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Path Integrals in Quantum Mechanics and Low-Dimensional QFT

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Abstract

The focus of this thesis is to introduce the path integral and some of its applications. One interpretation of quantum mechanics is that a microscopic system which moves from an initial- to a final state moves through each possible intermediate state. The path integral uses the principle of least action to sum over all such intermediate states to find the evolution of a quantum mechanical system. We compare the path integral approach to that of the Schrödinger equation and show that the two give an equivalent description of quantum mechanics.

To demonstrate the usefulness of the path integral, we introduce low-dimensional quantum field theory (QFT). In particular, we discuss Feynman diagrams. The idea behind Feynman diagrams is to sum over all possible weak interactions between fields to evaluate the properties of a system through the path integral. We also carry out a computation of a low energy effective action in a 0-dimensional model. The result of the computation shows that there is free energy also in a vacuum. Finally, we briefly generalize some of the previous discussion to 1-dimensional QFT. To give an example of a practical application, we give a qualitative discussion of how the path integral can be applied to statistical mechanics to predict the behaviour of superfluids.

Sammanfattning

Målet med den här rapporten är att introducera konceptet vägintegral och några av dess applikationer. En tolkning av kvantmekanik är att ett mikroskopiskt system som går från ett initialt- till ett slutgiltigt tillstånd kommer att passera genom alla möjliga mellanliggande tillstånd. Vägintegralen använder sig av principen om minsta verkan för att summera över alla sådana mellanliggande tillstånd för att hitta utvecklingen hos ett system. Vi kommer att jämföra vägintegralen med Schrödingers ekvation och visa att de två ger en ekvivalent beskrivning av kvantmekaniken.

För att demonstrera vägintegralens användbarhet introducerar vi lågdimensionell kvantfältteori. Vi diskuterar speciellt Feynmandiagram. Idén bakom Feynmandiagram är att summera över alla möjliga svaga interaktioner mellan fält för att utvärdera fysikaliska egenskaper hos system med hjälp av vägintegraler. Vi kommer också att utvärdera en effektiv verkan i 0-dimensionell kvantfältteori. Resultatet visar att det finns fri energi även i ett vakuum. Slutligen generaliserar vi delar av vår tidigare diskussion till 1-dimensionell kvantfältteori. Som ett exempel på praktiska applikationer för vi en kvalitativ diskussion kring hur vägintegraler kan användas inom statistisk mekanik för att förutsäga egenskaper hos superfluidier.

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1 Introduction

Quantum mechanics was originally formulated using Hamiltonian mechanics. This was the natural choice over Lagrangian mechanics since Hamiltonian mechanics is described by a set of canonical coordinates and momenta in phase space. (For an introduction to analytical mechanics, see Goldstein et al. [14]). In quantum mechanics, we can use Hermitian *operators* in Hilbert space, denoted by a hat, which satisfy similar commutation relations as those for the classical canonical variables. To go from the classical theory to the quantum theory, we make the exchange [25]

$$\{A, B\} \rightarrow \frac{[\hat{A}, \hat{B}]}{i\hbar}.$$

Here, $\{\}$ denotes a Poisson bracket. If A and B are functions of some coordinates q_i and conjugate momenta p_i , the Poisson bracket has the property $\{A, B\} = \frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial B}{\partial q_i} \frac{\partial A}{\partial p_i}$. The index i implies a sum over all variables. In the quantum mechanical case, $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ is a commutator, and \hat{A} and \hat{B} are constructed from operators. We may also formulate a Hamiltonian from such operators, and this Hamiltonian generates the time evolution of our system. This relatively simple transition from the classical theory to the quantum theory motivates the use of Hamiltonian formalism in quantum mechanics.

When Dirac proposed what was to become the path integral in 1933 [6], he did it with the intention of implementing Lagrangian formalism in quantum mechanics. Why, if Hamiltonian formalism works so well, would we switch to Lagrangian formalism? Partly because the latter can be considered more fundamental. Lagrangian mechanics is based on the action principle, and there is no equivalent action principle involving the coordinates and conjugate momenta in Hamiltonian mechanics. The Lagrangian is constructed from the kinetic energy and the potential energy of a system. The same cannot always be said about the Hamiltonian. Second, the Lagrangian formalism is more suitable for special relativity. This is because the action is a scalar quantity, and therefore invariant under coordinate transformations, e.g. Lorentz transformations. The Hamiltonian formalism is not compatible with special relativity: it involves a fixed time which is taken to be the same in all reference frames. Under a Lorentz transformation, the time parameter changes, and Hamiltonian mechanics breaks down. Lagrangian mechanics instead treats time and space on equal footing. This is useful when we want to combine quantum mechanics and special relativity, for example in quantum field theory, or QFT.

The complete formulation of the path integral was realized by Feynman in 1942 [10]. Feynman also showed that the path integral is equivalent to the Schrödinger equation in evaluating the time-evolution of a quantum mechanical system. We will prove the same in this thesis. The idea of the path integral is to sum, or integrate, over all possible paths for a system as it evolves from an initial state to a final state. This integral gives us the probability amplitude for the evolution of the system. Each path is weighed by a phase factor where the phase is given by the classical action. This approach to quantum

mechanics is attractive not only for the discussion about Lagrangian mechanics above, but also from a theoretical standpoint. One way to interpret quantum mechanics is to imagine that a quantum mechanical system takes not one path from a state to another, but every possible intermediate path simultaneously.

The path integral is however rarely used in non-relativistic quantum mechanics. But it has many other applications, notably in QFT. QFT treats fields, such as the electromagnetic field, and combines quantum mechanics, classical field theory and special relativity. It is a theory which revolves around counting all possible ways that a process can occur, and the path integral is well suited for this. In this thesis, we introduce path integrals in QFT through the partition function, which is a central equation in QFT containing much information about the physical properties of a system. However, it is often difficult to evaluate these path integrals. To simplify computation, one can use several tools, e.g. perturbation theory, which involves Feynman diagrams. The idea behind Feynman diagrams is to sum over all possible weak interactions between fields to evaluate terms in perturbation expansions. Another important aspect of QFT is symmetries. In general, finding symmetries of the action puts constraints on the dynamics of a system and helps us evaluate its physical properties. The specific symmetry which will be discussed in this thesis is supersymmetry, i.e. a symmetry between bosonic- and fermionic fields. For QFT:s possessing this symmetry, computations often simplify.

Today, the path integral is one of the cornerstones in many field theories. It has applications in e.g. statistical mechanics and string theory [18] [3]. One specific application is brought up in this thesis: the predictive power of the path integral for the behaviour of superfluids. A superfluid is a fluid which adopts exotic behaviours at low temperatures. For example, at a specific temperature, its heat capacity grows exponentially and it no longer experiences friction.

In conclusion, it is well worth the time to gain some understanding of the path integral and its role in modern physics. This thesis is a literature study of path integrals in quantum mechanics and QFT. It aims to explain the following questions at the level of a bachelor student.

- Why was the path integral introduced in quantum mechanics and how is it defined?
- What are the fundamental properties of the path integral in quantum mechanics?
- How can one prove equivalence between the path integral and the Schrödinger equation in quantum mechanics?
- How is the path integral used in QFT, specifically in the formulation of the partition function?
- How do Feynman diagrams and supersymmetry facilitate evaluation of path integrals?

- How can path integrals be used in statistical mechanics to predict the behaviour of superfluids?

As an illustration of the above points, we will perform a computation using path integrals. More specifically, we study an effective action in a 0-dimensional QFT and evaluate some properties of the system using both classical mechanics and QFT. We then compare the results.

We also seek a deeper understanding of quantum theories throughout, from the point of view of this new formalism.

2 Important Concepts in Quantum Mechanics

We begin with some background theory. In section 2.1, we discuss the Lagrangian formalism and how one can apply it to quantum mechanics. The discussion is based mainly on Dirac's original article on the subject from 1933 [6]. It also involves some input from Feynman's PhD thesis from 1942 [10] and Brown's summary of Feynman's PhD thesis [1]. This provides some of the mathematical foundation for the path integral.

In sections 2.2-2.5, we discuss wave-particle duality and the strange nature of quantum mechanical systems, which gives a more intuitive understanding of the path integral. The discussion is based on Feynman and Hibbs [11, ch. 1-5].

2.1 The Lagrangian in Quantum Mechanics

In the introduction, we discussed reasons for wanting to introduce Lagrangian formalism in quantum mechanics. However, there are issues with translating Lagrangian mechanics directly to quantum mechanics. (We give a brief summary of the central equations in Lagrangian- and Hamiltonian mechanics in Appendix A.) In Lagrangian mechanics, the time evolution of a system is obtained from the Euler-Lagrange equations. These equations involve partial derivatives of the Lagrangian $L = L(q, \dot{q}, t)$ with respect to some generalized coordinates q, \dot{q} . In quantum mechanics, these variables are replaced with operators, and it is not obvious how to define derivatives of operators; the derivative is itself an operator, and operators do not act on other operators.

Thus we cannot directly apply the Euler-Lagrange equations in quantum mechanics. Instead we must introduce the Lagrangian by another method. Dirac suggested we find a generating function which gives a time-transformation of the variables of our system, to find its evolution. To achieve this, we begin with classical mechanics and a more general transformation: that from some independent variables (q, p) to some other independent variables (Q, P) , such that

$$\begin{aligned} Q &= Q(q, p, t), \\ P &= P(q, p, t). \end{aligned} \tag{2.1}$$

For simplicity, we examine the case with only one coordinate and one conjugate momenta. The variables in equation (2.1) must fulfill

$$\boxed{\begin{aligned} P &= -\frac{\partial F}{\partial Q}, \\ p &= \frac{\partial F}{\partial q}. \end{aligned}} \quad (2.2) \quad \boxed{\begin{aligned} P &= \frac{\partial L}{\partial \dot{Q}}, \\ p &= \frac{\partial L}{\partial \dot{q}}. \end{aligned}} \quad (2.3)$$

The equations (2.2) is the general formalism of canonical transformations given some generating function $F(q, Q, t)$. The equations (2.3) are the definitions of conjugate momenta, see for example Goldstein et al. [14]. To find a transformation *in time*, we impose $(Q, P) = (q_i, p_i)$, in which (q_i, p_i) is the coordinate and conjugate momentum at the initial time t_i , and $(q, p) = (q_f, p_f)$, where (q_f, p_f) is the coordinate and conjugate momentum at a later time t_f . We also introduce q_k as the coordinate at some time in the interval $[t_i, t_f]$. We note that equations (2.2) are fulfilled if we let

$$\boxed{F = S = \int_{t_i}^{t_f} L(q, \dot{q}, t) dt.} \quad (2.4)$$

A demonstration of this is given below. It may be skipped by the reader.

We demonstrate that equation (2.4) fulfills the desired relations (2.2) by considering the expression

$$\frac{\partial S}{\partial q_k} = \int_{t_i}^{t_f} \left(\frac{\partial L}{\partial q} \frac{\partial q}{\partial q_k} + \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial q_k} \right) dt. \quad (2.5)$$

We use integration by parts on the second term in the integrand

$$\begin{aligned} \int_{t_i}^{t_f} \frac{\partial L}{\partial \dot{q}} \frac{\partial \dot{q}}{\partial q_k} dt &= \{\text{EL-equations, Appendix A}\} = \left[\frac{\partial L}{\partial \dot{q}} \frac{\partial q}{\partial q_k} \right]_{t_i}^{t_f} - \int_{t_i}^{t_f} \frac{\partial L}{\partial q} \frac{\partial q}{\partial q_k} dt \\ &= \{\text{Equation (2.3)}\} = p_f \frac{\partial q_f}{\partial q_k} - p_i \frac{\partial q_i}{\partial q_k} - \int_{t_i}^{t_f} \frac{\partial L}{\partial q} \frac{\partial q}{\partial q_k} dt. \end{aligned} \quad (2.6)$$

We use equation (2.6) to rewrite equation (2.5) and obtain

$$\frac{\partial S}{\partial q_k} = p_f \frac{\partial q_f}{\partial q_k} - p_i \frac{\partial q_i}{\partial q_k}.$$

By setting $q_k = q_i, q_f$ we obtain

$$\boxed{\begin{aligned} p_i &= -\frac{\partial S}{\partial q_i}, \\ p_f &= \frac{\partial S}{\partial q_f}. \end{aligned}}$$

which agrees with equations (2.2).

The above discussion about transformations has involved only classical mechanics. We return to quantum mechanics, where a canonical transformation between two coordinate representations is given by some transformation function $\langle q|Q\rangle$. We can write

$$\langle q|\hat{q}|Q\rangle = q \langle q|Q\rangle, \quad (2.7)$$

$$\langle q|\hat{p}|Q\rangle = -i\hbar \frac{\partial}{\partial q} \langle q|Q\rangle, \quad (2.8)$$

$$\langle q|\hat{Q}|Q\rangle = Q \langle q|Q\rangle, \quad (2.9)$$

$$\langle q|\hat{P}|Q\rangle = i\hbar \frac{\partial}{\partial Q} \langle q|Q\rangle. \quad (2.10)$$

\hat{q}, \hat{Q} simply pick out the position eigenvalue and \hat{p} acts as a derivative. For a derivation of this, see Sakurai and Napolitano [25, p. 52]. Equation (2.10) follows naturally from the property demonstrated in equation (2.8), since $\langle q|\hat{P}|Q\rangle = \overline{\langle Q|\hat{P}|q\rangle} = \overline{-i\hbar \frac{\partial}{\partial Q} \langle Q|q\rangle} = i\hbar \frac{\partial}{\partial Q} \langle q|Q\rangle$. This holds since \hat{p} is a hermitian operator.

Equations (2.7)-(2.10) have great implications. If we consider some function $\hat{g} = \hat{g}(\hat{q}, \hat{Q}, t)$, then equation (2.7) and (2.9) imply

$$\langle q|\hat{g}(\hat{q}, \hat{Q}, t)|Q\rangle = g(q, Q, t) \langle q|Q\rangle. \quad (2.11)$$

This is easily seen for every function which can be rewritten as a power series. Again, \hat{q}, \hat{Q} are operators and q, Q are variables in equation (2.11).

We make an ansatz for our transformation function, $\langle q|Q\rangle = e^{\frac{i}{\hbar}U}$, where U is a function of the form $U = U(q, Q, t)$. We get, from equation (2.8) and (2.10)

$$\begin{aligned} \langle q|\hat{p}|Q\rangle &= \frac{\partial}{\partial q} U(q, Q) \langle q|Q\rangle, \\ \langle q|\hat{P}|Q\rangle &= -\frac{\partial}{\partial Q} U(q, Q) \langle q|Q\rangle. \end{aligned} \quad (2.12)$$

Comparison between (2.12) and (2.11) gives

$$\hat{p} = \frac{\partial \hat{U}}{\partial \hat{q}}, \quad \hat{P} = -\frac{\partial \hat{U}}{\partial \hat{Q}}. \quad (2.13)$$

Equation (2.13) implies that \hat{U} is the quantum analogue of our generating function F in equation (2.2). By equation (2.4), we also have $F = S$, so that our transformation function is given by

$$\langle q_f | q_i \rangle = e^{\frac{i}{\hbar} U}, \quad (2.14)$$

where U is the quantum analogue of the classical action. $U(q_i, q_f, t)$ is a function of the coordinate at the initial time and the coordinate at the final time. It is reasonable to postulate that equation (2.14) holds only for infinitesimal time intervals $[t, t + \epsilon]$, since in this case, both the velocity and the position of the system can be expressed in terms of the initial- and final coordinates. This is because we can set the velocity to be constant and the position to be an intermediate point.

Dirac also introduced a classical analogue to $\langle q_f | q_i \rangle$ called $A(t_f, t_i)$, where

$$A(t_f, t_i) = \exp \left[\frac{i}{\hbar} L dt \right],$$

where L is the classical Lagrangian. Also $A(t_f, t_i)$ is valid only for an infinitesimal transformation. To achieve a finite transformation in time, we must apply many such consecutive infinitesimal transformations. In the classical case, we get

$$A(tT) = A(tt_m)A(t_m t_{m-1})A(t_{m-1} t_{m-2})A(t_{m-2} t_{m-3}) \dots A(t_1 T).$$

The corresponding finite transformation in quantum mechanics can be constructed by considering some finite transformation from t to T and introducing a complete basis at every intermediate timestep. According to the mathematical formalism of quantum mechanics, the resulting expression is given by

$$\langle q_t | q_T \rangle = \int \int \dots \int \langle q_t | q_m \rangle dq_m \langle q_m | q_{m-1} \rangle dq_{m-1} \langle q_{m-1} | q_{m-2} \rangle dq_{m-2} \dots \langle q_2 | q_1 \rangle dq_1 \langle q_1 | q_T \rangle. \quad (2.15)$$

Equation (2.15) implies that the path taken by a quantum mechanical system is not deterministic. At each intermediate step between the initial and final time, we must integrate over all possible positions for our system.

The above discussion by Dirac comes very close to Feynman's final formulation of the path integral, although Dirac's transformation function is missing a normalizing factor. Also, while Dirac argued that U in equation (2.14) is the quantum analogue of the classical action, Feynman showed in his PhD thesis that it is actually equivalent to the classical action. We prove the same in section 3.4.

2.2 Wave-Particle Duality and a Brief History of Quantum Theory

Particles can be described as both localized particles and as waves: which description is the most accurate depends on the system we choose to investigate and also on the way in which we measure it. Historically, the concept of wave-particle duality has been widely discussed, and the debate was first settled for photons. The wave nature of light was well explained by Maxwell's equations, first formulated in 1865 [20] and the theory of quantized light was proposed by Planck as he attempted to solve the problem of black-body radiation in 1901 [23]. The combined theory of wave-particle duality for photons was proposed by Einstein as he discovered the photoelectric effect in 1905 [8]. Later, de Broglie proposed in his PhD thesis in 1924 that the theory of wave-particle duality should be extended to all particles [21]. Later experiments confirmed this for electrons [5] and other particles. The complete theory of wave-particle duality is part of today's quantum mechanics, developed in the 1920s [15].

Later in this report, we discuss quantum field theory, QFT. The foundations of QFT was laid out as early as 1927 by Paul Dirac as he attempted to quantize the electromagnetic field [7][19]. Quantum fields showed early promise as they could describe both antimatter and annihilation- and creation of particles. QFT also combined special relativity and quantum mechanics, which was another reason for its development [29]. The formulation of QFT continued throughout the 1900s and is the subject of much current research. Feynman made many important contributions, among others his Feynman diagrams which appeared in print for the first time in 1949 [12]. They will be discussed in section 5.1.

2.3 The Double-Slit Experiment

A famous demonstration of wave-particle duality is the double-slit experiment, first performed with photons in 1801 by Thomas Young [30][28]. However, Young argued at the time that the result of his experiment was proof of the wave nature of light, rather than of wave-particle duality.

The experiment is conducted as follows. Particles are emitted from a source and allowed to pass through two narrow slits in a wall, and then strike a detector. Each particle is detected at some location in the detector, thus the particles behave as localized particles when we measure their spatial position. The original experiment in 1801 was not sophisticated enough to detect individual particles, which explains Young's original conclusion. If we leave our detector on for some time, we are left with a pattern made up of many detected particles. If we allow the particles to pass through only one of the slits, we observe a smooth distribution in the detector, with a maximum in front of the open slit. If we allow the particles to pass through both slits, we observe bands of alternating high and low intensity. This behaviour is observed even if we allow just one particle at a time to pass through the experiment. Since the intensity from both slits in our experiment cannot be explained as the superposition of intensities from slit 1 and slit

2, each particle cannot have passed through just one slit or the other. Rather, it seems that the particles must be described as a non-localized waves, able to pass through both slits simultaneously. This behaviour is illustrated in figure (1).

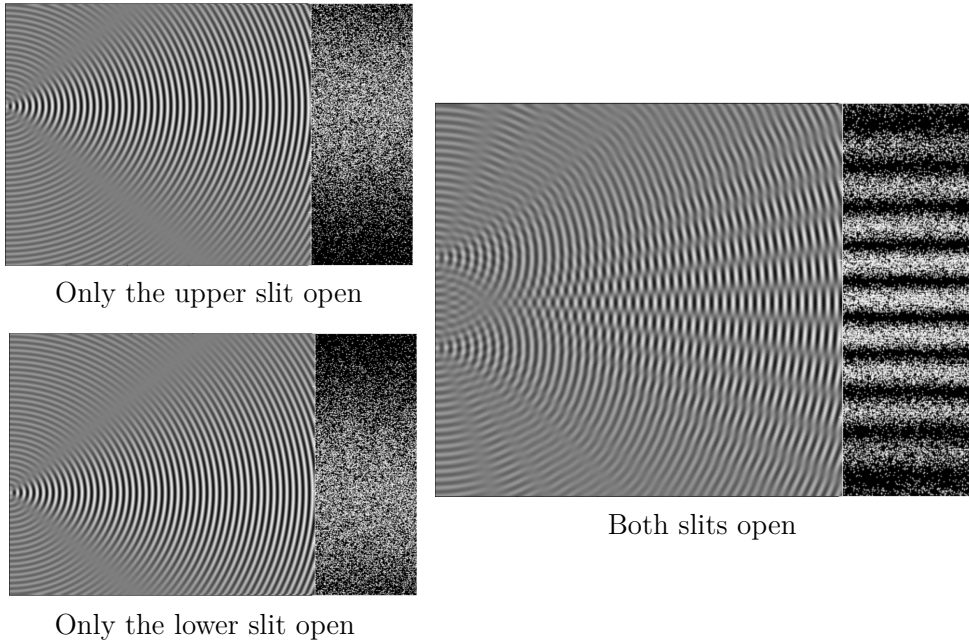


Figure 1: Illustration of the double-slit experiment, where the slits are on the left hand side and the detector is on the right hand side, with white dots representing detected particles. The figures were generated in Python.

We denote the amplitude of a particle wave just before it strikes some point in the detector Φ . We think of the slits as two particle sources, where the amplitude for arriving in the detector after passing through the upper slit is denoted by Φ_1 and similarly Φ_2 for the lower slit. In general, to obtain the intensity of a wave, we square its amplitude. If our two sources are independent, we obtain the intensity in the detector as $I = |\Phi_1|^2 + |\Phi_2|^2$. If the two sources are not independent, but are instead interfering, we must add the amplitudes before taking the square as in

$$I = |\Phi_1 + \Phi_2|^2. \quad (2.16)$$

This is indeed the equation which describes the observed pattern in figure (1), with both slits open. Our particles are then best described as interfering waves as they pass through the experiment and as localized particles when they strike the detector. This is a clear demonstration of wave-particle duality.

We can of course determine which of the two slits a particle passes through on its way to the detector. We could for example place a light source after the slits. A photon from the light source then interacts with each particle just after it passes through one of the slits, and alerts us of its position. However, we disturb the momentum of the particle

in the process, and smear out the interference pattern to where it is no longer visible. The resulting pattern in the detector is the superposition of two smooth distributions: the one which results from keeping only slit 1 open, and the one from keeping only slit 2 open. It seems as though our measuring which slit the particles pass through results in the particles passing through only one slit at a time.

2.4 The Uncertainty Principle in Experiments

The discussion in the previous section demonstrates a general rule for all experiments. It is well expressed in Feynman and Hibbs [11, p.9]:

"Any determination of the alternative taken by a process capable of following more than one alternative destroys the interference between alternatives."

This is another version of Heisenberg's uncertainty principle. In the case of the double-slit experiment, it is easy to see that the statement above is compatible with the original statement by Heisenberg, $\Delta x \Delta p \geq \frac{\hbar}{2}$. When we try to determine the position of a particle with a light source, we necessarily introduce an uncertainty in its momentum. This means that we alter the trajectory of the particle, and we disturb the pattern in the detector.

2.5 The Kernel

The amplitudes in equation (2.16) can be written as $\Phi_i(b, a)$, where the index i again denotes the amplitude for a specific path through the experiment. The argument (b, a) specifies the endpoint and the starting point for the path. In other words, $b = (x_b, t_b)$ denotes that the path ends at the point x_b at the fixed time t_b . The initial point is similarly given by $a = (x_a, t_a)$. The total amplitude $\Phi(b, a) = \Phi_1(b, a) + \Phi_2(b, a)$ is the sum of the amplitudes for alternative paths through the experiment. In our case, it consists of the paths 1 and 2, as illustrated in figure (2). The amplitude $\Phi(b, a)$ is also associated with an intensity through equation (2.16). Properly normalized, the intensity gives the probability for any one particle to go from point x_a to point x_b in the time interval $t_b - t_a$. We therefore refer to $\Phi(b, a)$ as a *probability amplitude*, assuming it is properly normalized.

We would now like to make a more general statement. We imagine putting more walls in between the source and the detector in the double-slit experiment. We also make some extra slits in the walls. To find the total amplitude to go from the detector at point a to the point b , we must sum over the amplitudes from all possible paths between the two points. The scenario is illustrated in figure (3), where examples of 3 possible paths are drawn. We call this total amplitude the *kernel*

$$K(b, a) = \sum_i \Phi_i(b, a), \quad (2.17)$$

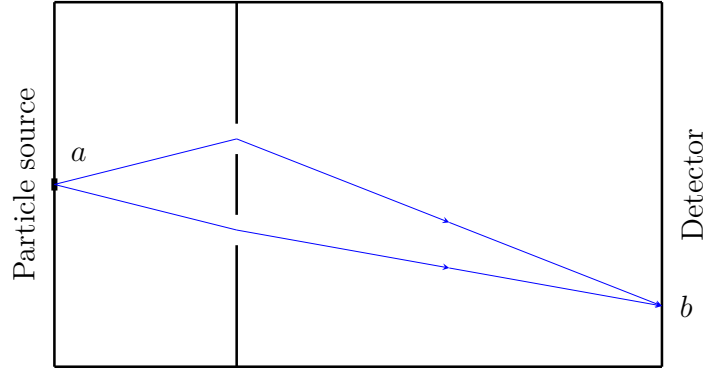


Figure 2: Two possible particle paths through the double-slit experiment.

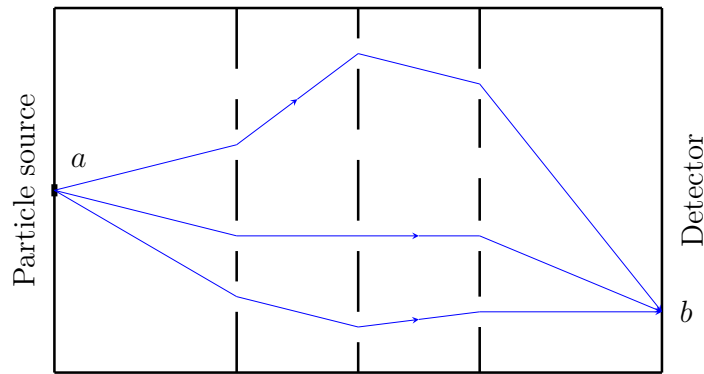


Figure 3: Three possible particle paths through a multiple-slit experiment.

If we keep putting up more walls and making more slits, eventually we have to sum over an infinite amount of paths through the space between a and b . The kernel in equation (2.17) is generalized to an integral

$$K(b, a) = C \int_a^b \mathcal{D}x(t) e^{\frac{i}{\hbar} S[b, a]}. \quad (2.18)$$

where C is some normalizing factor, and the notation $\mathcal{D}x(t)$ tells us that we must integrate over every possible path from (x_a, t_a) to (x_b, t_b) . The chosen path will in turn affect the value of $S[a, b]$, which is path-dependent. Equation (2.18) is Feynman's path integral. It is similar to Dirac's equation (2.15), except it involves the classical action, and it has been normalized to give the probability amplitude for the time evolution of our system.

Let us discuss some properties of the kernel in equation (2.18). We assume there is some intermediate time t_c , with $t_a < t_c < t_b$, when the system is at some point x_c . We want to know how to express the amplitude for several events occurring in succession. Probabilities for successive events multiply, and it follows that the associated probability amplitudes also multiply. We can write

$$K(b, a) = \int_{-\infty}^{\infty} K(b, c)K(c, a)dx_c. \quad (2.19)$$

Note that we must integrate over all possible positions x_c since the system may go through any possible point at time t_c .

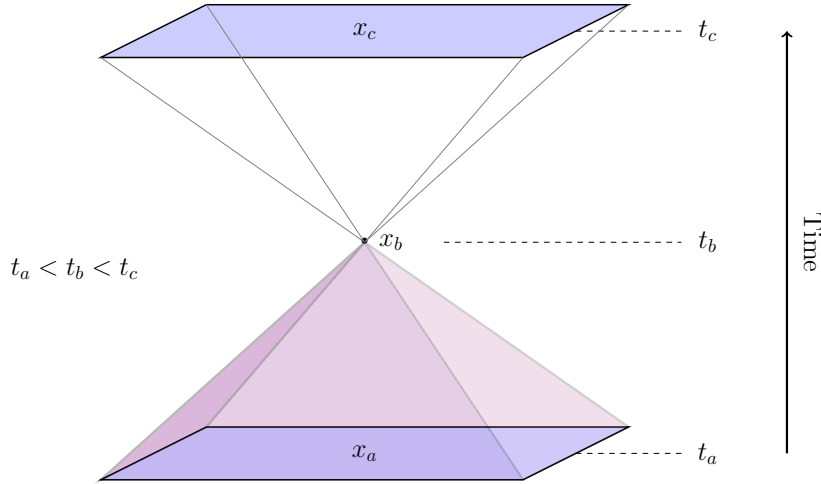


Figure 4: Evolution of a quantum mechanical system through time, from an infinite set of points x_a at time t_a to a final point (x_b, t_b) . The purple cone indicates that all states at the earlier time t_a influences the probability to arrive at (x_b, t_b) . However, no points at the later time t_c influences the probability to arrive at (x_b, t_b) , by causality.

Also, we want the kernel to be 0 for $t_a > t_b$. This is a statement about causality: events prior to t_b should affect the system at t_b , but later events should not. We put this restriction on the kernel in general

$$K(b, a) = 0 \text{ if } t_a > t_b. \quad (2.20)$$

One more thing: how is the kernel $K(b, a)$ related to the wave function of a system, $\psi(x, t)$? The absolute value squared of the wave function is the probability for the system to be in some state, much like the absolute value squared of the kernel. The difference between the two is that a kernel also carries information about some previous point in time; it is the amplitude that a system is in some state at t_b *given that it was in some previous state at t_a* . The wave function carries only information about the system at one specific time. We give some intuition for the relation between the two by the following relation

$$\psi(x_b, t_b) = \int_{-\infty}^{\infty} K(b, a)\psi(x_a, t_a)dx_a. \quad (2.21)$$

On the right hand side, we have the probability amplitude $\psi(x_a, t_a)$ for the system to be at the initial point (x_a, t_a) . We integrate this initial state against the amplitude $K(a, b)$ to go from point (x_a, t_a) to (x_b, t_b) and obtain the amplitude $\psi(x_b, t_b)$ for the system to arrive at the final point (x_b, t_b) .

We can visualize both equation (2.21) and the restriction (2.20) as in figure (4). We have a quantum mechanical system which evolves in time. If we want to find the amplitude for the system to be at (x_b, t_b) , we consider all possible initial points (x_a, t_a) and their associated amplitude $\psi(x_a, t_a)$. We integrate our initial states against the kernel $K(b, a)$, here visualized by the pink cone. By doing so, we obtain the amplitude for the system to be at (x_b, t_b) . No states at a later time t_c can contribute to this amplitude by causality, i.e. $K(b, c) = 0$. The blue planes are supposed to extend to infinity.

3 The Path Integral in Quantum Mechanics

This section is concerned with the validity of the path integral. In section 3.1 we show that the path integral behaves as expected in the classical limit, and in section 3.2-3.3 we evaluate the kernel of a free particle in position- and momentum basis. This gives us a concrete example of how to evaluate a path integral. It also shows that where we interpret the results, they correspond to our physical reality. Finally, in section 3.5, we show that the path integral formulation is equivalent to the Schrödinger formulation of quantum mechanics.

The discussion in section 3 is based on Feynman and Hibbs [11, ch. 2-4].

3.1 The Path Integral in the Classical Limit

It is important to emphasize that some paths give a negligible contribution to the path integral in equation (2.18). Let's consider a macroscopic system. This action in the argument of the exponential function is of the order of magnitude of a classical system. The action is divided by \hbar , which is of the order of magnitude of a microscopic system. Therefore, each path is weighed by a rapidly oscillating function $e^{\frac{i}{\hbar}S}$. When we change the path slightly, the action changes only slightly. However, the phase of the oscillating function changes drastically, since the action is again divided by \hbar . Therefore, every small step along a path gives alternating positive and negative contributions to the amplitude. In every such point, a neighboring path gives an equal contribution of opposite sign. Contributions from neighboring paths cancel everywhere *but for the path where the action stays constant when we alter the path slightly*. This corresponds to the extremum of the action, i.e. the classical path. As a result, in the classical limit, equation (2.18) reduces to some kernel

$$K(b, a) \propto e^{\frac{i}{\hbar}S_c},$$

where S_c is the action for the classical path.

The above reasoning applies also in the classical limit when we take $\hbar \rightarrow 0$. In conclusion, the path integral reduces to the classical path in the classical limit, as expected.

In the case of microscopic systems, the difference in the action as we change our path slightly is of the order of magnitude of microscopic systems, i.e. of the order of magnitude of \hbar . Therefore, many paths contribute to equation (2.18). However, the largest contributions are still given by those paths which minimize the action. That is, even for quantum mechanical systems, a longer path contributes a smaller probability amplitude, since this requires more kinetic energy. A path which passes through a large positive potential also contributes a smaller probability amplitude. For example, the probability is negligible that a particle moves through a wall in the double-slit experiment. Further support for this reasoning is given in section 4.2 when we discuss Wick-rotations.

3.2 Evaluation of the Path Integral for a Free Particle

Most of the time, path integrals are difficult to evaluate, and we must use some trick. In this section, we introduce a general method for evaluating the path integral of a particle in some potential V . The action is given by

$$S[b, a] = \int_{t_a}^{t_b} \left(\frac{1}{2} m \dot{x}^2 - V(x, t) \right) dt. \quad (3.1)$$

We use the property introduced in equation (2.19) and divide our time interval into not 2 steps, but infinitely many steps. For the sake of computation, we denote the number of time intervals N , where each interval is of length ϵ . We will later take $N \rightarrow \infty$, and consequently $\epsilon \rightarrow 0$. For small time intervals, the action can be approximated by $S_i[x_i, x_{i-1}, \epsilon] = \epsilon L_i \left(\frac{x_i - x_{i-1}}{\epsilon}, \frac{x_i + x_{i-1}}{2} \right)$. Here the velocity is approximated by $\frac{x_i - x_{i-1}}{\epsilon}$ and the position is approximated by $\frac{x_i + x_{i-1}}{2}$. We write

$$K(b, a) = \lim_{\epsilon \rightarrow 0} \frac{1}{A^N} \int \dots \int e^{\frac{i}{\hbar} \epsilon L_1} \dots e^{\frac{i}{\hbar} \epsilon L_N} dx_1 \dots dx_{N-1}. \quad (3.2)$$

That is, we approximate the paths between t_i and $t_i + \epsilon$ as straight lines and at each time t_i we integrate over all possible positions for the particle. The approximations introduced by these finite timesteps will not affect the solution when we eventually let $\epsilon \rightarrow 0$. It is also implicit that $x_0 = x_a$ and $x_N = x_b$. A is a normalization factor associated with each time step and our first task is to find an explicit expression for it. We start from equation (2.21) and write

$$\psi(x_2, t + \epsilon) = \int_{-\infty}^{\infty} K(2, 1) \psi(x_1, t) dx_1 = \frac{1}{A} \int_{-\infty}^{\infty} e^{\frac{i}{\hbar} \epsilon L_2} \psi(x_1, t) dx_1, \quad (3.3)$$

where ϵ is a small time interval. We use equation (3.1) to expand upon equation (3.3)

$$\psi(x_2, t + \epsilon) = \frac{1}{A} \int_{-\infty}^{\infty} \exp \left[\frac{i}{\hbar} \frac{m(x_2 - x_1)^2}{2\epsilon} - \frac{i}{\hbar} \epsilon V \left(\frac{x_2 + x_1}{2}, t \right) \right] \psi(x_1, t) dx_1. \quad (3.4)$$

The first term in the exponent involves a factor $\frac{1}{\epsilon}$. This term will in most cases result in a quickly oscillating function which forces the integral to zero. The only instance where this is not the case is when $|x_2 - x_1| \ll 1$. We therefore make the substitution $x_1 - x_2 = \eta$ and note that x_2 is fixed, i.e. $dx_1 = d(\eta + x_2) = d\eta$. We rewrite equation (3.4) with our new variable η

$$\psi(x, t + \epsilon) = \frac{1}{A} \int_{-\infty}^{\infty} \exp \left(\frac{im\eta^2}{2\hbar\epsilon} \right) \exp \left[-\frac{i}{\hbar} \epsilon V \left(\frac{2x + \eta}{2}, t \right) \right] \psi(x + \eta, t) d\eta, \quad (3.5)$$

where we have also made the substitution $x_2 \rightarrow x$. Those paths where $\eta \ll 1$ give the only notable contributions to the integral. This is intuitive from a physical standpoint, since we consider a very small timestep and it is unlikely that the particle travels far. We may expand equation (3.5) as a power series in η and ϵ

$$\begin{aligned} \psi(x, t) + \epsilon \frac{\partial \psi}{\partial t} = \frac{1}{A} \int_{-\infty}^{\infty} \exp \left(\frac{im\eta^2}{2\hbar\epsilon} \right) \left[1 - \frac{i}{\hbar} \epsilon V(x, t) \right] \\ \left[\psi(x, t) + \eta \frac{\partial \psi(x, t)}{\partial x} + \frac{\eta^2}{2} \frac{\partial^2 \psi(x, t)}{\partial x^2} \right] d\eta, \end{aligned} \quad (3.6)$$

where we have kept terms up to order ϵ and η^2 . This is done since the integrand in equation (3.5) involves an oscillating function with a phase $\frac{m\eta^2}{2\hbar\epsilon}$. The main contribution to the integral comes from a phase up to 2π radians, i.e. when η goes from 0 to $2\pi\sqrt{\frac{2\hbar\epsilon}{m}}$. Thus, those terms which make a significant contribution to the integral must fulfill $\eta^2 \sim \epsilon$.

The entirety of equation (3.6) will be used later, in section 3.4. In our search for A , we consider only the term of order 0 in ϵ and η . We do this because it simplifies the expression, and it is allowed since the equality in (3.6) must hold for any value of ϵ , also for $\epsilon \rightarrow 0$, and consequently $\eta \rightarrow 0$. We obtain

$$\psi(x, t) = \frac{1}{A} \psi(x, t) \int_{-\infty}^{\infty} \exp \left[\frac{im\eta^2}{2\hbar\epsilon} \right] d\eta = \{\text{Appendix B.1}\} = \psi(x, t) \frac{1}{A} \sqrt{\frac{2\pi i \hbar \epsilon}{m}}. \quad (3.7)$$

From equation (3.7), we conclude $A = \left(\frac{2\pi i \hbar \epsilon}{m} \right)^{\frac{1}{2}}$.

Our final expression for the path integral of a particle in an arbitrary potential is given by this normalizing factor together with equation (3.2)

$$K(b, a) = \lim_{\epsilon \rightarrow 0} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{N}{2}} \int \dots \int \prod_{i=1}^N \exp \left[\frac{i}{\hbar} \left(\frac{m(x_{i-1} - x_i)^2}{2\epsilon} - \epsilon V \left(\frac{x_{i-1} + x_i}{2}, t \right) \right) \right] x_1 \dots x_{N-1}. \quad (3.8)$$

We see now the purpose of splitting our time interval into steps. As long as our potential consists of at most quadratic terms in x , we are left with a product of Gaussian integrals as in equation (3.8), and they are often easy to solve.

We cannot proceed further unless we specify the potential. Depending on our choice, the path integral may become very difficult to evaluate. We choose $V = 0$ for simplicity. For a free particle, then, we get from equation (3.8)

$$K(b, a) = \lim_{\epsilon \rightarrow 0} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{N}{2}} \dots \int \underbrace{\left[\underbrace{\int \exp \left(\frac{im[(x_0 - x_1)^2 + (x_1 - x_2)^2]}{2\hbar\epsilon} \right) dx_1}_{I_1} \exp \left(\frac{im(x_2 - x_3)^2}{2\hbar\epsilon} \right) dx_2 \right]}_{I_2} \dots \quad (3.9)$$

We denote $k = \frac{m}{2\hbar\epsilon}$ and evaluate I_1

$$\begin{aligned} I_1 &= \exp(ik(x_0^2 + x_2^2)) \int_{-\infty}^{\infty} \exp(ik(2x_1^2 - 2x_1(x_0 + x_2))) dx_1 = \{\text{Appendix B.3}\} \\ &= \exp\left(\frac{ik}{2}(x_0 - x_2)^2\right) \sqrt{\frac{1}{2}} \left(\frac{\pi}{k}\right)^{\frac{1}{2}}. \end{aligned} \quad (3.10)$$

We use this result to calculate I_2 from equation (3.9) in a similar way. We obtain

$$I_2 = \exp\left(\frac{ik}{3}(x_0 - x_3)^2\right) \sqrt{\frac{1}{3}} \left(\frac{\pi}{k}\right)^{\frac{1}{2}}. \quad (3.11)$$

We notice a possible pattern in equation (3.10) and (3.11)

$$I_n = f(n) = \sqrt{\frac{1}{n+1}} \left(\frac{2\pi\hbar\epsilon}{m} \right)^{\frac{n}{2}} \exp\left(\frac{im}{2(n+1)\hbar\epsilon}(x_0 - x_{n+1})^2\right). \quad (3.12)$$

To establish this relation, we must show $I_{n+1} = f(n+1)$. We know from equation (3.9) that I_{n+1} is given by

$$I_{n+1} = \int I_n \exp\left(\frac{im}{2\hbar\epsilon}(x_n - x_{n+1})^2\right) dx_n. \quad (3.13)$$

We compute (3.13) explicitly in the same way that we did I_1, I_2 , and this gives exactly $I_{n+1} = f(n+1)$. Since we proved in equation (3.10) and (3.11) that the formula holds for $n = 1$ and $n = 2$, it must hold also for all $n > 2$. Finally, we can solve equation (3.9) with the help of equation (3.12)

$$K(b, a) = \lim_{\epsilon \rightarrow 0} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{N}{2}} I_{N-1} = \lim_{\epsilon \rightarrow 0} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{1}{2}} \sqrt{\frac{1}{N}} \exp \left(\frac{im}{2\hbar N \epsilon} (x_0 - x_N)^2 \right). \quad (3.14)$$

We set $(x_0, t_0) = (x_a, t_a)$ and $(x_N, t_N) = (x_b, t_b)$. We recall also that $N = \frac{t_N - t_0}{\epsilon} = \frac{t_b - t_a}{\epsilon}$. Using these relations, (3.14) can be written as

$$K(b, a) = \left(\frac{m}{2\pi i \hbar (t_b - t_a)} \right)^{\frac{1}{2}} \exp \left(\frac{im(x_b - x_a)^2}{2\hbar(t_b - t_a)} \right). \quad (3.15)$$

Equation (3.15) is the final expression for the kernel of a free particle. It will be studied further in the next section.

3.3 Momentum Representation of the Path Integral

We know that a state in quantum mechanics can be expressed in both position basis $\psi(x, t)$ and momentum basis $\Phi(p, t)$. We can do the same for kernels. A momentum representation $\tilde{K}_p(p_2, t_2; p_1, t_1)$ gives the amplitude for a system to have a certain momentum p_2 at some time t_2 , given that it had some momentum p_1 at an earlier time t_1 . The kernel obeys

$$\Phi(p_2, t_2) = \int \tilde{K}_p(p_2, t_2; p_1, t_1) \Phi(p_1, t_1) dp_1, \quad (3.16)$$

in analogy with (2.21).

However, we want to take it one step further. Since one of our goals is to give a description of quantum mechanics which is compatible with special relativity, there is a point in also transforming the variable of time to energy, and obtain $K_p(p_2, E_2; p_1, E_1)$. We can then describe our kernel using either the variables (x, t) or the variables (p, E) , similar to how we group position with time and momentum with energy in special relativity. We have

$$\Phi_E(p_2, E_2) = \frac{1}{2\pi \hbar} \int K_p(p_2, E_2; p_1, E_1) \Phi_E(p_1, E_1) dp_1, \quad (3.17)$$

where the factor $\frac{1}{2\pi \hbar}$ is inserted by convention. To find an expression which allows us to move from one representation of the kernel to another, we use the known Fourier transforms from position basis to momentum basis and back

$$\psi(x, t) = \frac{1}{2\pi\hbar} \int e^{\frac{ipx}{\hbar}} \Phi(p, t) dp, \quad \Phi(p, t) = \int e^{-\frac{ipx}{\hbar}} \psi(x, t) dx. \quad (3.18)$$

The equations in (3.18) along with equations (2.21) and (3.16) give us

$$\tilde{K}_p(p_2, t_2; p_1, t_1) = \iint e^{-\frac{ip_2x_2}{\hbar}} K(x_2, t_2; x_1, t_1) e^{\frac{ip_1x_1}{\hbar}} dx_2 dx_1. \quad (3.19)$$

How would we construct a similar transformation from time to energy? From the Schrödinger equation, we have $\langle t|\hat{H}|E\rangle = i\hbar \frac{\partial}{\partial t} \langle t|E\rangle$. This expression can be used to write $\langle t|\hat{H}|E\rangle = E \langle t|E\rangle = i\hbar \frac{\partial}{\partial t} \langle t|E\rangle \implies \langle t|E\rangle = Ae^{-\frac{itE}{\hbar}}$, where we set $A = \frac{1}{2\pi\hbar}$.

We find our desired Fourier transforms as

$$\begin{aligned} \langle t|\Phi\rangle &= \int \langle t|E\rangle \langle E|\Phi\rangle dE, & \langle E|\Phi\rangle &= \int \langle E|t\rangle \langle t|\Phi\rangle dt, \\ \Phi(p, t) &= \int \frac{1}{2\pi\hbar} e^{-\frac{itE}{\hbar}} \Phi_E(p, E) dE, & \Phi_E(p, E) &= \int e^{\frac{itE}{\hbar}} \Phi(p, t) dt. \end{aligned} \quad (3.20)$$

Equations (3.20) together with (3.16), (3.17) and (3.19) give

$$K_p(p_2, E_2; p_1, E_1) = \iiint e^{-\frac{ip_2x_2}{\hbar}} e^{\frac{iE_2t_2}{\hbar}} K(x_2, t_2; x_1, t_1) e^{\frac{ip_1x_1}{\hbar}} e^{-\frac{iE_1t_1}{\hbar}} dt_2 dx_2 dt_1 dx_1. \quad (3.21)$$

This is the final expression for the transform between our two basis representations of the kernel. Now, we would like to obtain the kernel for the free particle in the (p, E) -basis. This will allow us to better interpret equation (3.15).

We begin by substituting equation (3.15) for $K(x_2, t_2; x_1, t_1)$ in equation (3.19)

$$\tilde{K}_p(p_2, t_2; p_1, t_1) = \iint \exp\left(-\frac{ip_2x_2}{\hbar}\right) \left(\frac{m}{2\pi i\hbar(t_2 - t_1)}\right)^{\frac{1}{2}} \exp\left(\frac{im(x_2 - x_1)^2}{2\hbar(t_2 - t_1)}\right) \exp\left(\frac{ip_1x_1}{\hbar}\right) dx_1 dx_2.$$

We use the computation in Appendix B.3 to simplify the above expression and arrive at

$$\begin{aligned} \tilde{K}_p(p_2, t_2; p_1, t_1) &= \exp\left(-\frac{ip_1^2}{2\hbar m}(t_2 - t_1)\right) \int \exp\left(-\frac{i}{\hbar}(p_2 - p_1)x_2\right) dx_2 \\ &= 2\pi\hbar\delta(p_2 - p_1) \exp\left(-\frac{ip_1^2}{2\hbar m}(t_2 - t_1)\right). \end{aligned} \quad (3.22)$$

The integral in equation (3.22) evaluates to the delta function, which seems reasonable considering that $\{e^{\frac{i}{\hbar}xp_n}\}$ is an orthogonal basis. The factor $2\pi\hbar$ is not so obvious, but we show that it is necessary below. This part may be skipped by the reader.

We look at Fourier transforms of some arbitrary functions G, F

$$F(x) = \frac{1}{2\pi\hbar} \int e^{\frac{ipx}{\hbar}} G(p) dp, \quad G(p) = \int e^{-\frac{ipx}{\hbar}} F(x) dx.$$

We use these equations to write

$$G(p) = \frac{1}{2\pi\hbar} \int e^{\frac{-ipx}{\hbar}} \left(\int e^{\frac{ip'x}{\hbar}} G(p') dp' \right) dx = \frac{1}{2\pi\hbar} \int G(p') \left(\int e^{-\frac{i}{\hbar}(p-p')x} dx \right) dp'.$$

Since G and p, p' are arbitrary, for the equality to hold, the equation in parenthesis must fulfill

$$\int e^{\frac{i}{\hbar}(p-p')x} dx = 2\pi\hbar \delta(p' - p), \quad (3.23)$$

which motivates equation (3.22).

We substitute equation (3.22) for \tilde{K}_p in equation (3.21)

$$K_p(p_2, E_2; p_1, E_1) = 2\pi\hbar \delta(p_2 - p_1) \iint \exp\left(\frac{iE_2 t_2}{\hbar}\right) \exp\left(-\frac{ip_1^2}{2\hbar m}(t_2 - t_1)\right) \exp\left(-\frac{iE_1 t_1}{\hbar}\right) dt_2 dt_1. \quad (3.24)$$

To evaluate this, we make a change of variables $t_2 = t_1 + \tau$. We recall that for $t_1 > t_2$, the kernel must equal zero. Therefore, t_1 runs from $-\infty$ to ∞ and τ runs from 0 to ∞ . We rewrite equation (3.24) using this change of variables

$$\begin{aligned} K_p(p_2, E_2; p_1, E_1) &= 2\pi\hbar \delta(p_2 - p_1) \int_{-\infty}^{\infty} e^{\frac{i}{\hbar}(E_2 - E_1)t_1} dt_1 \int_0^{\infty} e^{\frac{i}{\hbar}(E_2 - \frac{p_1^2}{2m})\tau} d\tau \\ &= \lim_{\epsilon \rightarrow 0} (2\pi\hbar)^2 \delta(p_2 - p_1) \delta(E_2 - E_1) \left(\frac{i}{\frac{1}{\hbar}E_2 - \frac{p_1^2}{2m} + i\epsilon} \right). \end{aligned} \quad (3.25)$$

The factor $2\pi\hbar\delta(E_2 - E_1)$ comes from the integral over t_1 , in analogy with equation (3.23). The integral over τ is more difficult to evaluate since it doesn't converge. We must make a slight rotation into the complex plane $\omega \rightarrow \omega + i\epsilon$, where $\omega = \frac{1}{\hbar} \left(E_2 - \frac{p_1^2}{2m} \right)$.

ϵ is some positive real-valued variable which we will later send to zero to return to our original problem. This method allows us to evaluate the integral

$$\int_0^\infty e^{i\omega\tau} d\tau = \{\omega \rightarrow \omega + i\epsilon\} = \lim_{\epsilon \rightarrow 0} \int_0^\infty e^{(i\omega - \epsilon)\tau} d\tau = \lim_{\epsilon \rightarrow 0} -\frac{1}{i\omega - \epsilon} = \lim_{\epsilon \rightarrow 0} \frac{i}{\omega + i\epsilon}. \quad (3.26)$$

However, we cannot immediately take the limit $\epsilon \rightarrow 0$, since it would introduce a factor $\frac{1}{\omega}$ in equation (3.25) and the kernel would diverge at $\omega = 0$. This is unfavourable, since the kernel is used as a propagator and we may want to integrate over it with respect to all values of p and E , and therefore all values of ω . We could imagine setting $\epsilon = 0$ and taking the principle part of any integral which includes $\omega = 0$. However, this doesn't work for a different reason: when we take the inverse of the transform in (3.25), we want to get back to the time-representation of our kernel. Such an inverse transform involves a factor

$$\int_{-\infty}^\infty \frac{i}{\omega + i\epsilon} e^{-i\omega\tau} d\omega. \quad (3.27)$$

We said earlier that by causality, our kernel should evaluate to zero when $t_1 > t_2$. Equation (3.27) evaluates to zero when $\tau = t_2 - t_1 < 0$ only if ϵ is *finite and positive* (see Appendix B.4). Because of this, we cannot immediately set $\epsilon = 0$, but we can rewrite equation (3.26) as

$$\frac{i}{\omega + i\epsilon} = \frac{i(\omega - i\epsilon)}{\omega^2 + \epsilon^2} = \frac{i\omega}{\omega^2 + \epsilon^2} + \frac{\epsilon}{\omega^2 + \epsilon^2}. \quad (3.28)$$

As $\epsilon \rightarrow 0$, we take the first term to be $\frac{i}{\omega}$. Whenever we integrate over this term, it is implied that we take the principal part of the integral. As $\epsilon \rightarrow 0$, the second term goes to zero everywhere except at $\omega = 0$. Thus we write the second term $c\delta(\omega)$ for some constant c . We find this constant by integration

$$c = \int_{-\infty}^\infty c\delta(\omega) d\omega = \int_{-\infty}^\infty \frac{\epsilon}{\omega^2 + \epsilon^2} d\omega = \left(\frac{\omega}{\epsilon} = u\right) = \int_{-\infty}^\infty \frac{1}{u^2 + 1} du = \left[\arctan\left(\frac{\omega}{\epsilon}\right)\right]_{-\infty}^\infty = \pi.$$

We conclude that the second term in equation (3.28) can be written $\pi\delta(\omega)$. The whole expression becomes

$$\lim_{\epsilon \rightarrow 0} \frac{i}{\omega + i\epsilon} = P.P. \left(\frac{i}{\omega}\right) + \pi\delta(\omega). \quad (3.29)$$

However, we are not satisfied with this expression until we know that it preserves causality. In other words, the equation integrated against $e^{-i\omega\tau}$ must evaluate to zero when $\tau < 0$. It turns out that this is the case since the second term integrated against $e^{-i\omega\tau}$

evaluates to π and the first term integrated against $e^{-i\omega\tau}$ when $\tau < 0$ evaluates to $-\pi$, see Appendix B.5.

We rewrite our kernel using equation (3.25) and (3.29)

$$\begin{aligned} K_p(p_2, E_2; p_1, E_1) &= \lim_{\epsilon \rightarrow 0} \frac{(2\pi)^2 \hbar^3 i \delta(p_2 - p_1) \delta(E_2 - E_1)}{E_1 - \frac{p_1^2}{2m} + i\epsilon} \\ &= 4\pi^2 \hbar^3 \delta(p_2 - p_1) \delta(E_2 - E_1) \left[P.P. \left(\frac{i}{E_1 - \frac{p_1^2}{2m}} \right) + \pi \delta \left(E_1 - \frac{p_1^2}{2m} \right) \right]. \end{aligned} \quad (3.30)$$

How do we make sense of equation (3.30)? First of all, we have two delta functions in the expression. We remember that we are considering a free particle in this case, and it is reasonable that the energy and the momentum of the particle remain unchanged as it moves through space with no force acting on it.

We can also obtain a better understanding of the term in brackets. We look back at the original expression for the kernel of a free particle in the (p, t) -basis, equation (3.22). It is an oscillating function in τ with frequency $\frac{p_1^2}{2m}$, defined only for $\tau = t_2 - t_1 > 0$. If we plot the real or imaginary part of \tilde{K}_p as a function of τ it should look something like in figure (5).

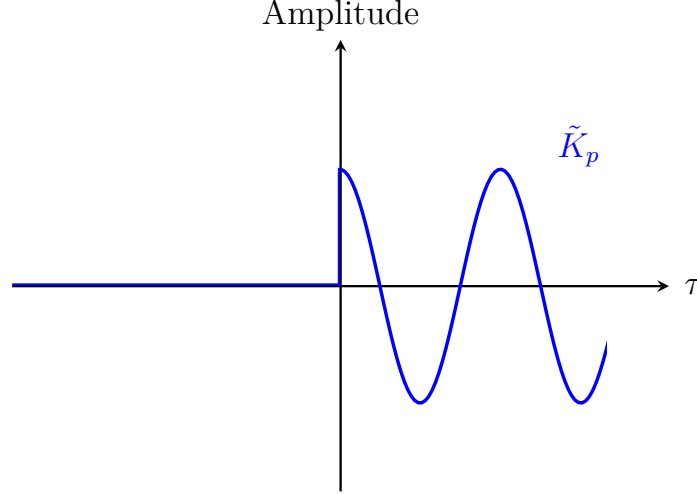


Figure 5: The kernel \tilde{K}_p of a free particle plotted against the time difference between the final- and initial state. The kernel is zero for $\tau < 0$ and for $\tau \geq 0$ it oscillates with constant frequency.

To go from the (p, t) -representation of the kernel to the (p, E) -representation, we performed a Fourier transform of the kernel in equation (3.22) with respect to time. The frequencies included in the Fourier transform were the energies of our system. Because

the kernel has a jump at $\tau = 0$, we must include all frequencies to recreate the curve. As the time difference τ increases, one frequency/energy begins to dominate. This frequency corresponds to $\frac{p^2}{2m}$, see equation (3.22). The above is intuitive also from a physical standpoint: when we treat energy as its own variable, independent from momentum, the energy doesn't necessarily correspond to the familiar expression $\frac{p^2}{2m}$. However, we can measure the energy more accurately as time passes (from the Heisenberg uncertainty principle), and it will in time approach $E = \frac{p^2}{2m}$.

This behaviour is implicit in equation (3.30) where the term $P.P. \left(\frac{i}{E_1 - \frac{p_1^2}{2m}} \right)$ accounts for the behaviour at $\tau = 0$ and the term $\delta \left(E_1 - \frac{p_1^2}{2m} \right)$ accounts for the behaviour at times $\tau > 0$.

3.4 The Path Integral in Relation to the Schrödinger Equation

We would like to prove that our path integral is equivalent to the Schrödinger equation for an infinitesimal time interval. We can do this for some arbitrary Lagrangian which is quadratic in \dot{x} . One might think this is a weakness in our proof, but most physical systems fit under this description. Also, we can read in Brown and Feynman [1, p.58] about considering only Lagrangians which are quadratic in \dot{x} :

"This is not a limitation, however, as it includes all the cases for which the Schroedinger equation has been experimentally verified."

We return to equation (3.6), which was derived from a Lagrangian of the required form. We evaluate each term on the right hand side which is at most of first order in ϵ or second order in η . The lowest order term has already been evaluated, in equation (3.7)

$$\frac{1}{A} \psi(x, t) \int_{-\infty}^{\infty} \exp \left[\frac{im\eta^2}{2\hbar\epsilon} \right] d\eta = \psi(x, t), \quad (3.31)$$

where we set $A = \left(\frac{2\pi i\hbar\epsilon}{m} \right)^{\frac{1}{2}}$. The term of first order in η evaluates to

$$\frac{1}{A} \frac{\partial \psi(x, t)}{\partial x} \int_{-\infty}^{\infty} \exp \left[\frac{im\eta^2}{2\hbar\epsilon} \right] \eta d\eta = 0, \quad (3.32)$$

since the integrand is an odd function. The two remaining terms evaluate to

$$\frac{1}{2A} \frac{\partial^2 \psi(x, t)}{\partial x^2} \int_{-\infty}^{\infty} \exp \left[\frac{im\eta^2}{2\hbar\epsilon} \right] \eta^2 d\eta = \{\text{Appendix B.2}\} = \frac{i\hbar\epsilon}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2}. \quad (3.33)$$

$$-\frac{i\epsilon}{A\hbar} V(x, t) \psi(x, t) \int_{-\infty}^{\infty} \exp \left[\frac{im\eta^2}{2\hbar\epsilon} \right] d\eta = \{\text{Appendix B.1}\} = -\frac{i}{\hbar} \epsilon V(x, t) \psi. \quad (3.34)$$

We rewrite equation (3.6) using equation (3.31)-(3.34)

$$\psi + \epsilon \frac{\partial \psi}{\partial t} = \psi + \frac{i\hbar\epsilon}{2m} \frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar} \epsilon V(x, t) \psi,$$

$$\boxed{i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x, t) \psi.} \quad (3.35)$$

Equation (3.35) is the Schrödinger equation and we have proven equivalence between the path integral and the Schrödinger equation for an infinitesimal time interval. This proof was first given by Feynman in 1942 [10] [1]. Since the Schrödinger equation was a well-established description of quantum mechanics at the time, it established also the path integral as a valid description of quantum mechanics. Further, Feynman argued as Dirac did in his article [6], see section 2.1. That is, to obtain a finite transformation, we integrate over each possible path between the initial- and final state of our system, and apply an infinitesimal path integral at each point. The resulting probability amplitude is given by the path integral in equation (2.18).

We would like to discuss one more aspect of the Schrödinger equation with respect to the path integral. We remember that the kernel is a special case of the wave function. Therefore, it should satisfy the Schrödinger equation

$$i\hbar \frac{\partial K(b, a)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 K(b, a)}{\partial x^2} + V(x, t) K(b, a). \quad (3.36)$$

However, this equation is not complete: the kernel is nonzero only for $t_a < t_b$, from equation (2.20). At $t_a = t_b$, we have a discontinuity in the kernel, and equation (3.36) fails to describe this behaviour. In order to examine what happens to $K(a, b)$ as $t_a = t_b$, we use equation (2.21) and take the limit as $t_b \rightarrow t_a$

$$\lim_{t_b \rightarrow t_a} \psi(x_b, t_b) = \psi(x_b, t_a) = \lim_{t_b \rightarrow t_a} \int_{-\infty}^{\infty} K(b, a) \psi(x_a, t_a) dx_a.$$

Thus we get $\lim_{t_b \rightarrow t_a} K(b, a) = \delta(x_a - x_b)$.

We can write equation (3.36) as

$$\frac{\partial K(b, a)}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 K(b, a)}{\partial x^2} - \frac{i}{\hbar} V(x, t) K(b, a) + \delta(x_a - x_b) \delta(t_a - t_b). \quad (3.37)$$

If we integrate the above function over an infinitesimal time interval around t_a , all terms in the right hand side go to zero except for $\delta(x_a - x_b)$, and we obtain the desired expression for the kernel at $t_a = t_b$. If we also impose $K(b, a) = 0$ when $t_a < t_b$, equation (3.37) uniquely defines the kernel. From Appendix C, we see that this equation tells us that the kernel is a Green's function for the Schrödinger equation.

Green's functions have the property that they propagate the effect of some "source" via integration. The kernel acts as a Green's function in that it propagates the effect of some initial state to some final state, under a given potential. Green's functions also obey the reciprocity relation $G(x_2, t_2; x_1, t_1) = G(x_1, t_2; x_2, t_1)$, see again Appendix C. This means that a source at the point x_1 has some influence on a state at point x_2 and this influence is the same if we interchange the position of the source and the response.

4 Important Concepts in QFT

The path integral rarely simplifies computations in non-relativistic quantum mechanics. We saw an example of this in the complicated computation of the free particle kernel in section 3.2. It would be nice to see some applications where the path integral is central and useful, and we therefore turn to QFT. In this section, we introduce some concepts and follow mainly Hori et al. [17, ch. 8-9]. We do not attempt mathematical rigor, but rather an intuitive understanding.

4.1 Manifolds and Riemannian Metric in Different Dimensions

The first important concept is a *manifold*, which is a topological space. A topological space, in turn, is a mathematical space where we can define convergence, continuity and connectedness. A manifold is a topological space that locally resembles Euclidian space, \mathbb{R}^n , which is the space that we are used to from classical mechanics. We note in particular that \mathbb{R}^n involves a flat spacetime, and that a circle is a simple example of a manifold: if we zoom in enough, it looks like a straight line, or \mathbb{R}^1 . The outline of a triangle is not a manifold: no matter how much we zoom in on the neighborhood of a corner, it will never resemble a straight line.

When we formulate a QFT, the starting point is our choice of manifold. Most of the time, we choose to work with a Riemannian manifold with a smooth metric on it. A metric is something which allows us to define angles and distances. A Riemannian manifold is just a space with a Riemannian metric, which gives a very intuitive definition of a distance: for a differentiable path we define a distance at every point in space as the length of an infinitesimal tangent vector at that point. This distance in spacetime can be written ds , with $ds^2 = d\vec{x}^2 + dt^2$ in Euclidean signature, or $ds^2 = d\vec{x}^2 - dt^2$ in Minkowski signature. Note that we work in natural units, i.e. $c = 1$. To obtain the length of some path, we walk an infinitesimal step along the tangent vector at each point of the path, as in

$$L[\gamma] = \int ds = \int |\dot{\gamma}(t)| dt,$$

where $L[\gamma]$ denotes the length of γ , and γ is a differentiable path. The distance between two points in our manifold is defined as the minimum of $L[\gamma]$ if γ runs between the points [27]. The Riemannian metric is applicable not just to 3 dimensions, so it generalizes our

familiar notion of distance.

Throughout this report, we have used Minkowski signature, since Minkowski space is the common choice for quantum mechanics. Now we want to move from Minkowski signature to Euclidean signature, since we will be considering QFT:s in Euclidean space, or Euclidean QFT:s. We can do so with a *Wick rotation*, i.e. a rotation into imaginary time $t \rightarrow it$. This rotation clearly transforms ds^2 in the desired way. A Wick rotation also results in a change in our path integral

$$\int e^{\frac{i}{\hbar}S} \mathcal{D}x \quad \rightarrow \quad \int e^{-S} \mathcal{D}x, \quad (4.1)$$

where we have switched to natural units for convenience.

It might be easier to evaluate path integrals in Euclidean space. In fact, the Wick rotation is very similar to our previous tricks for evaluating integrals in this report, see Appendix B. In the appendix, we use the Cauchy integral theorem to change the interval of integration from the real line to some contour in the complex plane. This allows us to go from an oscillating function to an exponentially decreasing one.

We stop briefly to comment on the nature of path integrals. It is obvious that the Euclidean signature path integral in equation (4.1) receives contributions mainly from those paths associated with a smaller value of the action. If the physics of our system are to remain the same under a change of coordinates, the same must hold for the path integral in Minkowski space. This further motivates our discussion in section 3.1.

Now to the dimension of our manifold. We deal mostly with 0-dimensional QFT in this report. Our manifold is then just a point, and there is no evolution in time and no spatial directions to move along. Also, we consider scalars rather than functions. 0-dimensional QFT:s are difficult to visualize and it is much more common to work in higher dimensions. However, many concepts can be easily introduced in 0 dimensions and then generalized to higher dimensions. That is what we aim to do here. Our action in 0 dimensions is given by

$$S(\phi_i),$$

where ϕ_i are scalars.

In 1-dimensional QFT, we consider one degree of freedom, often taken to be time. Another word for 1-dimensional QFT is quantum mechanics, where our manifolds correspond to the worldlines of particles. The action becomes

$$S[L(\phi_i(t), t)] = \int L(\phi_i(t), t) dt,$$

where ϕ_i are functions of time.

In higher dimensional QFT:s, we integrate over fields. For example in 4-dimensional QFT, the action can be written

$$S[L(\phi_i(x, y, z, t), t)] = \iiint L(\phi_i(x, y, z, t), t) dx dy dz dt,$$

where ϕ_i are fields. At each given time they take on a value for every point in 3-dimensional space.

There exist many fields, where the most familiar are bosonic fields and fermionic fields. Excitations of bosonic fields are bosonic particles and excitations of fermionic fields are fermionic particles. There is some intuition to this, since an excitation of a field means that energy is added to the field. Energy can only exist in quanta when we're dealing with quantum theories. So, we can never add an infinitesimal amount of energy to a quantum field, only a finite amount: a particle, which moves around as the field's energy distribution changes with time.

4.2 The Partition Function and Correlation Functions

We introduce the *partition function*

$$Z[\alpha, \epsilon] := \int \mathcal{D}\phi e^{-S[\phi, \alpha, \epsilon]}, \quad (4.2)$$

which is just a path integral in Euclidean space. In the above expression, we have included only one field ϕ . The notation in the exponent which includes variables α, ϵ will be useful in the following sections. α indicates the presence of a mass term, which can be thought of as a kinetic energy term. ϵ indicates the presence of an additional term, e.g. an interaction between fields, or a source. The partition function can be normalized as $\frac{Z[\alpha, \epsilon]}{Z[\alpha, 0]}$, where $Z[\alpha, 0]$ is the partition function for the corresponding free theory, where we include only the mass term. This notation will become more intuitive in the following sections.

Equation (4.2) is very similar to the partition function in statistical mechanics, although it looks different at first glance. We discuss this relationship more in section 6.3.

The partition function often encodes all information about a system, as it is the generator of correlation functions. The correlation function of some function $f(\psi)$ is defined as

$$\langle f(\phi) \rangle := \int \mathcal{D}\phi f(\phi) e^{-S[\phi, \alpha]}. \quad (4.3)$$

Equation (4.3), if normalized, is an expectation value averaged over all fields in a theory (in our case, only one field). The factor $e^{-S}/Z[\alpha, 0]$ is a probability density.

Often it is useful to express the correlation function as a derivative of the partition function. To achieve this, we add a term to the action $S \rightarrow S - af(\psi)$, take the derivative of the partition function w.r.t a and set it equal to zero

$$Z[\alpha, a] = \int d\phi e^{-S[\phi, \alpha] + af(\phi)} \implies \langle f(\phi) \rangle = \left. \frac{\partial Z[\alpha, a]}{\partial a} \right|_{a=0}. \quad (4.4)$$

4.3 Grassmann Variables

We construct wave functions in quantum mechanics to obey the Pauli exclusion principle, i.e. two fermions cannot coexist in the same state. Similarly in QFT, two fermionic fields cannot coexist in the same state. Say we would like to express a path integral in a theory involving fermionic fields. Such an integral involves fermionic fields in the argument of an exponential function. The exponential function can in turn be expanded in a power series, where the n :th term involves $n - 1$ factors of the same fermionic field. Thus all terms except the first two are ill-defined. In order to solve this problem and express a path integral involving fermionic fields, we introduce a new mathematical tool: Grassmann variables. They are denoted θ_n and are also called fermionic variables/fields. They exist alongside bosonic variables/fields, ψ_m , which behave like ordinary variables. Grassmann variables, on the other hand, are anti-commuting

$$\theta_a \theta_b = -\theta_b \theta_a, \quad (4.5)$$

and obey strange integration rules

$$\int d\theta_1 d\theta_2 \dots d\theta_n = 0, \quad (4.6)$$

$$\int \theta_1 \theta_2 \dots \theta_n d\theta_1 d\theta_2 \dots d\theta_n = 1, \quad (4.7)$$

where the ordering of the variables in equation (4.7) is important. The value of the integral picks up a factor (-1) for each transposition of two neighboring fields θ_i, θ_{i+1} . Removing one or more of the fields θ_a from equation (4.7) means again that the integral evaluates to zero.

We note that equation (4.5) implies $(\theta_a)^2 = 0$. Equation (4.5) also implies that a *pair* of Grassmann variables obey the same commutator relationship as a bosonic variable

$$\theta_c(\theta_a \theta_b) = -\theta_a \theta_c \theta_b = (\theta_a \theta_b) \theta_c.$$

The above formalism solves our issue with path integrals involving fermionic fields, since a power series in Grassmann variables will terminate. To demonstrate this, we consider a 0-dimensional QFT with only two fermionic fields and one bosonic field, with the action $S[\psi, \theta_1, \theta_2] = f(\psi) - g(\psi)\theta_1\theta_2$. f and g are arbitrary functions. In general, we expect the action to behave like an ordinary variable, i.e. we don't want it to act like a fermionic variable. Therefore, each term in an action function must include an *even* number of fermionic fields. By this reasoning, the above expression for $S[\psi, \theta_1, \theta_2]$ is the most general action for our chosen set of fields. Any term involving only one of the fermionic fields would be fermionic itself, and any term of higher order than two in the fermionic fields would equal zero, since $(\theta_a)^2 = 0$.

The path integral resulting from this action involves a term $e^{f(\psi)\theta_1\theta_2}$, which can be expanded in a Taylor series like any ordinary function, since the exponent is bosonic. The resulting expansion terminates, and can be written

$$e^{f(\psi)\theta_1\theta_2} = \sum_{n=0}^{\infty} \frac{(f(\psi)\theta_1\theta_2)^n}{n!} = 1 + f(\psi)\theta_1\theta_2.$$

5 The Path Integral in 0-Dimensional QFT

In this section, we explore some basic applications of the partition function in 0-dimensional QFT; in particular, how to simplify calculations of partition functions and correlation functions using Feynman diagrams and supersymmetry. In 0 dimensions, we do not consider each possible path through spacetime, since there is no spacetime to move through. Rather, the partition function in equation (4.2) reduces to a Lebesgue integral over the real line. The discussion in section 5 follows Hori et al. [17, ch. 9].

5.1 Feynman Diagrams

We consider a *free theory*, since it is easy to work with. This means that our action involves only terms which are quadratic in the fields. A quadratic term is called a *mass term*, analogous to a kinetic energy term in higher dimensional QFT - although in 0 dimensions, we have no actual kinetic energy since we have no time evolution. A term which is more than quadratic in the fields corresponds to an interaction between fields. We may introduce weak interactions in our free theory as *perturbations*, or small higher-order terms. We consider an example

$$S(\psi, \alpha, \epsilon) = \frac{\alpha}{2}\psi^2 + i\epsilon\psi^3, \tag{5.1}$$

The perturbation consists of the second term, where ϵ is a small, bosonic variable. We also note

$$Z(\alpha, 0) = \int_{-\infty}^{\infty} d\psi e^{-\frac{\alpha}{2}\psi^2} = \sqrt{\frac{2\pi}{\alpha}}, \quad (5.2)$$

so that we can use this factor to normalize our partition function later on.

We write out the partition function associated with the action in equation (5.1) and choose to normalize it. Since ϵ is small, we also make an expansion in ϵ

$$Z(\alpha, \epsilon) = \frac{1}{Z(\alpha, 0)} \int d\psi e^{-\frac{\alpha}{2}\psi^2 - i\epsilon\psi^3} = \frac{1}{Z(\alpha, 0)} \int d\psi e^{-\frac{\alpha}{2}\psi^2} \sum_{m=0}^{\infty} \frac{(-i\epsilon\psi^3)^m}{m!} \quad (5.3)$$

The above expression can be written $Z(\alpha, \epsilon) = \frac{1}{Z(\alpha, 0)} \sum_{m=0}^{\infty} \frac{(-i\epsilon)^m}{m!} \langle (\psi^3)^m \rangle_{\epsilon=0}$, where the subscript signifies that these correlation functions are evaluated with ϵ set to zero. To compute these correlation functions, we use the method introduced in equation (4.4), with a modified partition function

$$Z(\alpha, j) = \frac{1}{Z(\alpha, 0)} \int d\psi e^{-\frac{\alpha}{2}\psi^2 + j\psi}. \quad (5.4)$$

We see that n consecutive derivatives of $Z(\alpha, j)$ with respect to j gives us the correlation function $\langle \psi^n \rangle_{\epsilon=0}$, given that we set $j = 0$ after performing the derivatives. j is here called a *source*. Sometimes our theories contain actual sources, but here it is only a temporary tool which we eventually set to zero. We solve equation (5.4) explicitly, and use our expression for the normalization factor in equation (5.2)

$$Z(\alpha, j) = \frac{1}{Z(\alpha, 0)} \int d\psi e^{-\frac{\alpha}{2}\psi^2 + j\psi} = e^{\frac{j^2}{2\alpha}}. \quad (5.5)$$

The expression (5.5) can in turn be used to calculate the correlation functions $\langle \psi^n \rangle_{\epsilon=0}$

$$\langle \psi^n \rangle_{\epsilon=0} = \frac{\partial^n Z(\alpha, j)}{\partial^n j} \Big|_{j=0} = \begin{cases} c \left(\frac{1}{\alpha}\right)^{\frac{n}{2}} & \text{if } n \text{ is even,} \\ 0 & \text{otherwise,} \end{cases} \quad (5.6)$$

where c is some constant. This result follows directly from equation (5.5), since the first derivative of $Z(\alpha, j)$ brings down a factor $\frac{j}{\alpha}$ from the exponent. Each consecutive derivative acts either on the exponential function, bringing down an additional factor of $\frac{j}{\alpha}$, or it acts on one of the j :s in front of the exponential function. Since we end our calculation by setting $j = 0$, the only terms which survive are the ones where an equal amount of derivatives have acted on the exponential as on the factors in front, so that there are no factors of j left. How do we actually calculate c in equation (5.6)? We show below how to do it for $n = 6$, i.e. the term with $m = 2$ in the expansion in

equation (5.3). The term with $m = 1$ is proportional to $\langle \psi^3 \rangle_{\epsilon=0}$, which is zero according to equation (5.6), so there is no need to evaluate it.

What the computation comes down to is to find all possible ways of combining the derivatives in equation (5.6) into pairs. One way to do it is to label each ψ by some number, i.e. we want to calculate $\langle \psi_1 \psi_2 \psi_3 \psi_4 \psi_5 \psi_6 \rangle_{\epsilon=0}$. We let each field ψ_i correspond to a source j_i . This numbering will make more physical sense in section 6.1 when we discuss 1-dimensional QFT. Here, it is only a mathematical tool.

We start easy by calculating the correlation function for the first two fields

$$\langle \psi_1 \psi_2 \rangle_{\epsilon=0} = \frac{\partial^2 Z(\alpha, j_i)}{\partial j_2 \partial j_1} \Big|_{j=0} = \frac{\partial}{\partial j_2} \left(\frac{j_1}{\alpha} e^{\frac{j_i^2}{2\alpha}} \right) \Big|_{j=0} = \left[\frac{\delta_{j_1, j_2}}{\alpha} e^{\frac{j_i^2}{2\alpha}} + \frac{j_1 j_2}{\alpha^2} e^{\frac{j_i^2}{2\alpha}} \right]_{j=0} = \frac{1}{\alpha}. \quad (5.7)$$

We can visualize each factor of ψ_i in the correlation function as a vertex with one "leg" emanating from it (corresponding to a derivative). We pair up these legs, where each such pairing produces a propagator. Each propagator corresponds to a δ in the final expression for our correlation function, see equation (5.7), and each propagator contributes a factor $\frac{1}{\alpha}$ to its value. Finally, the number of possible ways of constructing these diagrams introduces a numerical factor. In the case of equation (5.7), we have two instances of ψ_i , so the pairing up of legs (or derivatives) can be done in only one way, as in figure (6). There is also only one propagator. This results in a factor $\frac{1}{\alpha}$ as the only contribution to the correlation function, in agreement with equation (5.7).



Figure 6: A Feynman diagram involving only one propagator.

For simplicity, we denote $\delta_{j_a, j_b} = \delta_{ab}$ from here on. If we carry out the computation in equation (5.7) again, but with all 6 fields, we obtain

$$\begin{aligned} \langle \psi_1 \psi_2 \psi_3 \psi_4 \psi_5 \psi_6 \rangle_{\epsilon=0} &= \left[\frac{\delta_{12} \delta_{34} \delta_{56}}{\alpha^3} e^{\frac{j_i^2}{2\alpha}} + \frac{\delta_{12} \delta_{35} \delta_{46}}{\alpha^3} e^{\frac{j_i^2}{2\alpha}} + \frac{\delta_{12} \delta_{45} \delta_{36}}{\alpha^3} e^{\frac{j_i^2}{2\alpha}} + \frac{\delta_{14} \delta_{25} \delta_{36}}{\alpha^3} e^{\frac{j_i^2}{2\alpha}} + \frac{\delta_{23} \delta_{45} \delta_{16}}{\alpha^3} e^{\frac{j_i^2}{2\alpha}} \right. \\ &\quad + 10 \text{ identical terms containing all different permutations of } \delta_{a,b} \\ &\quad \left. + \text{terms involving one or more factors of } j_i \right]_{j=0} \\ &= \frac{15}{\alpha}. \end{aligned} \quad (5.8)$$

Instead of performing this calculation, we can visualize each factor of ψ^3 in $\langle(\psi^3)^n\rangle$ as a vertex with 3 legs emanating from it (each one corresponding to a derivative). The expression in equation (5.8) corresponds to two factors of ψ^3 . The different possible Feynman diagrams in this case are given in figure (7). The legs (1,2,3) can be connected to the legs (4,5,6) to make two different shapes, A and B. To make the shape in A, we take one of the blue legs, say 1, and connect it to one of the pink legs. There are three ways to do this. Then, we pair up leg 2 with one of the remaining pink legs. In total, we can construct diagram A in $(3 \cdot 2 \cdot 1 = 3!)$ different ways. To construct diagram B, we must choose which one of the 3 blue legs connects to one of the pink legs. There are then 3 different pink legs to connect this blue leg to. Finally, there is only one choice of how to connect the remaining 4 legs. The total amount of combinations that form diagram B is (3^2) . In conclusion, diagram A and B contribute a total amount $\frac{1}{\alpha}(3! + 3^2) = \frac{15}{\alpha}$ to the correlation function, which is consistent with our explicit calculation (5.8).

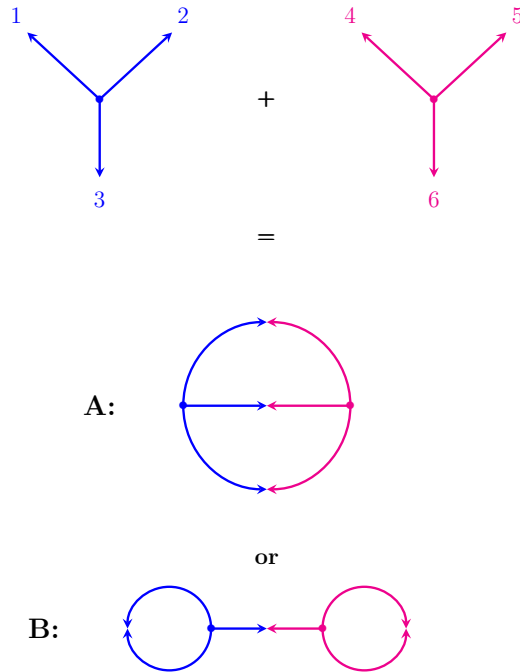


Figure 7: Feynman diagrams in a vacuum state.

Since we have no sources in our original problem, equation (5.1), we are effectively in a vacuum. If we read our Feynman diagrams in figure (7) from left to right and let this be the direction of time, we see that they are consistent with the vacuum interpretation: our initial- and final state consists of nothing. Fields are simply created from the vacuum and then annihilate.

We conclude from equations (5.3), (5.2) and (5.8) that our normalized partition function is given by

$$Z(\alpha, \epsilon) = 1 + 15 \frac{(-i\epsilon)^2}{2} \left(\frac{1}{\alpha}\right)^3 + \text{higher order corrections.}$$

This was a very simple example where the use of Feynman diagrams was not necessary for computation; we were able to find the terms in our perturbation expansion directly. This is often difficult. Instead, a deeper analysis of a given perturbed action gives us all possible Feynman diagrams, and we can then reconstruct the perturbation expansion *from our Feynman diagrams*. From here on, we focus only on the latter step, i.e. how to translate between Feynman diagrams and terms in a perturbation expansion.

Let us briefly analyze the action in equation (5.1). The mass term $\frac{\alpha}{2}\psi^2$ is quadratic in the field. The power series which would result from expanding such a term is represented by diagrams with two legs per vertex. This produces Feynman diagrams like the one in figure (8).



Figure 8: Feynman diagrams involving only one propagator per vertex.

This is clearly a field which propagates without interacting with other fields, so the mass term is analogous to a kinetic term, as we discussed in the beginning of this section. The term $i\epsilon\psi^3$ is instead a perturbation term, which represent self-interactions in the field ψ , shown visually in figure (7).

From the above discussion, we may draw some general conclusions, so that in the future we can more easily interpret Feynman diagrams as terms in a perturbation expansion. To make such an analysis, we must also examine the action which describes our system. For example, a mass term of the form $\frac{\alpha}{2}\psi^2$ in the action implies

- Each factor $\frac{1}{\alpha}$ in the perturbation expansion corresponds to a propagator of ψ , represented by a line.

The term $i\epsilon\psi^3$ implies

- Each factor ϵ in the perturbation expansion corresponds to a vertex. Each factor of ψ corresponds to a leg emanating from the vertex.

If we have a term $j\psi$ in our action, this corresponds to a system with sources, where the field ψ interacts once with each source. By the general logic of this section, we conclude

- Each factor j in the perturbation expansion corresponds to an external vertex (a vertex connected to only one propagator of ψ), with a circle at the vertex indicating a source.

Numerical factors which arise from all the possible ways of constructing a Feynman diagram are called symmetry factors. We saw an example of such a factor in equation (5.8).

Computation of the Dynamics of a System with and without Quantum Corrections

We demonstrate some concepts from the previous sections by analyzing a system using both classical methods and QFT. By comparing these approaches, we deduce the effect of quantum corrections.

We consider the action

$$S(\psi, \zeta) = \frac{a}{2}\psi^2 + \frac{1}{2}\psi^2\zeta + j\psi, \quad (5.9)$$

where a is a constant, j is a source, ψ is a dynamic field and ζ is a small, non-dynamic field. Dynamic fields are those which describe the evolution of a system. There is no term in the action which is quadratic in ζ , so this field cannot propagate; only perturb our system.

We use the action in (5.9) to find the classical equations of motion of ψ and the classical free energy. We then use the path integral to evaluate the QFT partition function and free energy. We use this free energy to find the one-particle irreducible (or 1PI) quantum effective action, which is the quantum analogue of the classical action. We then compute the equations of motion of ψ again, this time including quantum mechanical corrections.

1. Calculating the classical equation of motion of ψ .

In the classical case, a system takes the path which minimizes the action, i.e. the equations of motion are found by evaluating $\delta S = 0$. In our 0-dimensional case, we have no time variable to sum over, so the variation of the action simply gives

$$\delta S = \frac{\partial S}{\partial \psi} \delta \psi = (a\psi + \psi\zeta + j)\delta \psi = 0 \quad \implies \quad \psi_{cl}(j, \zeta) = -\frac{j}{a + \zeta}.$$

2. Calculating the classical free energy F_{cl} .

The classical free energy is given by a Legendre transform of the action, $F_{cl}(j, \zeta) = [j\psi - S(\psi, \zeta)]_{\psi=\psi_{cl}}$. In our case

$$F_{cl}(j, \zeta) = \left[-\frac{a}{2}\psi^2 - \frac{1}{2}\psi^2\zeta \right]_{\psi=\psi_{cl}} = -\frac{j^2}{2(a + \zeta)}. \quad (5.10)$$

3. Expanding F_{cl} and interpreting the terms as tree diagrams.

We expand our expression (5.10) in powers of ζ , using the power expansion $\frac{1}{1+x} = 1 - x + x^2 - x^3 + \dots$

$$F_{cl} = -\frac{j^2}{2a} \left(1 - \frac{\zeta}{a} + \frac{\zeta^2}{a^2} - \frac{\zeta^3}{a^3} + \dots \right). \quad (5.11)$$

We draw the corresponding Feynman diagrams in figure (9). The term $\psi^2\zeta$ represents an interaction between two different fields. According to the rules in section 5.1, we represent the interaction as tri-valent vertices. Solid lines represent propagators of ψ , corresponding to a factor $\frac{1}{a}$ in the perturbation terms. A dashed line represents a perturbation from the non-dynamical field ζ , corresponding to a factor ζ . Since ζ cannot propagate, there are no internal dashed lines. Finally, the circles represent sources and can only exist as external vertices connected by solid lines since they interact only once with ψ . These circles correspond to a factor j .

$$\begin{aligned}
 F_{cl} = & \text{[Diagram 1: two circles connected by a solid line]} + \text{[Diagram 2: two circles connected by a solid line, with a dashed line from the vertex]} + \text{[Diagram 3: two circles connected by a solid line, with two dashed lines from the vertices]} + \text{[Diagram 4: two circles connected by a solid line, with three dashed lines from the vertices]} + \dots \\
 = & -\frac{j^2}{2a} + \frac{j^2\zeta}{2a^2} - \frac{j^2\zeta^2}{2a^3} + \frac{j^2\zeta^3}{2a^4} - \dots
 \end{aligned}$$

Figure 9: Tree diagrams corresponding to each term in the power expansion of F_{cl} .

4. Computing the partition function and the free energy.

Now we move to QFT. The partition function in Euclidean signature is given by

$$\begin{aligned}
 Z[j, \zeta] &= \int_{-\infty}^{\infty} \exp \left[-\left(\frac{a}{2} \psi^2 + \frac{1}{2} \psi^2 \zeta + j\psi \right) \right] d\psi = \int_{-\infty}^{\infty} \exp \left[-\left(\frac{a}{2} + \frac{1}{2} \zeta \right) \psi^2 - j\psi \right] d\psi \\
 &= \sqrt{\frac{2\pi}{a + \zeta}} \exp \left(\frac{j^2}{2(a + \zeta)} \right). \quad (5.12)
 \end{aligned}$$

The free energy is given by $F(j, \zeta) = -\log Z(j, \zeta)$. We use this expression and equation (5.12) to obtain

$$F(j, \zeta) = -\frac{1}{2} \log \left(\frac{2\pi}{a + \zeta} \right) - \frac{j^2}{2(a + \zeta)}. \quad (5.13)$$

We conclude from a comparison between (5.10) and (5.13) that the free energy obtained from the QFT partition function includes one extra term compared to the classical free

energy.

5. Expanding the free energy in a power series and interpreting the terms as Feynman diagrams.

We use equation (5.13) along with the power expansion $\log(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \dots$ to obtain

$$F(j, \zeta) = -\frac{1}{2} \log \left(\frac{2\pi}{a} \right) + \underbrace{\frac{1}{2} \left(\frac{\zeta}{a} - \frac{\zeta^2}{2a^2} + \frac{\zeta^3}{3a^3} - \frac{\zeta^4}{4a^4} + \dots \right)}_A - \underbrace{\frac{j^2}{2} \left(1 - \frac{\zeta}{a^2} + \frac{\zeta^2}{a^3} - \frac{\zeta^3}{a^4} + \dots \right)}_B. \quad (5.14)$$

The first term in equation (5.14) is just a constant. The expansion which we call B is identical to the expression for F_{cl} in equation (5.11) and is represented by the same Feynman diagrams as in figure (9). Expansion A is represented as Feynman diagrams in figure (10).

$$\begin{aligned} F &= \dots + \text{[diagram: circle with two external dashed lines]} + \text{[diagram: circle with two external dashed lines]} + \text{[diagram: circle with four external dashed lines]} + \text{[diagram: circle with four external dashed lines]} + \dots \\ &= \dots + \frac{\zeta}{2a} - \frac{\zeta^2}{4a^2} + \frac{\zeta^3}{6a^3} - \frac{\zeta^4}{8a^4} + \dots \end{aligned}$$

Figure 10: Feynman diagrams corresponding to terms in the power expansion of F .

There are no sources present in these diagrams: only loops with propagators of ψ and interactions between ψ and ζ . Following from the discussion in section 5.1, these are vacuum Feynman diagrams. Our conclusion is that the free energy in the quantum theory gets an extra contribution from vacuum fluctuations.

6. Obtaining the 1PI quantum effective action and the equation of motion of ψ .

Classically, the free energy is given by the Legendre transform of the action, $F_{cl} = [j\psi - S]_{\psi=\psi_{cl}}$. In QFT, we instead write $F = [j\psi - \Gamma]_{\psi=\psi_c}$ where $\Gamma(\psi, \zeta)$ is the 1PI effective action. Γ is the generator of 1PI irreducible Feynman diagrams, in the same way that the partition function is the generator of correlation functions, as demonstrated by equation (5.6). 1PI irreducible Feynman diagrams are those which cannot be separated into two independent diagrams by disconnecting any one internal line. Γ can also be minimized to give the equations of motion ψ_c . Equations of motion are implicitly classical, since they assume a deterministic time evolution. However, the equations of

motion obtained from Γ are semi-classical, since they include quantum corrections. Such corrections arise from higher order Feynman diagrams, i.e. loop diagrams, which are by construction 1PI irreducible.

In this way, Γ is the quantum analogue of the classical action, and ψ_c is obtained by considering the variation

$$\begin{aligned}\delta\Gamma = 0 &= \frac{\partial(j\psi_c)}{\partial j}\delta j + \frac{\partial F}{\partial j}\delta j \\ \implies \psi_c &= \frac{\partial}{\partial j}F.\end{aligned}\tag{5.15}$$

We use equation (5.15) and our expression for the free energy (5.13) to obtain

$$\psi_c(j, \zeta) = -\frac{j}{a + \zeta}.\tag{5.16}$$

ψ_c is thus identical to our expression for ψ_{cl} (5.10). This is because our expression for the QFT free energy was identical to the expression for the classical free energy, apart from one extra term without sources. From equation (5.15), we see that only those terms which contain sources determine the equations of motion. Along the same line, if we set $j = 0$ in equation (5.16), we find that ψ_c is static.

Our final task is to find the 1PI quantum effective action for our system. We use equation (5.16) and (5.13) to obtain

$$\Gamma(\psi_c, \zeta) = -\frac{1}{2}\log\left(\frac{2\pi}{a + \zeta}\right) + \frac{j^2}{2(a + \zeta)} = -\frac{1}{2}\log\left(\frac{2\pi}{a + \zeta}\right) + \frac{a}{2}\psi_c^2 + \frac{1}{2}\psi_c^2\zeta.\tag{5.17}$$

Γ in equation (5.17) is similar to the classical action in equation (5.3). However, $\Gamma(\psi, \zeta)$ contains the extra term $-\frac{1}{2}\log\left(\frac{2\pi}{a + \zeta}\right)$, which accounts for quantum corrections. Also, Γ includes no sources. This is a result of our formalism: we are here interested in the behaviour of ψ rather than in the sources, and we obtained the above expression free from sources by performing a suitable Legendre transform.

5.2 Supersymmetry

In section 5.1, we used perturbation theory to evaluate the partition function. In this section, we examine QFT:s which are constructed to possess supersymmetry. This quality allows us to evaluate the partition function and other quantities exactly.

To demonstrate supersymmetry, we consider a system of two fermionic fields and one bosonic field with the action from section 4.3

$$S(\psi, \theta_1, \theta_2) = f(\psi) - \theta_1 \theta_2 g(\psi),$$

This time, we specify the action further, by putting $f(\psi) = \frac{1}{2}h'(\psi)^2$ and $g(\psi) = h''(\psi)$, where h is a function called the *superpotential*. The resulting action $S[\psi, \theta_1, \theta_2] = \frac{1}{2}h'(\psi)^2 - \theta_1 \theta_2 h''(\psi)$ is invariant under some transformations which *exchange bosonic- and fermionic fields*. Such transformations are called supersymmetry transformations. In our case, the following is a supersymmetry transformation

$$\begin{aligned}\delta\psi &= \epsilon_1 \theta_1 + \epsilon_2 \theta_2, \\ \delta\theta_1 &= \epsilon_2 h', \\ \delta\theta_2 &= -\epsilon_1 h'.\end{aligned}\tag{5.18}$$

ϵ_i are fermionic variables, and they are small, to generate an infinitesimal transformation. The corresponding transformation of the action is given by

$$\begin{aligned}\delta S &= \delta\psi \frac{\partial S}{\partial\psi} + \delta\theta_1 \frac{\partial S}{\partial\theta_1} + \delta\theta_2 \frac{\partial S}{\partial\theta_2} \\ &= (\epsilon_1 \theta_1 + \epsilon_2 \theta_2)(h'h'' - \theta_1 \theta_2 h''') + (\epsilon_2 h')(-\theta_2 h'') + (-\epsilon_1 h')(\theta_1 h'') = 0,\end{aligned}\tag{5.19}$$

where the ordering of the terms is important and we have taken into consideration the rule $\theta_a^2 = 0$ and the commutation relations for fermionic fields. We have also used the convention that derivatives be taken as $\frac{\partial}{\partial\theta_2}(\theta_1 \theta_2) = -\theta_1$. From equation (5.19), we see that the action is invariant under the transformation (5.18). One can easily show that also the measure is invariant. In conclusion, (5.18) generates a supersymmetry and the partition function is invariant under the transformation.

We demonstrate some useful consequences of supersymmetry in the following sections.

5.3 Deformation Invariance

We begin with an important consequence of supersymmetry: deformation invariance. In the context of this thesis, it means that our superpotential $h(\psi)$ from section 5.2 can be altered in ways that leave the partition function unchanged. This simplifies many calculations.

To prove deformation invariance, we first introduce another property of symmetric QFT:s, namely that correlation functions evaluate to zero for variations of fields, if the action is invariant under the variation. In our case, this means that the correlation function $\langle \delta\gamma \rangle = 0$ for any function $\gamma(\psi, \theta_1, \theta_2)$, where δ is a supersymmetry transformation. We prove this as follows

$$\begin{aligned}\langle \delta\gamma \rangle &= \int \delta\gamma e^{-S} d\psi d\theta_1 d\theta_2 = \int \delta(\gamma e^{-S}) d\psi d\theta_1 d\theta_2 \\ &= \int \left(\delta\psi \frac{\partial(\gamma e^{-S})}{\partial\psi} + \delta\theta_1 \frac{\partial(\gamma e^{-S})}{\partial\theta_1} + \delta\theta_2 \frac{\partial(\gamma e^{-S})}{\partial\theta_2} \right) d\psi d\theta_1 d\theta_2 = 0.\end{aligned}\quad (5.20)$$

The second equality follows from the property $\delta S = 0 \implies \delta(\gamma e^{-S}) = \delta\gamma e^{-S} + \gamma\delta(e^{-S}) = \delta\gamma e^{-S}$. The final equality in equation (5.20) is a consequence of several things. First, each term in γ contains at most one factor of each fermionic field. Therefore, the derivative of γ w.r.t. θ_1 or θ_2 will eliminate one of the fermionic fields from each term. By the rules of Grassman integration, equation (4.6), the integral of the resulting terms goes to zero. We are then left with only the last term $\frac{\partial(\gamma e^{-S})}{\partial\psi} \delta\psi$, where $\delta\psi$ can be moved outside the integral and the remaining expression is easily rewritten as a total derivative in ψ . The integral reduces to the evaluation of (γe^{-S}) at $\pm\infty$. We expect that the action goes to infinity far away, so also these boundary terms go to zero. The result in equation (5.20) thus holds as long as the supersymmetry transformation does not change the behaviour of S at infinity, since this could alter the behaviour of the boundary terms.

We would like to use the property in equation (5.20) to show that $\langle \delta_\rho S \rangle = 0$, where δ_ρ is the specific transformation given by a change in the superpotential $h \rightarrow h + \sigma\rho$, where $\rho = \rho(\psi)$, and σ is an infinitesimal bosonic parameter. Our end goal is to show that this transformation of the superpotential does not affect the partition function. Indeed, we see that $\langle \delta_\rho S \rangle = 0$ implies invariance of the partition function by the following

$$\begin{aligned}\langle \delta_\rho S \rangle &= \int \delta_\rho S e^{-S} d\psi d\theta_1 d\theta_2 = \int \frac{\partial}{\partial h}(S) \delta_\rho h e^{-S} d\psi d\theta_1 d\theta_2 = - \int \frac{\partial}{\partial h}(e^{-S}) \delta_\rho h d\psi d\theta_1 d\theta_2 \\ &= - \delta_\rho \left(\int e^{-S} d\psi d\theta_1 d\theta_2 \right).\end{aligned}$$

Thus $\langle \delta_\rho S \rangle = 0 \implies \delta_\rho Z = 0$. We remind ourselves of our expression for S , $S(\psi, \theta_1, \theta_2) = \frac{1}{2}h'(\psi)^2 - \theta_1\theta_2 h''(\psi)$. To prove $\langle \delta_\rho S \rangle = 0$, we begin by writing out S under the transformation δ_ρ

$$\delta_\rho S = S(h) - S(h + \sigma\rho) = \frac{1}{2}(\sigma^2 \rho'^2 + 2\sigma h' \rho') - \sigma \rho'' \theta_1 \theta_2.$$

We assume the term of second order in σ is negligible and write

$$\delta_\rho S = \sigma h' \rho' - \sigma \rho'' \theta_1 \theta_2. \quad (5.21)$$

We consider a suitable function $g(\psi, \theta_1) = \rho'(\psi)\theta_1$. The variation δg under our supersymmetry is identical to $\delta_\rho S$. We show this by utilizing the transformation in (5.18) along with the restriction $\epsilon_1 = \epsilon_2 = \epsilon$

$$\delta g = \delta\psi\rho''\theta_1 + \delta\theta_1\rho' = \sigma\rho'h' - \sigma\rho''\theta_1\theta_2. \quad (5.22)$$

By equation (5.20), $\langle\delta g\rangle = 0$. Also, a comparison between equation (5.22) and (5.21) gives $\langle\delta_\rho S\rangle = \langle\delta g\rangle = 0$. We have proven that the partition function is unchanged under the infinitesimal transformation $h \rightarrow h + \sigma\rho$. This implies invariance also for $h \rightarrow h + \rho$, since a finite transformation is achieved from many consecutive infinitesimal transformations. As a reminder, ρ is a bosonic function whose only restriction is that the behaviour of the action cannot be dominated by ρ at infinity.

We will see a consequence of this deformation invariance in the next section.

5.4 Localization

The idea behind localization is that in some supersymmetric QFT:s, the partition function receives contributions only from a limited amount of paths (or in 0 dimensions, a limited amount of points). Contributions from the remaining paths cancel against each other due to boson-fermion cancellations. As we saw in section 5.1, calculations in QFT often come down to approximations using perturbation theory. However, when a QFT allows for localization, we may use this technique to evaluate many quantities *exactly*.

To show that localization applies in our case, we return again to deformation invariance. Say our superpotential h is a polynomial. Then the transformation $h \rightarrow h + \rho$ does not change the behavior of S at infinity as long as ρ is a polynomial of at most the same degree as h . We could for example set $\rho = \beta h(\psi)$, where β is a real constant. This corresponds to rescaling our superpotential by some constant, $h \rightarrow \lambda h$.

If we allow λ to grow, the first term in our action $S(\psi, \theta_1, \theta_2) = \frac{1}{2}\lambda^2 h'(\psi)^2 - \theta_1\theta_2\lambda h''(\psi)$ quickly becomes the dominant term, i.e. we can effectively write $S(\psi, \theta_1, \theta_2) = \frac{1}{2}\lambda^2 h'(\psi)^2$ as $\lambda \rightarrow \infty$. As a consequence, our partition function goes to zero everywhere but at the points where $h'(\psi) = 0$. This happens to correspond to the points where our fermionic fields are unchanged by the supersymmetry transformation, see (5.18). The statement holds true for every QFT with supersymmetry, as stated in Hori et al. [17, p. 158]

"This is the localization principle: *The path-integral is localized at loci where the R.H.S of the fermionic transformation under supersymmetry is zero.*"

Since the partition function is independent of our choice of λ , it will receive contributions only from the points ψ_0 where $h'(\psi_0) = 0$, even if we go back to our original problem with $\lambda = 1$. We do so, and try to find an expression for Z . We consider the case where h is a polynomial of degree n with $n - 1$ distinct critical points. Around each of the points ψ_0 , we can expand h and keep only the first two non-zero terms

$$h(\psi) = h(\psi_0) + \frac{a_0}{2}(\psi - \psi_0)^2,$$

where $a_0 = h''$. Our normalized partition function is then of the form

$$\begin{aligned} Z &= \frac{1}{Z_0} \sum_{\psi_0} \int e^{-\frac{1}{2}a_0^2(\psi-\psi_0)^2 + a_0\theta_1\theta_2} d\psi d\theta_1 d\theta_2 = \frac{1}{\sqrt{2\pi}} \sum_{\psi_0} \int e^{-\frac{1}{2}a_0^2(\psi-\psi_0)^2} (1 + a_0\theta_1\theta_2) d\psi d\theta_1 d\theta_2 \\ &= \frac{1}{\sqrt{2\pi}} \sum_{\psi_0} \int a_0 e^{-\frac{1}{2}a_0^2(\psi-\psi_0)^2} d\psi = \sum_{\psi_0} \frac{a_0}{|a_0|} = \sum_{\psi_0} \frac{h''(\psi_0)}{|h''(\psi_0)|}. \end{aligned} \quad (5.23)$$

Z_0 is the partition function for the corresponding free theory. We see that when we consider localization, the evaluation of our partition function reduces to counting the number of critical points of the superpotential. Each root contributes a term ± 1 , where the sign depends on the slope of $h'(\psi_0)$.

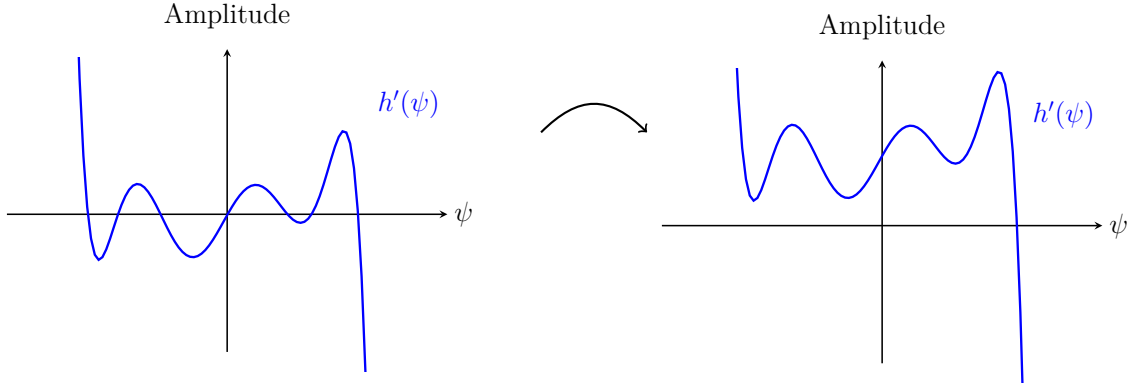


Figure 11: Some polynomial $h'(\psi)$, where $h(\psi)$ is of degree $n = 8$. The function has been shifted by the addition of a constant.

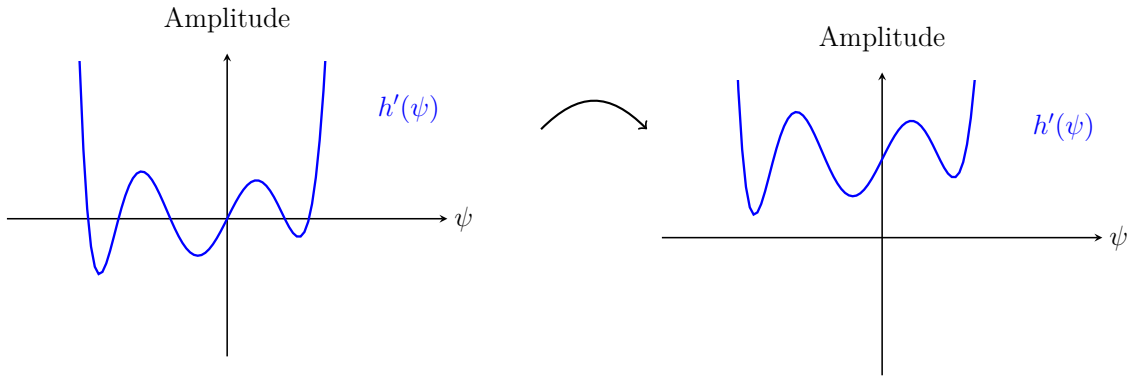


Figure 12: Some polynomial $h'(\psi)$, where $h(\psi)$ is of degree $n = 7$. The function has been shifted by the addition of a constant.

We can simplify the expression in equation (5.23) even further. To do this, we consider some deformation of our superpotential again. We set $\rho = b\psi$, and thus $h' \rightarrow h' + b$, where b is some real constant. If we let b grow large enough, the number of critical points $h'(\psi_0)$ reduces to one for an even degree n of h , or zero for an odd degree n of h , see figure (11). In the latter case, our partition function reduces to zero. In the first case, our partition function reduces to ± 1 , where the sign is determined by $h''(\psi)$ at our only remaining critical point. This sign is in turn decided by the sign in front of the leading term in h . We conclude that the evaluation of the partition function is sensitive only to the nature of the superpotential. If the superpotential is a polynomial, it is sensitive only to its degree, and the nature of its extremum points.

In other words, the evaluation of the partition function may simplify significantly when we construct a supersymmetric QFT. As a consequence, the computation of many correlation functions also simplify. We will see an example of this in the next section.

5.5 Landau-Ginzburg Supersymmetry

In this section, we again treat supersymmetry, with the addition that our fields are complex. We include twice as many fields, $(\psi, \theta_1, \theta_2) \rightarrow (\psi, \bar{\psi}, \theta_1, \theta_2, \bar{\theta}_1, \bar{\theta}_2)$, where the overline denotes a complex conjugate.

We choose a new action

$$S(\psi, \bar{\psi}, \theta_1, \theta_2, \bar{\theta}_1, \bar{\theta}_2) = |W'|^2 - W''\theta_1\theta_2 - \bar{W}''\bar{\theta}_1\bar{\theta}_2,$$

where $W = W(\psi)$ is a complex differentiable function and our new superpotential. We consider two supersymmetry transformations

$$\begin{aligned} \delta\psi &= \epsilon_1\theta_1 + \epsilon_2\theta_2 & \delta\bar{\psi} &= 0, \\ \delta\theta_1 &= \epsilon_2\bar{W}' & \delta\bar{\theta}_1 &= 0, \\ \delta\theta_2 &= -\epsilon_1\bar{W}' & \delta\bar{\theta}_2 &= 0. \end{aligned} \tag{5.24}$$

and

$$\begin{aligned} \bar{\delta}\psi &= 0 & \bar{\delta}\bar{\psi} &= \bar{\epsilon}_1\bar{\theta}_1 + \bar{\epsilon}_2\bar{\theta}_2, \\ \bar{\delta}\theta_1 &= 0 & \bar{\delta}\bar{\theta}_1 &= \bar{\epsilon}_2W', \\ \bar{\delta}\theta_2 &= 0 & \bar{\delta}\bar{\theta}_2 &= -\bar{\epsilon}_1W', \end{aligned} \tag{5.25}$$

where δ denotes a transformation which transforms only the fields and not to the complex conjugated fields. $\bar{\delta}$ denotes a separate transformation which transforms only the complex conjugated fields. ϵ_i are again small, fermionic variables. If we also set $\epsilon_1 = \epsilon_2$, $\bar{\epsilon}_1 = \bar{\epsilon}_2$, we see from the transformations in (5.24) and (5.25) that $\delta^2 = \bar{\delta}^2 = 0$.

We see this by noting that each term in $(\delta\theta_i)^2$ and $(\delta\psi)^2$ contains a factor of $\epsilon^2 = 0$. The same logic applies to the transformations of the complex conjugated fields.

We have already proven that localization can be applied to supersymmetric QFT:s such as this one. In analogy with the supersymmetric QFT in section 5.4, the partition function simplifies also in this case to include only those points where the superpotential has a critical point, $W'(\psi_0) = 0$. However, the expression for the partition function doesn't necessarily look the same as it did in equation (5.23). To evaluate the partition function in this QFT, we again expand the superpotential around its critical points and write $W(\psi) = W(\psi_0) + \frac{\alpha}{2}(\psi - \psi_0)^2$, with $\alpha = W''$. We also set $\psi = x + iy$, where x and y are real, bosonic variables. Our partition function reduces to

$$\begin{aligned}
 Z &= \frac{1}{2\pi} \sum_{\psi_0} \int \exp \left[- \left(|\alpha(\psi - \psi_0)|^2 - \alpha\theta_1\theta_2 - \bar{\alpha}\bar{\theta}_1\bar{\theta}_2 \right) \right] d\psi d\bar{\psi} d\theta_1 d\theta_2 d\bar{\theta}_1 d\bar{\theta}_2 \\
 &= \frac{1}{2\pi} \sum_{\psi_0} |\alpha|^2 \int \exp \left(-|\alpha|^2 |\psi - \psi_0|^2 \right) d\psi d\bar{\psi} \\
 &= \left(d\psi d\bar{\psi} = \text{abs} \left(\det \begin{vmatrix} \frac{\partial \psi}{\partial x} & \frac{\partial \psi}{\partial y} \\ \frac{\partial \bar{\psi}}{\partial x} & \frac{\partial \bar{\psi}}{\partial y} \end{vmatrix} \right) dx dy = 2 dx dy \right) \\
 &= \frac{1}{2\pi} \sum_{\psi_0} |\alpha|^2 2 \int e^{|\alpha|^2 x^2} dx \int e^{|\alpha|^2 y^2} dy = \frac{1}{2\pi} \sum_{\psi_0} |\alpha|^2 \frac{2\pi}{|\alpha|^2} = \sum_{\psi_0} 1. \tag{5.26}
 \end{aligned}$$

To obtain the expression on the last line, we use the property $\int \exp(-|\alpha|^2 |\psi - \psi_0|^2) d\psi d\bar{\psi} = \int \exp(-|\alpha|^2 |\psi|^2) d\psi d\bar{\psi}$, which holds since a change of variables $\psi \leftrightarrow \psi - \psi_0$ leaves the integral unchanged. We see from equation (5.26) that our complex-valued supersymmetry has reduced the partition function to counting the number of critical points of W . As opposed to equation (5.23) in section 5.4, here we don't have to consider the nature of the critical points.

We also want to investigate how to evaluate correlation functions using localization. We note first that a function $f(\psi, \bar{\psi}, \theta_1, \theta_2, \bar{\theta}_1, \bar{\theta}_2)$ which is invariant under at least one of the two supersymmetry transformations in (5.24) and (5.25) is in general easier to evaluate than a function which is not invariant. We explain why this is. Consider f and assume it is invariant under the δ -transformation. Assume also that δ_ρ denotes the transformation $W \rightarrow \lambda W$. By writing out $\langle f \rangle$ we see that $-\delta_\rho \langle f \rangle = \langle f \delta_\rho S \rangle = \langle f \delta h \rangle = \{ \delta f = 0 \} = \langle \delta(fh) \rangle = 0$. Here, $h = h(\psi, \bar{\psi}, \theta_1, \theta_2, \bar{\theta}_1, \bar{\theta}_2)$ is some function which fulfills $\delta h = \delta_\rho S$, similar to the function g we found in section 5.3 to prove deformation invariance. Since $\delta_\rho \langle f \rangle = 0$, we may apply localization also to this correlation function and evaluate it only in those points ψ_0 where $W' = 0$.

An example of a function which is invariant is any function of only ψ or $\bar{\psi}$, i.e. some function $\beta(\psi)$ or $\omega(\bar{\psi})$. β and ω are automatically invariant under one of our supersymmetry transformations, since $\delta\bar{\psi} = 0, \delta\psi = 0$, see (5.24) and (5.25). It turns out that functions of the type $\beta(\psi)$ or $\omega(\bar{\psi})$ are the *only* functions of the bosonic fields

which are invariant. To see this, we note that the function $\psi\bar{\psi}$ is not invariant, since $\delta(\psi\bar{\psi}) = \delta\psi\bar{\psi} + \psi\delta\bar{\psi} \neq 0$, and the same goes for $\bar{\delta}(\psi\bar{\psi})$. By the same reasoning, no function $\psi^n\bar{\psi}^m$; $n, m \neq 0$ is invariant.

We evaluate the correlation function of $\beta(\psi)$ similarly to how we evaluated the expression for Z in equation (5.26)

$$\langle\beta(\psi)\rangle = \frac{1}{2\pi} \sum_{\psi_0} \int \beta(\psi_0) \exp \left[- \left(|\alpha(\psi - \psi_0)|^2 - \alpha\theta_1\theta_2 - \bar{\alpha}\bar{\theta}_1\bar{\theta}_2 \right) \right] d\psi d\bar{\psi} d\theta_1 d\theta_2 d\bar{\theta}_1 d\bar{\theta}_2 = \sum_{\psi_0} \beta(\psi_0).$$

Again, supersymmetry has simplified an otherwise complicated computation. We read in David Skinner's lecture notes on QFT [26]

"In the absence of experimental evidence for a supersymmetric extension of the Standard Model, the close connections between supersymmetric QFTs and deep mathematics and the fact that supersymmetry helps tame otherwise intractable path integrals now provide the main reason for studying supersymmetry."

It is interesting to note that supersymmetry has many applications beyond trying to extend the Standard Model, although the search for supersymmetric particles is still very much ongoing.

Finally, we mention the importance of functions like $\beta(\psi)$. From now on, we refer to them not as functions, but as fields. Fields such as β which are invariant under the $\bar{\delta}$ -transformation are called *chiral fields*. Chiral fields have certain properties. Most importantly, we may evaluate their correlation functions exactly. Also, the product of two chiral fields, ζ and ν , is also a chiral field

$$\delta(\zeta\nu) = \delta(\zeta)\nu + \zeta\delta(\nu) = 0.$$

The same logic tells us that the addition of two chiral fields is also a chiral field. Under our constraint $\epsilon_1 = \epsilon_2 = \epsilon$, we saw that $\bar{\delta}^2 = 0$, so we may also construct *trivially chiral fields* of the form $\mu = \bar{\delta}\kappa$, where κ is some arbitrary field. It will always hold that $\bar{\delta}\mu = 0$ and $\langle\mu\rangle = 0$.

In general, a QFT is well described by the various correlation functions involving its fields. We could try to calculate the correlation function of any arbitrary field in our theory, but this often proves difficult, and we must turn to perturbation theory. It may therefore be useful to construct a QFT whose main building blocks are chiral fields. Trivially chiral fields like the ones mentioned previously, $\mu = \bar{\delta}\kappa$, are then those fields which play no physically significant role in the theory, since they do not affect the correlation function if added to a chiral field. Often, two chiral fields differ only by the addition of a trivially chiral field, and we can in principle treat those two fields as equivalent. This treatment helps us focus on the essential properties of a theory and only consider relevant degrees of freedom.

6 The Path Integral in 1-Dimensional QFT

In a sense we're now returning to the beginning of this report, since 1-dimensional QFT is another word for quantum mechanics. One difference from the 0-dimensional case is that we have boundaries to our manifold, and we always assume some boundary conditions.

In sections 6.1 and 6.2 we show very briefly how one may generalize Feynman diagrams and supersymmetry from 0 dimensions to 1 dimension. Section 6.2 also introduces supercharges, which are conserved quantities under supersymmetry. The discussion mostly follows Hori et al. [17, ch. 10]. Section 6.3 discusses the use of path integrals in statistical mechanics and thermal QFT, with applications to superfluids. The section is based on Feynman and Hibbs [11, ch. 10] and several articles where path integrals are used to model Helium-4, [2] [4] [24].

6.1 Feynman Diagrams

We will not perform any explicit calculations related to Feynman diagrams - we will simply give an idea of how to generalize some concepts from section 5.1 to 1 dimension.

In 1-dimensional QFT, we have a time variable, which means that our system can evolve and our equations may involve time derivatives. We consider an action similar to that in equation (5.1)

$$S[\psi, \epsilon] = \int \left(\frac{\alpha}{2} \dot{\psi}^2 + i\epsilon \psi^3 + j\psi \right) dt.$$

Now, the first term is an actual kinetic term and the second is a potential term. We have also included a source term. We choose to write out the corresponding partition function and expand it in a power series in ϵ

$$\begin{aligned} Z &= \int \mathcal{D}x(t) e^{-\int \left(\frac{\alpha}{2} \dot{\psi}(t)^2 + i\epsilon \psi(t)^3 + j(t)\psi(t) \right) dt} \\ &= \int \mathcal{D}x(t) e^{-\int \left(\frac{\alpha}{2} \dot{\psi}(t)^2 + j(t)\psi(t) \right) dt} \left(1 - i\epsilon \int \psi(t_1)^3 dt_1 + \frac{(-i\epsilon)^2}{2} \int \int \psi(t_1)^3 \psi(t_2)^3 dt_1 dt_2 + \dots \right) \\ &= \int \mathcal{D}x(t) e^{-\int \left(\frac{\alpha}{2} \dot{\psi}(t)^2 + j(t)\psi(t) \right) dt} \\ &\quad + \sum_{n=1}^{\infty} \frac{(-i\epsilon)^n}{n!} \int \int \dots \int dt_1 dt_2 \dots dt_n \left[\int \mathcal{D}x(t) e^{-\int \left(\frac{\alpha}{2} \dot{\psi}(t)^2 + j(t)\psi(t) \right) dt} \psi(t_1)^3 \psi(t_2)^3 \dots \psi(t_n)^3 \right]. \end{aligned}$$

The last expression in brackets may be rewritten as correlation functions, although we must here employ functional derivatives. For example

$$\begin{aligned}
 \langle \psi(t_1) \rangle_{\epsilon=0} &= \frac{\delta Z}{\delta j(t_1)} = \int \mathcal{D}x(t) \frac{\delta}{\delta j(t_1)} e^{-\int (\frac{\alpha}{2} \dot{\psi}(t)^2 + j(t)\psi(t)) dt} \\
 &= \int \mathcal{D}x(t) \left(\int \frac{\delta j(t)}{\delta j(t_1)} \psi(t) dt \right) e^{-\int (\frac{\alpha}{2} \dot{\psi}(t)^2 + j(t)\psi(t)) dt} \\
 &= \int \mathcal{D}x(t) \psi(t_1) e^{-\int (\frac{\alpha}{2} \dot{\psi}(t)^2 + j(t)\psi(t)) dt},
 \end{aligned}$$

in analogy to equation (5.6). The integrals involved in correlation functions are clearly more difficult to evaluate in 1 dimension than in 0 dimensions. Constructing Feynman diagrams to facilitate the calculations works in much the same way that it did in section 5.1. However, we see that the numbering of the fields is more intuitive in 1 dimension: here, a vertex represents an interaction at *a specific point in time*. When we move to still higher dimensions, vertices exist at different points in *spacetime*.

6.2 Supersymmetry and Supercharges

We consider a supersymmetric 1-dimensional QFT, or rather, supersymmetric quantum mechanics. We choose for our fields one bosonic field x , a complex fermionic field θ and its complex conjugate $\bar{\theta}$. We consider the action

$$S[x, \theta, \bar{\theta}] = \int \left(\frac{1}{2} \dot{x}^2 - \frac{1}{2} (h'(x))^2 + \frac{i}{2} (\bar{\theta} \dot{\theta} - \dot{\bar{\theta}} \theta) - h''(x) \bar{\theta} \theta \right) dt,$$

and a supersymmetry transformation

$$\begin{aligned}
 \delta x &= \epsilon \bar{\theta} - \bar{\epsilon} \theta, \\
 \delta \theta &= \epsilon (\dot{x} + h'(x)), \\
 \delta \bar{\theta} &= \bar{\epsilon} (-i\dot{x} + h'(x)),
 \end{aligned} \tag{6.1}$$

where ϵ is a complex fermionic variable given by $\epsilon = \epsilon_1 + i\epsilon_2$, with $\epsilon_1, \epsilon_2 \in \mathbb{R}$. Also, ϵ has no time-dependence. We see that the transformation in (6.1) simplifies to that in (5.18) if we allow the terms involving time derivatives to go to zero. This is equivalent to going from a 1-dimensional manifold to a 0-dimensional manifold. For this to generate a symmetry, the action must be invariant under the transformation. This is equivalent to saying that the Lagrangian can change by at most a total time derivative under the transformation. By evaluating δS , we can show

$$\begin{aligned}
 \delta S &= \int \left(\delta x \frac{\partial L}{\partial x} + \delta \dot{x} \frac{\partial L}{\partial \dot{x}} + \delta \theta \frac{\partial L}{\partial \theta} + \delta \dot{\theta} \frac{\partial L}{\partial \dot{\theta}} + \delta \bar{\theta} \frac{\partial L}{\partial \bar{\theta}} + \delta \dot{\bar{\theta}} \frac{\partial L}{\partial \dot{\bar{\theta}}} \right) dt \\
 &= \int \frac{\epsilon}{2} \frac{d}{dt} (\dot{x} \bar{\theta} + i h' \bar{\theta}) dt + \int \frac{\bar{\epsilon}}{2} \frac{d}{dt} (-\dot{x} \theta + i h' \theta) dt = 0.
 \end{aligned} \tag{6.2}$$

Since $\epsilon, \bar{\epsilon}$ do not depend on time, we move them outside of the integrals, and we are left with two integrals involving a total time derivative. The whole expression goes to zero.

Furthermore, Noether's theorem tells us that for every differentiable symmetry of the action, there exists a corresponding conservation law [22] [14, ch.13]. Supersymmetry in particular leads to conserved *supercharges*. We show now that our supersymmetric QFT involves two distinct supercharges Q and \bar{Q} .

First of all, we introduce a method of finding such conserved quantities. If we first consider some transformation involving a constant term ϵ , as in (6.1), the action is invariant under this transformation. If we instead let ϵ be a function of time, this is not necessarily the case. We instead arrive at some expression

$$\delta S = \int \dot{\epsilon} \kappa dt, \quad (6.3)$$

where κ is a conserved quantity. The reason why this works is because we have to include extra terms in our expression for δL when we allow ϵ to depend on time. These terms involve a factor of $\dot{\epsilon}$, and we arrive at an expression like the one in equation (6.3). We may then use integration by parts to rewrite equation (6.3), resulting in an integrand on the form $\epsilon \dot{\kappa}$. From the principle of least action, this expression must equal zero for all ϵ . Thus, $\dot{\kappa} = 0$.

To find the quantity which is conserved in our case, we set $\epsilon = \epsilon(t)$ in equation (6.1). We have already concluded that $\delta L = \frac{\epsilon}{2} \frac{d}{dt} (\dot{x} \bar{\theta} + i h' \bar{\theta}) dt + \frac{\bar{\epsilon}}{2} \frac{d}{dt} (-\dot{x} \theta + i h' \theta)$ when ϵ is constant in time, see equation (6.2). Now that ϵ is time-dependent, we can no longer move ϵ and $\bar{\epsilon}$ out of the integral, and these terms remain. We must also include additional terms in δL , namely those including $\dot{\epsilon}$ in $\delta \dot{x}$, $\delta \dot{\theta}$ and $\delta \dot{\bar{\theta}}$. By considering all the above, we obtain a new expression for δS after some algebra

$$\delta S = \int \left(-i \dot{\epsilon} (\bar{\theta} h'(x) + i \bar{\theta} \dot{x}) - i \dot{\bar{\epsilon}} (\theta h'(x) - i \theta \dot{x}) \right) dt. \quad (6.4)$$

A comparison between equation (6.3) and (6.4) reveals that our conserved supercharges are given by

$$\begin{aligned} Q &= \bar{\theta} (i \dot{x} + h'(x)), \\ \bar{Q} &= \theta (-i \dot{x} + h'(x)), \end{aligned}$$

where \bar{Q} is the complex conjugate of Q .

6.3 The Partition Function in Statistical Mechanics and Thermal QFT

Partition functions in QFT are closely related to those in statistical mechanics. This means that the mathematical structure of statistical mechanics and QFT is quite similar and the theory behind QFT is often useful when we analyze many-particle systems. In this section, we give an example of how one can apply QFT to statistical mechanics. We examine specifically the *canonical* partition function from statistical mechanics and its analogue in thermal QFT. The canonical partition function describes a system at fixed temperature, volume and number of particles which can exchange heat with its environment. The analogous field theory is QFT at a fixed temperature, thermal QFT. At the end of this section, we give a non-rigorous discussion about how thermal QFT may be used to predict the behaviour of superfluids.

In statistical mechanics our canonical partition function is given by a sum over the probabilities for the system to be in a given energy state. In a quantum mechanical system with quantized energy levels, we write this as the trace over the Boltzmann function

$$Z = \text{tr}(e^{-\beta H}).$$

We rewrite the above using the general Hamiltonian for a particle in a potential

$$Z = \int dx \langle x | e^{-\beta(\frac{p^2}{2m} + V(x))} | x \rangle. \quad (6.5)$$

It is implied that p and x are operators in the above expression. We would like to rewrite equation (6.5) into something similar to a path integral. In order to do so, we must first rewrite the exponential function as in $e^{-\beta(\frac{p^2}{2m} + V(x))} \rightarrow e^{-\beta\frac{p^2}{2m}} e^{-\beta V(x)}$. However, x and p do not commute. The Baker-Campbell-Hausdorff formula (BCH formula) tells us that in general $e^{f(p)} e^{g(x)} = e^{f(p) + g(x) + \frac{1}{2}[f(p), g(x)] + \dots}$, for some operators f and g . We can easily prove the BCH formula by expanding the logarithm of $e^A e^B$, where A and B are operators

$$\begin{aligned} \log(e^A e^B) &= \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} (e^A e^B - 1)^n = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} \left(\sum_{m=0}^{\infty} \sum_{k=0}^{\infty} \frac{A^m B^k}{m! k!} - 1 \right)^n \\ &= \underbrace{(A + B + AB + \dots)}_{n=1} - \underbrace{\frac{1}{2}(A^2 + B^2 + AB + BA + \dots)}_{n=2} + \dots = A + B + \frac{1}{2}[A, B] + \dots \end{aligned}$$

Thus, if $f(p)$ and $g(x)$ are infinitesimal, we can approximate $e^{f(p)+g(x)} = e^{f(p)} e^{g(x)}$.

We do what we have done previously in this thesis, and split an interval into smaller pieces. We take β in equation (6.5) to be the length of some interval and split it into N pieces, each of length ϵ . This allows us to write $e^{-\beta(\frac{p^2}{2m}+V(x))} = (e^{-\epsilon\frac{p^2}{2m}}e^{-\epsilon V(x)})^N$ as $N \rightarrow \infty$ and $\epsilon \rightarrow 0$. We use this expression to rewrite equation (6.5), and we insert the identity operator in position- and momentum basis at each step along our interval β

$$\begin{aligned}
 Z &= \lim_{N \rightarrow \infty} \int dx \langle x | (e^{-\epsilon\frac{p^2}{2m}} e^{-\epsilon V(x)})^N | x \rangle \\
 &= \lim_{N \rightarrow \infty} \int dx \int dx_1 \int \frac{dp_1}{2\pi} \dots \int dx_N \int \frac{dp_N}{2\pi} \langle x | e^{-\epsilon\frac{p^2}{2m}} | p_1 \rangle \langle p_1 | e^{-\epsilon V(x)} | x_1 \rangle \langle x_1 | e^{-\epsilon\frac{p^2}{2m}} | p_2 \rangle \\
 &\quad \langle p_2 | e^{-\epsilon V(x)} | x_2 \rangle \dots \langle x_{N-1} | e^{-\epsilon\frac{p^2}{2m}} | p_N \rangle \langle p_N | e^{-\epsilon V(x)} | x_N \rangle \langle x_N | x \rangle \\
 &= \lim_{N \rightarrow \infty} \prod_{i=1}^N \int dx_i \int \frac{dp_i}{2\pi} e^{-\epsilon(\frac{p_i^2}{2m} + V(x_i))} \langle x_{i-1} | p_i \rangle \langle p_i | x_i \rangle \Big|_{x_0=x_N} \\
 &= \lim_{N \rightarrow \infty} \prod_{i=1}^N \int dx_i \int \frac{dp_i}{2\pi} e^{-\epsilon(\frac{p_i^2}{2m} + V(x_i) + ip_i(x_{i-1} - x_i))} \Big|_{x_0=x_N}, \tag{6.6}
 \end{aligned}$$

where the constraint $x_0 = x_N$ follows from the integration $\int dx \langle x_n | x \rangle = \int dx \delta(x - x_N)$, and a change in notation $x \rightarrow x_0$.

We integrate over each p_i in expression (6.6) to obtain

$$\begin{aligned}
 Z &= \lim_{N \rightarrow \infty} \prod_{i=1}^N \sqrt{\frac{m}{2\pi\epsilon}} \int dx_i e^{-\epsilon\frac{m}{2} \left(\frac{x_i - x_{i-1}}{\epsilon} \right)^2 + \epsilon V(x_i)} \Big|_{x_0=x_N} = \lim_{N \rightarrow \infty} \prod_{i=1}^N \sqrt{\frac{m}{2\pi\epsilon}} \int dx_i e^{-\epsilon L(x_i, \dot{x}_i)} \Big|_{x_0=x_N} \\
 &= \boxed{\int_{x(0)}^{x(\beta)} \mathcal{D}x e^{-S[x, \dot{x}]} \Big|_{x(0)=x(\beta)}}. \tag{6.7}
 \end{aligned}$$

Here, we interpret ϵ as an infinitesimal piece of the "time interval" β , and we denote $\dot{x} = \frac{x_i - x_{i-1}}{\epsilon}$. This is only an analogy since we observe the similarity between the path integral in equation (3.2) and equation (6.7), although the latter is Wick-rotated and expressed in natural units. Note that the interval over which the path integral runs is not a true time interval here, so we are not considering a true motion between states.

Equation (6.7) is the partition function in thermal QFT. The expression agrees with our general formula for partition functions (4.2), but here we have additional constraints. Namely, the initial- and final state for the path integral must coincide and our interval is given by β , which in turn depends on the temperature T , as $\beta = \frac{1}{kT}$. Observe also

that we must integrate over all initial (final) states in equation (6.7). This differs from path integrals in previous sections, where we have assumed a fixed initial state. In statistical mechanics, we are interested in systems that exist in one of many states, each with a given probability. Therefore we must consider every possible initial position for a particle in this case.

We imagine a many-particle system: a liquid. The initial (final) state for the system then consists of a particle distribution. One possible path for such a system is illustrated in figure (13), part A. Each blue dot represents an initial position for a particle, to which it returns at the end of the interval. Now let's assume our liquid consists of indistinguishable bosons. For such particles, the final state in equation (6.7) looks the same if we interchange two or more bosons. In figure (13), part B, we illustrate one such path, which includes a permutation of final positions. In conclusion, both figure A and B illustrate allowed paths for the system, and both must be considered as we evaluate equation (6.7).

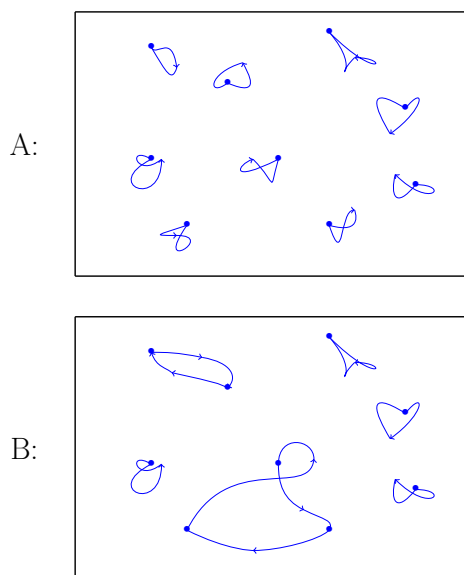


Figure 13: Two possible paths for particles in a liquid, from an initial state to an identical final state, where the dots represent initial/final positions. All particles are indistinguishable bosons.

Sidenote: if we consider fermions instead of bosons, some permutations of final positions give positive contributions to the partition function, and other permutations give negative contributions. For simplicity, we stick to the treatment of bosons in this example. Note also that all integer spin particles are bosons. Our discussion therefore applies to helium-4, which is a boson.

Normally, the paths which contribute most to the partition function are those which minimize the action, i.e. the shortest possible paths. When we evaluate equation (6.7), we mainly consider paths that move a very short distance away from the initial (final)

state. Paths such as those in figure (13), part B, force the particles to travel a longer distance. In other words, paths which involve permutations generally contribute less to the partition function. We can see just how suppressed such contributions are by considering equation (6.7), which for a system of particles is proportional to

$$Z \propto \int \mathcal{D}x(u) \exp \left(-\frac{m}{2} \sum_i \int_0^\beta \dot{x}_i^2 du \right) \approx \int \sum_P \rho(x_i) \exp \left(-\frac{m}{2\beta} \sum_i |x_i - P(x_i)|^2 \right) dx_i. \quad (6.8)$$

Here, $P(x_i)$ denotes the new final position of x_i after a permutation. In the last step, we approximate the paths from initial to final position as straight lines. We also assume some type of lattice model for the liquid, which enables us to introduce a particle density $\rho(x_i)$. The sum over P represents a sum over all possible permutations of final positions, and the sum over i is a sum over all particles in our liquid. This is a very crude approximation, but it works for our qualitative discussion.

From equation (6.8), we see that a path which includes a permutation of just two particles contributes to the partition function with a term proportional to $C = \exp \left(\frac{-mkTd_i^2}{\hbar^2} \right)$, where the factor \hbar^2 has been introduced by dimensional analysis. T is the temperature of the liquid. d_i is the distance travelled from initial to final state for particle i . This distance is at least of the order of magnitude of the average distance between particles. A path involving permutations of N particles includes a factor C^N , and its contribution is much suppressed. However, there are also $N!$ possible permutations involving the N particles, so the contribution is not necessarily negligible. For low enough temperatures and small enough spacing between particles, C may be large enough that contributions from paths involving permutations compares to those from paths without permutations. A deeper analysis of equation (6.7) for Helium-4 reveals that for a specific temperature, permutations involving an arbitrary amount of particles suddenly contribute noticeably to the partition function [2]. This behaviour arises very suddenly, and completely changes the behaviour of the liquid, since most information about the system is encoded in the partition function. Among other things, the liquid starts to flow without friction and its heat capacity grows exponentially. The liquid becomes a *superfluid*, and this is due to quantum mechanical effects at low temperatures, as we have discussed here.

To give an example of how these permuted paths might affect the properties of a liquid, we investigate the heat capacity. Heat capacity is defined in terms of the partition function as

$$C_v = T \frac{\partial^2 (kT \ln Z)}{\partial T^2} = kT \frac{1}{Z} \frac{\partial Z}{\partial T} - kT^2 \frac{1}{Z} \frac{\partial Z}{\partial T} \frac{1}{Z} \frac{\partial Z}{\partial T} + kT^2 \frac{1}{Z} \frac{\partial^2 Z}{\partial T^2}. \quad (6.9)$$

If we perform the derivatives in expression (6.9) on equation (6.8), the resulting expression for C_v contains two terms which are proportional to $\langle d_i^2 \rangle$ and $\langle d_i^4 - \langle d_i^2 \rangle^2 \rangle$ respectively, again with $d_i = |x_i - P(x_i)|$. We see that the first term is the average squared

distance travelled for each particle, and the second is the average of the difference between the quadratic distance and the average squared distance. When the partition function receives a majority of its contributions from paths without permutations, all distances d_i are small and of the same magnitude. However, at some low temperature we suddenly include particle paths of all different lengths in our computation. The above terms increase drastically, along with the heat capacity.

We excluded the potential term from the partition function in equation (6.8), and we made several other approximations throughout this section. A deeper analysis is required to accurately predict the quantitative behaviour of superfluids. This was done by Feynman in 1953 [9] [4], as he took into consideration the strong interaction between atoms by considering only paths which do not cross over other atoms. Such paths are achieved by allowing obstructing atoms to move a small distance out of the way. Since this requires additional kinetic energy, it introduces an extra factor in the partition function, i.e. a multiplicative factor in the integrand of equation (6.8). Feynman also argues that for a chosen set of particles, only permutations between closest neighbors contribute noticeably to the partition function. This can be shown mathematically, from analyzing the multiplicative factor just mentioned. In conclusion, the problem of modeling superfluids reduces to considering a lattice model of a liquid and a partition function similar to that in equation (6.8). We then evaluate the contributions from different paths for the particles in the system. Permutations are taken into consideration by constructing polygons between lattice sites. A numerical simulation based on the above reasoning was performed by Elser and Ceperley in 1987 [24]. They employed Monte Carlo methods to construct polygons in lattices models of Helium-4 (which enters a superfluid phase around 2 Kelvin). Many more have conducted similar studies, and a summary of similar articles was published by Ceperley in 1995 [2]. Resulting predictions for e.g. energy, specific heat and superfluid pressure show good agreement with experiment.

7 Conclusions

We introduced the subject of path integrals with a discussion about Hamiltonian vs. Lagrangian mechanics, where the more fundamental nature of Lagrangian mechanics provided one of the motivations for introducing the path integral in quantum mechanics. Another motivation came from the need of a formulation of quantum mechanics compatible with special relativity. We gave the mathematical definition of the path integral, $K(b, a) = \int \mathcal{D}x(t) e^{\frac{i}{\hbar} S}$, and also discussed interference between alternative paths in quantum mechanical systems for a more intuitive interpretation. We gave a summary of the properties of the path integral. Our discussion showed that the path integral behaves as expected in the classical limit, that the path integral preserves causality and that it treats consecutive events in a consistent manner. A common method for evaluating path integrals was introduced, i.e. splitting time intervals into infinitesimal pieces. With this method, we obtained an expression for the kernel of a free particle and for a particle in an arbitrary potential. The latter result led to Feynman's proof of equivalence between the path integral and the Schrödinger equation. We argue that

this proof validates the path integral formulation of quantum mechanics.

In later sections, we introduced 0-dimensional QFT. We discussed partition functions and correlation functions in particular, and Feynman diagrams and supersymmetry as tools to evaluate these functions. We also solved a simple problem in 0-dimensional QFT: for a given action, we found the free energy and the equations of motion by classical means, and then by taking quantum mechanical corrections into account. Our results showed that these corrections were in fact vacuum fluctuations.

We moved to 1-dimensional QFT and found that our theories apply also in this case, although computations become more complex. We also showed that the canonical partition function in statistical mechanics can be rewritten to give the partition function in thermal QFT. The result led to a practical application of the path integral in many-particle systems as we attempted to quantitatively describe the behaviour of superfluids. By studying articles on the subject, we saw that many successful simulations have been performed using path integrals to predict the behaviour of Helium-4 in the transition from fluid to superfluid.

Modern applications of the path integral far exceed those discussed in this report. What started out as a mathematical curiosity by Dirac has developed into a useful tool in many fields. One might ask whether theoretical physics is worth the effort when many new theories lack obvious applications. The efforts by Dirac and Feynman, and many others, show that there may be unexpected applications down the road. An interesting continuation of this thesis would be to investigate QFT in higher dimensions and how path integrals are applied in e.g. string theory, to see if path integrals could be a piece of the puzzle in finding a theory of quantum gravity.

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A The Central Equations in Lagrangian and Hamiltonian Mechanics

We give a brief recap of the central equations in Lagrangian- and Hamiltonian mechanics. First: *Functionals* are functions which acts on functions. One example is the action

$$S[L(q_i, \dot{q}_i, t)] = \int_a^b L(q_i, \dot{q}_i, t) dt, \quad \text{where } L = T - V. \quad (\text{A.1})$$

The principle of least action applied to equation (A.1) leads to the *Euler-Lagrange equations*

$$\boxed{\frac{\partial L}{\partial q_i} - \frac{\partial}{\partial t} \left(\frac{\partial L}{\partial \dot{q}_i} \right) = 0.} \quad (\text{A.2})$$

For a derivation, see Goldstein et al. [14, ch. 2].

Hamiltonian mechanics is closely related to Lagrangian mechanics. The Hamiltonian is defined as

$$H(q_i, p_i, t) = p_i \dot{q}_i - L(q_i, \dot{q}_i, t), \quad (\text{A.3})$$

where the indices in the first term on the RHS implies a sum over all variables. The Hamiltonian often evaluates to the total energy of a system, but not always. We may solve for L in equation (A.3) and insert this expression in equation (A.2). If we consider q_i and p_i to be our new variables, we obtain

$$\begin{aligned} \frac{\partial}{\partial p_i} (p_i \dot{q}_i - H(q_i, p_i, t)) - \frac{\partial}{\partial t} \left(\frac{\partial}{\partial \dot{p}_i} (p_i \dot{q}_i - H(q_i, p_i, t)) \right) &= 0 \rightarrow \dot{q}_i = \frac{\partial H}{\partial p_i}, \\ \frac{\partial}{\partial q_i} (p_i \dot{q}_i - H(q_i, p_i, t)) - \frac{\partial}{\partial t} \left(\frac{\partial}{\partial \dot{q}_i} (p_i \dot{q}_i - H(q_i, p_i, t)) \right) &= 0 \rightarrow \dot{p}_i = -\frac{\partial H}{\partial q_i}. \end{aligned}$$

The resulting equations are called *Hamilton's equations*

$$\boxed{\begin{aligned} \dot{q}_i &= \frac{\partial H}{\partial p_i}, \\ \dot{p}_i &= -\frac{\partial H}{\partial q_i}. \end{aligned}}$$

B Cauchy's Theorem over Infinite Domains

We state Cauchy's theorem here as expressed in Gamelin [13, p.110].

Cauchy's Theorem. Let D be a bounded domain with piecewise smooth boundary. If $f(z)$ is an analytic function on D that extends smoothly to ∂D , then

$$\int_{\partial D} f(z) dz = 0. \quad (\text{B.1})$$

For a proof, see the same book by Gamelin. In the following sections, we perform some computations using Cauchy's theorem, to be used in the main text. Throughout, we use the notation $z = x + iy$.

B.1 Complex-Valued Gaussian Integral

Assume we have an integral of the form

$$\int_{-\infty}^{\infty} e^{iax^2} dx, \quad (\text{B.2})$$

where x is a real variable and a is a real constant.

We choose a closed contour in the complex plane as in figure (14).

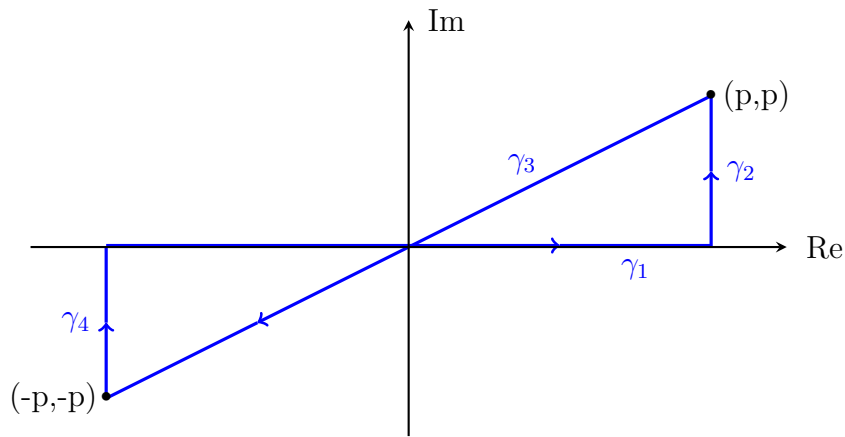


Figure 14: Closed directed curve in the complex plane.

The closed contour is made up of curves γ_i . We let I_i denote the integral of e^{iaz^2} w.r.t. z over the corresponding curve γ_i . By Cauchy's integral theorem (B.1) we have

$$I_1 + I_2 + I_3 + I_4 = 0 \implies I_1 = -I_2 - I_3 - I_4, \quad (\text{B.3})$$

I_1 is given by

$$I_1 = \int_{-p}^p e^{iax^2} dx, \quad (\text{B.4})$$

so that I_1 with $p \rightarrow \infty$ corresponds to the integral which we aim to evaluate, see (B.2). We express the integrals I_2 and I_4 as

$$I_2 = \{z = p + iy\} = \int_0^p e^{ia(p+iy)^2} idy.$$

$$I_4 = \{z = -p + iy\} = \int_{-p}^0 e^{ia(-p+iy)^2} idy = \int_0^p e^{ia(p+iy)^2} idy = I_2. \quad (\text{B.5})$$

We find an upper bound to this integral

$$|I_2| = \left| \int_0^p e^{ia(p+iy)^2} dy \right| \leq \int_0^p e^{-2apy} dy = \frac{1 - e^{-2ap^2}}{2ap}. \quad (\text{B.6})$$

From equation (B.6) and (B.5), we conclude $\lim_{p \rightarrow \infty} |I_2| = \lim_{p \rightarrow \infty} |I_4| = 0$.

The integral I_3 evaluates to

$$I_3 = \{z = x + ix\} = (1 + i) \int_p^{-p} e^{-2ax^2} dx. \quad (\text{B.7})$$

We let $p \rightarrow \infty$ and evaluate equation (B.7) as a Gaussian integral

$$\lim_{p \rightarrow \infty} I_3 = (1 + i) \int_{\infty}^{-\infty} e^{-2ax^2} dx = -(1 + i) \sqrt{\frac{\pi}{2a}} = -\sqrt{2} (e^{i\frac{\pi}{2}})^{\frac{1}{2}} \sqrt{\frac{\pi}{2a}} = -\sqrt{\frac{i\pi}{a}}. \quad (\text{B.8})$$

We combine our results from (B.3), (B.4) and (B.8) to get

$$\boxed{\int_{-\infty}^{\infty} e^{iax^2} dx = -\lim_{p \rightarrow \infty} I_3 = \sqrt{\frac{i\pi}{a}}.} \quad (\text{B.9})$$

B.2 Complex-Valued Gaussian Integral with a Quadratic Term

Assume we have an integral of the form

$$\int_{-\infty}^{\infty} x^2 e^{iax^2} dx.$$

This can be written as

$$\lim_{p \rightarrow \infty} \int_{-p}^p x^2 e^{iax^2} dx = -i \frac{d}{da} \left(\int_{-p}^p e^{iax^2} dx \right) = \{\text{Equation (B.9)}\} = -i \frac{d}{da} \left(\sqrt{\frac{i\pi}{a}} \right) = \frac{1}{2a^{\frac{3}{2}}} \sqrt{-i\pi}.$$

Our final result is

$$\boxed{\int_{-\infty}^{\infty} x^2 e^{iax^2} dx = \frac{1}{2a^{\frac{3}{2}}} \sqrt{-i\pi}.$$

B.3 Complex-Valued Gaussian Integral with a Linear Term in the Exponent

Assume we have an integral of the form

$$\int_{-\infty}^{\infty} e^{i(ax^2+bx)} dx.$$

We solve this by completing the square in the exponent

$$\int_{-\infty}^{\infty} e^{i\left(\sqrt{a}x + \frac{b}{2\sqrt{a}}\right)^2 - i\frac{b^2}{4a}} dx = \{y = \sqrt{a}x + \frac{b}{2\sqrt{a}}\} = \frac{1}{\sqrt{a}} \exp\left(-\frac{ib^2}{4a}\right) \int_{-\infty}^{\infty} e^{iy^2} dy = \sqrt{\frac{i\pi}{a}} \exp\left(-\frac{ib^2}{4a}\right),$$

where the last equality follows from equation (B.9). Our final result is

$$\boxed{\int_{-\infty}^{\infty} e^{i(ax^2+bx)} dx = \sqrt{\frac{i\pi}{a}} \exp\left(-\frac{ib^2}{4a}\right).$$

B.4 Integral of a Complex-Valued Exponential Function

Assume we have an integral of the form

$$I = \int_{-\infty}^{\infty} \frac{i}{x + i\epsilon} e^{-ix\tau} dx, \quad (\text{B.10})$$

where x is a real variable and τ and ϵ are real constants. We choose a closed contour as in figure (15).

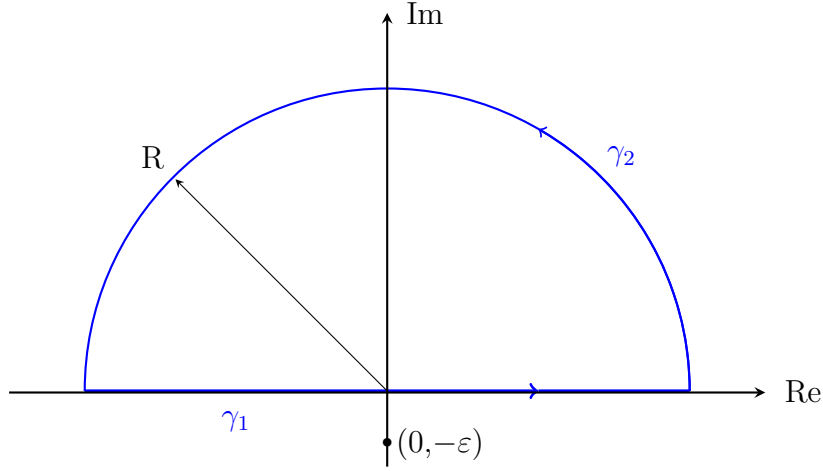


Figure 15: Closed directed contour in the complex plane with a pole at $(0, -\epsilon)$.

We let I_i denote the integral of equation $\frac{i}{z + i\epsilon} e^{-iz\tau}$ w.r.t. z over the corresponding curve γ_i . Since the integrand consists of an exponential function multiplied by the inverse of a polynomial, it is analytic everywhere except at $z = -i\epsilon$. Thus, the integrand is analytic inside our closed contour, as long as $\epsilon > 0$. By Cauchy's theorem (B.1), we have

$$I_1 + I_2 = 0 \quad \rightarrow \quad I_1 = -I_2.$$

We note also that the integral I_1 as $R \rightarrow \infty$ is our original problem (B.10).

We evaluate I_2 as the radius $R \rightarrow \infty$

$$\lim_{R \rightarrow \infty} I_2 = \lim_{R \rightarrow \infty} \int_{\gamma_2} \frac{i}{x + iy + i\epsilon} e^{-i\tau x} e^{\tau y} dz. \quad (\text{B.11})$$

As $R \rightarrow \infty$, either $|x|$ or y or both go to infinity along the curve γ_2 . We impose $\tau < 0$, which forces the integral in equation (B.11) to zero when $y \rightarrow \infty$. Similarly, the oscillating function $e^{-i\tau x}$ forces the integral to zero when $|x| \rightarrow \infty$, since this oscillating function is integrated against a bounded function. Our result is then $I_1 = -I_2 = 0$ and the solution to our problem

$$I = \int_{-\infty}^{\infty} \frac{i}{w + i\epsilon} e^{-iw\tau} dw = 0, \quad \text{if } \tau < 0.$$

B.5 The Principal Part of the Integral of a Complex-Valued Exponential Function

Assume we have an integral of the form

$$I = P.P. \int_{-\infty}^{\infty} \frac{e^{-i\tau x}}{x} dx = \lim_{\epsilon \rightarrow 0} \left(\int_{-\infty}^{-\epsilon} \frac{e^{-i\tau x}}{x} dx + \int_{\epsilon}^{\infty} \frac{e^{-i\tau x}}{x} dx \right),$$

where τ is a constant, with $\tau < 0$ and x is a real variable. We choose a closed contour as in figure (16). We let I_i denote the integral of the function $e^{-i\tau z}/z$ with respect to z over the corresponding curve γ_i .

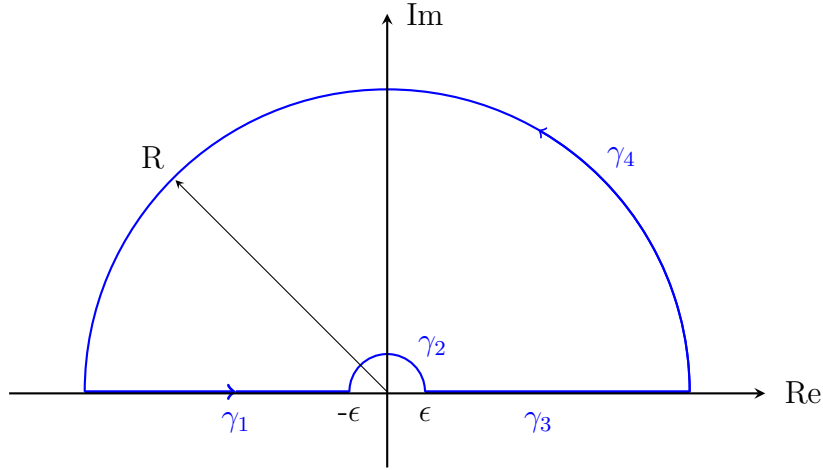


Figure 16: Closed directed curve in the complex plane.

Using Cauchy's theorem (B.1), we can write

$$I = I_1 + I_3 = -I_2 - I_4, \quad (\text{B.12})$$

where it is implied that we take $R \rightarrow \infty$ and $|\epsilon| \rightarrow 0$ as we evaluate the integrals $I_1 - I_4$.

By the same argument as in section B.4, we find that $I_4 = 0$ as $R \rightarrow \infty$. The integral I_2 is evaluated as

$$\begin{aligned} \lim_{|\epsilon| \rightarrow 0} I_2 &= \lim_{|\epsilon| \rightarrow 0} \int_{\gamma_2} \frac{e^{-iz\tau}}{z} dz = \{e^{-iz\tau} = 1, \text{ to the lowest order in Taylor series}\} = \\ &= \lim_{|\epsilon| \rightarrow 0} \int_{\gamma_2} \frac{1}{z} dz = \{z = |\epsilon|e^{i\theta}\} = i \int_{\pi}^0 d\theta = -i\pi. \end{aligned} \quad (\text{B.13})$$

From equation (B.12) and (B.13) we obtain

$$\boxed{P.P. \int_{-\infty}^{\infty} \frac{e^{-iz\tau}}{z} dz = i\pi, \quad \text{if } \tau < 0.}$$

C An Introduction to Green's Functions

The concept of Green's functions is used in the main text when we discuss the Schrödinger equation. Green's functions are used to solve inhomogeneous linear differential equations, such as

$$L[u(\bar{x}, t)] = Q(\bar{x}, t), \quad (\text{C.1})$$

where Q is a source, and L is an operator, $L = ik_1 \frac{\partial}{\partial t} + k_2 \nabla^2$, with $k_1, k_2 \in \mathbb{R}$. We also impose some inhomogeneous boundary conditions $u(\bar{x}_a, t) = \alpha$, $u(\bar{x}_b, t) = \beta$ and the initial condition $u(\bar{x}, 0) = g(\bar{x})$. The function $u(\bar{x}, t)$ is then the response to the source Q , under the given boundary- and initial conditions.

The Green's function $G(\bar{x}, t; \bar{x}_0, t_0)$ is defined by

$$L[G(\bar{x}, t; \bar{x}_0, t_0)] = \delta(\bar{x} - \bar{x}_0)\delta(t - t_0), \quad (\text{C.2})$$

with corresponding *homogeneous* boundary conditions as those for u at \bar{x}_a, \bar{x}_b . $G(\bar{x}, t; \bar{x}_0, t_0)$ is then the response at (\bar{x}, t) to a concentrated source at (\bar{x}_0, t_0) . By causality, this response should be zero if $t < t_0$, i.e. we impose $G(\bar{x}, t; \bar{x}_0, t_0) = 0$ if $t < t_0$. The Green's function defined in equation (C.2) can then be used to solve the problem in equation (C.1). The explicit solution is

$$\begin{aligned} u(\bar{x}, t) = & \int_0^t \iiint G(\bar{x}, t; \bar{x}_0, t_0) Q(\bar{x}_0, t_0) d^3 x_0 dt_0 - ik_1 \iiint G(\bar{x}, t; \bar{x}_0, 0) g(\bar{x}) d^3 x_0 \\ & + k_2 \int_0^t \oint u(\bar{x}_0, t_0) \nabla_{\bar{x}_0} G(\bar{x}, t; \bar{x}_0, t_0) \cdot \hat{n} dS_0 dt_0. \end{aligned}$$

(C.3)

A derivation of this will follow below. First, we focus on the expression in equation (C.3) and see that the Green's function propagates the effect of each nonhomogeneous part of our problem to give the response $u(\bar{x}, t)$. The first term gives the influence from the source Q . The second term gives the influence from the initial condition. The third

term gives the influence from the boundary conditions. This is a general property of Green's functions: they propagate the effect of some function via integration.

There is one more property of Green's functions which we should discuss: *the reciprocity theorem*

$$\boxed{G(\bar{x}_1, t_1; \bar{x}_0, t_0) = G(\bar{x}_0, t_1; \bar{x}_1, t_0)}, \quad (\text{C.4})$$

This formula tells us that the location of the source and the location of the response can be interchanged, and the influence from the source remains the same. Below follows a derivation of equation (C.3) and (C.4).

First, we introduce an adjoint operator $L^* = -ik_1 \frac{\partial}{\partial t} + k_2 \nabla^2$. We also consider a Green's function where we let the time of the source vary instead of the time of the response, $G(\bar{x}, t_1; \bar{x}_1, t)$. Note that the influence on some function at time t from a source at time t_0 depends only on the elapsed time, so we can consider the time interval $[t, t_1]$ as well as $[-t_1, -t]$. Using this fact, we rewrite our source-varying Green's function $G(\bar{x}, t_1; \bar{x}_1, t) = G(\bar{x}, -t; \bar{x}_1, -t_1)$. This is identical to our original Green's function, equation (C.2), but with the opposite sign for the time variable. We see that our source-varying Green's function fulfills $L^*[G(\bar{x}, t_1; \bar{x}_1, t)] = \delta(\bar{x} - \bar{x}_1)\delta(t - t_1)$.

We also consider two arbitrary functions $u(\bar{x}, t)$, $v(\bar{x}, t)$ and employ a method often used to solve similar problems. We write

$$\int_{t_i}^{t_f} \iiint [uL^*(v) - vL(u)] d^3x dt = \int_{t_i}^{t_f} \iiint \left[-ik_1 \left(u \frac{\partial v}{\partial t} + v \frac{\partial u}{\partial t} \right) - k_2 (v \nabla^2 u - u \nabla^2 v) \right] d^3x dt. \quad (\text{C.5})$$

We rewrite the first term in the integrand on the RHS using integration by parts

$$\begin{aligned} \int_{t_i}^{t_f} \iiint ik_1 \left(u \frac{\partial v}{\partial t} + v \frac{\partial u}{\partial t} \right) d^3x dt &= ik_1 \iiint uv \Big|_{t_i}^{t_f} d^3x + \int_{t_i}^{t_f} \iiint ik_1 \left(-v \frac{\partial u}{\partial t} + u \frac{\partial v}{\partial t} \right) d^3x dt \\ &= ik_1 \iiint uv \Big|_{t_i}^{t_f} d^3x. \end{aligned} \quad (\text{C.6})$$

We see that the adjoint operator L^* was introduced since L is not self-adjoint. If we had used L in place of L^* in equation (C.6), we would have been left with an additional integral on the right hand side.

We also rewrite the second term in the integrand on the RHS of equation (C.5) using Green's Second Identity, which is derived from the divergence theorem as

$$\begin{aligned}
\oint (u\nabla v - v\nabla u) \cdot \hat{n} dS &= \iiint \nabla \cdot (u\nabla v - v\nabla u) d^3x \\
&= \iiint (\nabla u \nabla v - \nabla v \nabla u) d^3x + \iiint (u\nabla^2 v - v\nabla^2 u) d^3x = \iiint (u\nabla^2 v - v\nabla^2 u) d^3x.
\end{aligned} \tag{C.7}$$

Here, \hat{n} is the normal unit vector to the boundary S . We use equation (C.7) and (C.6) to rewrite (C.5) as

$$\int_{t_i}^{t_f} \iiint [uL^*(v) - vL(u)] d^3x dt = -ik_1 \iiint uv \Big|_{t_i}^{t_f} d^3x - k_2 \int_{t_i}^{t_f} \oint (v\nabla u - u\nabla v) \cdot \hat{n} dS dt. \tag{C.8}$$

This will be an important result moving forward.

To finish our proof, we set $u = u(\bar{x}, t)$, $v = G(\bar{x}, t_0; \bar{x}_0, t)$ and $t_f = t_{0+}$, $t_i = 0$ in equation (C.8). t_{0+} here means that we integrate an infinitesimal slice of time beyond t_0 . Note also that v is a source-varying Green's function. We obtain

$$\begin{aligned}
&\int_0^{t_{0+}} \iiint (u(\bar{x}, t) \delta(\bar{x} - \bar{x}_0) \delta(t - t_0) - G(\bar{x}, t_0; \bar{x}_0, t) Q(\bar{x}, t)) d^3x dt \\
&= -ik_1 \iiint u(\bar{x}, t) G(\bar{x}, t_0; \bar{x}_0, t) \Big|_0^{t_{0+}} d^3x \\
&\quad - k_2 \int_0^{t_{0+}} \oint (G(\bar{x}, t_0; \bar{x}_0, t) \nabla u(\bar{x}, t) - u(\bar{x}, t) \nabla G(\bar{x}, t_0; \bar{x}_0, t)) \cdot \hat{n} dS dt. \tag{C.9}
\end{aligned}$$

The first term in the integrand on the LHS in equation (C.9) evaluates to $u(\bar{x}_0, t_0)$. The term $\int_0^{t_{0+}} \oint (G(\bar{x}, t_0; \bar{x}_0, t) \nabla u(\bar{x}, t) \cdot \hat{n}) dS dt$ evaluates to zero since G equals zero at the boundary. Also, the term $ik_1 \iiint u(\bar{x}, t_{0+}) G(\bar{x}, t_0; \bar{x}_0, t_{0+}) d^3x$ evaluates to zero by causality, since $t_{0+} > t_0$.

We rewrite equation (C.9) according to the above discussion. One can also show that we may now set $t_{0+} = t_0$. Finally, a change of variables $(x_0, t_0) \leftrightarrow (x, t)$, along with the reciprocity relation in equation (C.4), allows us to obtain the expression in (C.3).

We prove the reciprocity formula (C.4) in a similar way. We again consider equation (C.8) and set $u = G(\bar{x}, t; \bar{x}_0, t_0)$, $v = G(\bar{x}, t_1; \bar{x}_1, t)$ and $t_f = \infty$, $t_i = -\infty$. We obtain

$$\begin{aligned}
&\int_{-\infty}^{\infty} \iiint (G(\bar{x}, t; \bar{x}_0, t_0) \delta(\bar{x} - \bar{x}_1) \delta(t - t_1) - G(\bar{x}, t_1; \bar{x}_1, t) \delta(\bar{x} - \bar{x}_0) \delta(t - t_0)) d^3x dt \\
&= ik_1 \iiint G(\bar{x}, t; \bar{x}_0, t_0) G(\bar{x}, t_1; \bar{x}_1, t) \Big|_{t=-\infty}^{\infty} d^3x + \text{integral of } G \text{ over boundary.}
\end{aligned}$$

The final term where we evaluate G at the boundary equals zero. The first term on the right hand side also equals zero from causality. Thus, by evaluating the left hand side, we obtain $G(\bar{x}_1, t_1; \bar{x}_0, t_0) - G(\bar{x}_0, t_1; \bar{x}_1, t_0) = 0$. This concludes the derivation of equation (C.4).

For similar proofs and a more in-depth discussion, see Haberman [16, ch.11].
