INTRODUCTION TO QUANTUM MECHANICS

Schrödinger Equation and Path Integral

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Preface

With the discovery of quantization by Planck in 1900, quantum mechanics is now more than a hundred years old. However, a proper understanding of the phenomenon was gained only later in 1925 with the fundamental Heisenberg commutation relation or phase space algebra and the associated uncertainty principle. The resulting Schrödinger equation has ever since been the theoretical basis of atomic physics. The alternative formulation by Feynman in terms of path integrals appeared two to three decades later. Although the two approaches are basically equivalent, the Schrödinger equation has found much wider usefulness, particularly in applications, presumably, in view of its simpler mathematics. However, the realization that solutions of classical equations, notably in field theory, play an important role in our understanding of a large number of physical phenomena, intensified the interest in Feynman's formulation of quantum mechanics, so that today this method must be considered of equal basic significance. Thus there are two basic approaches to the solution of a quantum mechanical problem, and an understanding of both and their usefulness in respective domains calls for their application to exemplary problems and their comparison. This is our aim here on an introductory level.

Throughout the development of theoretical physics two types of forces played an exceptional role: That of the restoring force of simple harmonic motion proportional to the displacement, and that in the Kepler problem proportional to the inverse square of the distance, i.e. Newton's gravitational force like that of the Coulomb potential. In the early development of quantum mechanics again oscillators appeared (though not really those of harmonic type) in Planck's quantization and the Coulomb potential in the Bohr model of the hydrogen atom. Again after the full and proper formulation of quantum mechanics with Heisenberg's phase space algebra and Born's wave function interpretation the oscillator and the Coulomb potentials provided the dominant and fully solvable models with a large number of at least approximate applications. To this day these two cases of interaction with nonresonant spectra feature as the standard and most important

illustrative examples in any treatise on quantum mechanics and — excepting various kinds of square well and rectangular barrier potentials — leave the student sometimes puzzled about other potentials that he encounters soon thereafter, like periodic potentials, screened Coulomb potentials and maybe singular potentials, but also about complex energies that he encounters in a parallel course on nuclear physics. Excluding spin, any problem more complicated is frequently dispensed with by referring to cumbersome perturbation methods.

Diverse and more detailed quantum mechanical investigations in the second half of the last century revealed that perturbation theory frequently does permit systematic procedures (as is evident e.g. in Feynman diagrams in quantum electrodynamics), even though the expansions are mostly asymptotic. With various techniques and deeper studies, numerous problems could, in fact, be treated to a considerable degree of satisfaction perturbatively. With the growing importance of models in statistical mechanics and in field theory, the path integral method of Feynman was soon recognized to offer frequently a more general procedure of enforcing first quantization instead of the Schrödinger equation. To what extent the two methods are actually equivalent, has not always been understood well, one problem being that there are few nontrivial models which permit a deeper insight into their connection. However, the aforementioned exactly solvable cases, that is the Coulomb potential and the harmonic oscillator, again point the way: For scattering problems the path integral seems particularly convenient, whereas for the calculation of discrete eigenvalues the Schrödinger equation. Thus important level splitting formulas for periodic and anharmonic oscillator potentials (i.e. with degenerate vacua) were first and more easily derived from the Schrödinger equation. These basic cases will be dealt with in detail by both methods in this text, and it will be seen in the final chapter that potentials with degenerate vacua are not exclusively of general interest, but arise also in recently studied models of large spins.

The introduction to quantum mechanics we attempt here could be subdivided into essentially four consecutive parts. In the **first part**, Chapters 1 to 14, we recapitulate the origin of quantum mechanics, its mathematical foundations, basic postulates and standard applications. Our approach to quantum mechanics is through a passage from the Poisson algebra of classical Hamiltonian mechanics to the canonical commutator algebra of quantum mechanics which permits the introduction of Heisenberg and Schrödinger pictures already on the classical level with the help of canonical transformations. Then the Schrödinger equation is introduced and the two main exactly solvable cases of harmonic oscillator and Coulomb potentials are treated in detail since these form the basis of much of what follows. Thus this first part

deals mainly with standard quantum mechanics although we do not dwell here on a large number of other aspects which are treated in detail in the long-established and wellknown textbooks.

In the **second part**, Chapters 15 to 20, we deal mostly with applications depending on perturbation theory. In the majority of the cases that we treat we do not use the standard Rayleigh–Schrödinger perturbation method but the systematic perturbation procedure of Dingle and Müller which is introduced in Chapter 8. After a treatment of power potentials, the chapter thereafter deals with Yukawa potentials, and their eigenvalues. This is followed by the important case of the cosine or Mathieu potential for which the perturbation method was originally developed, and the behaviour of the eigenvalues is discussed in both weak and strong coupling domains with formation of bands and their asymptotic limits. The solution of this case — however in nonperiodic form — turns out to be a prerequisite for the complete solution of the Schrödinger equation for the singular potential $1/r^4$ in Chapter 19, which is presumably the only such singular case permitting complete solution and was achieved only recently. The earlier Chapter 17 also contains a brief description of a similar treatment of the elliptic or Lamé potential. The following Chapter then deals with Schrödinger potentials which represent essentially anharmonic oscillators. The most prominent examples here are the double well potential and its inverted form. Using perturbation theory, i.e. the method of matched asymptotic expansions with boundary conditions (the latter providing the so-called nonperturbative effects), we derive respectively the level-splitting formula and the imaginary energy part for these cases for arbitrary states. In the final chapter of this part we discuss the large order behaviour of the perturbation expansion with particular reference to the cosine and double well potentials.

In **part three** the path integral method is introduced and its use is illustrated by application to the Coulomb potential and to the derivation of the Rutherford scattering formula. Thereafter the concepts of instantons, periodic instantons, bounces and sphalerons are introduced and their relevance in quantum mechanical problems is discussed (admittedly in also trespassing the sharp dividing line between quantum mechanics and simple scalar field theory). The following chapters deal with the derivation of level splitting formulas (including excited states) for periodic potentials and anharmonic oscillators and — in the one-loop approximation considered — are shown to agree with those obtained by perturbation theory with associated boundary conditions. We also consider inverted double wells and calculate with the path integral the imaginary part of the energy (or decay width). The potentials with degenerate minima will be seen to re-appear throughout the text, and the elliptic or Lamé potential — here introduced earlier as a generaliza-

tion of the Mathieu potential — re-appears as the potential in the equations of small fluctuations about the classical configurations in each of the basic cases (cosine, quartic, cubic). All results are compared with those obtained by perturbation theory, and whenever available also with the results of WKB calculations, this comparison on a transparent level being one of the main aims of this text.

The introduction of collective coordinates of classical configurations and the fluctuations about these leads to constraints. Our **fourth and final part** therefore deals with elementary aspects of the quantization of systems with constraints as introduced by Dirac. We then illustrate the relevance of this in the method of collective coordinates. In addition this part considers in more detail the region near the top of a potential barrier around the configuration there which is known as a sphaleron. The physical behaviour there (in the transition region between quantum and thermal physics) is no longer controlled by the Schrödinger equation. Employing anharmonic oscillator and periodic potentials and re-obtaining these in the context of a simple spin model, we consider the topic of transitions between the quantum and thermal regimes at the top of the barrier and show that these may be classified in analogy to phase transitions in statistical mechanics. These considerations demonstrate (also with reference to the topic of spin-tunneling and large-spin behaviour) the basic nature also of the classical configurations in a vast area of applications.

Comparing the Schrödinger equation method with that of the path integral as applied to identical or similar problems, we can make the following observations. With a fully systematic perturbation method and with applied boundary conditions, the Schrödinger equation can be solved for practically any potential in complete analogy to wellknown differential equations of mathematical physics, except that these are no longer of hypergeometric type. The particular solutions and eigenvalues of interest in physics are — as a rule — those which are asymptotic expansions. This puts Schrödinger equations with e.g. anharmonic oscillator potentials on a comparable level with, for instance, the Mathieu equation. The application of path integrals to the same problems with the same aims is seen to involve a number of subtle steps, such as limiting procedures. This method is therefore more complicated. In fact, in compiling this text it was not possible to transcribe anything from the highly condensed (and frequently unsystematic) original literature on applications of path integrals (as the reader can see, for instance, from our precise reference to unavoidable elliptic integrals taken from Tables). An expected observation is that — ignoring a minor deficiency — the WKB approximation is and remains the most immediate way to obtain the dominant contribution of an eigenenergy, it is, however, an approximation whose higher

order contributions are difficult to obtain. Nonetheless, we also consider at various points of the text comparisons with WKB approximations, also for the verification of results.

In writing this text the author considered it of interest to demonstrate the parallel application of both the Schrödinger equation and the path integral to a selection of basic problems; an additional motivation was that a sufficient understanding of the more complicated of these problems had been achieved only in recent years. Since this comparison was the guide-line in writing the text, other topics have been left out which are usually found in books on quantum mechanics (and can be looked up there), not the least for permitting a more detailed and hopefully comprehensible presentation here. Throughout the text some calculations which require special attention, as well as applications and illustrations, are relegated to separate subsections which — lacking a better name — we refer to as Examples.

The line of thinking underlying this text grew out of the author's association with Professor R. B. Dingle (then University of Western Australia, thereafter University of St. Andrews), whose research into asymptotic expansions laid the ground for detailed explorations into perturbation theory and large order behaviour. The author is deeply indebted to his one-time supervisor Professor R. B. Dingle for paving him the way into this field which — though not always at the forefront of current research (including the author's) — repeatedly triggered recurring interest to return to it. Thus when instantons became a familiar topic it was natural to venture into this with the intent to compare the results with those of perturbation theory. This endeavour developed into an unforeseen task leading to periodic instantons and the exploration of quantum-classical transitions. The author has to thank several of his colleagues for their highly devoted collaboration in this latter part of the work over many years, in particular Professors J.–Q. Liang (Taiyuan), D. K. Park (Masan), D. H. Tchrakian (Dublin) and Jian–zu Zhang (Shanghai). Their deep involvement in the attempt described here is evident from the cited bibliography.*

H. J. W. Müller–Kirsten

*In the running text references are cited like e.g. Whittaker and Watson [283]. For ease of reading, the references referred to are never cited by mere numbers which have to be identified e.g. at the end of a chapter (after troublesome turning of pages). Instead a glance at a nearby footnote provides the reader immediately the names of authors, e.g. like E. T. Whittaker and G. N. Watson [283], with the source given in the bibliography at the end. As a rule, formulas taken from Tables or elsewhere are referred to by number and/or page number in the source, which is particularly important in the case of elliptic integrals which require a relative ordering of integration limits and parameter domains, so that the reader is spared difficult and considerably time-consuming searches in a source (and besides, shows him that each such formula here has been properly looked up).

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