S} \left\langle \bar{\theta}_{i_1} \theta_{j_1} \bar{\theta}_{i_2} \theta_{j_2} \cdots \bar{\theta}_{i_n} \theta_{j_n} \right\rangle = \left[\frac{\partial}{\partial \bar{\eta}_{j_1}} \frac{\partial}{\partial \eta_{i_1}} \cdots \frac{\partial}{\partial \bar{\eta}_{j_n}} \frac{\partial}{\partial \eta_{i_n}} \mathcal{Z}_{\mathrm{G}}(\eta, \bar{\eta}) \right] \Big|_{\eta = \bar{\eta} = 0}, \quad (1.76)$$

and, using the result (1.72),

$$\left\langle \bar{\theta}_{i_1} \theta_{j_1} \bar{\theta}_{i_2} \theta_{j_2} \cdots \bar{\theta}_{i_n} \theta_{j_n} \right\rangle = \left\{ \frac{\partial}{\partial \bar{\eta}_{j_1}} \frac{\partial}{\partial \eta_{i_1}} \cdots \frac{\partial}{\partial \bar{\eta}_{j_n}} \frac{\partial}{\partial \eta_{i_n}} \exp\left[-\sum_{i,j=1}^n \bar{\eta}_j \Delta_{j_i} \eta_i\right] \right\} \Big|_{\eta=\bar{\eta}=0}.$$
 (1.77)

After explicit differentiation (which is the same as integration), one obtains

$$\left\langle \bar{\theta}_{i_1} \theta_{j_1} \cdots \bar{\theta}_{i_n} \theta_{j_n} \right\rangle = \det \Delta_{j_l i_k} = \det \left\langle \bar{\theta}_{i_k} \theta_{j_l} \right\rangle$$
$$= \sum_{\substack{\text{permutations } P \\ \text{of } \{j_1, \dots, j_n\}}} \operatorname{sgn}(P) \Delta_{j_{P_1} i_1} \Delta_{j_{P_2} i_2} \cdots \Delta_{j_{P_n} i_n}, \qquad (1.78)$$

where sgn(P) is the signature of the permutation P, which is Wick's theorem for Grassmann algebras. The result differs from the expression (1.30), obtained in the case of complex commuting variables, only by the factor sgn(P).

Perturbative expansion. Expressions (1.73) and (1.74) form the basis of perturbation theory. To calculate the integral

$$\mathcal{Z}(\eta,\bar{\eta}) = \int \prod_{i} \mathrm{d}\bar{\theta}_{i} \mathrm{d}\theta_{i} \exp\left[\sum_{i,j=1}^{n} S_{ij}\bar{\theta}_{i}\theta_{j} + V(\bar{\theta},\theta) + \sum_{i=1}^{n} \left(\bar{\eta}_{i}\theta_{i} + \bar{\theta}_{i}\eta_{i}\right)\right],\tag{1.79}$$

one can formally expand in a power series in V and integrate term by term. One then finds

$$\mathcal{Z}(\eta,\bar{\eta}) = \exp\left[V\left(-\frac{\partial}{\partial\eta},\frac{\partial}{\partial\bar{\eta}}\right)\right]\mathcal{Z}_{\mathrm{G}}(\eta,\bar{\eta}).$$
(1.80)

1.7.2 Pfaffian and determinant

One can also calculate Gaussian integrals of the form

$$\mathcal{Z}(\mathbf{A}) = \int \mathrm{d}\theta_{2n} \cdots \mathrm{d}\theta_2 \mathrm{d}\theta_1 \, \exp\left(\frac{1}{2} \sum_{i,j=1}^{2n} \theta_i A_{ij} \theta_j\right),\tag{1.81}$$

where, since the product $\theta_i \theta_j$ is antisymmetric in (ij), the matrix **A** can be chosen to be antisymmetric:

$$A_{ij} + A_{ji} = 0. (1.82)$$

Expanding the exponential in a power series, one notes that only the term of order n that contains all products of degree 2n in θ ,

$$\mathcal{Z}(\mathbf{A}) = \frac{1}{2^n n!} \int \mathrm{d}\theta_{2n} \cdots \mathrm{d}\theta_1 \left(\sum_{i,j} \theta_i A_{ij} \theta_j\right)^n,\tag{1.83}$$

gives a non-zero contribution. In the expansion of the product, only the terms containing a permutation of $\theta_1 \cdots \theta_{2n}$ do not vanish. Then, ordering all terms to factorize the product $\theta_1 \theta_2 \cdots \theta_{2n}$, one finds

$$\mathcal{Z}(\mathbf{A}) = \frac{1}{2^n n!} \sum_{\substack{\text{permutations } P \\ \text{of } \{i_1, \dots, i_{2n}\}}} \operatorname{sgn}(P) A_{i_1 i_2} A_{i_3 i_4} \cdots A_{i_{2n-1} i_{2n}}, \quad (1.84)$$

where $sgn(P) = \pm 1$ is the signature of the permutation P. The quantity in the right-hand side is called the *Pfaffian* of the antisymmetric matrix A:

$$\mathcal{Z}(\mathbf{A}) = \mathrm{Pf}(\mathbf{A}). \tag{1.85}$$

With Grassmann integral techniques, one can prove the classical algebraic identity,

$$Pf^{2}(\mathbf{A}) = \det \mathbf{A}.$$
(1.86)

Indeed, $\mathcal{Z}^2(\mathbf{A})$ can be written as

$$\mathcal{Z}^{2}(\mathbf{A}) = \int \mathrm{d}\theta_{2n} \cdots \mathrm{d}\theta_{1} \,\mathrm{d}\theta'_{2n} \cdots \mathrm{d}\theta'_{1} \,\exp\left[\frac{1}{2} \sum_{i,j} \left(\theta_{i} A_{ij} \theta_{j} + \theta'_{i} A_{ij} \theta'_{j}\right)\right].$$
(1.87)

We change variables, setting

$$\eta_k = \frac{1}{\sqrt{2}} \left(\theta_k + i \theta'_k \right), \quad \bar{\eta}_k = \frac{1}{\sqrt{2}} \left(\theta_k - i \theta'_k \right)$$

The Jacobian is $(-1)^n$. Also

$$\theta_i \theta_j + \theta_i' \theta_j' = \bar{\eta}_i \eta_j - \bar{\eta}_j \eta_i , \qquad (1.88)$$

$$\mathrm{d}\eta_{2n}\cdots\mathrm{d}\eta_1\mathrm{d}\bar{\eta}_{2n}\cdots\mathrm{d}\bar{\eta}_1 = (-1)^{n^2}\prod_i\mathrm{d}\eta_i\mathrm{d}\bar{\eta}_i\,.$$
 (1.89)

Using the antisymmetry of the matrix \mathbf{A} , one then finds

$$\mathrm{Pf}^{2}(\mathbf{A}) = \int \mathrm{d}\eta_{1} \mathrm{d}\bar{\eta}_{1} \cdots \mathrm{d}\eta_{2n} \mathrm{d}\bar{\eta}_{2n} \, \exp\left(\sum_{i,j} \bar{\eta}_{i} A_{ij} \eta_{j}\right) = \det \mathbf{A} \, .$$

Wick's theorem. One can prove another version of Wick's theorem for expectation values with the weight $\exp[\sum_{ij} \theta_i A_{ij} \theta_j/2]$. One finds

$$\left\langle \theta_{i_1} \theta_{i_2} \cdots \theta_{i_{2p}} \right\rangle = \sum_{\substack{\text{all possible pairings} \\ P \text{ of } \{i_1, \dots, i_{2p}\}}} \operatorname{sgn}(P) \left\langle \theta_{i_{P_1}} \theta_{i_{P_2}} \right\rangle \cdots \left\langle \theta_{i_{P_{2p-1}}} \theta_{i_{P_{2p}}} \right\rangle, \tag{1.90}$$

where sgn(P) is the signature of the permutation P.

1.8 Legendre transformation

The Legendre transformation relates Hamiltonian and Lagrangian in classical mechanics, the free energy and the thermodynamic potential in statistical physics, and the generating functionals of connected correlation and vertex functions (to which contribute only oneline-irreducible Feynman diagrams). We recall here the definition (assuming for simplicity a finite number of variables) and explain a few basic properties.

We consider a real function $W(\mathbf{h})$ of n variables h_i , which has first- and second-order partial derivatives, and such that the matrix of elements $\partial^2 W/\partial h_i \partial h_j$ is positive:

$$orall \mathbf{v} \in \mathbb{R}^n ext{ and } |\mathbf{v}| > 0, \quad \sum_{i,j} v_i rac{\partial^2 W}{\partial h_i \partial h_j} v_j > 0.$$

The Legendre transform of the function $W(\mathbf{h})$ is a function $\Gamma(\mathbf{m})$ defined by the two equations,

$$W(\mathbf{h}) + \Gamma(\mathbf{m}) = \sum_{i} h_{i} m_{i} , \qquad (1.91a)$$

$$m_i = \frac{\partial W}{\partial h_i} \,. \tag{1.91b}$$

The positivity of the matrix of second derivatives ensures that, when equation (1.91b) can be inverted, it has a unique solution $\mathbf{h}(\mathbf{m})$.

The Legendre transformation is involutive. Indeed, a differentiation of equation (1.91a) with respect to **m** yields

$$\frac{\partial \Gamma}{\partial m_i} - h_i + \sum_j \frac{\partial h_j}{\partial m_i} \left. \frac{\partial}{\partial h_j} \left(W(\mathbf{h}) - \sum_i h_i m_i \right) \right|_{\mathbf{m} \text{ fixed}} = 0,$$

and, thus,

$$h_i = \frac{\partial \Gamma}{\partial m_i} \,. \tag{1.92}$$

Then, comparing the derivatives of equation (1.92) with respect to **m** with the derivatives of (1.91b) with respect to **h**, one finds that the matrix $\partial^2 \Gamma / \partial m_i \partial m_j$ is the inverse of the matrix $\partial^2 W / \partial h_i \partial h_j$:

$$\sum_{k} \frac{\partial^2 W}{\partial h_i \partial h_k} \frac{\partial^2 \Gamma}{\partial m_k \partial m_j} = \delta_{ij} , \qquad (1.93)$$

and, thus, the matrix $\partial^2 \Gamma / \partial m_i \partial m_j$ is also positive.

Stationarity of $W + \Gamma$. If $W(\mathbf{h})$ depends on one additional parameter μ , one finds

$$\frac{\partial\Gamma}{\partial\mu}\Big|_{\mathbf{m}\,\mathrm{fixed}} + \frac{\partial W}{\partial\mu}\Big|_{\mathbf{h}\,\mathrm{fixed}} + \sum_{i} \frac{\partial h_{i}}{\partial\mu} \frac{\partial}{\partial h_{i}}\Big|_{\mathbf{m}\,\mathrm{fixed}} \left(W(\mathbf{h}) - \sum_{i} h_{i}m_{i}\right) = 0\,,$$

and, thus,

$$\frac{\partial \Gamma}{\partial \mu} \bigg|_{\mathbf{m} \text{ fixed}} + \left. \frac{\partial W}{\partial \mu} \right|_{\mathbf{h} \text{ fixed}} = 0.$$
 (1.94)

Legendre transformation and real steepest descent method. We consider the generating function $W(\mathbf{h})$ of the cumulants of a distribution e^{-S} :

$$e^{W(\mathbf{h})} = \int d^n x \, e^{-S(\mathbf{x}) + \mathbf{h} \cdot \mathbf{x}} \,. \tag{1.95}$$

We recall that, in the perturbative sense, $W(\mathbf{b})$ is the sum of connected contributions (equation (1.18)). We calculate W by the steepest descent method. The saddle point equation is

$$-\frac{\partial S(\mathbf{x})}{\partial x_i} + h_i = 0, \qquad (1.96)$$

and, in the leading order approximation,

$$W(\mathbf{h}) + S(\mathbf{x}) - \mathbf{h} \cdot \mathbf{x} = 0.$$
(1.97)

Moreover, the matrix of second derivatives must be positive when the saddle point is real. Therefore, at leading order, $W(\mathbf{h})$ and $S(\mathbf{x})$ are related by a Legendre transformation and $\Gamma(\mathbf{m}) = S(\mathbf{m})$. Up to a trivial constant shift, the relation is exact in the case of Gaussian distributions.

In the sense of power series, the Legendre transformation generalizes to complex and Grassmann variables.

2 Euclidean path integrals and quantum mechanics (QM)

In most of this work, we study QM and quantum field theory (QFT) in Euclidean formulation. This means that we mainly discuss matrix elements of the quantum statistical operator $e^{-\beta H}$, where H is the quantum Hamiltonian and β the inverse temperature, rather than those of the quantum evolution operator $e^{-iHt/\hbar}$.

The statistical operator, which is proportional to the density matrix at thermal equilibrium $e^{-\beta H}/\mathcal{Z}$, where $\mathcal{Z}(\beta) = \operatorname{tr} e^{-\beta H}$ is the quantum partition function, describes 'evolution' in imaginary time, and, in this sense, most of its algebraic properties are the same as those of the real time evolution operator, explicit expressions being obtained by analytic continuation $\beta \mapsto it/\hbar$ [3]. Therefore, in this chapter, to keep track of the \hbar factors of real-time evolution, we first set $\beta = t/\hbar$.

Our basic tools to study first QM, and then QFT, are *functional integrals* [4], that is, *path* [5, 6, 7] and *field integrals*.

The path integral formulation of QM is well-suited to the study of systems with an arbitrary number of degrees of freedom. It makes a smooth transition between non-relativistic QM and QFT possible.

Another property plays an essential role in this work: the Euclidean field-integral formulation emphasizes the deep connection between QFT and the statistical physics of macroscopic systems [8], in particular, systems with short-range interactions near a continuous phase transition.

The operator $e^{-\beta H}$ has a useful property: it provides a tool to study the structure of the quantum ground state. For example, if H is bounded from below, the ground state energy E_0 is given by

$$E_0 = -\lim_{\beta \to \infty} \frac{1}{\beta} \ln \operatorname{tr} e^{-\beta H}.$$
(2.1)

In addition, if the ground state is unique and isolated, $e^{-\beta H}$ projects, for β large, onto the ground state vector $|0\rangle$ (in the quantum bra-ket notation):

$$e^{-\beta H} \underset{\beta \to \infty}{\sim} e^{-\beta E_0} \left| 0 \right\rangle \left\langle 0 \right|.$$
(2.2)

Therefore, the corresponding Euclidean functional integral often leads to a simple and intuitive understanding of the structure of the ground state of systems with a large number of degrees of freedom. Moreover, it gives a natural interpretation to barrier penetration effects in the semi-classical approximation.

Also, it is generally easier to define mathematically the path integral representing the operator $e^{-\beta H}$ (the Feynman–Kac formula) than $e^{-iHt/\hbar}$.

The main disadvantage of the Euclidean presentation of QM is that classical expressions have a somewhat unusual form, because time is imaginary. We shall speak of *Euclidean action*, *Euclidean Lagrangian*, and *Euclidean time*.

In this chapter, first we derive the path integral representation of the matrix elements of the quantum statistical operator for Hamiltonians of the simple separable form $p^2/2m + V(q)$. The path integral makes it possible to define a functional measure and, correspondingly, expectation values called correlation functions, which are generalized moments and related to quantum observables, after an analytic continuation in time.

Quantum Field Theory and Critical Phenomena 5E. Fifth edition. Jean Zinn-Justin, Oxford University Press (2021). © Jean Zinn-Justin. DOI: 10.1093/oso/9780198834625.003.0002 Note that, in the Euclidean formulation, when the potential becomes time dependent, the direct quantum interpretation is lost (going back to real time, one finds a potential depending on an imaginary time) while the path integral may still have an interpretation in the framework of one-dimensional classical statistical physics.

We calculate explicitly the path integral corresponding to the Euclidean action of harmonic oscillators to which is added a time-dependent external force. The result can then be used to generate Gaussian correlation functions, but also to reduce the evaluation of path integrals, in the case of analytic potentials, to perturbation theory.

We show, in a first example, that path integrals are especially well-suited to the study of the classical limit, by relating quantum and classical partition functions. We use the semi-classical approximation of the partition function to derive Bohr–Sommerfeld's quantization condition.

In the Appendix, we describe a useful representation of the two-point function.

2.1 Markovian evolution and locality

Markovian evolution. Let U(t, t'), t > t', be a bounded continuous operator in Hilbert space, which describes evolution between two times t' and t, and satisfies the Markov property,

$$U(t, t'')U(t'', t') = U(t, t'), \quad t \ge t'' \ge t', \quad \text{with} \quad U(t', t') = \mathbf{1}.$$
(2.3)

This property is also characteristic of the kind of stochastic processes we examine in Chapter 34, and implies that the evolution between t'' and time t depends only on the state of a system at time t'', but not on the details of preceding evolution.

We further assume that U(t, t') is differentiable with a continuous derivative and set

$$\left. \frac{\partial U(t,t')}{\partial t} \right|_{t=t'} = -K(t)/\hbar \,.$$

Differentiating equation (2.3) with respect to t, in the limit t'' = t, one obtains,

$$\hbar \frac{\partial U}{\partial t}(t,t') = -K(t)U(t,t').$$
(2.4)

The Markov property (2.3) makes it possible to express the operator U(t'', t') as a product of operators corresponding to arbitrarily small time intervals $\varepsilon = (t'' - t')/n$. Indeed,

$$U(t'',t') = \prod_{m=1}^{n} U[t'+m\varepsilon,t'+(m-1)\varepsilon], \quad \text{with} \quad n\varepsilon = t''-t', \quad (2.5)$$

where the product is time ordered according to the rule (2.3).

The operator K. So far, the arguments are rather general. We now specialize the operator K. If K is anti-Hermitian, of the form K = iH, where H is a quantum Hamiltonian, then U is unitary and has the form of a quantum evolution operator. Moreover, when the operator K is time independent, it is the generator of time translations, and the formal solution of equation (2.4) is $U(t, t') = e^{-i(t-t')H/\hbar}$.

By contrast, in this chapter, we mostly choose K Hermitian and positive. Moreover, if K is time independent, and of the form of a quantum Hamiltonian H, and if we set $t - t' = \hbar\beta$, then U is a quantum statistical operator of the form $e^{-\beta H}$, proportional to the density matrix at thermal equilibrium at temperature $T = 1/\beta$.

In this case, we still call the variable t time (or Euclidean time), although from the point of view of quantum evolution it is an imaginary time. Indeed, the continuation $t \mapsto it$ formally transforms the statistical into the evolution operator.

When K is time dependent, the direct connection with quantum physics is lost. However, the formalism can still be applied to classical statistical physics in the continuum, where t is a position and the operator $U(t + \varepsilon, t)$ the analogue of the transfer matrix.

Nevertheless, the algebraic part of the calculations that follow applies to all situations.

Note that, in Chapter 34, other operators (Fokker–Planck Hamiltonians) appear that, in general are neither Hermitian nor anti-Hermitian.

Position operator and matrix elements. We introduce a distinguished basis, the basis in which the quantum position operator \hat{q} is diagonal. Using the standard QM bra-ket notation, we denote by $|q\rangle$ the eigenvector of the quantum operator \hat{q} with eigenvalue q.

In terms of matrix elements, equation (2.5) becomes

$$\langle q'' | U(t'', t') | q' \rangle = \int \prod_{k=1}^{n-1} \mathrm{d}q_k \prod_{k=1}^n \langle q_k | U(t_k, t_{k-1}) | q_{k-1} \rangle,$$
 (2.6)

with the conventions

$$t_k = t' + k\varepsilon, \quad q_0 = q', \quad q_n = q''.$$

In the expression, we take the limit $n \to \infty$ at $n\varepsilon$ fixed, reducing the calculation of $\langle q''|U(t'',t')|q'\rangle$ to the asymptotic evaluation of the matrix elements $\langle q|U(t+\varepsilon,t)|q'\rangle$ for $\varepsilon \to 0$.

Locality of short-time evolution. If the operator K is local in the basis in which the position operator \hat{q} is diagonal, which means that its matrix elements $\langle q_1|K(t)|q_2\rangle$ have a support restricted to $q_1 = q_2$, then, for $\varepsilon \to 0$, only the matrix elements of $\langle q'|U|q\rangle$ with |q - q'| small contribute significantly to expression (2.6), and one can define a *path* integral representation of $\langle q''|U(t'', t')|q'\rangle$.

In particular, this property holds for operators of the form $K(t) \equiv K(\hat{p}, \hat{q}; t)$, where \hat{p} and \hat{q} are the momentum and position quantum operators with the commutation relation $[\hat{q}, \hat{p}] = i\hbar$, such that the classical quantity K(p, q; t) is polynomial in p and analytic in q.

2.2 Statistical operator: Path integral representation

We apply the preceding considerations to the special class of local Hamiltonians of the separable form:

$$H = \hat{\mathbf{p}}^2 / 2m + V(\hat{\mathbf{q}}, t), \quad [\hat{q}_{\alpha}, \hat{p}_{\beta}] = i\hbar\delta_{\alpha\beta}, \qquad (2.7)$$

where $\hat{\mathbf{p}}$ and $\hat{\mathbf{q}}$ are *d*-component quantum operators, and *m* is the mass of a particle. We specialize to the separable form, because the quantization of the corresponding classical Hamiltonian,

$$H_{\rm cl.} = \mathbf{p}^2 / 2m + V(\mathbf{q}, t),$$
 (2.8)

does not involve the problem of products of non-commuting operators. More general operators are discussed starting with Chapter 3.

We have seen that, to calculate the matrix elements of the evolution operator, we need to evaluate them only for short time intervals, with enough precision, and then use equation (2.6).

2.2.1 Short-time evolution

In the $|\mathbf{q}\rangle$ basis, equation (2.4), expressed in terms of the matrix elements $\langle \mathbf{q} | U | \mathbf{q}' \rangle$, takes the form of a Schrödinger equation in imaginary time:

$$-\hbar \frac{\partial}{\partial t} \langle \mathbf{q} | U(t,t') | \mathbf{q}' \rangle = \left[-\frac{\hbar^2}{2m} \nabla_{\mathbf{q}}^2 + V(\mathbf{q},t) \right] \langle \mathbf{q} | U(t,t') | \mathbf{q}' \rangle, \qquad (2.9)$$

 $(\nabla_{\mathbf{q}} \equiv (\partial/\partial q_1, \dots, \partial/\partial q_d))$ with the boundary condition $(\delta^{(d)}$ is the *d*-dimensional Dirac function),

$$\langle \mathbf{q} | U(t',t') | \mathbf{q}' \rangle = \delta^{(d)} (\mathbf{q} - \mathbf{q}').$$

When the potential V vanishes, $\langle \mathbf{q} | U(t,t') | \mathbf{q}' \rangle$ is obtained by a Fourier transformation:

$$\langle \mathbf{q} | U(t,t') | \mathbf{q}' \rangle = \int \frac{\mathrm{d}^d p}{(2\pi\hbar)^d} \exp\left[\frac{1}{\hbar} \left(i(\mathbf{q}-\mathbf{q}') \cdot \mathbf{p} - (t-t')\mathbf{p}^2/2m\right)\right]$$
$$= \left(\frac{m}{2\pi\hbar(t-t')}\right)^{d/2} \exp\left[-\frac{1}{\hbar}\frac{m\left(\mathbf{q}-\mathbf{q}'\right)^2}{2(t-t')}\right].$$
(2.10)

To solve equation (2.9) in the small $\varepsilon = t - t'$ limit, we set

$$\langle \mathbf{q} | U(t,t') | \mathbf{q}' \rangle = \exp \left[-\sigma(\mathbf{q},\mathbf{q}';t,t')/\hbar \right]$$

From equation (2.9), we infer

$$\frac{\partial \sigma}{\partial t} = -\frac{1}{2m} (\nabla_{\mathbf{q}} \sigma)^2 + V(\mathbf{q}, t) + \frac{\hbar}{2m} \nabla_{\mathbf{q}}^2 \sigma \,.$$

The function σ is dominated by the free contribution. We thus expand it for ε small as,

$$\sigma(\mathbf{q},\mathbf{q}';t,t') = m \frac{(\mathbf{q}-\mathbf{q}')^2}{2\varepsilon} + \frac{d}{2}\hbar\ln(2\pi\hbar\varepsilon/m) + \sigma_1(\mathbf{q},\mathbf{q}';t,t') + o(\varepsilon), \qquad (2.11)$$

where $\sigma_1 = O(\varepsilon)$. Neglecting higher-order terms, we obtain the equation $(\partial_t \equiv \partial/\partial t)$,

$$[(t-t')\partial_t + (\mathbf{q} - \mathbf{q}') \cdot \nabla_{\mathbf{q}}]\sigma_1 = (t-t')V(\mathbf{q}, t).$$
(2.12)

We introduce the linear trajectory

$$\mathbf{q}(\tau) = \mathbf{q}' + \frac{\tau - t'}{t - t'} (\mathbf{q} - \mathbf{q}'), \qquad (2.13)$$

which goes from \mathbf{q}' to \mathbf{q} at constant velocity and note that it is a solution of the homogeneous part of equation (2.12) as a function of q and t at τ fixed. The solution of equation (2.12) can then be written as

$$\sigma_1(\mathbf{q}, \mathbf{q}'; t, t') = \int_{t'}^t \mathrm{d}\tau \, V\big(\mathbf{q}(\tau), \tau). \tag{2.14}$$

The free contribution can also be expressed in terms of the trajectory (2.13) as

$$\frac{1}{2}m(\mathbf{q} - \mathbf{q}')^2 / (t - t') = \frac{1}{2} \int_{t'}^t \mathrm{d}\tau \, m \dot{\mathbf{q}}^2(\tau)$$

 $(\dot{q} \equiv dq/dt)$. This leads to the expression

$$\left\langle \mathbf{q} \right| U(t,t') \left| \mathbf{q}' \right\rangle = \left(\frac{m}{2\pi\hbar\varepsilon} \right)^{d/2} \exp\left\{ -\frac{1}{\hbar} \int_{t'}^{t} \mathrm{d}\tau \left[\frac{1}{2}m\dot{\mathbf{q}}^{2}(\tau) + V(\mathbf{q}(\tau),\tau) \right] + o(\varepsilon) \right\}.$$
(2.15)

It can be verified that the normalization is such that, for $\varepsilon \to 0$, $\langle \mathbf{q} | U(t,t') | \mathbf{q}' \rangle$ has $\delta^{(d)}(\mathbf{q} - \mathbf{q}')$ as a limit.



Fig. 2.1 A continuous, piecewise, linear path contributing to the integral (2.16)

2.2.2 The path integral

From equation (2.6), one derives

$$\langle \mathbf{q}'' | U(t'', t') | \mathbf{q}' \rangle = \lim_{n \to \infty} \left(\frac{m}{2\pi\hbar\varepsilon} \right)^{dn/2} \int \prod_{k=1}^{n-1} \mathrm{d}^d q_k \, \exp\left[-\mathcal{S}(\mathbf{q}, \varepsilon)/\hbar\right], \tag{2.16}$$

with

$$\mathcal{S}(\mathbf{q},\varepsilon) = \int_{t'}^{t''} \mathrm{d}t \left[\frac{1}{2} m \dot{\mathbf{q}}^2(t) + V(\mathbf{q}(t),t) \right] + no(\varepsilon), \qquad (2.17)$$

where $\mathbf{q}(t)$ now is the piecewise, linear, continuous trajectory defined by (Fig. 2.1),

$$\mathbf{q}(t) = \mathbf{q}_k + \frac{t - t_k}{t_{k+1} - t_k} (\mathbf{q}_{k+1} - \mathbf{q}_k), \text{ for } t_k \le t \le t_{k+1}.$$

In terms of the function $\mathbf{q}(t)$, which interpolates in time the variables $\mathbf{q}_k \equiv \mathbf{q}(t_k)$, the integral over the variables \mathbf{q}_k is also the integral over points of the path $\mathbf{q}(t)$.

One can then verify that higher orders in ε in equation (2.17) give vanishing contributions in the small ε , $n\varepsilon$ fixed, limit and, therefore,

$$\lim_{\substack{\varepsilon \to 0 \\ \text{at } n\varepsilon \text{ fixed}}} \mathcal{S}(\mathbf{q},\varepsilon) = \mathcal{S}(\mathbf{q}) \equiv \int_{t'}^{t''} \mathrm{d}t \left[\frac{1}{2} m \dot{\mathbf{q}}^2(t) + V(\mathbf{q}(t),t) \right].$$
(2.18)

We call $S(\mathbf{q})$ Euclidean action. It is expressed as a time integral of the Euclidean Lagrangian (the Lagrangian in imaginary time when V(q) does not depend on time explicitly), Legendre transforms of the Hamiltonian (2.8) (see Section 1.8).

The continuum limit of expression (2.16) can thus, formally, be written as

$$\langle \mathbf{q}'' | U(t'', t') | \mathbf{q}' \rangle = \int_{\mathbf{q}(t') = \mathbf{q}'}^{\mathbf{q}(t'') = \mathbf{q}''} \left[\mathrm{d}\mathbf{q}(t) \right] \exp\left[-\mathcal{S}(\mathbf{q})/\hbar\right].$$
(2.19)

The right-hand side is called *path integral*, because the integral involves a summation over all paths satisfying the prescribed boundary conditions, with a weight $\exp\left[-S/\hbar\right]$.

Notation. Note that we shall always write the integration measure $[d\mathbf{q}(t)]$ with brackets to distinguish path integrals from ordinary integrals.

Moreover, in the symbol $[d\mathbf{q}(t)]$ is buried an infinite normalization factor,

$$\mathcal{N} = \left(\frac{m}{2\pi\hbar\varepsilon}\right)^{dn/2}.$$
(2.20)

Therefore, we calculate only *expectation values*, which amounts to normalizing a path integral by dividing it by a reference path integral with the same kinetic term, the free motion $V \equiv 0$, or the harmonic oscillator, for example.

Brownian trajectories. The most singular term in σ (equation (2.11)) for $\varepsilon \to 0$ is $m(q-q')^2/2\varepsilon$ (independently of the potential). The support of the matrix element $\langle \mathbf{q} | U(t,t') | \mathbf{q}' \rangle$ is thus restricted to $|\mathbf{q}' - \mathbf{q}| = O(\sqrt{\varepsilon})$. For $|\mathbf{q}' - \mathbf{q}| = O(\sqrt{\varepsilon})$,

$$\sigma_1(\mathbf{q},\mathbf{q}';t') = \varepsilon V\big((\mathbf{q}+\mathbf{q}')/2,t'\big) + O(\varepsilon^2) = \frac{1}{2}\varepsilon\big(V(\mathbf{q})+V(\mathbf{q})'\big) + O(\varepsilon^2) = \varepsilon V(\mathbf{q},t) + O(\varepsilon^{3/2}),$$

because the potential is assumed to be analytic (we could generalize to piecewise-analytic potentials). Hence, a replacement of σ_1 in the expression (2.14), for instance, by $\varepsilon V(\mathbf{q}, t)$, modifies σ by a contribution of order $\varepsilon^{3/2}$, which is negligible.

This support property shows that in the action (2.18) the two terms play quite different roles. The kinetic term $\int dt \dot{\mathbf{q}}^2$ selects the class of paths contributing to the path integral, those for which $[\mathbf{q}(t+\varepsilon) - \mathbf{q}(t)]^2 / \varepsilon$ remains finite when ε goes to 0. More precisely, one finds that the expectation value of $[\mathbf{q}(t+\varepsilon) - \mathbf{q}(t)]^2$ is proportional to $|\varepsilon|\hbar/m$ for $\varepsilon \to 0$ (see Section A2.2 for a proof in the continuum limit). The kinetic term really is a part of the functional measure. It is essential to the very existence of the path integral.

By contrast, the potential weights paths according to the value of $\mathbf{q}(t)$ at each time, and determines the physical properties of the theory.

Brownian paths and leading contributions. The paths contributing to the path integral are typical of the Brownian motion (for details see Chapter 34); in particular, they are continuous but not differentiable, in contrast with what the formal expression (2.18)suggests. Still, the notation (2.18) is useful because the paths that give the largest contributions to the path integral (2.19) are in the neighbourhood of the paths that minimize the action (2.18) and, thus, solutions of the classical, Euclidean equations of motion. These paths are such that (functional derivatives are defined in Section 2.5.3)

$$\frac{\delta S}{\delta q_i(t)} = 0$$

,

and the operator associated with the kernel $\delta^2 S / \delta q_i(t_1) \delta q_j(t_2)$ is positive. These paths are classical, differentiable Euclidean paths. This observation is at the basis of *semi-classical approximations*.

Quantum evolution and path integral. When the potential is time independent, the path integral representing the matrix elements of the time-evolution operator can be recovered by an analytic continuation to real time $t \mapsto it$. One then formally obtains,

$$\langle \mathbf{q}^{\prime\prime} | U(t^{\prime\prime}, t^{\prime}) | \mathbf{q}^{\prime} \rangle = \int_{\mathbf{q}(t^{\prime})=\mathbf{q}^{\prime\prime}}^{\mathbf{q}(t^{\prime\prime})=\mathbf{q}^{\prime\prime}} [\mathrm{d}\mathbf{q}(t)] \exp(i\mathcal{A}(\mathbf{q})/\hbar), \qquad (2.21)$$

where \mathcal{A} is the classical action, time integral of the Lagrangian,

$$\mathcal{A}(\mathbf{q}) \equiv \int_{t'}^{t''} \mathrm{d}t \, \mathcal{L}\big(\mathbf{q}(t), \dot{\mathbf{q}}(t)\big), \quad \text{with} \quad \mathcal{L}\big(\mathbf{q}(t), \dot{\mathbf{q}}(t)\big) = \frac{1}{2}m\dot{\mathbf{q}}^2(t) - V\big(\mathbf{q}(t)\big). \tag{2.22}$$

2.3 Explicit evaluation of a path integral: The harmonic oscillator

This work will exhibit later numerous examples of situations where functional integrals play an essential role. Here, we begin with a simple problem, the calculation of the path integral associated with the Hamiltonian of the one-dimensional quantum harmonic oscillator. This example illustrates that Gaussian path integrals can be calculated explicitly in the continuum, without returning to the limiting process involving discrete time intervals.

We consider the quantum Hamiltonian ($\omega > 0$ constant),

$$H = \frac{1}{2m}\hat{p}^2 + \frac{1}{2}m\omega^2\hat{q}^2.$$
 (2.23)

The corresponding Euclidean classical action is

$$\mathcal{S}_{0}(q) = \int_{t'}^{t''} \left[\frac{1}{2} m \dot{q}^{2}(t) + \frac{1}{2} m \omega^{2} q^{2}(t) \right] \mathrm{d}t \,, \tag{2.24}$$

which is a quadratic form in q(t). When inserted into equation (2.19), the expression leads to the Gaussian integral,

$$\langle q'' | U_0(t'', t') | q' \rangle = \int_{q(t')=q'}^{q(t'')=q''} [\mathrm{d}q(t)] \exp\left[-\mathcal{S}_0(q)/\hbar\right].$$
 (2.25)

First, to determine the dependence on the boundary conditions q', q'', we change variables $q(t) \mapsto r(t)$ (a constant shift at fixed t) setting,

$$q(t) = q_c(t) + r(t),$$

in which q_c is the solution of the classical (Euclidean) equation of motion,

$$m\ddot{q}_c(t) - m\omega^2 q_c(t) = 0$$
, with $q_c(t') = q'$, $q_c(t'') = q''$. (2.26)

The new path r(t) then satisfies the boundary conditions

$$r(t') = r(t'') = 0. (2.27)$$

The action becomes

$$S_0(q) = S_0(q_c) + S_0(r) + m \int_{t'}^{t''} \left[\dot{q}_c(t) \dot{r}(t) + \omega^2 q_c(t) r(t) \right] dt$$

Integrating by parts, $\int \dot{q}_c \dot{r} = r \dot{q}_c - \int r \ddot{q}_c$, taking into account equation (2.26) and the boundary conditions (2.27), one notes that the terms linear in r cancel and the action (2.24) reduces to

$$\mathcal{S}_0(q) = \mathcal{S}_0(q_c) + \mathcal{S}_0(r)$$

One obtains

$$\langle q'' | U_0(t'', t') | q' \rangle = \mathcal{N}(\omega, \tau) e^{-S_0(q_c)/\hbar}, \qquad (2.28)$$

where

$$\mathcal{N}(\omega,\tau) = \int \left[\mathrm{d}r(t) \right] \exp\left[-\frac{m}{2\hbar} \int_{t'}^{t''} \mathrm{d}t \left(\dot{r}^2(t) + \omega^2 r^2(t) \right) \right], \tag{2.29}$$

with r(t') = r(t'') = 0.

Evaluation of the classical action. Setting $\tau = t'' - t'$, one can write the solution of equation (2.26) as

$$q_c(t) = \frac{1}{\sinh(\omega\tau)} \left[q' \sinh\left(\omega(t''-t)\right) + q'' \sinh\left(\omega(t-t')\right) \right].$$
(2.30)

To calculate $S_0(q_c)$ one can again integrate by parts, $\int \dot{q}^2 dt = q\dot{q} - \int q\ddot{q} dt$, and use the equation of motion (2.26). The result is

$$S_0(q_c) = \frac{m\omega}{2\sinh\omega\tau} \left[\left(q^{\prime 2} + q^{\prime \prime 2} \right) \cosh\omega\tau - 2q^\prime q^{\prime \prime} \right].$$
(2.31)

The remaining path integral. To complete the calculation, one still must evaluate the last Gaussian integral over r(t). The integral no longer depends on q', q'' and yields a normalization factor, function only of ω and t'' - t'. Since this involves an infinite normalization factor, we postpone the calculation until Section 2.6.1. The final result is

$$\langle q'' | U_0(t'',t) | q' \rangle = \left(\frac{m\omega}{2\pi\hbar \sinh \omega \tau} \right)^{1/2} \\ \times \exp\left\{ -\frac{m\omega}{2\hbar \sinh \omega \tau} \left[\left(q'^2 + q''^2 \right) \cosh \omega \tau - 2q'q'' \right] \right\}.$$
(2.32)

2.4 Partition function: Classical and quantum statistical physics

In this section, Hamiltonians are assumed to be *time independent* and to have a discrete spectrum.

2.4.1 The quantum partition function

The quantum partition function $\mathcal{Z}(\beta) = \operatorname{tr} e^{-\beta H}$ has a path integral representation that is immediately inferred from the representation of the statistical operator. One finds

$$\mathcal{Z}(\beta) = \operatorname{tr} e^{-\beta H} \equiv \operatorname{tr} U(\hbar\beta/2, -\hbar\beta/2) = \int dq \, \langle q | \, U(\hbar\beta/2, -\hbar\beta/2) \, | q \rangle$$
$$= \int [dq(t)] \exp\left[-\mathcal{S}(q)/\hbar\right], \tag{2.33}$$

where the paths now satisfy periodic boundary conditions: $q(-\hbar\beta/2) = q(\hbar\beta/2)$, and one integrates over all values of $q(\hbar\beta/2)$. It is actually convenient to rescale time $t \mapsto t/\hbar$. The action then reads

$$\mathcal{S}(q)/\hbar = \int_{-\beta/2}^{\beta/2} \mathrm{d}t \left[\frac{1}{2} m \dot{\mathbf{q}}^2(t) / \hbar^2 + V(\mathbf{q}(t)) \right].$$
(2.34)

The harmonic oscillator. Equation (2.28) makes it possible to relate the normalization of the path integral to the partition function $\mathcal{Z}_0(\beta)$ of the harmonic oscillator. Taking the trace of $U_0(\hbar\beta/2, -\hbar\beta/2)$, one finds

$$\mathcal{Z}_{0}(\beta) = \operatorname{tr} U_{0}(\hbar\beta/2, -\hbar\beta/2) \equiv \int \mathrm{d}q \, \langle q | \, U_{0}(\hbar\beta/2, -\hbar\beta/2) \, | q \rangle$$
$$= \mathcal{N}(\omega, \beta) \left(\frac{\pi\hbar}{m\omega \tanh(\beta\hbar\omega/2)} \right)^{1/2}. \tag{2.35}$$

The large β limit. One can also set the boundary conditions at t = 0 and $t = \beta$. Since the action is time-translation invariant the result is the same. However, in the formal large β limit (relevant for the ground-state energy), in the first case one obtains an explicitly time-translation invariant formalism on the whole real line while in the second case, one is led to integrate over paths on the positive real line with the boundary condition q(0) = 0. The first formalism is clearly simpler.

2.4.2 Classical and quantum statistical physics

We consider a *classical* one-dimensional lattice model, where the real variable q_k characterizes the configuration at site k. We choose a lattice with n sites and periodic boundary conditions $(q_n = q_0)$. The partition function is defined by

$$\mathcal{Z}(n,\varepsilon) = \int \left(\prod_{k=1}^{n} e^{-\varepsilon V(q_k)} \, \mathrm{d}q_k\right) \exp\left[-\mathcal{E}(q,\varepsilon)\right],\tag{2.36}$$

where the configuration energy, divided by the temperature, is given by

$$\mathcal{E}(q,\varepsilon) = \frac{1}{2\varepsilon} \sum_{k=1}^{n} \left(q_k - q_{k-1}\right)^2.$$
(2.37)

The partition function can also be considered as a time-discretized form of the path integral (2.33). The parameter ε plays, somewhat, the role of the temperature, and V(q) determines the distribution of q on each site.

We introduce the function

$$S(q,q') = \frac{1}{2\varepsilon} (q-q')^2 + \frac{1}{2} \varepsilon V(q) + \frac{1}{2} \varepsilon V(q'), \qquad (2.38)$$

and the kernel

$$\mathcal{T}(q,q') = \mathrm{e}^{-S(q,q')}$$

Using the bra-ket notation of QM, one can express the kernel in terms of elements of a *transfer matrix* \mathbf{T} , which has also the form of a quantum operator,

$$\mathcal{T}(q,q') = \langle q' | \mathbf{T} | q \rangle \tag{2.39}$$

In terms of \mathbf{T} , the partition function (2.36) can be written as

$$\mathcal{Z}(n,\varepsilon) = \operatorname{tr} \mathbf{T}^n.$$
(2.40)

In one dimension, one expects a non-trivial collective behaviour only at low temperatures, where $\varepsilon \to 0$. Then, one finds

$$\mathbf{T} \underset{\varepsilon \to 0}{\sim} \sqrt{2\pi\varepsilon} \,\mathrm{e}^{-\varepsilon \mathbf{H}},\tag{2.41}$$

where **H** is a quantum Hamiltonian, which in terms of the quantum position and momentum operators (with $\hbar = 1$ and $[\hat{q}, \hat{p}] = i$), takes the form

$$\mathbf{H} = \frac{1}{2}\hat{p}^2 + V(\hat{q}).$$

For $\varepsilon \to 0$, the eigenvalues and eigenvectors of the transfer matrix are related in a simple way to those of **H**. In the thermodynamic limit $n \to \infty$, the transfer matrix is dominated by its largest eigenvalue, which corresponds to the ground state energy E_0 of **H**. The free energy $\mathcal{W} = \ln \mathcal{Z}$ per unit length is

$$\frac{1}{n}\mathcal{W} = \frac{1}{n}\ln\mathcal{Z}(n,\varepsilon) \sim -\varepsilon E_0 + \frac{1}{2}\ln(2\pi\varepsilon)$$

On the other hand, combining equations (2.40) and (2.41), one infers that, when $\varepsilon \to 0$ with $n\varepsilon = \beta$ fixed, $\mathcal{Z}(n,\varepsilon)$ becomes proportional to the quantum partition function

$$\mathcal{Z}(\beta) = \operatorname{tr} e^{-\beta \mathbf{H}} = \lim_{\varepsilon \to 0} (2\pi\varepsilon)^{n/2} \mathcal{Z}(n,\varepsilon).$$

We have found an interesting relation between quantum statistical physics in zero dimension (one particle) and classical statistical physics in one dimension. This relation extends to higher space dimensions: *d*-dimensional classical statistical physics and (d-1)dimensional quantum statistical physics. Finally, we observe that the large β limit, which is the zero-temperature limit of the quantum model, is also the thermodynamic limit of the classical model.

2.5 Correlation functions. Generating functional

In the classical statistical model (2.36), the *m*-point correlation function is given by

$$\langle q_{i_1}q_{i_2}\cdots q_{i_m}\rangle_n = \mathcal{Z}^{-1}(n,\varepsilon) \int \left(\prod_{k=1}^n \mathrm{d}q_k \mathcal{T}(q_{k-1},q_k)\right) q_{i_1}q_{i_2}\cdots q_{i_m}.$$
 (2.42)

We assume the order $0 < i_1 \le i_2 \le \cdots \le i_m < n$, and we express the *m*-point correlation function in terms of the transfer matrix (2.39). We then integrate over all *q* variables except $q_{i_1}, q_{i_2}, \ldots, q_{i_m}$ and find,

$$\langle q_{i_1} q_{i_2} \cdots q_{i_m} \rangle_n = \mathcal{Z}^{-1}(n, \varepsilon) \int \prod_{s=1}^m \mathrm{d}q_{i_s} \langle q_{i_1} | \mathbf{T}^{n-i_m+i_1} | q_{i_m} \rangle q_{i_m} \\ \times \langle q_{i_m} | \mathbf{T}^{i_m-i_{m-1}} | q_{i_{m-1}} \rangle q_{i_{m-1}} \cdots \langle q_{i_2} | \mathbf{T}^{i_2-i_1} | q_{i_1} \rangle q_{i_1} .$$

The position operator \hat{q} is diagonal in the $|q\rangle$ basis and, therefore,

$$\langle q' | \mathbf{T}^r | q \rangle q = \langle q' | \mathbf{T}^r \hat{q} | q \rangle$$

We conclude the n-point function can be rewritten as,

$$\langle q_{i_1}q_{i_2}\cdots q_{i_m}\rangle_n = \mathcal{Z}^{-1}(n,\varepsilon)\operatorname{tr} \mathbf{T}^{n-i_m+i_1}\hat{q} \,\mathbf{T}^{i_m-i_{m-1}}\hat{q}\cdots \mathbf{T}^{i_2-i_1}\hat{q}$$

For $\varepsilon \to 0$, we can introduce the Hamiltonian **H**. It is also convenient to change notation, associating discrete values of a continuous variable t to site positions by $t_k = \varepsilon i_k$ (and $\beta = n\varepsilon$). We then obtain

$$Z^{(m)}(t_1, t_2, \dots, t_m) \equiv \langle q(t_1)q(t_2)\cdots q(t_m) \rangle_{\beta}$$

$$\sim_{\varepsilon \to 0} \mathcal{Z}^{-1}(\beta) \operatorname{tr} \left[e^{-(\beta - t_n + t_1)\mathbf{H}} \hat{q} e^{-(t_m - t_{m-1})\mathbf{H}} \hat{q} \cdots e^{-(t_2 - t_1)\mathbf{H}} \hat{q} \right]. (2.43)$$

From the direct definition (2.42), it follows that correlation functions have, for $\varepsilon \to 0$, $n\varepsilon = \beta$, $\varepsilon i_k = t_k$ fixed, the path integral representation

$$\langle q(t_1)q(t_2)\cdots q(t_m)\rangle_{\beta} = \mathcal{Z}^{-1}(\beta)\int [\mathrm{d}q]\,q(t_1)\cdots q(t_m)\,\mathrm{e}^{-\mathcal{S}(q)},$$
 (2.44)

with

$$\mathcal{S}(q) = \int_{-\beta/2}^{\beta/2} \mathrm{d}t \left[\frac{1}{2} \dot{q}^2(t) + V(q(t)) \right].$$

Note here that the analogy between classical and quantum statistical physics is not complete. Indeed, the classical correlation functions have no direct quantum analogue. Only the expectation values $\langle q^m(t) \rangle$ are both quantum and classical observables. However, this does not prevent the analogy between quantum and classical systems to extend to a less trivial subset of correlation functions in higher space dimensions, in the case of systems isotropic in space.

Moreover, the analytic continuations of the classical correlation functions $t_k \mapsto it_k$ are the dynamic correlation functions of the quantum theory.

2.5.1 Thermodynamic limit

In the classical statistical model, the limit $\beta \to \infty$ (zero temperature of the quantum model) is the thermodynamic limit. Assuming that the ground state is unique (this is always true in QM with a finite number of degrees of freedom and a regular potential), one finds

$$\langle q(t_1)q(t_2)\cdots q(t_m)\rangle = \langle 0|\,\hat{q}\,\,\mathrm{e}^{-(t_m-t_{m-1})(\mathbf{H}-E_0)}\,\hat{q}\cdots \mathrm{e}^{-(t_2-t_1)(\mathbf{H}-E_0)}\,\hat{q}\,|0\rangle\,.$$
 (2.45)

In particular, the expectation value of q(t) then is

$$\langle q(t) \rangle = \langle 0 | \hat{q} | 0 \rangle.$$

The connected two-point correlation function (the generalized second cumulant) is defined by

$$W^{(2)}(t_1, t_2) = \left\langle \left(q(t_1) - \langle q \rangle \right) \left(q(t_2) - \langle q \rangle \right) \right\rangle = \left\langle q(t_1)q(t_2) \right\rangle - \left\langle q \right\rangle^2.$$
(2.46)

Then,

$$W^{(2)}(t_1, t_2) = \langle 0 | \hat{q} e^{-(t_2 - t_1)(\mathbf{H} - E_0)} \hat{q} | 0 \rangle - \langle 0 | \hat{q} | 0 \rangle^2$$

Denoting by E_k , $E_0 < E_1 < E_2 \cdots$ the successive eigenvalues of **H**, and $|k\rangle$ the corresponding eigenvectors, one finds for large separations $|t_2 - t_1| \rightarrow \infty$,

$$W^{(2)}(t_1, t_2) = e^{-|t_2 - t_1|(E_1 - E_0)} \left(\langle 0| \, \hat{q} \, |1\rangle \right)^2 + O\left(e^{-|t_2 - t_1|(E_2 - E_0)} \right).$$

The connected two-point function decreases exponentially with a rate which, in lattice units, is

$$W_{i_1 i_2}^{(2)} \propto e^{-\varepsilon (E_1 - E_0)|i_2 - i_1|}$$

The decay of the two-point function is traditionally characterized by the *correlation* length ξ . Here, one finds

$$\xi = \frac{1}{E_1 - E_0} \frac{1}{\varepsilon} \,.$$

In the continuum limit $\varepsilon \to 0$, the correlation length in lattice units diverges. Keeping the variables t_1, t_2, \ldots, β fixed when $\varepsilon \to 0$, corresponds to measuring distances on the lattice in correlation length units, that is, in macroscopic units.

The existence of a non-trivial large-distance physics is the direct consequence of the divergence of the correlation length. A continuum limit can thus be defined, which is somewhat *universal* in the sense that it does not depend on the initial lattice structure, and on the precise way time is discretized. This is the first example of a situation we encounter again in the context of second order phase transitions.

Ground state degeneracy. With the conditions we have assumed, the ground state is unique. The existence and some properties of phase transitions, which we start discussing in Chapter 14, are related to a possible ground state degeneracy.

2.5.2 Generating functional of correlation functions

We consider a path integral defined in terms of the Euclidean action S(q), to which we add a coupling to an external force [9],

$$S(q,b) = S(q) - \int \mathrm{d}t \, b(t)q(t)$$

and satisfying periodic boundary conditions, $q(-\beta/2) = q(\beta/2)$. Then,

$$\mathcal{Z}(b,\beta) \equiv \operatorname{tr} U(\hbar\beta/2, -\hbar\beta/2) = \int [\mathrm{d}q(t)] \,\mathrm{e}^{-\mathcal{S}(q,b)/\hbar} \,. \tag{2.47}$$

The quantity $\mathcal{Z}(b,\beta)$ is the generating functional of correlation functions: if one expands the path integral in powers of b(t), one finds

$$\mathcal{Z}(b,\beta) = \mathcal{Z}(0,\beta) \sum_{n=0} \frac{1}{n!} \int \mathrm{d}t_1 \cdots \mathrm{d}t_n \, Z^{(n)}(t_1,\dots,t_n) b(t_1) \cdots b(t_n), \tag{2.48}$$

where

$$Z^{(n)}(t_1,\ldots,t_n) \equiv \langle q(t_1)\cdots q(t_n)\rangle = \frac{1}{\mathcal{Z}(0,\beta)} \int [\mathrm{d}q(t)] \,\mathrm{e}^{-\mathcal{S}(q,0)/\hbar} \,q(t_1)\cdots q(t_n).$$
(2.49)

2.5.3 Functional differentiation and correlation functions

In this chapter, and in many places in the work, we use functional derivatives. We define them here.

To recover the correlation functions $Z^{(n)}$ (equation (2.48)) from the generating functional $\mathcal{Z}(b)$, we can use the *functional differentiation* operator $\delta/\delta b(t)$. Functional differentiation obeys the standard algebraic rules (linearity and Leibniz's rule):

$$\frac{\delta}{\delta(t)} \left[\mathcal{Z}_1(b) + \mathcal{Z}_2(b) \right] = \frac{\delta}{\delta b(t)} \mathcal{Z}_1(b) + \frac{\delta}{\delta b(t)} \mathcal{Z}_2(b),
\frac{\delta}{\delta b(t)} \left[\mathcal{Z}_1(b) \mathcal{Z}_2(b) \right] = \mathcal{Z}_1(b) \frac{\delta}{\delta b(t)} \mathcal{Z}_2(b) + \mathcal{Z}_2(b) \frac{\delta}{\delta b(t)} \mathcal{Z}_1(b),$$
(2.50)

and, in addition,

$$\frac{\delta}{\delta b(t)}b(u) = \delta(t-u), \qquad (2.51)$$

where $\delta(x)$ is Dirac's δ -function.

For example, a functional differentiation with respect to b(t) of $\mathcal{Z}(b,\beta)$ (equation (2.47)), yields

$$\hbar \frac{\delta}{\delta b(t_1)} \mathcal{Z}(b,\beta) = \int \left[\mathrm{d}q \right] q(t_1) \exp\left[-\mathcal{S}(q,b)/\hbar\right]$$

Therefore, by differentiating p times with respect to b(t), one can generate any product $q(t_1) \cdots q(t_p)$. Taking the $b \equiv 0$ limit, one obtains correlation functions corresponding to the Euclidean action S(q),

$$\hbar^{p} \prod_{j=1}^{p} \frac{\delta}{\delta b(t_{j})} \mathcal{Z}(b,\beta) \bigg|_{b=0} = \int \left[\mathrm{d}q \right] \prod_{j=1}^{p} q(t_{j}) \exp\left[-\mathcal{S}(q)/\hbar\right]$$
(2.52a)

$$\equiv \mathcal{Z}(b \equiv 0, \beta) \langle q(t_1)q(t_2)\cdots q(t_p) \rangle . \qquad (2.52b)$$

More generally, a differential operator $\mathcal{F}(\hbar\delta/\delta b(t))$ generates in the right-hand side the expectation value of the functional $\mathcal{F}(q)$.

2.6 Harmonic oscillator. Correlation functions and Wick's theorem

We consider the Hamiltonian (harmonic oscillator coupled to an external force)

$$H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 q^2 - qb(t).$$
(2.53)

The Hamiltonian corresponds to the Euclidean action

$$S_{\rm G}(q,b) = \int_{-\tau/2}^{\tau/2} \mathrm{d}t \left[\frac{1}{2} m \dot{q}^2(t) + \frac{1}{2} m \omega^2 q^2(t) - b(t)q(t) \right].$$
(2.54)

We now calculate explicitly the Gaussian path integral corresponding to the action (2.54) (see equation (2.19)), with *periodic boundary conditions*,

$$\mathcal{Z}_{\rm G}(b,\beta) \equiv \operatorname{tr} U(\tau/2, -\tau/2) = \int_{q(\tau/2)=q(-\tau/2)} [\mathrm{d}q(t)] \exp[-\mathcal{S}_{\rm G}(q,b)/\hbar].$$
(2.55)

This quantity is also the generating functional of statistical correlation functions (equation (2.47)) of the Gaussian model discussed in Section 2.3.

To eliminate the linear term from the action, we adapt the method followed in Section 1.1. We change variables $q(t) \mapsto r(t)$ setting

$$q(t) = q_c(t) + r(t), \quad q_c(\tau/2) = q_c(-\tau/2) \Rightarrow r(\tau/2) = r(-\tau/2).$$
 (2.56)

The action becomes

$$S_{\rm G}(q,b) = S_0(r) + S_{\rm G}(q_c,b) + \int_{-\tau/2}^{\tau/2} {\rm d}t \left[m\dot{r}(t)\dot{q}_c(t) + m\omega^2 r(t)q_c(t) - b(t)r(t) \right].$$

In the term linear in r, we integrate by parts, and use the periodic boundary conditions (2.56). Then,

$$\begin{split} \int_{-\tau/2}^{\tau/2} \mathrm{d}t \, \dot{r}(t) \dot{q}_c(t) &= r(\tau/2) \dot{q}_c(\tau/2) - r(-\tau/2) \dot{q}_c(-\tau/2) - \int_{-\tau/2}^{\tau/2} \mathrm{d}t \, r(t) \ddot{q}_c(t) \\ &= r(\tau/2) \big(\dot{q}_c(\tau/2) - \dot{q}_c(-\tau/2) \big) - \int_{-\tau/2}^{\tau/2} \mathrm{d}t \, r(t) \ddot{q}_c(t). \end{split}$$

The term linear in r vanishes if the function $q_c(t)$ satisfies the classical equation

$$-\ddot{q}_c(t) + \omega^2 q_c(t) = b(t)/m \,,$$

with the boundary condition $\dot{q}_c(\tau/2) = \dot{q}_c(-\tau/2)$. The solution can be written as

$$q_c(t) = \frac{1}{m} \int_{-\tau/2}^{\tau/2} \Delta(t-u)b(u) \mathrm{d}u \,,$$

where the function Δ is the solution of the equation

$$-\ddot{\Delta}(t) + \omega^2 \Delta(t) = \delta(t),$$

with the periodic boundary conditions $\Delta(\tau/2) = \Delta(-\tau/2), \dot{\Delta}(\tau/2) = \dot{\Delta}(-\tau/2).$

One finds

$$\Delta(t) = \frac{1}{2\omega \sinh(\omega\tau/2)} \cosh(\omega(\tau/2 - |t|)).$$
(2.57)

In the limit $\tau \to \infty$, the function reduces to

$$\Delta(t) = \frac{1}{2\omega} e^{-\omega|t|} \,. \tag{2.58}$$

The classical action becomes

$$S_{\rm G}(q_c, b) = \int_{-\tau/2}^{\tau/2} \mathrm{d}t \left[\frac{1}{2} m \dot{q}_c^2(t) + \frac{1}{2} m \omega^2 q_c^2(t) - b(t) q_c(t) \right] = -\frac{1}{2} \int_{-\tau/2}^{\tau/2} \mathrm{d}t \, q_c(t) b(t)$$
$$= -\frac{1}{2m} \int_{-\tau/2}^{\tau/2} \mathrm{d}t \, \mathrm{d}u \, b(t) \Delta(t-u) b(u).$$

The remaining integral over r(t) just yields tr $U_0(\tau/2, -\tau/2)$ (equation (2.32)). After setting $\tau = \hbar\beta$, one finds (equation (2.35)),

$$\operatorname{tr} U_0(\tau/2, -\tau/2) = \mathcal{Z}_0(\beta)$$

where $\mathcal{Z}_0(\beta)$ is the partition function of the harmonic oscillator. Therefore,

$$\frac{\mathcal{Z}_{\mathcal{G}}(b,\beta)}{\mathcal{Z}_{0}(\beta)} = e^{-\mathcal{S}_{\mathcal{G}}(q_{c},b)/\hbar} = \exp\left[\frac{1}{2m\hbar} \int_{-\hbar\beta/2}^{\hbar\beta/2} \mathrm{d}u \,\mathrm{d}v \,\Delta(v-u)b(v)b(u)\right].$$
(2.59)

2.6.1 Correlation functions, Wick's theorem

Replacing $\mathcal{Z}_{G}(b,\beta)$ by the explicit expression (2.59), and differentiating twice, one obtains the two-point correlation function

$$\langle q(t)q(u)\rangle_0 = \mathcal{Z}_0^{-1}(\beta)\hbar^2 \left. \frac{\delta^2}{\delta b(t)\delta b(u)} \mathcal{Z}_{\mathcal{G}}(b,\beta) \right|_{b\equiv 0} = \frac{\hbar}{m} \Delta(t-u).$$
(2.60)

More generally, the arguments of Section 1.1 apply: as a characteristic property of the Gaussian measure, all correlation functions can be expressed in terms of the two-point function as stated by Wick's theorem (1.14) (ℓ must be even):

$$\langle q(t_1)q(t_2)\cdots q(t_\ell)\rangle_0 = \sum_{\substack{\text{all possible pairings}\\P \text{ of }\{1,2,\dots,\ell\}}} \langle q(t_{P_1})q(t_{P_2})\rangle_0 \cdots \langle q(t_{P_{\ell-1}})q(t_{P_\ell})\rangle_0 .$$
(2.61)

Harmonic oscillator: The partition function. We can now determine the dependence of the partition function $\mathcal{Z}_0(\beta)$ on the parameter ω . Indeed, differentiating the path integral, one obtains

$$\frac{\partial}{\partial\omega}\ln\mathcal{Z}_0(\beta) = -\frac{m\omega}{\hbar} \int_{-\hbar\beta/2}^{\hbar\beta/2} \mathrm{d}t \left\langle q^2(t) \right\rangle_0 = -\frac{\hbar\beta}{2} \frac{\cosh(\omega\hbar\beta/2)}{\sinh(\omega\hbar\beta/2)}.$$
(2.62)

Hence,

$$\mathcal{Z}_0(\beta) = \mathcal{N}' \frac{1}{\sinh(\beta \hbar \omega/2)}$$

For dimensional reasons, \mathcal{N}' is a pure number. It can be obtained by taking the limit $\beta \to \infty$, where one should find $e^{-\beta E_0}$. The complete result, thus, is

$$\mathcal{Z}_0(\beta) = \frac{1}{2\sinh(\beta\hbar\omega/2)} = \frac{\mathrm{e}^{-\beta\hbar\omega/2}}{1 - \mathrm{e}^{-\beta\hbar\omega}},\qquad(2.63)$$

which, indeed, is the partition function of the harmonic oscillator. This also completes the calculation of the normalization in expression (2.32), as a consequence of the relation (2.35).

2.6.2 Harmonic oscillator: Paths and square integrable functions

Sometimes, mainly in semi-classical calculations (solitons, instantons), an alternative method of calculation is useful, which we explain here in the example of the harmonic oscillator. Since we expect problems with infinite normalizations, we first work with the discretized form and then describe it in the continuum. We set here $\hbar = m = 1$. Then,

$$\mathcal{S}_0(q) = \sum_{k=1}^n \left[\frac{\left(q_k - q_{k-1}\right)^2}{2\varepsilon} + \frac{1}{2}\varepsilon\omega^2 q_k^2 \right], \text{ with } q_0 = q_n.$$

Due to the periodic boundary conditions, the system is translation invariant, and thus the quadratic form in the variables q_k is simple to diagonalize. We introduce a discrete Fourier representation, setting

$$q_k = \frac{1}{\sqrt{n}} \sum_{\ell=0}^{n-1} e^{2i\pi k\ell/n} c_\ell , \qquad (2.64)$$

with the reality conditions

$$c_0 = \bar{c}_0, \quad \bar{c}_{n-\ell} = c_\ell.$$
 (2.65)

Then,

$$\mathcal{S}_0(q) = \sum_{\ell=0}^{n-1} \bar{c}_\ell \left[\left(1 - \cos(2\pi\ell/n) \right) / \varepsilon + \frac{1}{2} \omega^2 \varepsilon \right] c_\ell , \qquad (2.66)$$

where the orthogonality relations

$$\frac{1}{n}\sum_{k=0}^{n-1} e^{2i\pi k\ell/n} = \begin{cases} 1 & \text{for } \ell = 0 \pmod{n}, \\ 0 & \text{otherwise }, \end{cases}$$

have been used. These relations also show that the transformation is unitary, and the Jacobian of the change of variables is a phase factor.

The integral now has the form (1.29), but the relation (2.65) implies that only about half of the complex variables are independent. One finds

$$\mathcal{Z}_{0} = (2\varepsilon)^{-n/2} \left[\prod_{\ell=0}^{n-1} \left(1 - \cos(2\pi\ell/n) \right) / \varepsilon + \frac{1}{2} \omega^{2} \varepsilon \right]^{-1/2}.$$
 (2.67)

The product can be calculated explicitly. Setting

$$\cosh\theta = 1 + \omega^2 \varepsilon^2 / 2 \,,$$

one obtains

$$\prod_{\ell=0}^{n-1} \left[\left(1 - \cos(2\pi\ell/n) \right) / \varepsilon + \frac{1}{2}\omega^2 \varepsilon \right] = \frac{2}{(2\varepsilon)^n} \left(\cosh n\theta - 1 \right).$$

In the $\varepsilon \to 0$ limit, with $n\varepsilon = \beta$ fixed, $n\theta \to \beta\omega$, and one recovers the partition function of the harmonic oscillator,

$$\mathcal{Z}_0(\beta) = \frac{\mathrm{e}^{-\beta\omega/2}}{1 - \mathrm{e}^{-\beta\omega}} \,.$$

Continuum calculation. The calculation with discrete variables suggests how to perform a continuum calculation. In the continuum limit, the change of variables (2.64) becomes the expansion of q(t) on normalized periodic square integrable functions:

$$q(t) = \frac{1}{\sqrt{\beta}} \sum_{\ell} c_{\ell} e^{2i\pi\ell t/\beta}, \quad \text{with} \quad c_{-\ell} = \bar{c}_{\ell}.$$

The Jacobian is unity and the measure simply

$$[\mathrm{d}q(t)] \mapsto \mathrm{d}c_0 \prod_{\ell>0} \mathrm{d}c_\ell \,\mathrm{d}\bar{c}_\ell \,. \tag{2.68}$$

The function \mathcal{S}_0 becomes

$$S_0 = \frac{1}{2}\omega^2 c_0^2 + \sum_{\ell \ge 1} \bar{c}_\ell (\omega^2 + 4\pi^2 \ell^2 / \beta^2) c_\ell \,.$$

The integration then is straightforward:

$$\mathcal{Z}_0(\beta) \propto \frac{1}{\omega} \prod_{\ell \ge 1} \left[(\omega^2 + 4\pi^2 \ell^2 / \beta^2) \right]^{-1}.$$
 (2.69)

The infinite product diverges and must be normalized. The free Hamiltonian is not available because the partition function does not exist. However, it is possible to compare different values of ω , or calculate the derivative

$$\frac{\partial}{\partial \omega} \ln \mathcal{Z}_0(\beta) = -\frac{1}{\omega} - \sum_{\ell > 0} \frac{2\omega}{\omega^2 + 4\pi^2 \ell^2 / \beta^2} = -\frac{\beta}{2 \tanh(\omega\beta/2)}$$

which is the result (2.62).

2.7 Perturbed harmonic oscillator

We now consider the Hamiltonian (in this section we set $\hbar = 1$)

$$H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2 + V_{\rm I}(q), \qquad (2.70)$$

where we assume only that $V_{I}(q)$ is expandable in powers of q:

$$V_{\rm I}(q) = \sum_n v_n q^n$$

The corresponding partition function is given by

$$\mathcal{Z}(\beta) = \int_{q(-\beta/2)=q(\beta/2)} [\mathrm{d}q] \exp\left\{-\int_{-\beta/2}^{\beta/2} \left[\frac{1}{2}\dot{q}^2(t) + \frac{1}{2}\omega^2 q^2(t) + V_\mathrm{I}(q(t))\right] \mathrm{d}t\right\}.$$
 (2.71)

To evaluate the path integral (2.71), one can generalize the identities (1.15) and (1.17). We apply identity (2.52a) to the path integral (2.55):

$$\mathcal{Z}(\beta) = \left\{ \exp\left[-\int_{-\beta/2}^{\beta/2} \mathrm{d}t \, V_{\mathrm{I}}\left(\frac{\delta}{\delta b(t)}\right) \right] \mathcal{Z}_{\mathrm{G}}(b,\beta) \right\} \bigg|_{b=0}.$$
(2.72)

We then replace the partition function $\mathcal{Z}_{G}(b,\beta)$ by its explicit expression (2.59), calculated in Section 2.6 (equation (2.59)),

$$\frac{\mathcal{Z}(\beta)}{\mathcal{Z}_0(\beta)} = \exp\left[-\int_{-\beta/2}^{\beta/2} \mathrm{d}t \, V_{\mathrm{I}}\left(\frac{\delta}{\delta b(t)}\right)\right] \exp\left[\frac{1}{2} \int \mathrm{d}u \, \mathrm{d}v \, b(u) \Delta(u-v) b(v)\right]\Big|_{b=0} \,. \tag{2.73}$$

If $V_{I}(q)$ is a polynomial, a more explicit form is obtained by expanding (2.73) in powers of $V_{I}(q)$. Perturbation theory is then reduced to calculating Gaussian expectation values:

$$\mathcal{Z}(\beta)/\mathcal{Z}_0(\beta) = \sum_{k=0} \frac{(-1)^k}{k!} \int \mathrm{d}t_1 \mathrm{d}t_2 \cdots \mathrm{d}t_k \left\langle V_{\mathrm{I}}(q(t_1)) \cdots V_{\mathrm{I}}(q(t_k)) \right\rangle_0 \,,$$

where $\langle \bullet \rangle_0$ means the expectation value with respect to the Gaussian measure. The arguments given in Section 1.1 immediately apply here also, and the successive terms in the expansion can be calculated using Wick's theorem (1.14), in the form (2.61). This is the basis of perturbation theory.

Equal-time correlation functions. The perturbative expansion involves the Gaussian expectation values of equal-time products, which, with the help of Wick's theorem, can be expressed in terms of $\langle q^2(t) \rangle_0$. Because the paths contributing to the path integrals are continuous, this expectation value is defined. However, equal-time expectation values containing time derivatives are not, because the paths are not differentiable. An example is provided by a particle in a magnetic field (see Section 3.3.1).

Example. The quartic anharmonic oscillator. We consider the Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2 + \lambda q^4, \qquad (2.74)$$

and expand the partition function to second order in λ :

$$\mathcal{Z}(\beta)/\mathcal{Z}_{0}(\beta) = 1 - \lambda \int_{-\beta/2}^{\beta/2} \mathrm{d}t \left\langle q^{4}(t) \right\rangle_{0} + \frac{1}{2} \lambda^{2} \int_{-\beta/2}^{\beta/2} \mathrm{d}t_{1} \mathrm{d}t_{2} \left\langle q^{4}(t_{1})q^{4}(t_{2}) \right\rangle_{0} + O\left(\lambda^{3}\right).$$

Then, using Wick's theorem (2.61), we infer

$$\left\langle q^{4}(t)\right\rangle_{0} = 3\left(\left\langle q^{2}(t)\right\rangle\right)_{0}^{2} = 3\Delta^{2}(0),$$

and

$$\begin{split} \left\langle q^{4}(t_{1})q^{4}(t_{2})\right\rangle_{0} &= 9\left(\left\langle q^{2}(t_{1})\right\rangle_{0}\right)^{2}\left(\left\langle q^{2}(t_{2})\right\rangle_{0}\right)^{2} + 72\left\langle q^{2}(t_{1})\right\rangle_{0}\left(\left\langle q(t_{1})q(t_{2})\right\rangle_{0}\right)^{2}\left\langle q^{2}(t_{2})\right\rangle_{0} \\ &+ 24\left(\left\langle q(t_{1})q(t_{2})\right\rangle_{0}\right)^{4} \\ &= 9\Delta^{4}(0) + 72\Delta^{2}(0)\Delta^{2}(t_{1}-t_{2}) + 24\Delta^{4}(t_{1}-t_{2}). \end{split}$$

Combining these expressions and using the periodicity of $\Delta(t)$, we find

$$\mathcal{Z}(\beta)/\mathcal{Z}_{0}(\beta) = 1 - 3\lambda\beta\Delta^{2}(0) + \frac{9}{2}\lambda^{2}\beta^{2}\Delta^{4}(0) + 36\beta\lambda^{2}\Delta^{2}(0)\int_{-\beta/2}^{\beta/2} \mathrm{d}t\,\Delta^{2}(t) + 12\lambda^{2}\beta\int_{-\beta/2}^{\beta/2} \mathrm{d}t\,\Delta^{4}(t) + O\left(\lambda^{3}\right).$$

$$(2.75)$$

In particular, the first three terms exponentiate, in agreement with the general result (1.18).

The classical limit and perturbation theory. A perturbative expansion can be generated for any decomposition of the potential into the sum of a quadratic term and a remainder, as in equation (2.70). However, if one wants to associate the perturbative expansion with a formal expansion in powers of \hbar , then one concludes from expression (2.19) that the action, and thus the potential, have to be expanded around a minimum. Denoting by q_0 a minimum of the potential, we then write

$$V(q) = V(q_0) + \frac{1}{2}V''(q_0)(q - q_0)^2 + V_{\rm I}(q - q_0)^2$$

The expansion in powers of the coefficients of $V_{\rm I}$ can then be organized as an expansion in powers of \hbar , called a *loop expansion*. Some problems associated with a possible degeneracy of the classical minimum are examined in Chapter 39.

Correlation functions and perturbation theory. We have explained how to calculate, in the form of a perturbative expansion, the path integral for any Hamiltonian of the form $p^2/2m + V(q)$ in terms of the path integral (2.55). The method can immediately be generalized to the corresponding correlation functions.

2.8 Semi-classical expansion

In the formal limit $\hbar \to 0$, one expects the quantum partition function to converge towards the classical partition function. We verify this property here by calculating the leading order and the first correction of the semi-classical expansion of the partition function (2.33). In particular, since \hbar has a dimension, the expansion parameter must take the form of \hbar divided by an action. The calculation exhibits the explicit expansion parameter.

We then use this result to generate semi-classical Wentzel–Kramers–Brillouin (WKB)like approximations for the spectrum.

2.8.1 Quantum partition function

For $\hbar \to 0$, the leading term in the action (2.34) is the kinetic term and the dominant contributions come from constant paths. It is thus convenient to first calculate the matrix elements

$$\langle q_0 | e^{-\beta H} | q_0 \rangle = \int_{q(-\beta/2)=q_0}^{q(\beta/2)=q_0} [dq(t)] \exp\left[-\mathcal{S}(q)/\hbar\right].$$
 (2.76)

In the path integral, we change variables $q(t) \mapsto q(t) + q_0$ in such a way that the integral becomes

$$\langle q_0 | e^{-\beta H} | q_0 \rangle = \int_{q(-\beta/2)=0}^{q(\beta/2)=0} [dq(t)] \exp\left[-\Sigma(q)\right],$$
 (2.77)

with

$$\Sigma(q) = \Sigma_0(q) + \int_{-\beta/2}^{\beta/2} dt \, V(q_0 + q(t)), \text{ and}$$
(2.78)
$$\Sigma_0(q) = \int_{-\beta/2}^{\beta/2} dt \, \frac{1}{2} m \dot{q}^2(t) / \hbar^2.$$

With these new boundary conditions, q(t) is of order \hbar and the potential can be expanded in powers of q as

$$V(q_0 + q(t)) = V(q_0) + V'(q_0)q(t) + \frac{1}{2}V''(q_0)q^2(t) + O(\hbar^3).$$

Then, we expand the integrand,

$$\begin{aligned} \langle q_0 | e^{-\beta H} | q_0 \rangle &= \mathcal{N}(\beta) e^{-\beta V(q_0)} \left[1 - V'(q_0) \int_{-\beta/2}^{\beta/2} \mathrm{d}t \, \langle q(t) \rangle \right. \\ &+ \frac{1}{2} (V'(q_0))^2 \int_{-\beta/2}^{\beta/2} \mathrm{d}t \, \mathrm{d}u \, \langle q(t)q(u) \rangle - \frac{1}{2} V''(q_0) \int_{-\beta/2}^{\beta/2} \mathrm{d}t \, \langle q^2(t) \rangle + O(\hbar^3) \right], \end{aligned}$$

and calculate the successive terms $(\langle \bullet \rangle)$ is a notation for the expectation value with respect to $e^{-\Sigma_0}$). First, we note that $\langle q(t) \rangle = 0$. The two-point function corresponding to Σ_0 , with the proper boundary conditions, is proportional to $\Delta(t, u) = \Delta(u, t)$, the solution of

$$\ddot{\Delta}(t,u) = \delta(t-u)$$
, with $\Delta(-\beta/2, u) = \Delta(\beta/2, u) = 0$

It follows that

$$\frac{m}{\hbar^2} \langle q(t)q(u) \rangle = \Delta(t,u) = -\frac{1}{2}|t-u| + \frac{1}{4}\beta - ut/\beta, \qquad (2.79)$$

a form that can be substituted in the expansion.

The normalization $\mathcal{N}(\beta)$ is given by

$$\mathcal{N}(\beta) = \langle q = 0 | e^{-\beta p^2/2m} | q = 0 \rangle$$

and is obtained from the free expression (2.10), where t - t' is replaced by $\hbar\beta$ (and d = 1). One finds

$$\mathcal{N}(\beta) = \frac{1}{\hbar} \sqrt{\frac{m}{2\pi\beta}}.$$
(2.80)

The complete result takes the form of the simple integral (after an integration by parts),

$$\mathcal{Z}(\beta) = \frac{1}{\hbar} \sqrt{\frac{m}{2\pi\beta}} \int \mathrm{d}q \exp\left[-\beta V(q) - \beta^2 \hbar^2 V''(q)/24m + O(\hbar^4)\right].$$
(2.81)

Discussion.

(i) For $\hbar \to 0$, one recovers the classical partition function with a Boltzmann weight obtained by integrating $e^{-\beta H(p,q)}$ over p, where H is the classical Hamiltonian, $H = p^2/2m + V(q)$:

$$\mathcal{Z}_{\rm cl.}(\beta) = \int \frac{\mathrm{d}p \,\mathrm{d}q}{2\pi\hbar} \,\mathrm{e}^{-\beta H(p,q)} = \frac{1}{\hbar} \sqrt{\frac{m}{2\pi\beta}} \int \mathrm{d}q \,\,\mathrm{e}^{-\beta V(q)}$$

(ii) Defining the *thermal wavelength* by

$$\lambda_{\rm th.} = \hbar \sqrt{\beta/m},$$

and a length scale typical of the variations of the potential, and which increases when $\beta \rightarrow 0$ (high temperature),

$$l_{\text{pot.}} \propto \sqrt{\left|\left\langle V(q)\right\rangle / \left\langle V''(q)\right\rangle \right|},$$

we note that the ratio between the classical term and the first quantum correction is of order $\lambda_{\rm th.}/l_{\rm pot.}$. At high temperatures (*i.e.*, β small), the thermal wavelength is small, and statistical systems have a classical behaviour. On the contrary, at low temperature, quantum effects eventually dominate. Note that this analysis applies to regular potentials, at this order twice differentiable, but not to other potentials like the idealized potentials often used in QM examples (square well, and so on).

(iii) Formally, the classical limit leads to a kind of *dimensional reduction*: the quantum partition function corresponds to a path integral, that is, an integral over one-dimensional objects. By contrast, the corresponding classical function is given by an integral over the zero mode, which is just one point, that is, of dimension 0.

2.8.2 WKB spectrum

The spectrum in the WKB limit, that is, a limit in which $\hbar \to 0$ at fixed energy (in contrast with perturbation theory where the energies are also of order \hbar), can be obtained from the semi-classical expansion of the partition function described in Section 2.8.1.

In the case of a Hamiltonian with a discrete spectrum, the partition function can be written as

$$\mathcal{Z}(\beta) = \operatorname{tr} e^{-\beta H} = \sum_{n=0} e^{-\beta E_n}.$$

The Laplace transform of $\mathcal{Z}(\beta)$ is then

$$G(E) = \int_0^\infty \mathrm{d}\beta \,\,\mathrm{e}^{\beta E} \,\mathcal{Z}(\beta) = \sum_n \frac{1}{E_n - E} \,,$$

where the result in the right-hand side is obtained by analytic continuation from sufficiently negatives values of the energy variable E.

After continuation to complex values of E, one obtains the eigenvalue distribution

$$\frac{1}{2i\pi} \left(G(E+i0) - G(E-i0) \right) = \sum_{n} \delta(E-E_n).$$

For what follows, it is convenient to consider the integrated distribution ($\theta(s)$ is the step function, $\theta(s) = 0$ for s < 0, $\theta(s) = 1$ for s > 0),

$$\int_{-\infty}^{E} dE' \frac{1}{2i\pi} (G(E'+i0) - G(E'-i0)) = \sum_{n} \theta(E-E_{n}).$$

In particular, if we choose $E = E_k$, a value of the spectrum, then

$$\int_{-\infty}^{E_k} dE' \frac{1}{2i\pi} \left(G(E'+i0) - G(E'-i0) \right) = k + 1/2, \qquad (2.82)$$

where we have set $\theta(0) = 1/2$, a prescription motivated by a more careful analysis.

Approximating $\mathcal{Z}(\beta)$ by the leading term of the semi-classical result (2.81), from equation (2.82) we infer

$$G_{\rm cl.}(E) = \frac{1}{\hbar} \sqrt{m/2} \int \mathrm{d}q \left[V(q) - E \right]^{-1/2}$$

We take the discontinuity of $G_{cl.}(E)$ on the cut. The exact discrete distribution is replaced by a continuous distribution, a result that is not surprising for a classical approximation. Nevertheless, from the integrated distribution, we can extract an approximation for the eigenvalues valid for large quantum numbers, because our approximation is also a high temperature approximation, where physical quantities are dominated by eigenvalues with large quantum numbers. We find

$$\frac{1}{2i} \int_{-\infty}^{E} \mathrm{d}E' \big(G_{\mathrm{cl.}}(E'+i0) - G_{\mathrm{cl.}}(E'-i0) \big) = \frac{1}{\hbar} \int \mathrm{d}q \,\theta \big(E - V(q) \big) \sqrt{2m[E - V(q)]}.$$

Equation (2.82) then yields the Bohr–Sommerfeld quantization condition:

$$\int \mathrm{d}q \,\theta \left(E_k - V(q) \right) \sqrt{2m[E_k - V(q)]} = \hbar \pi \left(k + \frac{1}{2} \right)$$

The left-hand side is finite for $\hbar \to 0$: one verifies that, indeed, this approximation is an approximation for large quantum numbers $E_k = O(1)$, $k\hbar = O(1)$, while the distance between eigenvalues goes to zero with \hbar .

The successive terms in the expansion of the partition function yield corrections to this leading order result.

A2 Additional remarks

A2.1 A useful relation between determinant and trace

In Section 1.6.5, we have used the identity $\ln \det = \operatorname{tr} \ln$. For general complex matrices, the proof of the identity is elementary, and is based on reducing the matrix to a triangular form, a transformation that is always possible.

To indicate how one can prove algebraically the result for operators, we consider the Gaussian path integral

$$\mathcal{Z}(\lambda) = \int [\mathrm{d}q(t)] \exp\left[-\frac{1}{2} \int \mathrm{d}t_1 \,\mathrm{d}t_2 \,q(t_1) K(t_1, t_2; \lambda) q(t_2)\right],\tag{A2.1}$$

where λ is a parameter, the complex kernel K representing the operator **K** is a symmetric function of (t_1, t_2) , and Re **K** is a strictly positive operator. The Gaussian integration yields,

$$\mathcal{Z}(\lambda) \propto \left[\det(\mathbf{K})\right]^{-1/2}$$
. (A2.2)

Using the definition (A2.1), we calculate the logarithmic derivative,

$$\frac{\mathrm{d}\ln \mathcal{Z}}{\mathrm{d}\lambda} = -\frac{1}{2} \left\langle \int \mathrm{d}t_1 \, \mathrm{d}t_2 \, q(t_1) \frac{\mathrm{d}K(t_1, t_2; \lambda)}{\mathrm{d}\lambda} q(t_2) \right\rangle,$$

where the expectation value $\langle \bullet \rangle$ refers to the Gaussian measure in expression (A2.1). Then,

$$\langle q(t_1)q(t_2)\rangle = \mathbf{K}^{-1}(t_1, t_2) \Rightarrow \frac{\mathrm{d}\ln \mathcal{Z}}{\mathrm{d}\lambda} = -\frac{1}{2}\operatorname{tr}\frac{\mathrm{d}\mathbf{K}}{\mathrm{d}\lambda}\mathbf{K}^{-1}$$

Therefore, comparing with the derivative of expression (A2.2), one obtains

$$\frac{\mathrm{d}\ln\mathcal{Z}}{\mathrm{d}\lambda} = -\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\lambda}\ln\det(\mathbf{K}) = -\frac{1}{2}\operatorname{tr}\frac{\mathrm{d}\mathbf{K}}{\mathrm{d}\lambda}\mathbf{K}^{-1}.$$

For an invertible, differentiable operator $\mathbf{M}(\lambda)$,

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\operatorname{tr}\ln\mathbf{M}(\lambda) = \operatorname{tr}\mathbf{M}^{-1}(\lambda)\frac{\mathrm{d}}{\mathrm{d}\lambda}\mathbf{M}(\lambda).$$
(A2.3)

It follows that

$$\frac{\mathrm{d}}{\mathrm{d}\lambda} \left[\ln \det(\mathbf{K}) - \operatorname{tr} \ln(\mathbf{K}) \right] = 0 \,.$$

Integrated, the equation implies, but only for any symmetric operator K, the identity

$$\ln \det \mathbf{K} = \operatorname{tr} \ln \mathbf{K} \,. \tag{A2.4}$$

The result can be generalized by replacing the path integral by field integrals, and also integrating over complex fields to remove the restriction to symmetric operators.

A2.2 The two-point function: An integral representation

The two-point correlation function plays a special role in QFT and statistical physics. It has a useful representation that reveals some of its properties.

We assume that the quantum Hamiltonian H is Hermitian, bounded from below and, to simplify the notation, has a discrete spectrum with a unique ground state.

The connected two-point function (equation (2.46)) can be written as

$$W^{(2)}(t) \equiv \langle q(0)q(t) \rangle = \langle 0 | \hat{q} e^{-|t|H} \hat{q} e^{|t|H} | 0 \rangle - (\langle 0 | \hat{q} | 0 \rangle)^2.$$

Introducing the basis in which H is diagonal, we can expand it as

$$W^{(2)}(t) = \sum_{n>0} |\langle 0| \hat{q} |n \rangle|^2 e^{-(\varepsilon_n - \varepsilon_0)|t|}, \text{ with } \varepsilon_0 < \varepsilon_1 \le \varepsilon_2 \cdots \le \varepsilon_n \cdots, \qquad (A2.5)$$

where the state vectors $|n\rangle$ and the energies ε_n are, respectively, the eigenfunctions and eigenvalues of H.

As a consequence of the Hermiticity of H, the eigenvalues are real and the exponentials in the sum of the right-hand side have positive coefficients. The expansion (A2.5) leads to the representation of the Fourier transform $\tilde{Z}^{(2)}(\omega)$ of the connected two-point function,

$$\widetilde{W}^{(2)}(\omega) = \int \mathrm{d}t \, W^{(2)}(t) \,\mathrm{e}^{i\omega t} = 2 \sum_{n>0} \frac{(\varepsilon_n - \varepsilon_0) \,|\langle 0|\,\hat{q}\,|n\rangle|^2}{\omega^2 + (\varepsilon_n - \varepsilon_0)^2} \,. \tag{A2.6}$$

Two properties of $\widetilde{W}^{(2)}(\omega)$ follow: it is a meromorphic function of ω^2 with poles only on the real negative axis. Moreover, the pole residues are all positive; it follows that $\widetilde{Z}^{(2)}(\omega)$ cannot decrease faster than $1/\omega^2$ for ω^2 large. More precisely, the limit of the derivative of $W^{(2)}(t)$, when $t \to 0_+$, is given by

$$\lim_{t \to 0_{+}} \frac{\mathrm{d}}{\mathrm{d}t} Z^{(2)}(t) = \langle 0 | \hat{q} [\hat{q}, H] | 0 \rangle.$$

Since the left-hand side is real, one can replace the operator in the right-hand side by its Hermitian part:

$$\lim_{t \to 0_{+}} \frac{\mathrm{d}}{\mathrm{d}t} Z^{(2)}(t) = \frac{1}{2} \langle 0 | [\hat{q} [\hat{q}, H]] | 0 \rangle \,.$$

For a Hamiltonian quadratic in the momentum variable of the form $H = \frac{1}{2m}\hat{p}^2 + O(\hat{p})$, the commutators can be evaluated explicitly, and one obtains

$$[\hat{q} [\hat{q}, H]] = -\frac{1}{m} \quad \Rightarrow \quad \lim_{t \to 0_+} \frac{\mathrm{d}}{\mathrm{d}t} Z^{(2)}(t) = -\frac{1}{2m} \,.$$

Combining this result with the representation (A2.5), one finds

$$\frac{1}{2m} = \sum_{n \ge 0} \left| \langle 0 | \, \hat{q} \, | n \rangle \right|^2 \, (\varepsilon_n - \varepsilon_0),$$

and, therefore, from (A2.6),

$$\widetilde{Z}^{(2)}(\omega) \underset{\omega \to \infty}{\sim} \frac{1}{m\omega^2}.$$

A2.3

The result is not surprising. The behaviour for ω large is related to short-time evolution and we have shown that the most singular part of the matrix elements of $e^{-\beta H}$ is then determined by the free part $p^2/2m$ of the Hamiltonian.

Finally, when the spectrum of H has a continuous part, the sum in (A2.6) is replaced by an integral, the poles are replaced by a cut with a positive discontinuity, but the other conclusions remain unchanged. The relativistic generalization of representation (A2.6) is called the Källen–Lehmann representation [10].

Thermal correlation functions. The preceding calculation can easily be generalized to the finite temperature, or finite length from the classical point of view:

$$Z^{(2)}(t) = Z^{-1}(\beta) \operatorname{tr} e^{-(\beta - |t|)H} \hat{q} e^{-|t|H} \hat{q}, \quad Z(\beta) = \operatorname{tr} e^{-\beta H}.$$

One verifies that the result is the same:

$$\lim_{t \to 0+} \frac{\mathrm{d}}{\mathrm{d}t} Z^{(2)}(t) = -\frac{1}{2m} \,.$$

This implies, in particular,

$$\left\langle \left(q(t+\varepsilon) - q(t) \right)^2 \right\rangle_{\varepsilon \to 0} \approx |\varepsilon| \frac{1}{m},$$

confirming that the generic paths contributing to the path integral are Brownian paths.

A2.3 Time-ordered products of operators

We express all expressions in the *real-time formalism* and use the framework of simple QM, because the generalization to QFT is just a matter of changing notation. We start from expression (2.44), after continuation to real time, and want to directly recover a form analogous to the operator form (2.43). We also immediately take the thermodynamic limit. We define the *n*-point correlation function as

$$Z^{(n)}(t_1, t_2, \dots, t_n) = \int [\mathrm{d}q] \, q(t_1) \cdots q(t_n) \, \mathrm{e}^{i\mathcal{A}(q)/\hbar} \,. \tag{A2.7}$$

We then order times,

$$t_1 \le t_2 \le \dots \le t_n \,, \tag{A2.8}$$

and decompose the time interval into (n+1) subintervals $(-\infty, t_1), (t_1, t_2), \ldots, (t_n, +\infty)$. The total action is the sum of the corresponding contributions:

$$\mathcal{A}(q) = \sum_{i=1}^{n+1} \int_{t_{i-1}}^{t_i} \left[\frac{1}{2} m \dot{q}^2(t) - V(q(t)) \right] \mathrm{d}t, \quad \text{with} \quad t_0 = -\infty, \quad t_{n+1} = +\infty.$$
 (A2.9)

We rewrite the path integral (A2.7) with the help of the identity

$$\prod_{i=1}^{n} q(t_i) = \int \prod_{i=1}^{n} \mathrm{d}q_i \,\delta\left[q(t_i) - q_i\right] q_i \,.$$

The path integral then factorizes into a product of path integrals corresponding to the different subintervals.

Returning to the very definition of the path integral (equations (2.18) and (2.19)), we note that the numerator in expression (A2.7) is exactly (recalling the ordering (2.3))

$$\langle 0 | e^{it_n H} \hat{q} e^{-i(t_n - t_{n-1})H} \hat{q} \cdots e^{-i(t_2 - t_1)H} \hat{q} e^{-it_1 H} | 0 \rangle.$$

Introducing the operator Q(t), the Heisenberg representation of the operator \hat{q} ,

$$Q(t) = e^{itH} \hat{q} e^{-itH}, \qquad (A2.10)$$

we can write

$$Z^{(n)}(t_1, t_2, \dots, t_n) = \langle 0 | Q(t_n) \cdots Q(t_1) | 0 \rangle.$$
 (A2.11)

The order of the operators on the right-hand side reflects the time ordering (A2.8).

We introduce a time-ordering operator T, which, to a set of time-dependent operators $A_1(t_1),...,A_l(t_l)$, associates the time-ordered product (T-product) of these operators. For example, for l = 2,

$$T[A_1(t_1)A_2(t_2)] = A_1(t_1)A_2(t_2)\theta(t_1 - t_2) + A_2(t_2)A_1(t_1)\theta(t_2 - t_1)A_2(t_2)\theta(t_1 - t_2)\theta(t_1 - t_2)\theta(t_2 - t_1)A_2(t_2)\theta(t_1 - t_2)\theta(t_2 - t_1)A_2(t_2)\theta(t_1 - t_2)\theta(t_1 - t_2)\theta$$

We can then rewrite expression (A2.11), irrespective now of the order between the times t_1, \ldots, t_n ,

$$Z^{(n)}(t_1, t_2, \dots, t_n) = \langle 0 | \operatorname{T} [Q(t_1)Q(t_2) \cdots Q(t_n)] | 0 \rangle.$$
 (A2.12)

The *n*-point function (A2.7) can be expressed as the vacuum expectation value of the time-ordered product of Heisenberg operators. These time-ordered products are the analytic continuation of the imaginary time correlation functions. They generate Green's functions from which one can derive scattering amplitudes (see Section 6.3.2).

More generally, at a finite temperature $1/\beta$, one finds the time-dependent correlation functions of quantum statistical physics

$$Z^{(n)}(t_1, t_2, \dots, t_n) = \mathcal{Z}^{-1}(\beta) \operatorname{tr} \left\{ e^{-\beta H} \operatorname{T} \left[Q(t_1) Q(t_2) \cdots Q(t_n) \right] \right\}.$$
(A2.13)

3 Quantum mechanics (QM): Path integrals in phase space

In Chapter 2, we have defined a path integral representation of the matrix elements of the quantum statistical operator $e^{-\beta H}$ in the case of Hamiltonians H of the separable form $p^2/2m + V(q)$. We will now extend the construction to Hamiltonians that are more general functions of phase-space variables [11–13]. This results in integrals over paths in phase space involving the action expressed in terms of the classical Hamiltonian H(p,q). However, in the case of general Hamiltonians, the path integral is not completely defined, and this reflects the problem that the classical Hamiltonian does not completely specify the quantum Hamiltonian due to the problem of ordering quantum operators in products.

When the Hamiltonian is a quadratic function of the momentum variables, the integral over momenta is Gaussian and can be performed. In the separable example, the path integral of Chapter 2 is recovered. In the case of the charged particle in a magnetic field a more general form is found. It is ambiguous, since a problem of operator ordering arises, and the ambiguity must be fixed. Hamiltonians that are general quadratic functions provide other important examples and, therefore, we analyse them thoroughly. Such Hamiltonians appear in the quantization of the motion on Riemannian manifolds. We find that the problem of ambiguities is even more severe. We illustrate the analysis by the quantization of the free motion on the sphere S_{N-1} .

In the Appendix, we discuss various additional issues related to quantization problems, including the path integral quantization of systems for which the action generating the classical equation of motion cannot be globally defined. The problem arises when phase space, as in the quantization of spin degrees of freedom, or ordinary space, as in the example of the magnetic monopole, have non-trivial topological properties.

3.1 General Hamiltonians: Phase-space path integral

We first recall how the *classical* equations of motion, in the Hamiltonian formalism and in real time, can be derived by a variational principle from an action function of phase-space variables, position, and conjugate momentum, which we denote by q, p. We then construct the corresponding path integral representation *first in real time*, then in imaginary time.

3.1.1 Hamiltonian and Lagrangian

The classical action corresponding to a Hamiltonian $\mathcal{H}(p,q;t)$ reads $(\dot{q} \equiv dq/dt)$

$$\mathcal{A}(p,q) = \int_{t_1}^{t_2} \mathrm{d}t \left[p(t)\dot{q}(t) - \mathcal{H}\left(p(t), q(t); t \right) \right], \tag{3.1}$$

with boundary conditions $q(t_1) = q_1$, $q(t_2) = q_2$. Indeed, varying the trajectory in phase space,

$$\frac{\delta \mathcal{A}(p,q)}{\delta p(t)} = \dot{q}(t) - \frac{\partial \mathcal{H}}{\partial p} = 0, \quad \frac{\delta \mathcal{A}(p,q)}{\delta q(t)} = -\dot{p}(t) - \frac{\partial \mathcal{H}}{\partial q} = 0, \quad (3.2)$$

one recovers the classical equations of motion in the Hamiltonian formulation.

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Legendre transformation. Hamiltonian and Lagrangian are related by a Legendre transformation (see Section 1.8). The Legendre transformation is defined here by (\dot{q} and q are considered as independent quantities)

$$\mathcal{H}(p,q;t) + \mathcal{L}(\dot{q},q;t) = p(t)\dot{q}(t), \quad \dot{q}(t) = \frac{\partial \mathcal{H}}{\partial p}.$$

One verifies that these equations imply

$$p(t) = \frac{\partial \mathcal{L}}{\partial \dot{q}}, \quad \frac{\partial \mathcal{L}}{\partial q} + \frac{\partial \mathcal{H}}{\partial q} = 0,$$

and equations (3.2) then are equivalent to the Euler-Lagrange equations derived from the action (3.1) expressed in terms of the Lagrangian,

$$\mathcal{A}(q) = \int_{t_1}^{t_2} \mathrm{d}t \, \mathcal{L}\big(\dot{q}(t), q(t); t\big)$$

3.1.2 QM: Path integral for time evolution

In classical mechanics, the Lagrangian is more intuitive, because it is expressed in terms of physical observables, unlike the Hamiltonian. However, QM is based on a Hamiltonian formalism, the Hamiltonian governing unitary time evolution.

For a general quantum Hamiltonian H function of position \hat{q} and conjugate momentum \hat{p} operators, with canonical commutation relation $[\hat{q}, \hat{p}] = i\hbar$, one can use the method of Section 2.1, based on evaluating the matrix elements of the evolution operator solution of

$$i\hbar\frac{\partial U}{\partial t}(t,t') = \hat{H}(t)U(t,t'), \quad U(t',t') = \mathbf{1}, \qquad (3.3)$$

001

for short time intervals. Rather, we postulate as an ansatz, a representation by a path integral over trajectories in phase space of the form

$$\langle q'' | U(t'', t') | q' \rangle = \int_{q(t')=q'}^{q(t'')=q''} [dp(t)dq(t)] \exp[i\mathcal{A}(p,q)/\hbar],$$
 (3.4)

where $\mathcal{A}(p,q)$ is the action (3.1), and \mathcal{H} a smooth function, classical limit of the quantum Hamiltonian \hat{H} . Expression (3.4) is especially aesthetic, since it involves only the invariant Liouville measure on phase space and the classical action. In particular, it is formally invariant under canonical transformations: transformations in phase space preserving the Poisson brackets,

$$(p,q) \mapsto (P(p,q), Q(p,q)), \text{ with } \{p,q\} = \{P,Q\}.$$

Again, the extension to several degrees of freedom is simple: one substitutes in the path integral representation (3.4), the corresponding classical action, and Liouville measure.

Verification. We evaluate the path integral for a short time interval $\tau = t'' - t'$ limit. The action becomes

$$\mathcal{A}(p,q) = p(q''-q') - \tau \mathcal{H}(p,q_{\mathrm{av.}}),$$

where q_{av} is some average value between q' and q''. In a time-discretized form, the measure in phase space is normalized with respect to $2\pi\hbar$. Then,

$$\langle q'' | U(t' + \tau, t') | q' \rangle \approx \int \mathrm{d}p \, \mathrm{e}^{ip(q'' - q')/\hbar} \left[1 - \frac{i\tau}{\hbar} \mathcal{H}(p, q_{\mathrm{av.}}) \right]$$
$$= \left[1 - \frac{i\tau}{\hbar} \mathcal{H}(-i\hbar\partial/\partial q, q_{\mathrm{av.}}) \right] \delta(q'' - q') = \langle q'' | (\mathbf{1} - i\tau \mathbf{H}/\hbar) | q' \rangle ,$$

where \mathbf{H} , in fact, can be any quantum operator that has the correct classical limit. Therefore, the path integral (3.4) is, formally, the correct expression, but it is ambiguous. Remarks

(i) The preceding discussion illustrates the problem that, since the path integral involves only the classical Hamiltonian, in the replacement of a quantum Hamiltonian by its classical limit, the order in products of non-commuting operators is lost and thus, the path integral, beyond its formal expression, is not defined.

A time-discretized form of the path integral involves a precise quantum Hamiltonian, but then this information is lost in the continuum limit. Therefore, the path integral must be supplemented with some additional information or limiting procedure.

(ii) The canonical invariance can be true only for a very restricted class of transformations. We will show elsewhere (Section A3.2) that in the case of a one-dimensional, one degree of freedom Hamiltonian \mathcal{H} , one can always find a canonical transformation that maps \mathcal{H} onto a free Hamiltonian:

$$p\dot{q} - \mathcal{H} \longmapsto P\dot{Q} - \frac{1}{2m}P^2.$$

One could then naively conclude that semi-classical approximations are always exact. It is easy to produce counter examples.

Phase space path integral for the statistical operator. The statistical operator is obtained by changing to imaginary time $t \mapsto -it$ in expression (3.4). One finds

$$\langle q'' | U(t'', t') | q' \rangle = \int_{q(t')=q'}^{q(t'')=q''} \left[\mathrm{d}p(t) \mathrm{d}q(t) \right] \exp\left[-\mathcal{S}(p,q) / \hbar \right],$$
 (3.5)

where $\mathcal{S}(p,q)$ is the Euclidean action in the Hamiltonian formalism,

$$\mathcal{S}(p,q) = \int_{t'}^{t''} \mathrm{d}t \left[-ip(t)\dot{q}(t) + \mathcal{H}(p(t),q(t);t) \right].$$
(3.6)

3.1.3 Separable Hamiltonians: Equivalence

First, we verify that in the case of a simple Hamiltonian like

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

where no commutation problem is involved, the real-time continuation of the path integral (2.19) is recovered after integration over p(t) in expression (3.4).

The classical action is

$$\mathcal{A}(p,q) = \int_{t'}^{t''} \mathrm{d}t \left[p(t)\dot{q}(t) - p^2(t)/2m - V(q(t)) \right].$$
(3.7)

In the path integral (3.4), the integral over the momentum variables p(t) is Gaussian. Following the strategy explained in Section 2.6, we change variables, $p(t) \mapsto r(t)$, with

$$p(t) = m\dot{q}(t) + r(t).$$
 (3.8)

The action becomes

$$\mathcal{A}(q,r) = \int_{t''}^{t'} \mathrm{d}t \left(-\frac{1}{2m} r^2(t) + \frac{1}{2} m \dot{q}^2(t) - V(q(t)) \right).$$

The path integral then factorizes into an integral over r(t),

$$\mathcal{N}(t',t'') = \int \left[\mathrm{d}r(t) \right] \exp\left(-\frac{i}{\hbar} \int_{t'}^{t''} \frac{r^2(t)}{2m} \mathrm{d}t\right),$$

that does not depend on the potential V(q), and yields only a normalization factor \mathcal{N} function of t' and t'', and an integral over q(t). One finds,

$$\langle q^{\prime\prime} | U(t^{\prime\prime}, t^{\prime}) | q^{\prime} \rangle = \int_{q(t^{\prime})=q^{\prime}}^{q(t^{\prime\prime})=q^{\prime\prime}} \left[\mathrm{d}q(t) \right] \exp\left(\frac{i}{\hbar} \mathcal{A}(q)\right),$$

with

$$\mathcal{A}(q) = \int_{t'}^{t''} \mathrm{d}t \left[\frac{1}{2} m \dot{q}^2(t) - V(q(t)) \right].$$
(3.9)

Therefore, we have verified explicitly the equivalence between the representations (3.4) and (2.21).

3.2 The harmonic oscillator. Perturbative expansion

We first consider the quantum harmonic oscillator coupled linearly to external sources. We then use the results to define a perturbative expansion for general Hamiltonians.

3.2.1 The quantum harmonic oscillator

As an example, we consider the Euclidean action

$$\mathcal{S}(p,q) = \int_{t'}^{t''} \mathrm{d}t \left[-ip(t)\dot{q}(t) + \mathcal{H}(p(t),q(t)) - a(t)p(t) - b(t)q(t) \right],$$
(3.10)

where \mathcal{H} is the Hamiltonian of the harmonic oscillator ($\omega > 0$ constant),

$$\mathcal{H}(p,q) = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2 \,,$$

and a(t), b(t) are external sources. We calculate the trace of the statistical operator at zero temperature, which corresponds to a path integral (3.5) with vanishing boundary conditions at infinite time. As we have done in Section 3.1.3, we first integrate over p(t), which amounts to substituting

$$p(t) = i\dot{q}(t) + a(t),$$

and, after an integration by parts, obtain

$$\mathcal{S}(q) = \int dt \left[\frac{1}{2} \dot{q}^2(t) + \frac{1}{2} \omega^2 q^2(t) - (b(t) - i\dot{a}(t))q(t) - \frac{1}{2}a^2(t) \right].$$

We then use the results (2.32) and (2.59) and find

$$\operatorname{tr} U(+\infty, -\infty) = \operatorname{tr} U_0 e^{-\mathcal{S}(a,b)/\hbar},$$

with (equation (2.58))

$$\mathcal{S}(a,b) = -\frac{1}{2} \int_{t'}^{t''} \mathrm{d}t \,\mathrm{d}u \big(b(t) - i\dot{a}(t) \big) \frac{1}{2\omega} \,\mathrm{e}^{-\omega|t-u|} \big(b(u) - i\dot{a}(u) \big) - \frac{1}{2} \int_{t'}^{t''} \mathrm{d}t \,a^2(t). \tag{3.11}$$

Differentiating twice $e^{-S(a,b)}$ with respect to a(t) and b(t), and then setting $a(t), b(t) \equiv 0$, we obtain the Gaussian two-point functions,

$$\begin{cases} \langle p(t)p(t') \rangle = \frac{1}{2}\omega e^{-\omega|t-t'|}, \\ \langle p(t)q(t') \rangle = -\frac{1}{2}i \operatorname{sgn}(t-t') e^{-\omega|t-t'|}, \\ \langle q(t)q(t') \rangle = \frac{1}{2\omega} e^{-\omega|t-t'|}, \end{cases}$$
(3.12)

where sgn(t) is the sign function: sgn(t) = 1 for t > 0, sgn(-t) = -sgn(t).

The free action limit. The $\omega = 0$ limit with boundaries at infinity does not exist (in another context, this is called an infrared divergence). Finite time boundary conditions are required. For simplicity, we choose conditions relevant for the partition function, $q(-\beta/2) = q(\beta/2) = 0$ (see Section 2.8.1). Then,

$$\Delta(t,t') = -\frac{1}{2}|t-t'| + \frac{1}{4}\beta - tt'/\beta, \qquad (3.13)$$

and

$$\begin{cases} \langle p(t)p(t')\rangle = 1/\beta, \\ \langle p(t)q(t')\rangle = -\frac{1}{2}i\operatorname{sgn}(t-t') - it'/\beta, \\ \langle q(t)q(t')\rangle = \frac{1}{4}\beta - \frac{1}{2}|t-t'| - tt'/\beta. \end{cases}$$
(3.14)

For more generic boundary conditions, $q(-\beta/2) = q'$, $q(\beta/2) = q''$,

$$\langle q(t) \rangle = q' + (t + \beta/2)(q'' - q')/\beta, \quad \langle p(t) \rangle = (q'' - q')/\beta,$$

and the *connected* two-point correlation functions are still given by equations (3.14).

3.2.2 Phase space path integral: Perturbative definition

We decompose a general Hamiltonian into the sum ($\omega > 0$ constant)

$$\mathcal{H}(p,q) = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2 + \mathcal{H}_{\text{Int.}}(p,q)$$

where $\mathcal{H}_{\text{Int.}}$ can be expanded as a series in p, q.

Perturbative expansion. We expand the path integral in powers of $\mathcal{H}_{\text{Int.}}$. The first term is given by the Gaussian expectation value $\langle H_{\text{Int.}} \rangle$. Wick's theorem implies that general Gaussian expectation values can be expressed in terms of the various Gaussian two-point functions.

If $\mathcal{H}_{Int.}$ is separable, that is,

$$\mathcal{H}_{\text{Int.}}(p,q) = \mathcal{H}_1(p) + \mathcal{H}_2(q), \qquad (3.15)$$

only the pp and qq two-point functions taken at t = t' are involved, and expectation values are defined. This corresponds to the case where no problem of ordering in products of quantum operators arises. However, when $\mathcal{H}_{Int.}$ contains products pq, the expectation value involves sgn(0) (equations (3.12)), which is not defined. This reflects the problem of operator ordering. From the path integration viewpoint, with the Gaussian measure associated with the harmonic oscillator, the paths in phase space that contribute are not regular enough. Finally, only the choice sgn(0) = 0 corresponds to a Hermitian Hamiltonian.

At higher orders, Wick's theorem again implies that all expectation values can be expressed in terms of Gaussian two-point functions. However, the singular terms correspond to equal-time contributions, *which are already present at leading order*.

3.3 Hamiltonians quadratic in momentum variables

We have outlined a few problems one faces when trying to define a general path integral in phase space. To show that expression (3.6) has, nevertheless, at least some heuristic value, we now discuss the example of more general Hamiltonians quadratic in momenta.

3.3.1 Quantization in a static magnetic field

The classical Hamiltonian of a particle (in \mathbb{R}^d) in a potential and a static magnetic field has the form,

$$\mathcal{H}_{\text{mag.}} = \frac{1}{2m} \left[\mathbf{p} + e\mathbf{A}(\mathbf{q}) \right]^2 + V(\mathbf{q}), \qquad (3.16)$$

where **A** is the vector potential and *e* the electric charge. The Hamiltonian is gauge invariant (see Chapter 21), that is, invariant in the changes $(\nabla \equiv (\partial/\partial q_1, \ldots, \partial/\partial q_d))$

$$\mathbf{A}(\mathbf{q}) \mapsto \mathbf{A}(\mathbf{q}) + \nabla \Lambda(\mathbf{q}), \quad \mathbf{p} \mapsto \mathbf{p} - e \nabla \Lambda(\mathbf{q}),$$
 (3.17)

which do not affect the magnetic field.

The quantization of the Hamiltonian leads to a problem of order of quantum operators in the product $\mathbf{p} \cdot \mathbf{A}(\mathbf{q})$ [14]. The order in the quantum Hamiltonian (\hat{X} denotes the quantum operator associated with the classical variable X),

$$\hat{H} = \frac{1}{2m} \left[\hat{\mathbf{p}}^2 + e\mathbf{A}(\hat{\mathbf{q}}) \cdot \hat{\mathbf{p}} + e\hat{\mathbf{p}} \cdot \mathbf{A}(\hat{\mathbf{q}}) + e^2 \mathbf{A}^2(\hat{\mathbf{q}}) \right] + V(\hat{\mathbf{q}}), \qquad (3.18)$$

is determined by the *condition of Hermiticity*. Indeed, a change in the order of operators is equivalent to the addition of an imaginary potential proportional to

$$\mathbf{A}(\mathbf{\hat{q}}) \cdot \mathbf{\hat{p}} - \mathbf{\hat{p}} \cdot \mathbf{A}(\mathbf{\hat{q}}) = i\hbar \,\nabla \cdot \mathbf{A}(\mathbf{\hat{q}}).$$

In the presence of a magnetic field, the phase of wave functions $\psi(\mathbf{q})$ can be changed at each point of space independently (a gauge symmetry). The U(1) gauge transformation,

$$\psi(\mathbf{q}) \mapsto \psi(\mathbf{q}) e^{-ie\Lambda(\mathbf{q})/\hbar},$$
(3.19)

can be cancelled by adding the gradient term (3.17) to the vector potential.

Path integral representation. The Euclidean action (3.6) becomes,

$$\mathcal{S}(\mathbf{p}, \mathbf{q}) = \int_{t'}^{t''} \mathrm{d}t \left[-i\mathbf{p}(t) \cdot \mathbf{q}(t) + \mathcal{H}_{\mathrm{mag.}} \left(\mathbf{p}(t), \mathbf{q}(t) \right) \right].$$
(3.20)

In the path integral,

$$\langle \mathbf{q}'' | U(t'', t') | \mathbf{q}' \rangle = \int_{\mathbf{q}(t')=\mathbf{q}'}^{\mathbf{q}(t'')=\mathbf{q}''} \left[\mathrm{d}\mathbf{p}(t) \mathrm{d}\mathbf{q}(t) \right] \exp\left[-\mathcal{S}(\mathbf{p}, \mathbf{q}) / \hbar \right], \tag{3.21}$$

the integral over momentum is still Gaussian. In the action, the terms linear in \mathbf{p} can be eliminated by the change of variables, $\mathbf{p}(t) \mapsto \mathbf{r}(t)$, with

$$\mathbf{p}(t) = im\dot{\mathbf{q}}(t) - e\mathbf{A}(\mathbf{q}(t)) + \mathbf{r}(t)$$

After integration over $\mathbf{r}(t)$, one obtains an integral over the path $\mathbf{q}(t)$ with the action

$$\mathcal{S}(\mathbf{q}) = \int_{t'}^{t''} \mathrm{d}t \left[\frac{1}{2} m \dot{\mathbf{q}}^2(t) + i e \mathbf{A} \left(\mathbf{q}(t) \right) \cdot \dot{\mathbf{q}}(t) + V \left(\mathbf{q}(t) \right) \right], \qquad (3.22)$$

in which one recognizes the Euclidean (or imaginary time) classical action integral of the Lagrangian, corresponding to the Hamiltonian (3.16).
Note that, in this example, the Euclidean action is not real, and thus does not define a positive measure. Actually, the imaginary contribution ensures consistency of the path integral with gauge invariance: the transformation (3.17) adds a total derivative to the Lagrangian and the variation of the action, δS is

$$\delta \mathcal{S} = ie \left[\Lambda(\mathbf{q}'') - \Lambda(\mathbf{q}') \right].$$

It follows that the matrix elements $\langle \mathbf{q}'' | U(t'', t') | \mathbf{q}' \rangle$ are multiplied by the phase factor $\exp\left[-ie\left(\Lambda(\mathbf{q}'') - \Lambda(\mathbf{q}')\right)/\hbar\right]$, consistently with the gauge transformation (3.19).

Hermiticity and the sgn(0) problem. From the analysis of Section 3.2.2, one expects a problem related to operator ordering, because the Hamiltonian is not separable (the analysis is inspired by section 5.2 of Ref. [6]).

To understand where the problem shows up, we expand the path integral corresponding to the action

$$\mathcal{S}(\mathbf{q}) = \int \mathrm{d}t \left[\frac{1}{2} \dot{\mathbf{q}}^2(t) + i e \mathbf{A} \left(\mathbf{q}(t) \right) \cdot \dot{\mathbf{q}}(t) + \frac{1}{2} \omega^2 \mathbf{q}^2(t) \right], \quad \omega > 0,$$

in powers of the charge e. At first order, we find a contribution which, using Wick's theorem, can be written as $(\langle \bullet \rangle$ is a notation for expectation value with weight e^{-S})

$$-\frac{ie}{\hbar}\int \mathrm{d}t \sum_{i,j} \left\langle \dot{q}_i(t)q_j(t) \right\rangle \left\langle \frac{\partial A_i}{\partial q_j} \right\rangle.$$

From equations (2.58, 2.60), we derive

$$\dot{q}_i(t_1)q_j(t_2)\rangle = -\frac{1}{2}\hbar\,\delta_{ij}\,\operatorname{sgn}(t_1-t_2)\,\mathrm{e}^{-\omega|t_1-t_2|}\,.$$

Therefore, formally

$$-\frac{ie}{\hbar}\int \mathrm{d}t\sum_{i,j}\left\langle \dot{q}_i(t)q_j(t)\right\rangle \left\langle \frac{\partial A_i}{\partial q_j}\right\rangle = \frac{1}{2}ie\,\mathrm{sgn}(0)\int \mathrm{d}t\left\langle \nabla\cdot\mathbf{A}\left(\mathbf{q}(t)\right)\right\rangle.$$

As expected, the result involves sgn(0), because the Hamiltonian is not separable and, thus, the path integral is not defined. This difficulty also reflects the property that, since the Brownian paths are not differentiable, a potential involving $\dot{\mathbf{q}}$ is not defined and a regularization is required (see Chapter 8). For example, one can add a term like $\nu^2(\ddot{q})^2$ in the action and take then the $\nu = 0$ limit.

Note that the assignment sgn(0) = 0 preserves invariance under time reversal. Moreover, equation (2.58) implies

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\langle q_i(t) q_j(t) \right\rangle = 0 \,.$$

Therefore, only the choice sgn(0) = 0 is consistent with the commutation between time derivative and averaging.

Another choice would be equivalent to the addition of a term $-\frac{1}{2}ie\operatorname{sgn}(0)\hbar\nabla\cdot\mathbf{A}(\mathbf{q})$ to the action, proportional to the commutator $[\hat{\mathbf{p}}, \mathbf{A}(\hat{\mathbf{q}})]$, showing the relation between this ambiguity and the problem of ordering operators. Such a term could be cancelled explicitly by modifying the action, resulting in a more complicate formalism.

Finally, the operator $e^{-\beta \hat{H}}$ is Hermitian when the Hamiltonian is Hermitian. From the point of view of the path integral, the hermiticity condition implies formally the invariance of the path integral under the simultaneous changes $S \to S^*$ (complex conjugation) and $t \to -t$ (transposition, and thus exchange of boundary conditions). By preserving this symmetry throughout the calculation, and, therefore, setting sgn(0) = 0, one ensures consistency with the (Hermitian) choice of quantization (3.18).

We meet this problem again in Sections 4.2, 4.6, and 37.6.1, and in Chapter 34, and it is implicit in field theories with derivative couplings, like gauge theories.

3.3.2 General quadratic Hamiltonians

A general Hamiltonian quadratic in \mathbf{p} can be derived from a general Lagrangian quadratic in the velocities. Because, in all examples we encounter, the quantization problem is initially formulated in terms of a classical Lagrangian, we consider the problem of quantizing a real-time Lagrangian in *n*-dimensional space of the form

$$\mathcal{L}(\dot{q},q) = \frac{1}{2} \sum_{\alpha,\beta} \dot{q}^{\alpha} g_{\alpha\beta}(q) \dot{q}^{\beta}, \quad 1 \le \alpha, \beta \le n, \qquad (3.23)$$

where $g_{\alpha\beta}(q)$ is a positive matrix. Interesting examples correspond to random motion on Riemannian manifolds, as we shall briefly discuss in Section 34.9. The tensor $g_{\alpha\beta}(q)$ then is the metric tensor (for details see Chapter 28). Field theoretical generalizations are studied in Chapters 19 and 29.

The corresponding classical Hamiltonian is obtained by a *Legendre transformation*. The conjugate momenta are

$$p_{\alpha} = \frac{\partial \mathcal{L}(\dot{q}, q)}{\partial \dot{q}^{\alpha}} = \sum_{\beta} g_{\alpha\beta}(q) \dot{q}^{\beta}$$

and, therefore, the Hamiltonian is

$$H(p,q) = \sum_{\alpha} p_{\alpha} \dot{q}^{\alpha} - \mathcal{L}(\dot{q},q) = \frac{1}{2} \sum_{\alpha,\beta} p_{\alpha} g^{\alpha\beta}(q) p_{\beta}, \qquad (3.24)$$

where the traditional notation $g^{\alpha\beta}$ for the matrix inverse of $g_{\alpha\beta}$ has been used:

$$\sum_{\gamma} g_{\alpha\gamma}(q) g^{\gamma\beta}(q) = \delta^{\beta}_{\alpha}$$

The Euclidean action reads

$$\mathcal{S}(p,q) = \int \mathrm{d}t \bigg[-i \sum_{\alpha} p_{\alpha}(t) \dot{q}_{\alpha}(t) + \frac{1}{2} \sum_{\alpha,\beta} p_{\alpha}(t) g^{\alpha\beta} \big(q(t) \big) p_{\beta}(t) \bigg].$$
(3.25)

Again the integration over p(t) is Gaussian and can be performed. Formally, one finds,

$$\operatorname{tr} U = \int \prod_{t} \frac{\mathrm{d}q(t)}{\sqrt{\det g^{\alpha\beta}(q(t))}} e^{-\mathcal{S}(q)}$$

with

$$\mathcal{S}(q) = \frac{1}{2} \int \mathrm{d}t \sum_{\alpha,\beta} \dot{q}^{\alpha}(t) g_{\alpha\beta}(q(t)) \dot{q}^{\beta}(t).$$
(3.26)

In S(q) we recognize the Euclidean action integral of the classical Lagrangian (3.23) after continuation to imaginary time. This is not surprising, since the integration over p_{α} is equivalent to a Legendre transformation.

However, in contrast with the preceding example, the Gaussian integration has generated a non-trivial q(t) dependent normalization factor,

$$\mathcal{N}(q) \propto \frac{1}{\sqrt{\det g^{\alpha\beta}(q(t))}},$$
(3.27)

which, when $g_{\alpha\beta}$ is the metric tensor on a Riemannian manifold, formally reconstructs the *covariant measure* on the manifold (see Section 28.3.1).

However, a difficulty appears with the evaluation of the normalization $\mathcal{N}(q)$. We rewrite the *p* integral with the action (3.25) as

$$\int [\mathrm{d}p(t)] \exp\left[-\frac{1}{2} \int \mathrm{d}t \, \mathrm{d}t' \sum_{\alpha,\beta} p_{\alpha}(t) K_{\alpha\beta}(t,t') p_{\beta}(t')\right],$$

with

$$K_{\alpha\beta}(t,t') \equiv \delta(t-t')g^{\alpha\beta}(q(t)).$$

Using the general identity (A2.4), $\ln \det \mathbf{K} = \operatorname{tr} \ln \mathbf{K}$, one finds formally

$$\mathcal{N}(\mathbf{q}) \propto \mathrm{e}^{\mathrm{tr}\ln\mathbf{K}} = \exp\left[\frac{1}{2} \delta(0)' \int \mathrm{tr}\ln\mathbf{g}\left[q(t)\right] \mathrm{d}t\right].$$
(3.28)

Due to the factor $\delta(0)$, the expression is not defined (δ being the Dirac δ -function). This difficulty is again related to the problem of ordering operators in products. If one performs a small \hbar (semi-classical) expansion of the path integral, one finds a divergent quantum correction (see Chapters 19, 29). This divergence is cancelled by the leading contribution coming from (3.28), as the calculation of Section 3.3.3 shows. However, the remaining finite part is not defined in the formal continuum time limit. It is possible to use a time-discretized form, which reflects a choice of quantization, to calculate it. Another direct way of understanding this difficulty is to notice that, since in expression (3.27) the difference |q - q'| is generically of order $\sqrt{|t - t'|}$, a replacement of $\mathbf{g}(\mathbf{q}_{av})$ by any other symmetric function of q and q', which has the same q = q' limit, changes this quantity at order |t - t'|, in general. The modification of $\mathcal{N}(\mathbf{q})$ then generates a finite quantum correction to the classical action, typical of a commutation of momentum and position operators. Some more details about this problem can be found in Section A37.2.

From the point of view of a statistical model corresponding to the discretized path integral, this means that the *continuum limit* is less universal than in the simpler flat $\mathbf{g} = \mathbf{1}$ case. It depends on a number of additional parameters related to the choice of quantization. However, in many examples, quantization is constrained by symmetry properties. The same symmetries then also determine the corresponding parameters.

3.3.3 Phase-space formalism: The $\delta(0)$ problem

If one expands around flat space, setting

$$q^{\alpha\beta} = \delta^{\alpha\beta} + h^{\alpha\beta},$$

adds to the action (3.25) either a harmonic oscillator term or finite time boundaries, it is possible to expand the path integral in powers of h. The propagators are given by equations (3.12) or (3.14) multiplied by $\delta^{\alpha\beta}$. Using Wick's theorem, one finds that the first-order correction has the form

$$-\frac{1}{2}\int \mathrm{d}t \sum_{\alpha,\beta} \left\langle p_{\alpha}(t)h^{\alpha\beta}(q(t))p_{\beta}(t)\right\rangle = -\frac{1}{2n}\int \mathrm{d}t \left\langle \mathbf{p}^{2}(t)\right\rangle \left\langle \mathrm{tr}\,\mathbf{h}(q(t))\right\rangle$$
$$-\frac{1}{2n^{2}}\sum_{\alpha,\beta} \left\langle \nabla_{\alpha}\nabla_{\beta}h^{\alpha\beta}(q(t))\right\rangle.$$

We note that no $\delta(0)$ contribution is generated, but only the unavoidable less singular sgn(0), resulting from the ambiguity in operator ordering appears in the perturbative expansion. The divergence thus results from the momentum integration. This exercise exhibits a situation in which the order of integrations in path integrals matters.

Finally, the first order is the most singular, because it contains the equal-time contributions. When the ambiguity is fixed, the full perturbative expansion is defined.

3.4 The spectrum of the O(2)-symmetric rigid rotator

To illustrate the discussion of Hamiltonians quadratic in momentum variables, we calculate the spectrum of the O(N) rigid rotator, using the path integral representation (this model is also the one-dimensional O(N) non-linear σ -model, see Chapter 19). We first examine the N = 2 case, which is simpler and can be treated exactly. The O(2) rotator actually provides an example of the peculiarities of the path integral when position space has non-trivial topological properties.

In the case of a general parametrization of the circle, the Hamiltonian is a quadratic function of momenta with a position-dependent coefficient, which leads to quantization problems. However, if the circle is parametrized by an angle θ , the Hamiltonian of the O(2) rotator becomes simply

$$H = -\frac{1}{2} \frac{\partial^2}{\left(\partial\theta\right)^2},\tag{3.29}$$

and would be a free Hamiltonian if θ were not an angular variable. As a consequence, the spectrum, instead of being continuous, is discrete. The eigenvalues are

$$E_l = \frac{1}{2}l^2, (3.30)$$

where l is an integer, the angular momentum.

The path integral representation of the matrix elements of the statistical operator $e^{-\beta H}$ is analogous to the path integral ($\dot{\theta} \equiv d\theta/dt$) of the free motion:

$$\langle \theta'' | e^{-\beta H} | \theta' \rangle = \int_{\theta(0)=\theta'}^{\theta(\beta)=\theta''} [d\theta(t)] \exp\left[-\frac{1}{2} \int_0^\beta (\dot{\theta}(t))^2 dt\right].$$
(3.31)

However, the cyclic character of the variable also modifies the evaluation of the path integral. The matrix elements $\langle \theta'' | e^{-\beta H} | \theta' \rangle$ are invariant under a translation of θ' and θ'' , and periodic in both angles. Therefore, the operator $e^{-\beta H}$ can be diagonalized in the basis of eigenfunctions $\psi_l = e^{il\theta}$:

$$e^{-\beta H_l} = \frac{1}{(2\pi)^2} \int_0^{2\pi} d\theta' d\theta'' e^{il(\theta'-\theta'')} \langle \theta''| e^{-\beta H} |\theta'\rangle, \text{ with } l \text{ integer } l$$

We now introduce the topological charge

$$Q = \frac{1}{2\pi} \int_0^\beta \mathrm{d}t \, \dot{q}(t).$$

The charge is topological, because it depends only on the end points of a trajectory. It characterizes the different classes of mappings of the circle onto itself. Indeed, if a trajectory goes from θ' to θ'' by winding q times around the circle, then

$$Q = q + \frac{\theta^{\prime\prime} - \theta^\prime}{2\pi} \,,$$

where the integer q is called the *winding number*.

We then consider the path integral

$$e^{-\beta H_l} = \int_{\theta(0)=\theta'}^{\theta(\beta)=\theta''} \exp\left\{-\int_0^\beta dt \left[\frac{1}{2} \left(\dot{\theta}(t)\right)^2 + il\dot{\theta}(t)\right]\right\},\tag{3.32}$$

where the trajectories go from θ' to θ'' while winding an arbitrary number of times around the circle. Since l is an integer, in the path integral the additional contribution is independent of the winding number.

Evaluation of the path integral. We first solve the classical equation of motion. We now find the family of trajectories which go from θ' to θ'' ,

$$\theta_c(t) = \theta' + t \left(\theta'' - \theta' + 2\pi q \right) / \beta, \quad \text{with } q \in \mathbb{Z}.$$
(3.33)

Trajectories corresponding to different winding numbers are topologically distinct, that is, they cannot be related by continuous deformation. Hence, they have all to be taken into account, because Brownian paths are continuous and, thus, fluctuations around one trajectory do not include any other one.

We then shift $\theta(t)$, setting $\theta(t) = \theta_c(t) + u(t)$. The path integral (3.31) becomes a sum of contributions of the form,

$$e^{-\beta H_l} = \sum_{q=-\infty}^{+\infty} \mathcal{N}(\beta) \int_0^{2\pi} \frac{d\theta' d\theta''}{(2\pi)^2} \exp\left[-\frac{1}{2\beta} \left(\theta'' - \theta' + 2\pi q\right)^2 + il(\theta' - \theta'')\right].$$
 (3.34)

The normalization $\mathcal{N}(\beta)$ is given by a path integral which is independent of θ' , θ'' and q. Since the integration over u(t) sums fluctuations around the classical trajectory, it is expected that the angular character of u(t) is irrelevant and, therefore,

$$\mathcal{N}(\beta) = \sqrt{2\pi/\beta}$$

We set

$$\theta'' = \theta' - 2\pi q + \varphi \,.$$

Then,

$$\exp\left[-\beta H_l\right] = \frac{1}{\sqrt{2\pi\beta}} \sum_{q=-\infty}^{+\infty} \int_{2\pi q}^{2\pi(q+1)} \mathrm{d}\varphi \,\mathrm{e}^{-il\varphi} \exp\left(-\frac{1}{2\beta}\varphi^2\right).$$

The sum yields the Gaussian integral

$$\exp\left(-\beta H_l\right) = \frac{1}{\sqrt{2\pi\beta}} \int_{-\infty}^{+\infty} \mathrm{d}\varphi \, \exp\left[-\left(il\varphi + \varphi^2/2\beta\right)\right] = \mathrm{e}^{-\beta l^2/2}$$

which is the exact spectrum (3.30).

It has been possible to perform an exact calculation because the O(2) group is Abelian, and the group manifold flat. The discussion of the general O(N) group is more involved, as we now show, because the group manifold has a curvature.

3.5 The spectrum of the O(N)-symmetric rigid rotator

The Hamiltonian of the O(N) rigid rotator can be written as

$$H = \frac{1}{2}\mathbf{L}^2,\tag{3.35}$$

where the vector \mathbf{L} , the angular momentum, represents the set of generators of the Lie algebra of the O(N) group. If the sphere is parametrized in terms of coordinates q^i , the Hamiltonian takes the form

$$H = \frac{1}{2} \sum_{i,j} g^{ij}(\mathbf{q}) p_i p_j , \qquad (3.36)$$

where $g^{ij}(\mathbf{q})$ is the inverse of the metric tensor on the sphere (see also Section 34.9).

For example, if the sphere is parametrized locally by a vector \mathbf{r} in \mathbb{R}^N of unit length and components $(\mathbf{q}, (1-\mathbf{q}^2)^{1/2})$, the inverse metric tensor reads

$$g^{ij}(\mathbf{q}) = \delta^{ij} - q^i q^j. \tag{3.37}$$

According to the discussion of Section 3.3.2, the corresponding path integral representation of $e^{-\beta H}$ is then

$$\langle \mathbf{q}^{\prime\prime} | e^{-\beta H} | \mathbf{q}^{\prime} \rangle = \int \left[\sqrt{g\left(\mathbf{q}(t)\right)} \mathrm{d}\mathbf{q}(t) \right] \exp\left[-\frac{1}{2} \int_{0}^{\beta} \mathrm{d}t \sum_{i,j} g_{ij}\left(\mathbf{q}(t)\right) \dot{q}^{i}(t) \dot{q}^{j}(t) \right], \quad (3.38)$$

in which $g(\mathbf{q})$ is the determinant of the matrix g_{ij} . The contribution to the measure coming from the Gaussian integration over the momenta p_i has formally generated the invariant measure on the sphere. The path integral (3.38) can also be expressed in terms of a vector \mathbf{r} of unit length as

$$\langle \mathbf{r}'' | e^{-\beta H} | \mathbf{r}' \rangle = \int_{\mathbf{r}(0)=\mathbf{r}'}^{\mathbf{r}(\beta)=\mathbf{r}''} \left[\mathrm{d}\mathbf{r}(t)\delta\left(1-\mathbf{r}^2(t)\right) \right] \exp\left[-\frac{1}{2}\int_0^\beta \mathrm{d}t\,\dot{\mathbf{r}}^2(t)\right].$$
(3.39)

Because, for N > 2, the sphere has curvature, it cannot be mapped onto a flat space and, thus, the Hamiltonian can no longer be mapped onto a free Hamiltonian. On the other hand, all loops on the sphere are contractible and there are no longer different topological classes.

High temperature expansion. We call θ the angle between \mathbf{r}' and \mathbf{r}'' :

$$\cos\theta = \mathbf{r}' \cdot \mathbf{r}'', \quad 0 \le \theta \le \pi$$

We introduce a matrix $\mathbf{R}(t)$, which acts on $\mathbf{r}(t)$ and rotates \mathbf{r}' onto \mathbf{r}'' in the plane $(\mathbf{r}', \mathbf{r}'')$ in a time β . Its restriction to the two-dimensional $(\mathbf{r}', \mathbf{r}'')$ plane has the form

$$\begin{bmatrix} \cos(\theta t/\beta) & \sin(\theta t/\beta) \\ -\sin(\theta t/\beta) & \cos(\theta t/\beta) \end{bmatrix}.$$

It is the identity in the subspace orthogonal to the $(\mathbf{r}', \mathbf{r}'')$ plane.

We then change variables, $\mathbf{r}(t) \mapsto \boldsymbol{\rho}(t)$, setting

$$\mathbf{r}(t) = \mathbf{R}(t)\boldsymbol{\rho}(t).$$

We call u and v the two components of ρ in the $(\mathbf{r}', \mathbf{r}'')$ plane, u being the component along \mathbf{r}' and $\rho_{\rm T}$ the component in the orthogonal subspace. With this notation, we find

$$\langle \mathbf{r}'' | e^{-\beta H} | \mathbf{r}' \rangle = \int_{\boldsymbol{\rho}(0)=\mathbf{r}'}^{\boldsymbol{\rho}(\beta)=\mathbf{r}'} \left[d\boldsymbol{\rho}(t)\delta\left(1-\boldsymbol{\rho}^2(t)\right) \right] \exp\left[-\mathcal{S}(\boldsymbol{\rho})\right], \qquad (3.40)$$

with

$$S(\boldsymbol{\rho}) = \frac{1}{2} \int_{0}^{\beta} dt \left[\dot{\boldsymbol{\rho}}_{T}^{2}(t) + \dot{u}^{2}(t) + \dot{v}^{2}(t) + \frac{\theta^{2}}{\beta^{2}} \left(u^{2}(t) + v^{2}(t) \right) + 2 \frac{\theta}{\beta} \left(\dot{v}(t)u(t) - \dot{u}(t)v(t) \right) \right], \qquad (3.41)$$

and the constraint

$$u^2 + v^2 + \rho_{\rm T}^2 = 1. \tag{3.42}$$

3.5

We take into account only fluctuations around the classical solution u = 1, $\rho_{\rm T} = 0$, v = 0, neglecting exponentially small contributions in β^{-1} .

We eliminate the variable u from the action (3.41) by solving the constraint (3.42):

$$u = \left(1 - v^2 - \boldsymbol{\rho}_{\mathrm{T}}^2\right)^{1/2}$$

and expand the action in powers of $\rho_{\rm T}$ and v. The leading order is

$$\mathcal{S}(\boldsymbol{\rho}) = \theta^2 / 2\beta \,,$$

a result that shows that the calculation is valid for $\theta = O(\sqrt{\beta})$. The next order is given by the Gaussian integration and requires the quadratic terms in $\rho_{\rm T}$ and v,

$$\frac{1}{2}\int_0^\beta \mathrm{d}t \left[\dot{\boldsymbol{\rho}}_{\mathrm{T}}^2(t) - (\theta^2/\beta^2) \boldsymbol{\rho}_{\mathrm{T}}^2(t) + \dot{v}^2(t) \right]$$

The integral over v(t) is independent of θ and can be absorbed into the normalization. The integrals over the components of $\rho_{\rm T}$ factorize and give identical results: the integral over $\rho_{\rm T}$ is the integral over one component to the power (N-2). Since each component satisfies the conditions

$$\rho_i(0) = \rho_i(\beta) = 0$$

we expand the functions $\rho_i(t)$ on the appropriate orthonormal basis:

$$\rho_i(t) = \sqrt{\frac{2}{\beta}} \sum_{n>0} \rho_{in} \sin(n\pi t/\beta).$$

The Gaussian integral over the variables ρ_{in} then yields

$$\langle \mathbf{r}'' | e^{-\beta H} | \mathbf{r}' \rangle \sim K(\beta) e^{-\theta^2/2\beta} \left[\prod_{n>0} \left(1 - \frac{\theta^2}{n^2 \pi^2} \right) \right]^{-(N-2)/2}$$

The normalization constant $K(\beta) = (2\pi\beta)^{-(N-1)/2}$ is independent of θ . The infinite product can be calculated:

$$\prod_{n>0} \left(1 - \frac{\theta^2}{n^2 \pi^2} \right) = \frac{\sin \theta}{\theta} \,,$$

and, therefore,

$$\langle \mathbf{r}'' | e^{-\beta H} | \mathbf{r}' \rangle \sim K(\beta) \left(\frac{\theta}{\sin \theta} \right)^{(N-2)/2} e^{-\theta^2/2\beta}.$$
 (3.43)

To extract the eigenvalues of H, we project the expression onto the orthogonal polynomials $P_l^N(\cos\theta)$ associated with the O(N) group, which satisfy

$$\int_0^{\pi} \mathrm{d}\theta \,(\sin\theta)^{N-2} P_l^N(\cos\theta) P_{l'}^N(\cos\theta) = \delta_{ll'}\,,\tag{3.44}$$

and which are proportional to the Gegenbauer polynomials $C_l^{(N-2)/2}$.

For β small, we need only the small θ expansion of these polynomials:

$$P_l^N(\cos \theta) = P_l^N(1) \left(1 - \frac{l(l+N-2)}{2(N-1)} \theta^2 + O\left(\theta^4\right) \right).$$

If we assume that, to each value of l, corresponds only one eigenvalue E_l of H, then the following expansion holds,

$$e^{-\beta E_l} \propto K(\beta) \int_0^{\pi} d\theta P_l^N(\cos \theta) \left(\theta \sin \theta\right)^{(N-2)/2} e^{-\theta^2/(2\beta)}$$
$$= e^{-\beta E_0} \left(1 - \frac{1}{2}l(l+N-2)\beta + O\left(\beta^2\right)\right), \qquad (3.45)$$

and, therefore,

$$E_l = E_0 + \frac{1}{2}l(l+N-2) + O(\beta).$$
(3.46)

Since E_l is independent of β , we can infer from this calculation the exact result, up to an additive constant E_0 .

Ambiguities and symmetry. Concerning this calculation, a comment is in order: we have explained in Section 3.3 that the path integrals (3.38, 3.39) are not defined, because the measure gives formally divergent contributions. We have stated that these divergences are cancelled by divergences in perturbation theory. As a consequence, the resulting expressions are ambiguous, and these ambiguities reflect the problem of operator ordering in the quantization of a classical Hamiltonian. Still, we have obtained here some non-trivial results. The reason is that at every stage of the calculation explicit O(N) invariance has been maintained. This chooses implicitly among all possible definitions of the path integral a subclass that corresponds to an O(N)-symmetric quantized Hamiltonian.

We see later, when discussing the non-linear σ -model (Chapter 19), that such a Hamiltonian is fully determined up to an additive constant. The ambiguities of the quantization here are entirely contained in E_0 .

A3 Quantization. Topological actions: Quantum spins, magnetic monopoles

Convention. In the Appendix, in order to recover the usual expressions of classical mechanics, we work in *real time*.

A3.1 Symplectic form and quantization: General remarks

In the Hamiltonian formulation of classical mechanics, the action has the form (3.6),

$$\mathcal{A}(p,q) = \int_{t'}^{t''} dt \left[p(t)\dot{q}(t) - H(p(t),q(t),t) \right].$$
(A3.1)

The term $\int p\dot{q} dt$ also represents the area in phase space between the classical trajectory C and the axis p = 0. In the notation of exterior calculus, it can be written as

$$\int_{\partial D} p(t)\dot{q}(t) \,\mathrm{d}t = \int_{D} \mathrm{d}p \wedge \mathrm{d}q \,, \tag{A3.2}$$

in which ∂D , the boundary of the domain D, contains the classical trajectory C and a fixed reference curve. If we now parametrize phase space differently, introducing new coordinates u_{α} , the right-hand side of the equation becomes

$$\int_D \mathrm{d}p \wedge \mathrm{d}q = \int_D \sum_{\alpha,\beta} \omega_{\alpha\beta}(u) \,\mathrm{d}u_\alpha \wedge \mathrm{d}u_\beta \,.$$

In the terminology of forms $\omega = \sum_{\alpha,\beta} \omega_{\alpha\beta} \, du_{\alpha} \wedge du_{\beta}$ is a 2-form (see Section 1.5), which, by construction, is obtained by differentiating a 1-form; here,

$$\omega = \mathrm{d}\omega',\tag{A3.3}$$

$$\omega' = p(u) \sum_{\alpha} \frac{\mathrm{d}q}{u_{\alpha}} \mathrm{d}u_{\alpha} = \sum_{\alpha} \omega_{\alpha} \mathrm{d}u_{\alpha} \,, \tag{A3.4}$$

and is called the *symplectic form*.

Since the square of the operator d acting on differential forms vanishes, the form ω is *closed*, that is, it satisfies

$$d\omega = 0. (A3.5)$$

Example. In Section 4.1, we discuss the holomorphic formalism. We introduce a complex parametrization of phase space (equation (4.39)) of the form

$$p - iq = -i\sqrt{2}z$$
, $p + iq = i\sqrt{2}\overline{z}$.

In terms of z, \bar{z} , the symplectic form becomes

$$\mathrm{d}p\wedge\mathrm{d}q=\frac{1}{i}\mathrm{d}z\wedge\mathrm{d}\bar{z}\,.$$

Preceding considerations immediately generalize to several degrees of freedom. Let u_{α} be 2n variables parametrizing a phase space for n degrees of freedom. The action \mathcal{A} in the Hamiltonian formulation can be written as

$$\mathcal{A}(u) = \int_{D} \omega - \int_{\partial D} \mathrm{d}t \, H\big(u(t), t\big), \tag{A3.6}$$

where ω , a symplectic form, is a *closed 2-form*,

$$\omega(u) = \sum_{\alpha,\beta} \omega_{\alpha\beta} \mathrm{d} u_{\alpha} \wedge \mathrm{d} u_{\beta} \,, \quad \text{with } \mathrm{d} \omega = 0 \,.$$

The condition $d\omega = 0$ is sufficient to ensure that the classical equations of motion depend only on the boundary ∂D of the domain D, but not on the interior, as was obvious for the initial action (A3.1). The equations of motion then take the form

$$\sum_{\beta} \omega_{\alpha\beta}(u) \dot{u}_{\beta}(t) = \frac{\partial H}{\partial u_{\alpha}(t)}.$$
(A3.7)

Locally, equation (A3.5) can be integrated in the same way as $dp \wedge dq$ can be integrated into p dq. However, if phase space has non-trivial topological properties, it cannot always be integrated globally, that is, the symplectic form is not *exact*. This property has peculiar consequences in QM, since the path integral involves the action explicitly in the form $e^{i\mathcal{A}/\hbar}$. For the path integral to make sense, this phase factor must be independent of the choice of the action \mathcal{A} .

This problem shows up in the example of the quantization of spin degrees of freedom discussed in Section A3.3.1.

Canonical invariance of the symplectic form. We consider the symplectic form

$$\Omega = \sum_i \mathrm{d} p_i \wedge \mathrm{d} q_i \,.$$

We introduce a smooth function $\Sigma(Q, q)$ and the transformation $(\mathbf{p}, \mathbf{q}) \mapsto (\mathbf{P}, \mathbf{Q})$ defined by,

$$p_i = \partial \Sigma / \partial q_i, \quad P_i = -\partial \Sigma / \partial Q_i.$$
 (A3.8)

First, we implement the transformation $\mathbf{p} \mapsto \mathbf{Q}$. The symplectic form becomes

$$\Omega = \sum_{i,j} \frac{\partial^2 \Sigma}{\partial q_i \partial Q_j} \mathrm{d}Q_j \wedge \mathrm{d}q_i \,.$$

Then, we implement the transformation $\mathbf{q} \mapsto \mathbf{P}$:

$$\mathrm{d}P_j = \sum_i \frac{\partial^2 \Sigma}{\partial Q_j \partial q_i} \mathrm{d}q_i \,,$$

and, therefore,

$$\Omega = \sum_j \mathrm{d} P_j \wedge \mathrm{d} Q_j \,.$$

A3.2 Classical equations of motion and quantization

We consider a general Hamiltonian $H(\mathbf{p}, \mathbf{q}, t)$ corresponding to the classical action,

$$\mathcal{A}(\mathbf{p},\mathbf{q}) = \int_{T'}^{T} \mathrm{d}t \left[\mathbf{p}(t) \cdot \dot{\mathbf{q}}(t) - H(\mathbf{p}(t),\mathbf{q}(t);t) \right], \qquad (A3.9)$$

with $q_i(T') = x'_i$ and $q_i(T) = x_i$.

We specialize to Hamiltonian systems (called integrable) for which the classical equations of motion can be solved with arbitrary boundary conditions. In particular, this implies that one can calculate explicitly the action for a classical trajectory as a function of initial time T' and position \mathbf{x}' , and final time T and position \mathbf{x} .

The action A_c corresponding to a trajectory $\{\mathbf{p}_c(t), \mathbf{q}_c(t)\}\$ in phase space, the solution of the classical of motions is a function of the initial and final positions, and time:

$$A_c(\mathbf{x}', \mathbf{x}; T) = \mathcal{A}(\mathbf{p}_c, \mathbf{q}_c). \tag{A3.10}$$

The analytic continuation of all expressions to imaginary time is simple.

It is well-known, and verified again in the next section (see equation (A3.19)), that the classical action A_c satisfies the Hamilton–Jacobi equations.

A3.2.1 Preliminary remarks

We first recall a few classical results. WE denote by $S(\mathbf{Q}, \mathbf{q}; t)$ a function satisfying the Hamilton–Jacobi equations:

$$\frac{\partial S}{\partial t} = -H\left(\frac{\partial S}{\partial \mathbf{q}}, \mathbf{q}; t\right),\tag{A3.11}$$

with $S(\mathbf{Q}, \mathbf{Q}; T') = 0$, and with additional implicit boundary conditions at t = T', which will be explained. We use S to generate a time-dependent canonical transformation in phase space, transforming the set (\mathbf{p}, \mathbf{q}) into (\mathbf{P}, \mathbf{Q}) :

$$p_i = \partial S / \partial q_i, \quad P_i = -\partial S / \partial Q_i.$$
 (A3.12)

The implicit boundary conditions follow from the conditions

$$t = T' \Rightarrow P_i = p_i \quad \text{and} \quad Q_i = q_i \,.$$
 (A3.13)

We use the relation (A3.11) and apply the first transformation (A3.12) to the action (A3.9). We obtain

$$\mathcal{A}(\mathbf{p},\mathbf{q}) = \int_{T'}^{T} \left(\sum_{i} \frac{\partial S}{\partial q_{i}} \dot{q}_{i}(t) + \frac{\partial S}{\partial t} \right) \mathrm{d}t \,. \tag{A3.14}$$

The quantities \mathbf{q} and \mathbf{Q} are time dependent. Expression (A3.14) can be rewritten as

$$\mathcal{A}(\mathbf{p},\mathbf{q}) = \int_{T'}^{T} \frac{\mathrm{d}}{\mathrm{d}t} S(\mathbf{q}(t),\mathbf{Q}(t);t) \mathrm{d}t - \int_{T'}^{T} \sum_{i} \frac{\partial S}{\partial Q_{i}} \dot{Q}_{i}(t) \mathrm{d}t.$$
(A3.15)

Finally, using the second equation (A3.12), one obtains

$$\mathcal{A}(\mathbf{p},\mathbf{q}) = S(\mathbf{x},\mathbf{Q}(T);T) + \int_{T'}^{T} P_i(t)\dot{Q}_i(t)dt. \qquad (A3.16)$$

The equations of motion are now trivial,

$$\dot{Q}_i = 0 \Longrightarrow Q_i(t) = Q_i(T'). \tag{A3.17}$$

The conditions (A3.13) determine the solution

$$Q_i(t) = x'_i \,. \tag{A3.18}$$

Therefore, we have shown that

$$A_c(\mathbf{x}', \mathbf{x}; T) \equiv S(\mathbf{x}, \mathbf{x}'; T), \qquad (A3.19)$$

and found a canonical transformation which maps the initial Hamiltonian system onto a trivial one with a vanishing Hamiltonian. By performing an additional inverse transformation based on a standard Hamiltonian, like a free Hamiltonian of the form

$$H = \frac{1}{2} \sum p_i^2, \qquad (A3.20)$$

or a harmonic oscillator,

$$H = \frac{1}{2} \sum_{i} \left(p_i^2 + q_i^2 \right), \qquad (A3.21)$$

we can map the original Hamiltonian system onto any convenient Hamiltonian.

A3.2.2 Liouville measure

The transformation (A3.12) leaves the Liouville measure in phase-space invariant. To prove it, we perform the transformation in two steps (a proof quite similar to the proof of canonical invariance given in Section A3.1). First, we go from p_i to Q_i :

$$\prod_{i} (\mathrm{d}p_{i}\mathrm{d}q_{i}) = \prod_{i} (\mathrm{d}q_{i}\mathrm{d}Q_{i}) \det\left(\frac{\partial^{2}S}{\partial q_{k}\partial Q_{l}}\right).$$
(A3.22)

We then eliminate q_i in favour of P_i :

$$\frac{\partial q_i}{\partial P_j} = \left(\frac{\partial P}{\partial q}\right)_{ij}^{(-1)} = -\left(\frac{\partial^2 S}{\partial q \partial Q}\right)_{ij}^{(-1)}.$$
(A3.23)

Therefore, the second Jacobian cancels the first one (the argument also shows the invariance of the symplectic form $\sum_i dp_i \wedge dq_i$ (see also Section A3.1).

The analysis suggests that we can perform two transformations (A3.12) on the path integral representation of the evolution operator, to reduce it to a path integral corresponding to a standard system for which the evolution operator is exactly known:

$$\langle \mathbf{x}' | U(T',T) | \mathbf{x} \rangle = \int \prod_{i} \left[\mathrm{d}q_i(t) \mathrm{d}p_i(t) \right] \exp\left[i\mathcal{A}(\mathbf{p},\mathbf{q}) \right],$$
 (A3.24)
with $q_i(T') = x'_i, \quad q_i(T) = x_i.$

In this way, it would seem that we are able to calculate exactly the evolution operator of any system for which we know how to solve the classical equations of motion with arbitrary boundary conditions. In particular, this would apply to systems with one degree of freedom, with a Hamiltonian H of the form

$$H = p^2/2m + V(q). (A3.25)$$

A3.2

Unfortunately, it is easy to verify that the result is wrong at least in one-dimensional QM. Actually, the whole procedure is somewhat ill-defined. Indeed, changes of variables on the path integral on phase space are even more ambiguous than transformations on ordinary path integrals in configuration space. We have given some indications of this problem in Section 3.1. Let us just mention that if we discretize time, we discover that the transformation is not really canonical, because to a variable $q(t_k)$ corresponds a momentum variable $p(t_k + \Delta t)$ of a slightly displaced time. This effect, invisible in the naive continuum limit, completely changes the result. It is thus necessary to work with the discretized form of the phase-space path integral, but this is cumbersome. On the other hand, the situation seems to be more favourable in quantum field theory. The problem we have described above comes mainly from commutation of quantum operators. We emphasize in Chapter 7 that the commutators are infinite in field theory and disappear in the renormalization. Therefore, one may expect, as this has been verified on a few examples with enough symmetries, that the semi-classical approximations of classically integrable field theories reproduce features of the exact solution.

A3.3 Topological actions

We now indicate how non-trivial topological properties of phase space, irrelevant from the point of view of classical mechanics, affect quantization.

In Section 3.4, we have evaluated the path integral in an example where space has non-trivial topological properties. We now discuss two other examples where topology plays an essential role, in the sense that the action which generates the classical equations of motion cannot be globally defined. We first quantize angular momentum operators in the path integral formalism, in a fixed representation. One of the peculiarities of this system is that phase space itself has non-trivial topological properties. The second example is provided by the magnetic monopole which gives a non-trivial topological structure to ordinary space. In both examples, one calls the action topological. Because a topological action cannot be globally defined, its amplitude is quantized, a property specific to QM. Indeed, in classical mechanics, a multiplication of the action by a constant does not affect the equations of motion.

A3.3.1 Spin dynamics and quantization

Classical spin dynamics. We consider a vector **S** in three dimensions of fixed length s: $\mathbf{S}^2 = s^2$. We give **S** the simple dynamics,

$$\frac{\mathrm{d}\mathbf{S}}{\mathrm{d}t} = \mathbf{H} \times \mathbf{S} \,, \tag{A3.26}$$

in which **H** is a constant vector. This equation is first order in time and involves two independent variables corresponding to a point on the sphere. These variables can be considered as a position and its conjugate momentum. Therefore, phase space is isomorphic to the sphere S_2 . The Hamiltonian is simply

$$\mathcal{H}(\mathbf{S}) = \mathbf{H} \cdot \mathbf{S} \,. \tag{A3.27}$$

More precisely, it is simple to verify that if one parametrizes \mathbf{S} as

 $\mathbf{S} = s(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta),$

then equation (A3.26) is generated by the action

$$\mathcal{A}(\theta,\varphi) = \int \left[s\dot{\varphi}(t)\cos\theta(t) - \mathcal{H}(\varphi(t),\theta(t)) \right] dt \,. \tag{A3.28}$$

QM: Path integrals in phase space

We note in the expression that $\cos \theta$ and φ play the role of conjugate variables. However, two remarks are in order: first we have integrated the symplectic 2-form but, for this purpose, we have been forced to introduce a parametrization of the sphere that is singular at $\theta = 0$ and π . When the trajectory contains the north or the south pole of the sphere, the integral is not defined. The 2-form cannot be integrated globally into a 1-form because the integral $\int d\varphi d\cos \theta$, which is the area on the sphere, is defined only mod (4π) .

In classical mechanics, these properties play no direct role, since only equations of motion are physical.

Note that the symplectic form has other useful representations (ϵ_{ijk} is the completely antisymmetric tensor, with $\epsilon_{123} = 1$),

$$\mathrm{d}\cos\theta\wedge\mathrm{d}\varphi = \frac{1}{2}s^{-3}\sum_{i,j,k}\epsilon_{ijk}S_i\mathrm{d}S_j\wedge\mathrm{d}S_k = 2i\sum_i\mathrm{d}z_i\wedge\mathrm{d}\bar{z}_i\,,$$

where z_i is a two-component complex vector of length 1, corresponding to the isomorphism between S_2 and the symmetric space CP_1 (see Section 39.5):

$$\mathbf{S} = s \sum_{i,j} ar{z}_i \boldsymbol{\sigma}_{ij} z_j \,, \,\, ext{with} \,\, \sum_i ar{z}_i z_i = 1 \,,$$

where σ is the set of Pauli matrices. In a special *gauge*, the vector **z** can also be written as

$$z_1 = e^{i\varphi/2} \cos(\theta/2),$$

$$z_2 = e^{-i\varphi/2} \sin(\theta/2).$$

A3.3.2 Quantization of spin degrees of freedom

We consider the path integral representation of the corresponding evolution operator in QM. The action itself now appears explicitly and the problem discussed in the preceding section becomes relevant. The path integral exists only if the integrand $e^{i\mathcal{A}/\hbar}$ is defined. Since the total area is defined only mod (4π) , the integrand must be invariant under such a change. This implies that $4\pi s$ must be a multiple of $2\pi\hbar$: the parameter s/\hbar is quantized and can take only half-integer values. This is a generic property in QM: the amplitude of *topological* contributions to the action, that is, contributions that are not globally defined, is *quantized*. The magnetic monopole of Section A3.3.3, or the Chern–Simons term in three-dimensional non-Abelian gauge theories, provide other examples of such a situation.

In the parametrization (A3.28), the action can be written as (we now set $\hbar = 1$)

$$\mathcal{A}(\theta,\varphi) = \int \left[\dot{\varphi}(t) \left(\gamma + \cos\theta(t)\right) - \mathcal{H}\left(\varphi(t),\theta(t)\right)\right] \mathrm{d}t\,,\qquad(A3.29)$$

an expression that differs from expression (A3.28) only by a total derivative: by choosing $\gamma = 1/2, 0$ for s half-integer, integer, respectively, one renders e^{iA} regular near $\theta = 0, \pi$.

To relate this action to the usual operator formulation of the angular momentum relations, we first note that, classically,

$$S_{\pm} = \mathrm{e}^{\pm i\varphi} \left(s^2 - S_z^2 \right)^{1/2}$$

After quantization, S_z becomes p_{φ} , the conjugate momentum of the angular variables φ :

$$S_z \equiv p_\varphi = \frac{1}{i} \frac{\mathrm{d}}{\mathrm{d}\varphi}.$$

It can be verified that the quantum operators S_{\pm} can be written as

$$S_{\pm} = e^{\pm i\varphi/2} \left(s^2 - p_{\varphi}^2\right)^{1/2} e^{\pm i\varphi/2}$$

Then, using

$$j(j+1) = \mathbf{S}^2 = S_z^2 + S_+ S_- S_z = s^2 - 1/4$$

we find the relation between the angular momentum j and the parameter s,

$$s = j + 1/2$$
. (A3.30)

In particular, since s is quantized, we recover a property of QM: quantization of spin.

If we denote by m the eigenvalues of S_z , we observe that, in the φ -configuration space, the corresponding eigenvectors have the form $e^{im\varphi}$, and the projector K on the basis is

$$K(\varphi'',\varphi') = \sum_{m=-j}^{m=j} e^{im(\varphi'-\varphi'')} = \frac{\sin\left[(j+1/2)\left(\varphi'-\varphi''\right)\right]}{\sin\left[(\varphi'-\varphi'')/2\right]}.$$
 (A3.31)

We can compare this expression with the short-time path integral representation, which leads to

$$K(\varphi'',\varphi') \propto \sum_{n} \int_{-s}^{s} \mathrm{d}p_{\varphi} \,\mathrm{e}^{ip_{\varphi}\left(\varphi'-\varphi''+2n\pi\right)},$$
$$\propto \sin\left[s\left(\varphi'-\varphi''\right)\right] \sum_{n} \frac{2(-1)^{n}}{\left(\varphi'-\varphi''+2n\pi\right)}.$$

The sum over *n* must be regularized, but the factor $\sin s(\varphi' - \varphi'')$ is consistent with equation (A3.31) and the identification (A3.30).

A final word of caution: although the path integral quantization of spin variables is quite useful to study the classical limit (which is also the limit $s \to \infty$), the problem of operator ordering in products leads to the usual ambiguities in explicit calculations.

A3.3.3 The magnetic monopole

Electromagnetism provides another example of the situation encountered in Section A3.3.1. In a magnetic system, the only physical quantity which appears in the classical equations of motion is the magnetic field. The contribution of the magnetic term to the action can be generally written as the integral of a 2-form (involving the magnetic field), since this form is closed:

$$\mathcal{A}_{\text{mag.}} = e \int \sum_{i,j} F_{ij}(x) \, \mathrm{d}x_i \wedge \mathrm{d}x_j \,, \text{ with } F_{ij}(x) = \sum_k \epsilon_{ijk} B_k(x).$$

Because the 2-form F is closed, one can integrate it locally by introducing a vector potential, which is a 1-form (see equation (3.22)):

$$F_{ij}(x) = \partial_i A_j(x) - \partial_j A_i(x), \quad \Rightarrow \ \mathcal{A}_{\text{mag.}} = e \int \mathbf{A}(\mathbf{x}) \cdot d\mathbf{x}.$$

However, if the 2-form F is not exact, the vector potential cannot be globally defined. This is precisely what happens when a magnetic field is generated by a magnetic monopole.

The formal duality symmetry between magnetic and electric fields in Maxwell's equations has led Dirac to speculate about the existence of yet undiscovered isolated magnetic charges, magnetic equivalents of electric charges. An isolated magnetic charge g creates a magnetic field **B** of the form

$$\mathbf{B} = g \frac{\mathbf{x}}{|\mathbf{x}|^3} \,.$$

The field \mathbf{B} is also a singular solution to the free static Maxwell's equations. It has an infinite energy and hence, in this form, it is irrelevant to physics. However, in non-Abelian gauge theories with spontaneous symmetry breaking, finite energy solutions (solitons) can be found, which coincide at large distance with Dirac's magnetic monopoles.

The integral of the magnetic field over a closed surface containing the magnetic charge is $4\pi g$, as one immediately verifies by using polar coordinates $\{r, \theta, \varphi\}$ with the monopole at the origin:

$$\int \sum_{i,j} F_{ij}(x) \mathrm{d}x_i \wedge \mathrm{d}x_j = g \int \frac{r}{r^3} \times r^2 \mathrm{d}\cos\theta \,\mathrm{d}\varphi = 4\pi g \,.$$

If the vector potential could be globally defined, the integral would obviously vanish. More directly, if one tries to calculate the corresponding vector potential, one finds, in a family of gauges,

$$A_i(x) = g \sum_{j,k} \epsilon_{ijk} n_k x_j \frac{\mathbf{n} \cdot \mathbf{x}}{r \left(r^2 - (\mathbf{n} \cdot \mathbf{x})^2\right)},$$

where \mathbf{n} is a constant unit vector. We observe that the potential is singular along the line of direction \mathbf{n} passing through the origin. This line of singularities is not physical and can be displaced, but not removed.

Again, this property has no classical consequences. However, in QM, since the classical action can be defined only (mod $4\pi eg$), the weight factor $e^{i\mathcal{A}}$ is only defined if

$$4\pi eg = 0 \pmod{2\pi} \Rightarrow 2eg = \text{integer},$$

in which we recognize Dirac's quantization condition.

Note that when this condition is fulfilled, parallel transport (see Section 21.7) is globally defined in \mathbb{R}^3 .

4 Quantum statistical physics: Functional integration formalism

In this chapter, we introduce the representation by functional integrals of the density matrix at thermal equilibrium in non-relativistic quantum mecanics (QM), with many degrees of freedom, in the grand canonical formulation.

A class of quantum Hamiltonians can be expressed in terms of creation and annihilation operators, instead of the more usual position and momentum operators, a method adapted to the study of perturbed harmonic oscillators. In the holomorphic formalism, these operators act by multiplication and differentiation on a Hilbert space of analytic functions. Alternatively, they can also be represented by kernels, functions of complex variables z, \bar{z} that, in the classical limit correspond to a complex parametrization of phase space. The formalism is adapted to the description of many-body boson systems.

A path integral representation of the density matrix at thermal equilibrium, where paths belong to complex spaces, instead of the more usual position–momentum phase space, corresponds to this formalism.

A parallel formalism can then be set-up to describe systems with many fermion degrees of freedom, with Grassmann variables replacing complex variables.

Both formalisms can be generalized to quantum gases of Bose and Fermi particles in the grand canonical formulation. *Field integral* representations of the corresponding quantum partition functions are then derived.

4.1 One-dimensional QM: Holomorphic representation

We briefly recall the main ideas and properties of the holomorphic representation. To motivate the construction, we consider the quantum harmonic oscillator

$$H_0 = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\omega^2\hat{q}^2, \quad \omega > 0, \qquad (4.1)$$

where \hat{q}, \hat{p} are the position and momentum operators, respectively, with the commutation relation $[\hat{q}, \hat{p}] = i\hbar$. We introduce the annihilation and creation operators a, a^{\dagger} defined by

$$\hat{p} - i\omega\hat{q} = -i\sqrt{2\hbar\omega} a$$
, $\hat{p} + i\omega\hat{q} = i\sqrt{2\hbar\omega} a^{\dagger} \Rightarrow [a, a^{\dagger}] = 1$. (4.2)

In terms of a, a^{\dagger} , the Hamiltonian takes the standard form $\hbar\omega(a^{\dagger}a+1/2)$. In what follows, we omit the constant energy shift $\hbar\omega/2$ and consider

$$H_0 = \hbar \omega a^{\dagger} a \,. \tag{4.3}$$

We then introduce a complex variable z and represent a^{\dagger} and a by the operators z and $\partial/\partial z$, acting by multiplication and differentiation on a complex vector space of analytic functions of the form

$$f(z) = \sum_{n=0}^{\infty} \frac{1}{n!} f_n z^n,$$
(4.4)

which have the same commutation relations

$$a^{\dagger} \mapsto z, \quad a \mapsto \partial/\partial z, \quad [\partial/\partial z, z] = 1.$$
 (4.5)

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The Hamiltonian H_0 is then represented by

$$H_0 = \hbar \omega z \frac{\partial}{\partial z} \,. \tag{4.6}$$

In this representation, the eigenfunctions of H_0 are the monomials z^n , since

$$\hbar\omega z \frac{\partial}{\partial z} z^n = n\hbar\omega z^n.$$

The action of the operator $U_0(t) = e^{-H_0 t/\hbar}$ (again we first keep the \hbar normalization of real-time evolution) on analytic functions is

$$U_0(t)f(z) = e^{-H_0t/\hbar} f(z) = f(e^{-\omega t} z).$$
(4.7)

4.1.1 Hilbert space of analytic functions

The vector space of analytic functions can be endowed with a structure of Hilbert space [15]: the scalar product of two functions g and f is defined by

$$(g,f) = \int \frac{\mathrm{d}\bar{z}\,\mathrm{d}z}{2i\pi} \,\mathrm{e}^{-z\bar{z}} \,\overline{g(z)} \,f(z), \tag{4.8}$$

where this type of complex integrals has been defined and discussed in Section 1.4.

With this scalar product, the operators z and $\partial/\partial z$ are Hermitian conjugate and the eigenfunctions of the harmonic oscillator form an orthogonal basis:

$$\int \frac{\mathrm{d}\bar{z}\,\mathrm{d}z}{2i\pi}\,\mathrm{e}^{-z\bar{z}}\,\bar{z}^n z^m = n!\,\delta_{mn}\,,\tag{4.9}$$

a result that follows, for instance, from Wick's theorem (1.30). In particular, the norm of a function of the form (4.4) is finite if

$$(f,f) = \sum_{n} \frac{1}{n!} |f_n|^2 < \infty$$

Therefore, square integrable functions belong to a subset of entire analytic functions.

Using the orthogonality relations (4.9), one defines an analogue of Dirac's δ -function:

$$f(0) = \int \frac{d\bar{z} dz}{2i\pi} e^{-z\bar{z}} f(z).$$
 (4.10)

4.1.2 Operator kernels

Since the functions $z^n/\sqrt{n!}$ form an orthonormal basis, the identity operator can be represented by the kernel

$$e^{z\bar{z}} = \sum_{n=0} \frac{\bar{z}^n}{\sqrt{n!}} \frac{z^n}{\sqrt{n!}}$$

This property is expressed by the identity

$$\int \frac{\mathrm{d}\bar{z}'\mathrm{d}z'}{2i\pi} \,\mathrm{e}^{\bar{z}'z} \,\mathrm{e}^{-z'\bar{z}'} f(z') = f(z), \tag{4.11}$$

which is a direct consequence of the identity (4.10).

More generally, any operator function of a and a^{\dagger} can first be written in 'normal' order by commuting all creation operators on the left of all annihilation operators. It becomes a linear combination of operators of the form

$$a^{\dagger m} a^n \mapsto z^m \left(\partial / \partial z \right)^n$$
,

in the representation (4.5). To a normal-ordered operator $O(z, \partial/\partial z)$, we then associate a kernel $\mathcal{O}(z, \bar{z})$, for which we also use the notation of matrix elements $\langle z | \mathcal{O} | \bar{z} \rangle$ (the bra-ket notation of QM) obtained by acting on the identity,

$$\mathcal{O}(z,\bar{z}) \equiv \langle z | \mathcal{O} | \bar{z} \rangle = O(z,\partial/\partial z) e^{z\bar{z}} = O(z,\bar{z}) e^{z\bar{z}} .$$
(4.12)

Acting with $O(z, \partial/\partial z)$ on both sides of equation (4.11), one infers

$$(Of)(z) = \int \frac{\mathrm{d}\bar{z}'\mathrm{d}z'}{2i\pi} \mathcal{O}(z,\bar{z}') \,\mathrm{e}^{-z'\bar{z}'} f(z').$$

The kernel associated with the product of the two operators is then given by

$$\int \frac{\mathrm{d}\bar{z}'\mathrm{d}z'}{2i\pi} \langle z|\mathcal{O}_2|\bar{z}'\rangle \,\mathrm{e}^{-z'\bar{z}'} \langle z'|\mathcal{O}_1|\bar{z}\rangle = \langle z|\mathcal{O}_2\mathcal{O}_1|\bar{z}\rangle.$$
(4.13)

From the form (4.8) of the scalar product, one also infers the expression of the trace of an operator,

$$\operatorname{tr} \mathcal{O} = \int \frac{\mathrm{d}\bar{z}\,\mathrm{d}z}{2i\pi} \,\mathrm{e}^{-z\bar{z}}\,\mathcal{O}(z,\bar{z}),\tag{4.14}$$

a form consistent with the cyclic property of the trace, as one can verify by taking the trace of equation (4.13).

With the definition (4.12), the matrix elements of the Hamiltonian (4.6) and the operator $U_0(t)$ are, respectively,

$$\langle z | H_0 | \bar{z} \rangle = \hbar \omega z \bar{z} e^{z \bar{z}}, \qquad \langle z | U_0(t) | \bar{z} \rangle = e^{z \bar{z} e^{-\omega t}}.$$
(4.15)

The partition function $\mathcal{Z}_0(\beta)$ corresponding to H_0 is the trace of $U_0(\hbar\beta)$. Using equations (4.14) and (4.15), one finds the expected result,

$$\mathcal{Z}_0(\beta) = \operatorname{tr} U_0(\hbar\beta) = \int \frac{\mathrm{d}\bar{z}\,\mathrm{d}z}{2i\pi} \,\mathrm{e}^{-z\bar{z}}\,\mathrm{e}^{z\bar{z}\,\mathrm{e}^{-\omega\hbar\beta}} = \frac{1}{1 - \mathrm{e}^{-\hbar\omega\beta}} \,. \tag{4.16}$$

Some properties of kernels.

(i) From the property that z and $\partial/\partial z$ are Hermitian conjugate, follows that Hermitian conjugation of operators is represented by the formal complex conjugation of kernels:

 $O \mapsto O^{\dagger} \quad \Leftrightarrow \quad \mathcal{O}(z, \bar{z}) \mapsto \overline{\mathcal{O}}(z, \bar{z}).$

Clearly, with this definition H_0 and $U_0(t)$ are Hermitian.

(ii) To an operator O that has the matrix elements O_{mn} in the harmonic oscillator basis, is associated the kernel $\sum_{m,n} O_{mn}(z^m/\sqrt{m!})(\bar{z}^n/\sqrt{n!})$.

(iii) A somewhat similar representation, in the case of phase-space variables, is the mixed position-momentum representation $\langle q | \mathcal{O} | p \rangle$, which is obtained by a Fourier transformation on one argument,

$$\langle q | \mathcal{O} | p \rangle = \int \mathrm{d}q' \, \mathrm{e}^{i p q' / \hbar} \langle q | \mathcal{O} | q' \rangle.$$

4.2 Holomorphic path integral

We now derive a path integral representation of the matrix elements of the solution of equation (2.4)

$$\hbar \frac{\partial U}{\partial t}(t,t') = -H(t)U(t,t'), \quad U(t',t') = \mathbf{1}, \qquad (4.17)$$

based on the holomorphic formalism, first in the example of the harmonic oscillator, and then for more general Hamiltonians [16, 17, 2] (see also the contribution of Faddeev in Ref. [12]). We expect the path integral to be related to the form (3.21) by a simple change of variables of the form (4.2) (quantum operators being replaced by classical variables), but the boundary conditions and boundary terms require a specific analysis.

4.2.1 The harmonic oscillator

We first expand the exact expression (4.15), for small Euclidean time ε , as

$$\langle z | U_0(\varepsilon) | \bar{z} \rangle = \exp\left(z\bar{z}(1-\omega\varepsilon) + O(\varepsilon^2)\right).$$
 (4.18)

To calculate U_0 for a finite time interval t'' - t', we then write it as

$$U_0(t'' - t') = \lim_{n \to \infty} U_0^n \left(\varepsilon = (t'' - t')/n \right)$$
(4.19)

and express the products in terms of kernels using the rule (4.13),

$$\langle z'' | U_0(t'',t') | \bar{z}' \rangle = \lim_{n \to \infty} \int \prod_{k=1}^{n-1} \frac{\mathrm{d}\bar{z}_k \mathrm{d}z_k}{2i\pi} \exp\left[-\mathcal{S}_{\varepsilon}(z,\bar{z})\right], \qquad (4.20)$$

with

$$S_{\varepsilon}(z,\bar{z}) = \left[-\sum_{k=1}^{n-1} \bar{z}_k \left(z_{k+1} - z_k \right) - \bar{z}_0 z_1 + \omega \varepsilon \sum_{k=0}^{n-1} \bar{z}_k z_{k+1} \right],$$
(4.21)

and the boundary conditions $\bar{z}_0 = \bar{z}', z_n = z''$.

In the formal continuum limit $n \to \infty$, $\varepsilon \to 0$, the expression (4.20) leads to the path integral representation

$$\langle z''| U_0(t'',t') |\bar{z}'\rangle = \int \left[\frac{\mathrm{d}\bar{z}(t)\mathrm{d}z(t)}{2i\pi}\right] \exp\left[-\mathcal{S}_0(z,\bar{z})\right],\tag{4.22}$$

with $(\dot{z}(t) \equiv dz/dt)$

$$S_0(z,\bar{z}) = -\bar{z}(t')z(t') + \int_{t'}^{t''} \mathrm{d}t \,\bar{z}(t) \left[-\dot{z}(t) + \omega z(t)\right],\tag{4.23}$$

and the boundary conditions z(t'') = z'', $\bar{z}(t') = \bar{z}'$. The path $\{z(t), \bar{z}(t)\}$ is a trajectory in phase space in the complex parametrization.

The symmetry of the action between initial and final times, which is not explicit, can be verified by an integration by parts of the term $\bar{z}\dot{z}$, but the validity of time integration within a path integral requires a specific prescription (and the boundary term becomes $-\bar{z}(t'')z(t'')$). The partition function. To calculate the trace of U_0 , we return to the discretized form, because boundary terms are involved. Using equation (4.14), we obtain

$$\mathcal{Z}_0(\beta) = \operatorname{tr} U_0(\hbar\beta/2, -\hbar\beta/2) = \lim_{n \to \infty} \int \prod_{k=1}^n \frac{\mathrm{d} z_k \mathrm{d} \bar{z}_k}{2i\pi} \exp\left[-\mathcal{S}_\varepsilon(\bar{z}, z)\right], \tag{4.24}$$

where S_{ε} now has different boundary terms,

$$\mathcal{S}_{\varepsilon}(\bar{z},z) = \sum_{k=1}^{n} \left[-\bar{z}_{k-1} \left(z_k - z_{k-1} \right) + \hbar \omega \varepsilon \bar{z}_{k-1} z_k \right], \qquad (4.25)$$

with the identification $\bar{z}_n = \bar{z}_0$ and $z_n = z_0$.

In the continuum limit, we obtain the path integral representation of the partition function

$$\mathcal{Z}_{0}(\beta) = \int \left[\frac{\mathrm{d}z(t)\mathrm{d}\bar{z}(t)}{2i\pi}\right] \exp\left[-\mathcal{S}_{0}(\bar{z},z)\right],\tag{4.26}$$

with

$$S_0(\bar{z}, z) = \int_{-\beta/2}^{\beta/2} \mathrm{d}t \, \bar{z}(t) \left[-\dot{z}(t) + \hbar\omega z(t)\right], \qquad (4.27)$$

and the periodic boundary conditions $z(-\beta/2) = z(\beta/2), \bar{z}(-\beta/2) = \bar{z}(\beta/2).$

4.2.2 Linear coupling to an external source: Generating functional The expression (4.26) generalizes simply to a system linearly coupled to external sources $\bar{b}(t)$ and b(t) with the Hamiltonian

$$H = \hbar \omega z \partial / \partial z - b(t) \partial / \partial z - \bar{b}(t) z.$$
(4.28)

At order ε , the solution $U_{\rm G}(t+\varepsilon,t)$ of equation (2.4) is $1-\varepsilon H(t)$ and, therefore,

$$\begin{aligned} \langle z | U_{\rm G}(t+\varepsilon,t) | \bar{z} \rangle &= {\rm e}^{\bar{z}z} \left[1 - \varepsilon \left(\omega z \bar{z} - b(t) \bar{z} - \bar{b}(t) z \right) \right] + O(\varepsilon^2) \\ &= \exp \left[\bar{z}z - \varepsilon \left(\omega z \bar{z} - b(t) \bar{z} - \bar{b}(t) z \right) \right] + O(\varepsilon^2) \end{aligned}$$

In the continuum limit, the action S_0 in the path integral (4.22) is replaced by the action

$$\mathcal{S}_{\rm G}(z,\bar{z}) = -\bar{z}(t')z(t') + \int_{t'}^{t''} \mathrm{d}t \left\{ \bar{z}(t) \left[-\dot{z}(t) + \omega z(t) \right] - \bar{z}(t)b(t) - \bar{b}(t)z(t) \right\}.$$
(4.29)

The trace of $U_{\rm G}$ takes the form (equation (4.14)),

$$\operatorname{tr} U_{\mathrm{G}}(\hbar\beta/2, -\hbar\beta/2) = \int \frac{\mathrm{d}\bar{z}\,\mathrm{d}z}{2i\pi} \,\mathrm{e}^{-z\bar{z}} \,U_{\mathrm{G}}(\hbar\beta/2, -\hbar\beta/2; z, \bar{z})$$
$$= \int \left[\frac{\mathrm{d}\bar{z}(t)\mathrm{d}z(t)}{2i\pi}\right] \exp\left[-\mathcal{S}_{\mathrm{G}}(z, \bar{z})\right], \tag{4.30}$$

with

$$\mathcal{S}_{\mathrm{G}}(z,\bar{z}) = \int_{-\beta/2}^{\beta/2} \mathrm{d}t \left\{ \bar{z}(t) \left[-\dot{z}(t) + \hbar\omega z(t) \right] - \bar{z}(t)b(t) - \bar{b}(t)z(t) \right\}$$

and the periodic boundary conditions $z(-\beta/2) = z(\beta/2), \ \bar{z}(-\beta/2) = \bar{z}(\beta/2).$

We leave the explicit calculation of the Gaussian path integral as an exercise, since an analogous calculation is presented in the fermion case. The result is

$$\operatorname{tr} U_{\mathrm{G}}(\hbar\beta/2, -\hbar\beta/2) = \mathcal{Z}_{0}(\beta) \exp\left[\int_{\beta/2}^{\beta/2} \mathrm{d}t \,\mathrm{d}u \,\bar{b}(u) \Delta(t-u)b(t)\right], \qquad (4.31)$$

where $\mathcal{Z}_0(\beta)$ is the partition function (4.16) of the harmonic oscillator and the function

$$\Delta(t) = \frac{1}{2} e^{-\hbar\omega t} \left[\operatorname{sgn}(t) + 1/\tanh(\hbar\omega\beta/2) \right], \qquad (4.32)$$

 $(\operatorname{sgn}(t) = 1 \text{ for } t > 0, \operatorname{sgn}(-t) = -\operatorname{sgn}(t), \operatorname{d}\operatorname{sgn}(t)/\operatorname{d}t = 2\delta(t))$ is the solution of the differential equation

$$\dot{\Delta}(t) + \hbar\omega\Delta(t) = \delta(t), \qquad (4.33)$$

in the interval $\left[-\beta/2,\beta/2\right]$ with periodic boundary conditions.

In particular, the Gaussian two-point function with weight e^{-S_0} (equation (4.27)), which we call propagator with reference to real propagation, and which is the basic element of perturbation theory, is given by

$$\langle \bar{z}(t_2)z(t_1)\rangle_0 = \mathcal{Z}_0^{-1}(\beta) \left. \frac{\delta^2}{\delta b(t_2)\delta \bar{b}(t_1)} \exp\left[\int_{\beta/2}^{\beta/2} \mathrm{d}t \,\mathrm{d}u \,\bar{b}(t)\Delta(u-t)b(u) \right] \right|_{b=\bar{b}\equiv 0}$$

= $\Delta(t_2-t_1).$ (4.34)

The Fourier representation of the propagator is

$$\Delta(t) = \frac{1}{2\pi} \int \frac{\mathrm{d}\kappa \,\mathrm{e}^{i\kappa t}}{i\kappa + \hbar\omega} \,. \tag{4.35}$$

Partition function. The partition function $\mathcal{Z}_0(\beta)$ (equation (4.26)) can be related to the propagator by the method of Section 2.6.2. Differentiating the path integral (4.26) with respect to ω , one finds

$$\frac{\partial \ln \mathcal{Z}_0(\beta)}{\partial \omega} = -\hbar \int_{-\beta/2}^{\beta/2} \mathrm{d}t \left\langle z(t)\bar{z}(t) \right\rangle_0 = -\hbar\beta \Delta(0)$$

A difficulty then arises, because $\Delta(t)$ is not continuous at t = 0; this, again, is the sgn(0) problem (a problem that can only be solved by a regularization of the path integral). Integrating, one obtains (using the limit $\beta \to \infty$ to determine the integration constant)

$$\mathcal{Z}_0(\beta) = rac{\mathrm{e}^{-\hbar\beta\omega\,\mathrm{sgn}(0)/2}}{2\sinh(\hbar\beta\omega/2)}.$$

The ambiguity due to sgn(0) has the nature of a constant shift of the Hamiltonian, a natural consequence of the order problem between the operators z and $\partial/\partial z$. The rule consistent with the normal order (4.3) is to set sgn(0) = -1 and yields

$$\mathcal{Z}_0(\beta) = \frac{1}{1 - \mathrm{e}^{-\hbar\beta\omega}} \,. \tag{4.36}$$

However, such a choice is inconvenient for perturbative calculations, because it breaks time reversal symmetry, and it is better to choose sgn(0) = 0. This corresponds to a symmetric form $\frac{1}{2}(z\partial/\partial z + \partial/\partial zz)$ and yields the standard harmonic oscillator. The additional contribution can then be cancelled, if necessary, by shifting physical parameters.

69

4.2.3 General one-dimensional Hamiltonian

Quite generally, one expresses the quantum Hamiltonian H(p,q) in terms of creation and annihilation operators and commutes all creation operators to the left (normal order). In the Hamiltonian $h(a^{\dagger}, a)$, one replaces operators by the corresponding classical variables, as explained in Section 4.1. One obtains the matrix elements $\langle z | U(t + \varepsilon, t) | \bar{z} \rangle$ at order ε and, following the method of Section 4.2.1, derives the path integral representation

$$\langle z'' | U(t'', t') | \bar{z}' \rangle = \int \left[\frac{\mathrm{d}\bar{z}(t)\mathrm{d}z(t)}{2i\pi} \right] \exp\left[-\mathcal{S}(z, \bar{z}) \right], \quad \text{with}$$

$$(4.37)$$

$$S(z(t), \bar{z}(t)) = -\bar{z}(t')z(t') + \int_{t'}^{t'} dt \left[-\bar{z}(t)\dot{z}(t) + h(z(t), \bar{z}(t))/\hbar \right], \quad (4.38)$$

and the boundary conditions $z(t'') = z'', \bar{z}(t') = \bar{z}'$.

Such a path integral can be used to generate a perturbative expansion. However, the expansion is plagued by singularities, reflections of the quantization problem and the order between the quantum operators z and $\partial/\partial z$. In particular, the undefined quantity $\Delta(0)$ appears. As we have already explained, normal order corresponds to the choice of $\operatorname{sgn}(0) = -1$, which is somewhat inconvenient, and it is preferable to choose $\operatorname{sgn}(0) = 0$ and to modify $h(z, \overline{z})$ to suppress the unwanted additional contributions.

Real parametrization of phase space. From the classical point of view, momentum and position variables (p,q) and complex variables (\bar{z}, z) are two different parametrizations of phase space related by

$$p - i\omega q = -i\sqrt{2\hbar\omega}\,\bar{z}\,,\qquad p + i\omega q = i\sqrt{2\hbar\omega}\,z\,.$$
(4.39)

Path integrals, because they involve classical Hamiltonians, extend somewhat this correspondence to QM. If, in the path integral over phase space derived in Chapter 3 (equation (3.21)), one changes variables $(p(t), q(t)) \mapsto (\bar{z}(t), z(t))$, where the variables are related at all times by the relations (4.39), one finds a form (4.37, 4.38), with

$$h(z,\bar{z}) = H\left(i(z-\bar{z})\sqrt{\hbar\omega/2}, (z+\bar{z})\sqrt{\hbar/2\omega}\right)$$

The differences come only from boundary terms and boundary conditions, and this justifies our starting from first principles again. But once the modifications are known, one can infer the holomorphic path integral directly from the phase-space integral.

Both formalisms may have problems generated by ordering operators in products. However, the transformation (4.39) is not innocuous, since even simple Hamiltonians of the form $p^2 + V(q)$ have quantization problems after the transformation.

Partition function. The partition function is given by

$$\mathcal{Z}(\beta) = \int \frac{\mathrm{d}\bar{z}\,\mathrm{d}z}{2i\pi} \,\mathrm{e}^{-z\bar{z}} \left\langle z \right| U(\hbar\beta/2, -\hbar\beta/2) \left| \bar{z} \right\rangle = \int \left[\frac{\mathrm{d}\bar{z}(t)\mathrm{d}z(t)}{2i\pi} \right] \exp\left[-\mathcal{S}(z, \bar{z}) \right] \,\mathrm{d}z$$

with

$$\mathcal{S}(z,\bar{z}) = \int_{-\beta/2}^{\beta/2} \mathrm{d}t \left[-\bar{z}(t)\dot{z}(t) + h(z(t)\bar{z}(t)) \right],$$

and the periodic boundary conditions $z(-\beta/2) = z(\beta/2), \ \bar{z}(-\beta/2) = \bar{z}(\beta/2).$

It can be calculated by expanding around the harmonic oscillator, $h(z, \bar{z}) = \omega z \bar{z} + h_{\rm I}(z, \bar{z})$, and evaluating perturbative terms by using Wick's theorem (1.30) together with the two-point function (4.32).

Remark. If the Hamiltonian has the form discussed in Chapter 2,

$$H = \frac{1}{2}\hat{p}^2 + \frac{1}{2}\omega^2\hat{q}^2 + V_{\rm I}(\hat{q}),$$

perturbation theory requires only the Gaussian two-point function of q(t), which is proportional to $z(t) + \bar{z}(t)$. We see from the action (4.29) that this sum can be generated by taking a real source b(t) ($\bar{b}(t) = b(t)$) and acting by functional differentiation with respect to b(t) on $U_{\rm G}$. Thus, the expressions (4.31) and (4.32) can be symmetrized in time. After the rescaling, $b(t) \mapsto b(t)\sqrt{\hbar/2\omega}$, one finds

$$\operatorname{tr} U_{\mathrm{G}}(\hbar\beta/2, -\hbar\beta/2) = \frac{1}{2\sinh(\omega\beta/2)} \exp\left[\frac{1}{2} \int \mathrm{d}t_1 \,\mathrm{d}t_2 \,b(t_1)\Delta(t_1 - t_2)b(t_2)\right],$$

with

$$\Delta(t) = \hbar \frac{\cosh \hbar \omega (\beta/2 - |t|)}{2\omega \sinh(\hbar \omega \beta/2)}$$

a result consistent with equation (2.57).

4.3 Several degrees of freedom. Boson interpretation

In the holomorphic formalism, a Hamiltonian H_0 , sum of ν independent harmonic oscillators with frequencies $\omega_i > 0$, can be expressed as the differential operator

$$H_0 = \sum_{i=1}^{\nu} \hbar \omega_i \, z_i \frac{\partial}{\partial z_i} \,,$$

acting on analytic functions of ν complex variables, which can be expanded in the form

$$\psi(\mathbf{z}) = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{i_1, i_2, \dots, i_n=1}^{\nu} \psi_{i_1 i_2 \dots i_n} z_{i_1} z_{i_2} \cdots z_{i_n} , \qquad (4.40)$$

where the coefficient $\psi_{i_1i_2...i_n}$ is symmetric in its *n* indices $i_1, i_2, ..., i_n$. The monomial $z_{i_1}z_{i_2}\cdots z_{i_n}$ is an eigenstate of H_0 with the energy $\hbar(\omega_{i_1}+\omega_{i_2}+\cdots+\omega_{i_n})$.

Many-body boson interpretation. Due to the additive character of the spectrum of the harmonic oscillator, the energy eigenvalues also have the interpretation of the total energy of non-interacting particles. In this alternative interpretation, one-particle states are associated with the energies $\hbar \omega_i$. Moreover, $\psi_{i_1 i_2...i_n}$ is then the component of $\psi(\mathbf{z})$ on an *n*-particle state and, since $\psi_{i_1 i_2...i_n}$ is symmetric in its *n* indices, these particles obey the Bose–Einstein statistics: the holomorphic formalism makes a description of general boson states, which are linear combinations of states with an arbitrary number of particles, possible.

We choose the functions $\Psi(\mathbf{z})$ to be normalizable with respect to the scalar product

$$(\psi_1, \psi_2) = \int \left(\prod_{i=1}^{\nu} \frac{\mathrm{d}z_i \,\mathrm{d}\bar{z}_i}{2i\pi} \,\mathrm{e}^{-z_i\bar{z}_i}\right) \overline{\psi_1(\mathbf{z})} \psi_2(\mathbf{z}),\tag{4.41}$$

which generalizes the scalar product (4.8). Then,

$$\|\Psi\|^2 = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{i_1, i_2, \dots, i_n} |\psi_{i_1 i_2 \dots i_n}|^2 < \infty.$$

4.4

The normalizable functions (4.40) belong to a Hilbert space of entire functions of ν variables. When $\|\Psi\| = 1$, the *n*th term in the sum gives the probability for the quantum system to be in an *n*-particle state, the factor 1/n! cancelling the over-counting of states implied by the unrestricted summation over all indices $\{i_k\}$.

The kernel of the identity is now

$$\mathcal{I}(z,\bar{z}) = \exp\left(\sum_{i=1}^{\nu} \bar{z}_i z_i\right).$$
(4.42)

The kernels of the Hamiltonian and the number operator N follow:

$$\langle z|H_0|\bar{z}\rangle = \mathcal{I}(z,\bar{z})\sum_i \hbar\omega_i z_i \bar{z}_i, \quad \langle z|N|\bar{z}\rangle = \mathcal{I}(z,\bar{z})\sum_i z_i \bar{z}_i.$$

The partition function for free bosons that can occupy ν different states of energy $\hbar\omega_i$ is then given by the path integral

$$\mathcal{Z}_{0}(\beta) = \int \left[\frac{\mathrm{d}z(t)\mathrm{d}\bar{z}(t)}{2i\pi}\right] \exp\left[-\mathcal{S}_{0}\left(\bar{\mathbf{z}},\mathbf{z}\right)\right],\tag{4.43}$$

$$\mathcal{S}_0(\bar{\mathbf{z}}, \mathbf{z}) = \int_{-\beta/2}^{\beta/2} \mathrm{d}t \, \sum_i \bar{z}_i(t) \left[-\dot{z}(t) + \hbar \omega_i z_i(t) \right]. \tag{4.44}$$

By adding to the action S_0 , a polynomial of higher degree in the variables z_i and \bar{z}_i , it is possible to describe interactions between bosons.

This formalism is well-suited to the study of quantum statistical systems of bosons in the grand canonical formulation, as discussed in Section 4.4.2.

4.4 The Bose gas. Field integral representation

We now consider a non-relativistic gas of bosons, that is, identical quantum particles obeying the Bose–Einstein statistics of mass m, in continuum space. For simplicity, we assume that the particles have no internal degrees of freedom, like spin.

A formalism with a fixed number of particles is useful for models where the *n*-body problem can be solved exactly, or approximately, but more cumbersome in general.

The grand canonical formalism, where the number of particles can vary, and is fixed only on average, is better adapted in many situations where collective effects are important, like in the theory of phase transitions.

4.4.1 Matrix density at thermal equilibrium: Fixed number of particles

The density matrix at thermal equilibrium for a fixed number of bosons, can be calculated from a *path integral*, simple extension of the form derived in Chapter 2, but where the boson character is taken into account.

We consider an n-particle Hamiltonian in d dimensions of the general form

$$H_n = T_n + \mathcal{V}_n(\mathbf{x}_1, \dots, \mathbf{x}_n), \quad \mathbf{x}_i \in \mathbb{R}^d,$$
(4.45)

where T_n is the kinetic term,

$$T_n = -\frac{\hbar^2}{2m} \sum_{i=1}^n \nabla_i^2, \qquad (4.46)$$

with $\nabla_i \equiv \nabla_{x_i} \equiv (\partial/\partial_{x_i^1}, \partial/\partial_{x_i^2}, \dots, \partial/\partial_{x_i^d})$, and where the potential $\mathcal{V}_n(\mathbf{x}_1, \dots, \mathbf{x}_n)$ is a symmetric function of the *n* positions. The Hamiltonian acts on square integrable symmetric wave functions of *n* positions, $\psi_n(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n)$, which belong to the Hilbert space \mathfrak{H}_n of *n*-particle boson states. Quantum statistical physics

The partition function is the trace of the statistical operator $e^{-\beta H}$, but, in the trace, the statistical properties of the quantum particles have to be taken into account. This implies that the trace in the partition function has to be restricted to the relevant subspace by the insertion of the corresponding projectors. The partition function can be expressed as a path integral of the form,

$$\mathcal{Z}(n,\beta) = \int [\mathrm{d}^d x_i(t)] \,\mathrm{e}^{-\mathcal{S}(x)/\hbar},\tag{4.47}$$

with

$$\mathcal{S}(x)/\hbar = \int_0^\beta \mathrm{d}t \left[\sum_i \frac{1}{2m\,\hbar^2} \left(\dot{\mathbf{x}}_i(t) \right)^2 + V_n \left(\mathbf{x}_1(t), \dots, \mathbf{x}_n(t) \right) \right],\tag{4.48}$$

but averaged over the n! different boundary conditions corresponding to all permutations P, $\mathbf{x}_i(\beta) = \mathbf{x}_{P(i)}(0)$.

4.4.2 Second quantization. Field integral representation

We now discuss the thermodynamics of a gas of quantum particles in the grand canonical formalism in which the number of particles is fixed only on average by tuning a parameter μ coupled to the number of particles and called *chemical potential*. Generalizing the formalism of Section 4.3, we use a representation of bosons often referred to as *second quantization*. We derive an expression for the partition function that has the form of a *field integral*, a generalization of the holomorphic path integral (4.44) of Section 4.3.

The *n*-particle potential. We consider here only potentials that are sums of one-body and two-body potentials (to simplify the notation, we now substitute $\mathbf{x} \mapsto x$):

$$\mathcal{V}_n(x_1, x_2, \dots, x_n) = \sum_{i=1}^n V_1(x_i) + \sum_{i < j \le n} V_2(x_i, x_j), \qquad (4.49)$$

 $(V_2(x,y) = V_2(y,x))$ but the generalization to other many-body potentials is simple.

4.4.3 Fock space

We consider the direct sum $\oplus \mathfrak{H}_n$, $n = 1, ..., \infty$ of Hilbert spaces. Since the wave functions are symmetric, we introduce a complex field $\varphi(x)$, and a generating functional of *n*-particle wave functions (see Section 2.5.3)

$$\Psi(\varphi) = \sum_{n=0} \frac{1}{n!} \left(\int \prod_{i} \mathrm{d}^{d} x_{i} \,\varphi(x_{i}) \right) \psi_{n}(x_{1}, \dots, x_{n}), \tag{4.50}$$

which generalizes expression (4.40). The scalar product of two functionals is given by the *field integral* (see Section 4.4.5)

$$(\Psi_1, \Psi_2) = \left\langle \overline{\Psi_1(\varphi)} \Psi_2(\varphi) \right\rangle \equiv \int [\mathrm{d}\varphi \,\mathrm{d}\bar{\varphi}] \,\overline{\Psi_1(\varphi)} \Psi_2(\varphi) \exp\left[-\int \mathrm{d}^d x \,\bar{\varphi}(x)\varphi(x)\right], \quad (4.51)$$

which generalizes expression (4.41), and which is normalized by the condition

$$(1,1) = \langle 1 \rangle \equiv \int [\mathrm{d}\varphi \,\mathrm{d}\bar{\varphi}] \exp\left[-\int \mathrm{d}^d x \,\bar{\varphi}(x)\varphi(x)\right] = 1.$$

Since the measure is Gaussian, to calculate expectation values one only needs the twopoint function. The kernel in the quadratic form is the identity. Its inverse is also the identity and, therefore,

$$\langle \bar{\varphi}(x)\varphi(y)\rangle = \delta^{(d)}(x-y)$$

Using then Wick's theorem, it is simple to verify that the norm of the functional Ψ is then given by

$$|\Psi|^2 = (\Psi, \Psi) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(\int \prod_i d^d x_i \right) |\psi_n(x_1, \dots, x_n)|^2.$$

When $\|\Psi\| = 1$, the *n*th term in the sum is the probability that the boson system is in an *n*-particle state. The complex vector space of functionals with finite norm is called a Fock space, and this formalism is often called second quantization.

4.4.4 Hamiltonian in Fock space

We denote by **H** the Hamiltonian in Fock space, whose restriction to *n*-particle states is H_n , **T** the kinetic term whose restriction is T_n , and \mathbf{V}_1 , \mathbf{V}_2 the one- and two-body potentials, respectively. Thus,

$$\mathbf{H} = \mathbf{T} + \mathbf{V}_1 + \mathbf{V}_2 \,. \tag{4.52}$$

We then represent the kinetic term \mathbf{T} and the potential terms \mathbf{V}_1 and \mathbf{V}_2 by operators acting on Ψ by functional differentiation.

We first calculate

$$\int d^d x \, \varphi(x) \nabla_x^2 \frac{\delta}{\delta \varphi(x)} \Psi(\varphi) = \int d^d x \, \varphi(x) \nabla_x^2 \sum_n \frac{1}{(n-1)!} \\ \times \int \left(\prod_{i < n} d^d x_i \, \varphi(x_i) \right) \psi_n(x_1, \dots, x_{n-1}, x).$$

The variable x in the right-hand side can be renamed x_n . A symmetrization of the coefficient of $\prod_{i \le n} \varphi(x_i)$ then yields a factor 1/n and the sum of all gradients squared. We have reconstructed, up to a factor, the kinetic term (4.46). We conclude that

$$\mathbf{T}\Psi(\varphi) = -\frac{\hbar^2}{2m} \int \mathrm{d}^d x \,\varphi(x) \nabla_x^2 \frac{\delta}{\delta\varphi(x)} \Psi(\varphi). \tag{4.53}$$

For the one-body potential V_1 , an analogous argument shows that

$$\mathbf{V}_{1}\Psi(\varphi) = \int \mathrm{d}^{d}x \,\varphi(x) V_{1}(x) \frac{\delta}{\delta\varphi(x)} \Psi(\varphi)$$

To generate a two-body potential, it is necessary to differentiate twice with respect to φ at two different points. It is simple to verify the representation

$$\mathbf{V}_{2}\Psi(\varphi) = \frac{1}{2} \int \mathrm{d}^{d}x \,\mathrm{d}^{d}y \,\varphi(x)\varphi(y)V_{2}(x,y) \frac{\delta^{2}}{\delta\varphi(x)\delta\varphi(y)}\Psi(\varphi). \tag{4.54}$$

We now have a representation of the full Hamiltonian **H** acting on generating functionals.

The representation of the operator number of particles N is given by

$$\mathbf{N} = \int \mathrm{d}^d x \,\varphi(x) \frac{\delta}{\delta\varphi(x)} \quad \Rightarrow \quad [\mathbf{N}, \mathbf{H}] = 0 \,. \tag{4.55}$$

In what follows, we consider as full Hamiltonian the sum $\mathbf{H} - \mu \mathbf{N}$, where the chemical potential μ determines the average value of \mathbf{N} .

Because, in this construction, the role of coordinates is played by fields $\varphi(x)$, we are constructing a non-relativistic (in general non-local) quantum field theory (QFT).

4.4.5 Kernels of operators and field integral representation

Within the holomorphic formalism, we now use functional methods to derive a representation of matrix elements of the statistical operator as *field integrals*, generalization of the path integrals discussed in Section 4.2.1: in the field integral, the summation over fields replaces the summation over paths. The form of the field integral actually follows rather directly from results already obtained in QM, provided one interprets the function $\varphi(x)$ as a set of complex variables depending on a continuous index x and $\Psi(\varphi)$ as an analytic 'functional' in the holomorphic formalism of Section 4.1. Note that the matrix elements of the statistical operator depend on two fields and represent an operator acting on the space of generating functionals.

We denote by $\bar{\varphi}(x)$ the field conjugate to $\varphi(x)$. The kernel of the identity operator $\mathcal{I}(\varphi, \bar{\varphi})$, generalization of expression (4.42) and consistent with the definition (4.51) of the scalar product, takes the form

$$\mathcal{I}(\varphi,\bar{\varphi}) = \exp\left[\int \mathrm{d}^d x \,\varphi(x)\bar{\varphi}(x)\right]. \tag{4.56}$$

The kernel associated with operators defined in terms of the field $\varphi(x)$ and functional derivatives is then obtained by acting on $\mathcal{I}(\varphi, \bar{\varphi})$. Note that the Hamiltonian here is directly written in normal order. Its matrix elements are

$$\langle \varphi | \mathbf{H} | \bar{\varphi} \rangle = \mathcal{I}(\varphi, \bar{\varphi}) \left\{ \int \mathrm{d}^d x \, \varphi(x) \left[-\frac{\hbar^2}{2m} \nabla^2 + V_1(x) \right] \bar{\varphi}(x) \right.$$

$$\left. + \frac{1}{2} \int \mathrm{d}^d x \, \mathrm{d}^d y \, \varphi(x) \varphi(y) V_2(x, y) \bar{\varphi}(x) \bar{\varphi}(y) \right\}.$$

$$(4.57)$$

The kernel associated with the particle number operator is

$$\langle \varphi | \mathbf{N} | \bar{\varphi} \rangle = \mathcal{I}(\varphi, \bar{\varphi}) \int \mathrm{d}^d x \, \varphi(x) \bar{\varphi}(x).$$
 (4.58)

Considering the space coordinate x as a continuous index, we can adapt the expressions of Section 4.2.1, in particular equation (4.38), to this more general situation, in much the same way as we have generalized the simple integrals of Chapter 1 to path integrals. We then obtain a field integral, because we no longer integrate over paths, but instead, over fields $\{\varphi(t, x), \bar{\varphi}(t, x)\}$. Here, one finds

$$\langle \varphi'' | \mathbf{U}(t'',t') | \bar{\varphi}' \rangle = \langle \varphi'' | e^{-(t''-t)(\mathbf{H}-\mu\mathbf{N})/\hbar} | \bar{\varphi}' \rangle = \int [\mathrm{d}\bar{\varphi}(t,x)\mathrm{d}\varphi(t,x)] e^{-\mathcal{S}(\varphi,\bar{\varphi})}, \quad (4.59)$$

with the boundary conditions $\bar{\varphi}(t,x') \equiv \bar{\varphi}'(x)$, $\varphi(t,x'') \equiv \varphi''(x)$, and the Euclidean action

$$S(\varphi,\bar{\varphi}) = -\bar{\varphi}(t,x')\varphi(t,x') + \int dt \, d^dx \, \bar{\varphi}(t,x) \left(-\frac{\partial}{\partial t} - \frac{\hbar}{2m} \nabla_x^2 + \frac{V_1(x) - \mu}{\hbar} \right) \varphi(t,x) + \frac{1}{2\hbar} \int dt \, d^dx \, d^dy \, \bar{\varphi}(t,x)\varphi(t,x)V_2(x,y)\bar{\varphi}(t,y)\varphi(t,y).$$
(4.60)

Setting $t = \hbar\beta$, one obtains the statistical operator and then the partition function,

$$\mathcal{Z}(\beta) = \int [\mathrm{d}\bar{\varphi}(t, x) \mathrm{d}\varphi(t, x)] \exp[-\mathcal{S}(\varphi, \bar{\varphi})], \qquad (4.61)$$

with the periodic boundary conditions

$$\bar{\varphi}(-\beta/2, x) = \bar{\varphi}(\beta/2, x), \quad \varphi(-\beta/2, x) = \varphi(\beta/2, x),$$

and the Euclidean action is

$$\mathcal{S}(\varphi,\bar{\varphi}) = \int \mathrm{d}t \,\mathrm{d}^d x \,\bar{\varphi}(t,x) \left(-\frac{\partial}{\partial t} - \frac{\hbar^2}{2m} \nabla_x^2 + V_1(x) - \mu \right) \varphi(t,x) + \frac{1}{2} \int \mathrm{d}t \,\mathrm{d}^d x \,\mathrm{d}^d y \,\bar{\varphi}(t,x) \varphi(t,x) V_2(x,y) \bar{\varphi}(t,y) \varphi(t,y).$$
(4.62)

We have derived a representation of the partition function in the form of a field integral for a *non-relativistic QFT* (see, for example, Ref. [19]). The generalization to a relativistic theory is then mainly a matter of implementing relativistic invariance.

U(1) symmetry. The particle number conservation has an interesting consequence for the field integral: it has a U(1) symmetry, corresponding to the transformations

$$\varphi(t,x) \mapsto e^{i\kappa} \varphi(t,x), \quad \bar{\varphi}(t,x) \mapsto e^{-i\kappa} \bar{\varphi}(t,x),$$

with κ any real constant. We show in Section 15.10 that interesting physics is associated with the spontaneous breaking of the symmetry.

4.4.6 The Gaussian model

As an illustration, we now calculate the partition function of the Gaussian model, which corresponds to a gas of independent particles in a one-body external potential V_1 . We begin with the free gas. We want to show that well-known results are recovered. Although functional methods are not required for these simple examples, their study will help us to take into account the effect of additional interactions.

Free Bose gas. In the absence of a potential, the partition function can be calculated exactly. To take advantage of translation invariance, we expand the fields $\varphi, \bar{\varphi}$ in Fourier modes. In *d*-space dimensions,

$$\bar{\varphi}(t,\mathbf{x}) = \int \mathrm{d}^d p \,\,\mathrm{e}^{i\mathbf{p}\cdot\mathbf{x}/\hbar}\,\tilde{\varphi}^*(t,\mathbf{p}), \quad \varphi(t,\mathbf{x}) = \int \mathrm{d}^d p \,\,\mathrm{e}^{-i\mathbf{p}\cdot\mathbf{x}/\hbar}\,\tilde{\varphi}(t,\mathbf{p}). \tag{4.63}$$

The Jacobian is trivial, and the action becomes

$$\mathcal{S}_{0}(\tilde{\varphi},\tilde{\varphi}^{*}) = (2\pi\hbar)^{d} \int \mathrm{d}t \,\mathrm{d}^{d}p \,\tilde{\varphi}^{*}(t,\mathbf{p}) \left(-\frac{\partial}{\partial t} + \frac{\mathbf{p}^{2}}{2m} - \mu\right) \tilde{\varphi}(t,\mathbf{p}).$$
(4.64)

We first calculate the partition function in a hypercubic box of linear size L with periodic boundary conditions and then take the thermodynamic limit. The fields $\varphi(t, \mathbf{x}), \bar{\varphi}(t, \mathbf{x})$ are periodic functions of period L of all space coordinates. After Fourier transformation, the corresponding momenta belong to the lattice

$$\mathbf{p} = 2\pi\hbar\mathbf{n}/L, \quad \mathbf{n} \in \mathbb{Z}^d,$$

and the action reads

$$\mathcal{S}_{0}(\tilde{\varphi}^{*},\tilde{\varphi}) = (2\pi\hbar)^{2d} \int \mathrm{d}t \sum_{\mathbf{n}} \tilde{\varphi}^{*}(t,\mathbf{p}) \left(-\frac{\partial}{\partial t} + \frac{\mathbf{p}^{2}}{2m} - \mu\right) \tilde{\varphi}(t,\mathbf{p}).$$
(4.65)

The field integral factorizes and the result is the product over all values of **n** of a partition function of the form (4.36). The free energy, $W_0(\beta) = \beta^{-1} \ln Z_0(\beta)$, is

$$\mathcal{W}_0(\beta) = -\frac{1}{\beta} \sum_{\mathbf{n} \in \mathbb{Z}^d} \ln\left(1 - e^{-\beta(\mathbf{p}^2/2m - \mu)}\right).$$
(4.66)

In the thermodynamic limit $L \to \infty$, the free energy per unit volume, which is the pressure Π , becomes $(d\mathbf{n} = d\mathbf{p}L/2\pi\hbar)$

$$\Pi = L^{-d} \mathcal{W}_0(\beta) = -\frac{1}{\beta} \int \frac{\mathrm{d}^d p}{(2\pi\hbar)^d} \ln\left(1 - \mathrm{e}^{-\beta(\mathbf{p}^2/2m-\mu)}\right).$$
(4.67)

Note that the Bose gas is stable only if the chemical potential is non-positive.

The derivative of $\ln \mathcal{Z}$ with respect to β , at $\beta \mu$ fixed, yields the average energy density

$$\langle H \rangle = -\frac{1}{L^d} \left. \frac{\partial \ln \mathcal{Z}}{\partial \beta} \right|_{\beta\mu \text{ fixed}} = \frac{1}{(2\pi\hbar)^d} \int \frac{\mathrm{d}^d p \ \mathbf{p}^2 / 2m}{\mathrm{e}^{\beta(\mathbf{p}^2/2m-\mu)} - 1} \,. \tag{4.68}$$

The derivative of $\ln \mathcal{Z}$ with respect to $\beta \mu$ (β fixed) yields the average particle number, and thus the gas density

$$\rho = L^{-d} \langle N \rangle = \frac{1}{L^d \beta} \int \mathrm{d}t \, \mathrm{d}^d x \, \langle \varphi(t, x) \bar{\varphi}(t, x) \rangle = \frac{1}{(2\pi\hbar)^d} \int \frac{\mathrm{d}^d p}{\mathrm{e}^{\beta(\mathbf{p}^2/2m-\mu)} - 1} \, \cdot \qquad (4.69)$$

This equation, called *equation of state*, is known to exhibit the phenomenon of Bose– Einstein condensation. At fixed temperature $T = 1/\beta$, when μ increases the density ρ increases. When the dimension d of space is larger than 2, since μ cannot become positive, ρ is bounded by the value ρ_c of the integral calculated for $\mu = 0$:

$$\rho \le \rho_c = \frac{1}{(2\pi\hbar)^d} \int \frac{\mathrm{d}^d p}{\mathrm{e}^{\beta \mathbf{p}^2/2m} - 1} = \zeta(d/2) \left(\frac{mT}{2\pi\hbar^2}\right)^{d/2},$$

where $\zeta(s)$ is Riemann's ζ -function. Conversely, at fixed density, the equation of state has a solution up to a minimal temperature T_0 given by

$$T_0 = \frac{2\pi\hbar^2}{m} \left(\frac{\rho}{\zeta(d/2)}\right)^{2/d}$$

To understand the physics at lower temperatures $T < T_0$, it is useful to return to a large but finite box, where the momentum modes are discrete. One then discovers that a macroscopic fraction of the free Bose gas condenses in the ground state, which corresponds to the zero-momentum mode. This is the phenomenon of *Bose–Einstein condensation*.

In two dimensions, because ρ_c diverges, there is no condensation.

General one-body potential. To calculate the Gaussian field integral, we replace the Fourier expansion (4.63) by an expansion on the eigenfunctions of the one-body Hamiltonian H_1 . The same arguments then lead to

$$\mathcal{W}(\beta) = -\operatorname{tr}\ln\left(1 - \mathrm{e}^{\beta\mu - \beta H_1}\right).$$

Similarly,

$$\langle N \rangle = \operatorname{tr} \left[1 - \mathrm{e}^{\beta \mu - \beta H_1} \right]^{-1}, \quad \langle H \rangle = \operatorname{tr} H_1 \left[1 - \mathrm{e}^{\beta \mu - \beta H_1} \right]^{-1}.$$

An analysis, based on the arguments of Section 2.8, shows that, in the semi-classical limit, the free energy becomes

$$\mathcal{W}(\beta) = -\frac{1}{\beta} \int \frac{\mathrm{d}^d p \,\mathrm{d}^d x}{(2\pi\hbar)^d} \ln\left(1 - \mathrm{e}^{\beta\mu - \beta H_1(p,x)}\right),$$

where $H_1(p, x)$ is the classical Hamiltonian.

A simple example is provided by a harmonic well, of the kind relevant for the magnetic traps of some Bose–Einstein condensation experiments. For simplicity, we assume that the trap is spherical. Then,

$$H_1 = \frac{1}{2m}\mathbf{p}^2 + \frac{1}{2}m\omega^2\mathbf{x}^2.$$

In the semi-classical limit, the average number of particles in the trap, for $\mu = 0$, is

$$\langle N \rangle = \frac{\zeta(d)}{(\hbar\beta\omega)^d}$$

an approximation valid for temperatures large enough, $T \gg \hbar \omega$. Condensation now occurs for any dimension d > 1 below the temperature

$$T_0 = 1/\beta = \hbar\omega(\langle N \rangle)^{1/d}.$$

At lower temperatures, the discrete nature of the quantum spectrum becomes relevant, the relation between particle numbers and chemical potential can be satisfied up to $\mu = d\hbar\omega/2$, and below T_0 particles accumulate in the ground state.

4.4.7 Pair potentials: The example of the $\delta(x)$ -function potential

When one is interested only in long-wavelength phenomena, one can often approximate a short-range pair-potential by a δ -function pseudo potential. The action then simplifies and becomes *local* (here, we assume $V_1 \equiv 0$):

$$\mathcal{S}(\varphi,\bar{\varphi}) = \int \mathrm{d}t \,\mathrm{d}^d x \left[\bar{\varphi}(t,x) \left(-\frac{\partial}{\partial t} - \frac{\hbar^2}{2m} \nabla^2 - \mu \right) \varphi(t,x) + \frac{g}{2} \left(\bar{\varphi}(t,x) \varphi(t,x) \right)^2 \right]. \tag{4.70}$$

For simple potentials, the strength g of the interaction is proportional to $\hbar^2 a^{d-2}/m$, where a is the s-wave scattering length. a must be positive, that is, correspond to a repulsive interaction, for the boson system to be stable.

Note that μ is no longer restricted to be negative. For $\mu > 0$, the minimum of the $\varphi, \overline{\varphi}$ potential now corresponds to a non-vanishing value of $|\varphi|$. This suggests the possibility of a phase transition.

In one space dimension, the model is exactly integrable and solvable by Bethe's Ansatz, in the sense that all eigenstates of the Hamiltonian are linear combinations of a finite number of plane waves. If thermal fluctuations are neglected, the model leads to a classical field equation, called non-linear Schrödinger equation, which is also integrable.

In three dimensions, the model is especially interesting: in the presence of the interaction, the condensation temperature of the Bose gas becomes the transition temperature for a phase transition where the U(1) symmetry is spontaneously broken. Therefore, it describes the physics of the helium superfluid transition (see Section 15.10). Quantum statistical physics

However, note that a Hamiltonian with a δ -function potential is only defined in one dimension. In higher dimensions, it leads to divergences that have to be dealt with (regularized, see Chapter 8) by adding an artificial short-distance structure. In two dimensions, the model is renormalizable, as power counting shows, and not renormalizable in higher dimensions (see Chapter 8).

In all dimensions d > 0, a problem of quantization also appears. Since

$$[\delta/\delta\varphi(x),\varphi(x)] = \delta^{(d)}(0)',$$

it leads to divergences. A careful derivation shows that normal order eliminates all divergences in one dimension.

Perturbative expansion. As an exercise, we calculate the correction of order g to the free energy. We need the Gaussian two-point $\langle \varphi \bar{\varphi} \rangle$ correlation function. In partial Fourier representation, from equations (4.64), (4.32), and (4.34), we infer $(\vartheta(t) = (1 + \operatorname{sgn}(t))/2)$,

$$\tilde{\Delta}(t,p) = \langle \tilde{\varphi}^*(t,p)\tilde{\varphi}(0,p)\rangle = \frac{\mathrm{e}^{-\omega(p)t}}{(2\pi\hbar)^d} \left(\vartheta(t) + \frac{1}{\mathrm{e}^{\beta\omega(p)} - 1}\right), \text{ with } \omega(p) = \frac{p^2}{2m} - \mu.$$

We recognize the sum of the two contributions generated by quantum and thermal fluctuations. After Fourier transformation over time, one finds (equation (4.35))

$$\tilde{\Delta}(\omega, p) = \frac{1}{(2\pi\hbar)^{d+1}} \frac{1}{i\omega + p^2/2m - \mu} \,. \tag{4.71}$$

Using Wick's theorem, one obtains

$$\mathcal{W}(\beta) = \mathcal{W}_0(\beta) - \frac{g}{2\beta} \int \mathrm{d}t \, \mathrm{d}^d x \left(\langle \varphi(t, x) \bar{\varphi}(t, x) \rangle \right)^2 + O(g^2).$$

Translation invariance implies that the two-point function at coinciding points is independent of t, x and thus the integral over space and Euclidean time generates a factor $L^d\beta$. Then one faces the sgn(0) problem. The convention dictated by normal order is

$$\Delta(0, \mathbf{p}) = \frac{1}{e^{\beta(p^2/2m-\mu)} - 1}$$

and the result is then simply the square of the leading order density:

$$\mathcal{W}(\beta) = \mathcal{W}_0(\beta) - gL^d \left[\frac{1}{(2\pi\hbar)^d} \int \frac{\mathrm{d}^d p}{\mathrm{e}^{\beta(p^2/2m-\mu)} - 1} \right]^2 + O(g^2).$$

High temperature. The periodic boundary conditions in the Euclidean time direction imply that the field can be expanded on a basis of periodic functions of period β ,

$$\varphi(t,x) = \sum_{\nu \in \mathbb{Z}} e^{2i\pi\nu t/\beta} \,\varphi_{\nu}(x), \quad \bar{\varphi}(t,x) = \sum_{\nu \in \mathbb{Z}} e^{2i\pi\nu t/\beta} \,\bar{\varphi}_{\nu}(x).$$

At high temperature, $\beta \rightarrow 0$, in the action the time derivative suppresses the contribution of all non-zero modes. In this limit, the field can be approximated by the zero mode. Note that high temperature is defined with respect to, for instance, the correlation length ξ that characterizes the decay of correlation functions in space directions. In terms of the thermal wavelength $\lambda_{\rm th}$, the condition, which can be written as

$$\lambda_{\rm th} = \hbar \sqrt{\beta/m} = \sqrt{\hbar^2/mT} \ll \xi \,, \label{eq:lambda}$$

is satisfied at high temperature for finite correlation length, or at finite temperature when the correlation length diverges, that is, near a second-order phase transition.

The action (4.70) can then be approximated as

$$\mathcal{S}(\varphi,\bar{\varphi}) = \beta \int \mathrm{d}^d x \left[\bar{\varphi}_0(x) \left(-\hbar^2 \nabla^2 / 2m - \mu \right) \varphi_0(x) + \frac{1}{2} g \left(\bar{\varphi}_0(x) \varphi_0(x) \right)^2 \right], \qquad (4.72)$$

an action that we study systematically in the context of Euclidean QFT, and which is relevant to the superfluid phase transition (see Section 15.10).

4.5 Fermion representation and complex Grassmann algebras

To construct a formalism for fermions parallel to the one describing bosons as in Section 4.3, we now introduce Grassmann algebras. Grassmann algebras together with the rules of differentiation and integration have been described in Sections 1.5–1.7. We assume that the fermions can occupy a finite number ν of states and their number is not fixed.

4.5.1 Analytic Grassmann functions, scalar product

We consider a Grassmann algebra \mathfrak{C} with two sets of generators $\{\theta_i, \bar{\theta}_i\}, i = 1, \ldots, \nu$. We generalize the considerations of Section 4.3 to fermions. 'Analytic' Grassmann functions are elements of the subalgebra \mathfrak{A} of functions of θ_i variables only:

$$\frac{\partial \psi}{\partial \bar{\theta}_i} = 0 \,, \quad \forall i \,.$$

Analytic Grassmann functions form a complex vector space of dimension 2^{ν} . This is in direct relation with Fermi–Dirac statistics for a system with ν states: each state can either be empty or occupied by one fermion. Analytic functions have an expansion of the form

$$\psi(\theta) = \sum_{n=0}^{\nu} \frac{1}{n!} \sum_{i_1, i_2, \dots, i_n} \psi_{i_1 i_2 \dots i_n} \theta_{i_1} \theta_{i_2} \cdots \theta_{i_n}$$

Since the product of Grassmann generators is antisymmetric, the complex coefficients $\psi_{i_1i_2...i_n}$, amplitude of the vector on an *n*-particle state, can be chosen antisymmetric in all indices and this enforces the Pauli principle for fermions.

Scalar product of Grassmann analytic functions. In the same way as for analytic complex functions (expression (4.41)), a scalar product between two analytic Grassmann functions ψ_1 and ψ_2 can be defined by (two different forms are possible, see *e.g.*, Ref. [18]),

$$(\psi_1, \psi_2) = \int \left(\prod_i \mathrm{d}\theta_i \mathrm{d}\bar{\theta}_i\right) \exp\left(\sum_i \bar{\theta}_i \theta_i\right) \,\psi_1^{\dagger}(\theta) \,\psi_2(\theta). \tag{4.73}$$

With this definition, the norm of a vector ψ is positive and given by

$$\|\psi\|^2 = (\psi, \psi) = \sum_{n=0}^{\nu} \frac{1}{n!} \sum_{i_1, i_2, \dots, i_n} |\psi_{i_1 i_2 \dots i_n}|^2.$$

If the function ψ has unit norm, the quantity $\frac{1}{n!} \sum_{i_1, i_2, \dots, i_n} |\psi_{i_1 i_2 \dots i_n}|^2$ is the probability to find the quantum system in an *n*-fermion state.

The ' δ '-function. In Grassmann algebras, the role of the Dirac δ -function is played by the function θ itself, since

$$\int \mathrm{d}\theta \,\theta f(\theta) = f(0),$$

in which f(0) means the constant part of the affine function $f(\theta)$. The $\delta(\theta)$ -function has the convenient integral representation, analogous to a Fourier transform,

$$f(0) = \int d\theta \, d\bar{\theta} \, e^{\bar{\theta}\theta} \, f(\theta). \tag{4.74}$$

4.5.2 Operator algebra and kernels

Operator algebra. We have already introduced in Section 1.6.1 the algebra of operators $\{\theta_i, \partial/\partial \theta_i\}$ acting by left multiplication and differentiation on the algebra \mathfrak{A} of Grassmann functions. They satisfy the commutation relations of the usual fermion annihilation and creation operators (see relations (1.48)) and are Hermitian conjugate with respect to the scalar product (4.73).

For example, a Hamiltonian H_0 for non-interacting fermions that can occupy ν states of energies $\hbar \omega_i$ is represented by

$$H_0 = \sum_{i=1}^{\nu} \hbar \omega_i \,\theta_i \frac{\partial}{\partial \theta_i} \,, \tag{4.75}$$

as one can verify by explicit calculation,

$$H_0 \sum_{i_1, i_2, \dots, i_n} \psi_{i_1 i_2 \dots i_n} \theta_{i_1} \theta_{i_2} \cdots \theta_{i_n} = \sum_{i_1, i_2, \dots, i_n} \hbar(\omega_{i_1} + \omega_{i_2} + \dots + \omega_{i_n}) \psi_{i_1 i_2 \dots i_n} \theta_{i_1} \theta_{i_2} \cdots \theta_{i_n} .$$

The operator number of particles N, which commutes with the Hamiltonian when the number of fermions is conserved, is obtained from H_0 by replacing all $\hbar\omega_i$ by 1:

$$N = \sum_{i=1}^{\nu} \theta_i \frac{\partial}{\partial \theta_i}.$$
(4.76)

The identity as a kernel. A representation of the identity $\mathcal{I}(\theta, \bar{\theta})$ as a kernel (element of \mathfrak{C}) follows from the existence of an orthonormal basis:

$$\mathcal{I}(\theta,\bar{\theta}) = \prod_{i} (1+\theta_i\bar{\theta}_i) = \exp\left(-\sum_{i}\bar{\theta}_i\theta_i\right).$$
(4.77)

A direct verification relies on the identity (4.74),

$$\int \prod_{i} \mathrm{d}\theta'_{i} \mathrm{d}\bar{\theta}'_{i} \mathcal{I}(\theta, \bar{\theta}') \exp\left(\sum_{i} \bar{\theta}'_{i} \theta'_{i}\right) f(\theta') = \int \prod_{i} \mathrm{d}\theta'_{i} \mathrm{d}\bar{\theta}'_{i} \exp\left(\sum_{i} \bar{\theta}'_{i} (\theta'_{i} - \theta_{i})\right) f(\theta')$$
$$= f(\theta). \tag{4.78}$$

Quantum statistical physics

Operator algebra and kernels. Using the anticommutation relations, we commute all multiplication operators to the left of all differentiation operators, writing all operators in *normal order*. We then use equation (4.78) to associate to each element of this operator algebra a kernel,

$$\theta_{i_1}\theta_{i_2}\dots\theta_{i_p}\frac{\partial}{\partial\theta_{j_1}}\frac{\partial}{\partial\theta_{j_2}}\dots\frac{\partial}{\partial\theta_{j_q}}\mathcal{I}(\theta,\bar{\theta}) = \theta_{i_1}\theta_{i_2}\dots\theta_{i_p}\bar{\theta}_{j_1}\bar{\theta}_{j_1}\dots\bar{\theta}_{j_q}\mathcal{I}(\theta,\bar{\theta}), \tag{4.79}$$

which belongs to the Grassmann algebra \mathfrak{C} .

Such an operator $O(\theta, \partial/\partial \theta)$ defined by its kernel $\mathcal{O}(\theta, \overline{\theta})$,

$$O(\theta, \partial/\partial\theta) \mapsto \mathcal{O}(\theta, \bar{\theta}) \equiv \langle \theta | \mathcal{O} | \bar{\theta} \rangle = O(\theta, \bar{\theta}) \mathcal{I}(\theta, \bar{\theta}), \tag{4.80}$$

then acts on a function as

$$(Of)(\theta) = \int \prod_{i} \mathrm{d}\theta'_{i} \mathrm{d}\bar{\theta}'_{i} \,\mathcal{O}(\theta, \bar{\theta}') \exp\left(\sum_{i} \bar{\theta}'_{i} \theta'_{i}\right) f(\theta'). \tag{4.81}$$

The kernel associated with the product $\mathcal{O}_2\mathcal{O}_1$ is given by

$$\langle \theta | \mathcal{O}_2 \mathcal{O}_1 | \bar{\theta} \rangle = \int \prod_i \mathrm{d}\theta'_i \mathrm{d}\bar{\theta}'_i \langle \theta | \mathcal{O}_2 | \bar{\theta}' \rangle \exp\left(\sum_i \bar{\theta}'_i \theta'_i\right) \langle \theta' | \mathcal{O}_1 | \bar{\theta} \rangle.$$
(4.82)

Trace. The trace of an operator is

$$\operatorname{tr} \mathcal{O} = \int \prod_{i} \mathrm{d}\bar{\theta}_{i} \mathrm{d}\theta_{i} \exp\left(-\sum_{i} \bar{\theta}_{i} \theta_{i}\right) \left\langle \theta \right| \mathcal{O} \left|\bar{\theta}\right\rangle.$$
(4.83)

Note the difference of sign in the exponentials between expressions (4.82) and (4.83). One can verify that the sign in (4.83) is consistent with the cyclic property of the trace.

Hamiltonian and number operator. The Hamiltonian (4.75) is then represented by

$$\langle \theta | H_0 | \bar{\theta} \rangle = \mathcal{I}(\theta, \bar{\theta}) \sum_i \hbar \omega_i \theta_i \bar{\theta}_i ,$$
 (4.84)

and the particle number operator by

$$\langle \theta | N | \bar{\theta} \rangle = \mathcal{I}(\theta, \bar{\theta}) \sum_{i} \theta_{i} \bar{\theta}_{i} .$$
 (4.85)

Complex conjugation and Hermitian conjugation of operators. The Hermitian conjugation for operator kernels is the Hermitian conjugation in the algebra \mathfrak{C} as defined by (equations (1.67)). One can verify that H_0 and N are Hermitian.

4.5.3 An example: One state system

As a consequence of the Pauli principle, the vector space for particles obeying the Fermi– Dirac statistics (fermions) that can occupy only one state reduces to a two-dimensional complex vector space: a state can only be empty (the vacuum) or occupied once.

A superposition of the zero-particle and one-particle states is represented by the affine complex function

$$\psi(\theta) = \psi_0 + \psi_1 \theta$$
, $(\psi_0, \psi_1) \in \mathbb{C}^2$.

If the function ψ is normalized by the scalar product (4.73), $\|\psi\|^2 = (\psi, \psi) = 1$, $|\psi_0|^2$ and $|\psi_1|^2$ represent the respective probability for the system to be in the vacuum state or in the occupied state. The Hamiltonian

$$H_0 = \hbar \omega \theta \frac{\partial}{\partial \theta}, \quad \omega > 0, \qquad (4.86)$$

has the eigenvalue 0 for the vacuum state and $\hbar\omega$ for the one-particle state. The corresponding kernel is

$$\langle \theta | H_0 | \bar{\theta} \rangle = \hbar \omega \theta \frac{\partial}{\partial \theta} e^{-\bar{\theta}\theta} = \hbar \omega \theta \bar{\theta} e^{-\bar{\theta}\theta} = -\hbar \omega \bar{\theta} \theta .$$
 (4.87)

One can verify that the matrix elements of the operator $U_0(t) = e^{-tH_0/\hbar}$ are

$$\langle \theta | U_0(t) | \bar{\theta} \rangle = e^{-\bar{\theta}\theta \, e^{-\omega t}}. \tag{4.88}$$

With our definition, both kernels are invariant under complex conjugation. From the explicit expression (4.88) and the definition (4.83), one infers the partition function

$$\mathcal{Z}_{0}(\beta) = \operatorname{tr} U_{0}(\hbar\beta) = \int \mathrm{d}\bar{\theta} \,\mathrm{d}\theta \,\,\mathrm{e}^{-\bar{\theta}\theta} \,\mathrm{e}^{-\hbar\omega} = 1 + \mathrm{e}^{-\hbar\omega\beta} \,\,. \tag{4.89}$$

Negative energy states. If, in the Hamiltonian (4.86), ω is negative, the occupied state has an energy lower than the vacuum. This means that the two states have been misidentified; they have to be interchanged. A simple transformation deals with the problem. In the kernel (4.87), one sets $\eta = \bar{\theta}, \bar{\eta} = \theta$.

4.6 Path integrals with fermions

The derivation of a path integral representation for the statistical operator of fermion systems closely follows the method of Sections 4.1 and 4.2.1, with the Grassmann variables replacing the complex variables.

We first construct a path integral representation for the statistical operator (4.88). Path integrals are certainly not required to deal with this simple example. However, the path integral representation is useful, because it can easily be generalized to an arbitrary number of possible fermion states.

We expand the exact expression (4.88) for a small time-interval ε as

$$\left\langle \theta \left| U_0(\varepsilon) \right| \bar{\theta} \right\rangle = \exp\left[-\bar{\theta} \theta \left(1 - \omega \varepsilon \right) + O\left(\varepsilon^2 \right) \right].$$
 (4.90)

The product form (4.82) makes it possible to write the statistical operator at finite time as

$$\left\langle \theta'' \left| U_0(t'',t') \right| \bar{\theta}' \right\rangle = \lim_{n \to \infty} \int \prod_{k=1}^{n-1} \mathrm{d}\theta_k \mathrm{d}\bar{\theta}_k \, \exp\left[-\mathcal{S}_{\varepsilon}(\theta,\bar{\theta}) \right], \tag{4.91}$$

with

$$S_{\varepsilon}(\theta,\bar{\theta}) = \bar{\theta}_0 \theta_1 + \sum_{k=1}^{n-1} \bar{\theta}_k \left(\theta_{k+1} - \theta_k\right) - \varepsilon \sum_{k=0}^{n-1} \omega \bar{\theta}_k \theta_{k+1}, \qquad (4.92)$$

where $\varepsilon = (t'' - t')/n$ and $\bar{\theta}_0 \equiv \bar{\theta}', \ \theta_n \equiv \theta''$.