Preface

Chapter 1

Introduction

In this thesis, some new aspects in dealing with path integrals are discussed, in particular the perturbatively defined quantum statistical path integral and the application of methods known from quantum field theory such as generating functionals in phase space. The expectation values appearing in perturbative expansions of path integrals are usually pictured by Feynman diagrams. We derive a graphical recursion relation to systematically construct topologically different Feynman diagrams with their correct multiplicities for the anharmonic oscillator as an quantum statistical example and for scattering processes in quantum electrodynamics, which illustrates the power of this method for quantum field theoretic problems. Generalizations and extensions of variational perturbation theory are used to calculate statistical properties of quantum systems and membranes.

1.1 Path Integrals

It was in 1948 when R.P. Feynman introduced the quantum mechanical path integral to calculate the transition amplitude for a charged particle in electromagnetic field [1]. With the path integral, the reinterpretation of the classically known notions "paths" and "orbits" became possible. Not only the paths which make the action extremal but also all other ways the particle may follow contribute to the transition amplitude with a phase factor which relates the action of a path to Planck's constant $\hbar$. In its Euclidean form, the statistical path integral is built up from Boltzmann factors indeed indicating the probability of a certain path of the particle [2–4].

The exact calculation of path integrals is only possible for systems whose action is quadratic in the canonical variables, for example position $x(\tau)$ and momentum $p(\tau)$. In quantum mechanics, the path integrals for the transition amplitudes of the free particle and the harmonic oscillator are exactly calculated by time-slicing. Explicitly evaluating the path integral for a system with a more complicated potential is impossible, if it cannot be brought into the necessary Gaussian form. This is, however, possible for a class of systems, where the path integral can be transformed to be of oscillator type, e.g. for the hydrogen atom by applying the Duru-Kleinert transformation [4]. In non-interacting quantum field theories, e.g. for Klein-Gordon or Dirac fields, the Lagrangian density is usually quadratic in the fields and their derivatives. Thus such path integrals are of Gaussian type and can easily be calculated. If quantum fields interact, functional integrals cannot be evaluated analytically in almost all cases.

1.2 Perturbative and Non-Perturbative Methods for the Calculation of Path Integrals

Nevertheless, the interest in functional integrals has grown rapidly. Path integrals for a physical system with weakly coupled interaction allow for a simple perturbation expansion, where the correlation functions can be graphically pictured by Feynman diagrams. The most famous example is the interaction of charged relativistic particles with an electromagnetic field, as described by quantum electrodynamics, where the coupling constant is $\alpha \approx 1/137$. For strong-coupling systems, path integrals are used for the development of nonperturbative methods. Strong-coupling theories are necessary for calculating critical exponents of a system near a phase transition [5], for describing confinement between quarks in quantum chromodynamics [6], or for the investigation of interacting strings [7]. Path integral Monte Carlo methods on a lattice were developed to combine the selective probability picture of path integrals with the great numerical power of supercomputers. Analytic non-perturbative methods for strongly coupled systems are usually used to perform resummations of perturbative expansions as, for example, by Padé or Borel methods. Alternatively, Feynman and Kleinert [8] as well as Giachetti and Tognetti [9] developed a variational approach to approximatively calculate path integrals for *arbitrarily* coupled quantum mechanical systems. Within the last decade, the precision has been strongly improved by extending it to higher-order variational perturbation theory [4, Chap. 5]. Additionally, considerable progress was achieved in applying it to calculate critical exponents from strong-coupling series of the Ginzburg-Landau theory of critical phenomena [5,10,11].

1.3 Contents of This Thesis

This thesis is divided into four parts. In **Part I**, a perturbative definition of the quantum statistical phase space integral is introduced. Conventional time-slicing methods for calculating path integrals yield integration measures, which are not well defined since these are infinite in the continuum limit. Moreover, it is difficult to prove reparametrization invariance of the path integral under coordinate transformations, in particular in curved spaces. A perturbative expansion of any phase space path integral, where the complete Hamiltonian is treated as perturbation, does not possess these problems, since the exactly solvable contribution has a regular measure and is trivially reduced to products of δ functions. It is interesting that this procedure leads directly to a high-temperature expansion for the partition function. We prove the applicability of this method by calculating the effective classical potential for the harmonic oscillator.

Since it is necessary to calculate expectation values of products of Hamiltonians, it is useful to introduce Feynman rules, which can also be applied, if the Hamiltonian contains nonpolynomial terms. This requires to generalize Wick's rule, too. Furthermore, the calculation of mixed position-momentum correlations must be considered. As examples, we study harmonic expectation values whose treatment is necessary for the harmonic variational perturbation theory. In the case of nonpolynomial perturbations, so-called smearing formulas replace the ordinary Wick decompositions of polynomial correlations into products of two-point correlation functions. We also discuss the role of zero-mode fluctuations for paths with periodic and fixed boundary conditions.

In high orders of perturbation theory, it becomes often difficult to determine all topologically different Feynman diagrams and their multiplicities. Usually this problem is attacked with the help of combinatorial considerations. A powerful alternative is presented in **Part II**. We derive recursion relations from which all Feynman diagrams in any order are systematically generated without introducing artificial currents. These relations can be completely expressed in a graphical way. This means that the Feynman diagrams of a certain theory in any order are generated by cutting, removing, and glueing operations on diagrams of previous orders of perturbation. We present recursion relations for the quantum mechanical anharmonic oscillator and investigate the applicability to quantum field theories, where we specialize to quantum electrodynamics.

The resummation of divergent perturbative series with harmonic variational perturbation theory is the central aspect of **Part III**. After a short introduction of variational perturbation theory, we first

generalize this theory to density matrices and calculate the particle densities for the double well and the pair distribution function of hydrogen for different temperatures. Another interesting system is the hydrogen atom in a uniform external magnetic field, since it destroys the isotropy of the Coulomb interaction between electron and proton. The calculation of the effective classical potential, which governs the quantum statistics of this system, is followed by a detailed treatment of the ground-state energy. This quantity has a power expansion for weak strengths of the magnetic field, but a complicated logarithmic behavior for strong magnetic fields. We use the variational approach to find an expression for the ground-state energy as a function of the magnetic field strength, which is valid for all strengths of the magnetic field although the asymptotic behavior is so extremely different. The results are in good agreement with known values from numerical calculations. Considering the strong-field asymptotics in detail, we go analytically beyond an estimate presented by Landau.

Another example, where variational perturbation theory yields very good results, is the strong-coupling calculation of the fluctuation pressure of a membrane between walls. This shall be discussed in **Part IV**. A fluid membrane is tensionless, and its shape is governed by the curvature energy. By thermal fluctuations, the membrane exerts a pressure upon the walls. The pressure law is ideal-gas-like and contains a dimensionless pressure constant, whose value is not exactly known. From our strong-coupling calculation we obtain a very precise value that lies well in the error bounds of former Monte Carlo simulations. We also evaluate the pressure constants for a stack of membranes, where our strong-coupling approach is applicable for any number of membranes. Compared with Monte Carlo simulations, where only constants for low numbers of membranes were computed, our results are in very good agreement.