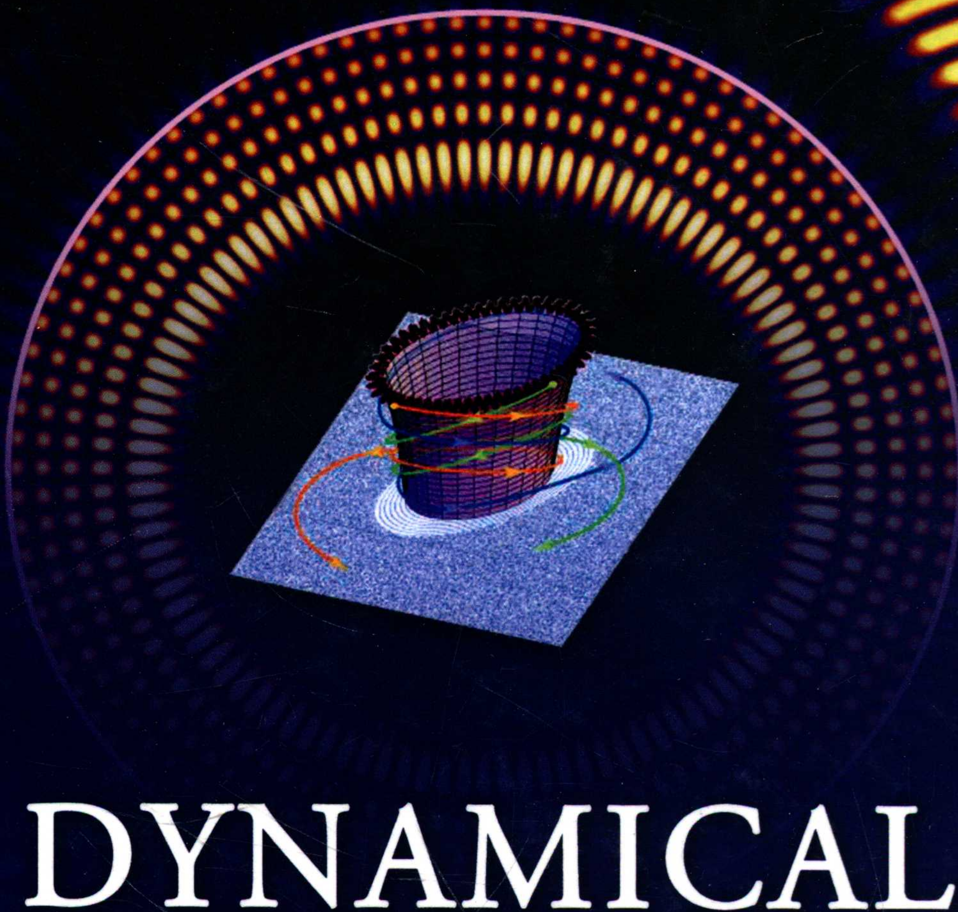
Edited by
Srihari Keshavamurthy
Peter Schlagheck



DYNAMICAL TUNNELING

Theory and Experiment

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Foreword

From my personal perspective, it is fundamentally interesting to consider physical phenomena which occur quantum mechanically, but not classically, or the reverse, occur classically, but not quantum mechanically. Tunneling falls squarely into this scheme and as such is quite a fascinating topic. Although tunneling was recognized a long, long time ago and was worked on extensively in many physical contexts, it has nevertheless gone through a revolution of sorts beginning in the very early 1980s during which it went from merely being fascinating to being way more fascinating, as I might be tempted to put it crudely. I would identify two advances at the heart of this revolution. The first is the conceptual introduction of dynamical tunneling by Davis and Heller. This generalization of barrier tunneling to tunneling through a separatrix allows for a unified picture of, say, what is happening in a rapidly rotating quantum pendulum tunneling between clockwise and counterclockwise motions, a problem without a clearly identifiable potential barrier, and a particle tunneling back and forth in a double well, a problem with a clearly identifiable potential barrier. The dynamics of either possesses a separatrix from a classical phase-space perspective. Generalizing a bit further from there, Ozorio de Almeida's treatment of tunneling induced by a classical resonance followed not long thereafter.

Davis and Heller were concerned with tunneling problems that necessarily require a multi-degree-of-freedom perspective. This is in fact what I call the second advance, that is, not shying away from such problems. Later in the 1980s, Wilkinson initiated analytical work on such systems and we began our studies on chaos-assisted tunneling (Lin and Ballentine were also seeing the same effects). Prior to this point, a number of multi-degree-of-freedom problems were properly solved via mapping back to a barrier problem in an effective single collective degree of freedom. Think of fission. However, once one begins to consider tunneling problems of an inescapable, multi-degree-of-freedom nature, then all the complex features of classical dynamics, regular and chaotic motion, homoclinic tangles, periodic orbits, diffusion, and so on, may rear their heads in a variety of ways, and as many of us have found over the years, they all seem to in some context or another. It is this realization which, in my view, greatly enriches the subject, and I have no sympathy for the notion that these "complexities" represent unfortunate complications. It also leads to an openness to consider new experimental problems, which may be found with ultracold atoms and optical lattices. Instead of avoiding multidimensional arrangements, there is a motivation for creating them or seeking them out.

Back in 1997, the National Institute for Nuclear Theory held an international program organized by Bohigas, Leggett, and Tomsovic entitled "Tunneling in Complex Systems" where a significant community interested in tunneling problems came together and discussed such topics as dynamical tunneling, chaos-assisted tunneling and ionization, chaotic tunneling, multidimensional complex trajectories, and possible or even speculative connections to various experiments involving magnetic systems or the decay of superdeformed nuclei. My feeling in hindsight is that it was clear that there was still an enormous amount we did not understand about dynamical tunneling problems at that time. Perhaps going a bit further, it was not at all obvious whether some of the known unsolved problems would be solved anytime soon either. Many appeared on their face to be rather intractable. In terms of an analytical theory, understanding chaos-assisted tunneling is yet to begin. My recollection is that this was also before most, if not all, of the beautiful work done with ultracold atoms and optical lattices.

Nevertheless, I guess it should not come as an enormous surprise that a great deal of progress has been made since then, but a pleasant surprise it has been. New ideas, new contexts, new theories, new experiments, they are all there. Personally, and among other things not being mentioned in a short foreword, I have been impressed with the work on resonance-assisted tunneling beginning with Ullmo's group and tunneling between regular and chaotic states from Ketzmerick's group, all of which are required for a complete theory of chaos-assisted tunneling. The experiments from Phillips' and Raizen's groups impress as well, though the effective size of $\hbar$ in those works muddies the interpretations. A book is most certainly called for and this one fits the bill; one where there is an overview and a consolidation of presentation of the current state of dynamical tunneling. Anyone generally interested in tunneling really should be familiar with the works presented here. I look forward to seeing this book in print.

Steven Tomsovic
Indian Institute of Technology Madras

Preface

Tunneling has remained a special phenomenon, a quintessential quantum effect, starting with the early days of quantum theory. Nearly a century's worth of theoretical and experimental studies have highlighted the crucial role of tunneling in various physical phenomena. The far-reaching implications of tunneling are evident in diverse fields including nuclear, atomic, molecular physics, and, more recently, in the area of mesoscopic science. Despite the obvious relevance of this topic to a wide range of disciplines, an interdisciplinary scientific community devoted to tunneling has not yet developed to a satisfactory degree. One may attribute this, at first glance, to the apparent simplicity of a generic tunneling process, which basically involves "only" a quantum particle that crosses a classical barrier due to the evanescent components of its wave function. The quantitative description of this seemingly simple process, however, can become rather intricate and rich if more than one particle and/or more than one spatial dimension are effectively involved. This is especially the case for "dynamical tunneling," which essentially denotes classically forbidden transitions through dynamical rather than energetic barriers, that is barriers that are formed by constraints of the underlying classical dynamics related to exact or approximate constants of motion. This book is devoted to the study of dynamical tunneling—mechanisms and consequences.

Apart from providing a resource for the state of the art along various research lines related to dynamical tunneling, the present book is also an attempt to establish and connect the "tunneling community" across the borders of the various fields and disciplines in physics. Previous steps in this direction include, among others, the book *Tunneling in Complex Systems* edited by Steven Tomsovic (World Scientific, 1998), as well as several international workshops, such as the "International Symposium of Complexified Dynamics, Tunneling and Chaos" (Kusatsu, Japan, 2005) and, most recently, the conference and summer school "Tunneling and Scattering in Complex Systems—From Single to Many Particle Physics" (Dresden, Germany, 2009). Incidentally, the selection of specific topics and contributors for this book coincides to a large extent with the spectrum of talks and lectures at this latter event in Dresden—although this book was not intended to serve as a proceeding of the Dresden conference. We were certainly not able to cover the entire breadth of the subject of dynamical tunneling in this book, but had to make a selection for the sake of coherence: semiclassical aspects of dynamical tunneling as well as tunneling with cold atoms and molecular manifestations are therefore more strongly represented than, for instance, nonclassical processes in electronic mesoscopic physics.

As always, this book would not have been possible without the support of a number of colleagues whom we would like to thank. Specifically, we are indebted to our contact persons at Taylor & Francis CRC, Lance Wobus and David Fausel, for their initiatives, encouragement, patience, and assistance in details concerning the formalities of the publication process. Thanks are also due to Shashi Kumar from Glyph International for his valuable technical help concerning the assembly of the individual chapters. P.S. would, further, like to take this opportunity and thank his co-organizers of the Dresden workshop, Arnd Bäcker and Markus Oberthaler, as well as the Max-Planck Institute for the Physics of Complex Systems for hosting and financing the workshop. He would also like to acknowledge support from the DFG Forschergruppe 760 "Scattering Systems with Complex Dynamics" which provided a unique framework for interdisciplinary research on complex dynamics in open systems in general and on dynamical tunneling in particular during the last three years. The success of the Forschergruppe is evident from at least two of the contributions (Chapters 6 and 8) that are a part of this volume.

Last but not least, we have to mention our contributors, the authors of the chapters of this book, who agreed to provide review articles on aspects of their specific research on dynamical tunneling.

Their willingness to participate in the cross-refereeing process of the book as well as constant words of encouragement has made our task easy. It has been a unique and wonderful experience for us. We thank them for their contributions and hope that this book will serve as a useful resource on various aspects of dynamical tunneling.

Srihari Keshavamurthy
Peter Schlagheck

Editors

Srihari Keshavamurthy is a theoretical chemist in the department of chemistry at the Indian Institute of Technology (IIT) Kanpur, India. He got his BSc degree from the University of Madras, India; MS from the Villanova University, Pennsylvania; and PhD from University of California, Berkeley. After a postdoc at Cornell University, he joined the IIT Kanpur in December 1996. His primary interest is to understand the mechanisms of chemical reaction dynamics and control from the classical-quantum correspondence perspective.

Peter Schlagheck is a theoretical physicist in the department of physics at the University of Liège, Belgium. He got his PhD in 1999 at the Technical University of Munich, Germany. After a postdoc at the Université Paris Sud, France from 1999 to 2001, he became an assistant at the University of Regensburg, Germany in 2002. In 2009, he obtained a faculty position at the University of Liège. His research interests include the transport of ultracold atoms and tunneling in the presence of chaos.

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Contents

1 An Overview of Dynamical Tunneling

Eric J. Heller

CONTENTS

This chapter represents a personal perspective on dynamical tunneling. It does not attempt to review all the significant recent developments in the subject, many of which are already represented in this volume. Rather, it weaves a path through some case histories, some simple but emblematic, others more complex and involving experimental counterparts.

The whole concept of tunneling is by its very nature semiclassical. Quantum amplitudes do what they need to do according to quantum mechanics, and it is up to us to label something as tunneling or not. We do so by comparison with classical mechanics, making tunneling an intrinsically semiclassical idea. Potential barrier tunneling, a process wherein quantum eigenstates penetrate regions of coordinate space which are classically forbidden, is the simplest kind of tunneling, found in every elementary textbook on quantum mechanics.

Dynamical tunneling got its name by its contrast with barrier tunneling. Classical mechanical trajectories sometimes refuse to go where they are allowed to by constraints other than potential barriers, constraints such as action or angular momentum. In other words, even in the absence of potential barriers, the dynamics may refuse to carry the trajectories from region A to region B, and if the quantum amplitudes respect no such constraint in the quantized version of the same system, we say the quantum system is "dynamically tunneling." It is well known, for example, that when a plane wave meets a potential barrier, some of it is backscattered even if the total energy lies above the highest point of the potential barrier. Even better known is the wave amplitude found in the shadow region behind a barrier. These are examples of dynamical tunneling, although in both cases historically these phenomena have been called "diffraction." The trouble with the term diffraction is that it is highly abused: one can find it describing all sorts of phenomena including scattering which is perfectly classically allowed.

We prefer the umbrella term suggested long ago by Bill Miller, namely "classically forbidden processes." Such processes are usefully divided into two types: barrier tunneling and dynamical tunneling.

One might easily get the impression in a book like this that quantum mechanics happily explores everywhere that classical trajectories do, and then some, due to tunneling. But of course this is not the case: certain types of Anderson localization represent quantum reluctance to go where classical trajectories do. A very simple example of quantum localization (which we take to be an umbrella term of which Anderson localization is one example) is a particle in a "box and corridor" shaped as in Figure 1.1. All but a measure zero of the classical orbits in this system manage to escape; however, it is intuitively obvious that the very lowest stationary states of the system are quantum mechanically localized to the vicinity of the box. The reason is that the zero point energy cost of being in the corridor is greater than the total energy of states which are confined to the larger box. Therefore, the first few quantum mechanical eigenstates will be confined to the box and a short distance into the corridor.

1.1 MIRRORS AND SHADOWS

An impenetrable segment of a barrier wall, illuminated by trajectories from in front, possesses a hard shadow, a refuge from the hail of projectiles. As is well known in all sorts of wave theories including quantum mechanics, waves do not respect such hard shadows. Since the dynamics (in this case ballistic straight-line trajectories) creates a hard shadow, penetration of the waves into the shadow region is an example of dynamical tunneling. An equally good but less commonly used example is the reflection from the front surface of the mirror, from one point to another, along a path that cannot be reached by a specular bounce.

Consider the source point A and the receiving point B as shown in Figure 1.2. According to the Kirchhoff approximation, we may consider the total illumination at B to be a sum of all the amplitudes which reach a point x on the mirror, and from there scatter to the point B. The amplitude

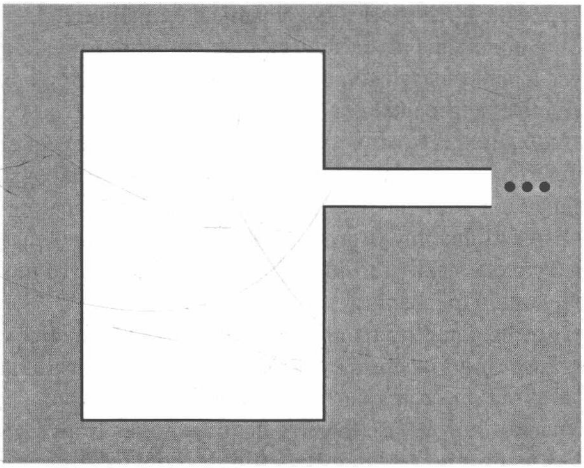

FIGURE 1.1 Box and corridor (the lines represent hard walls, the potential is flat inside, and the corridor extends forever to the right) which supports many bound states below the energy of the first state which propagates down the corridor. All but a set of measure zero trajectories escape, however, independent of their energy.

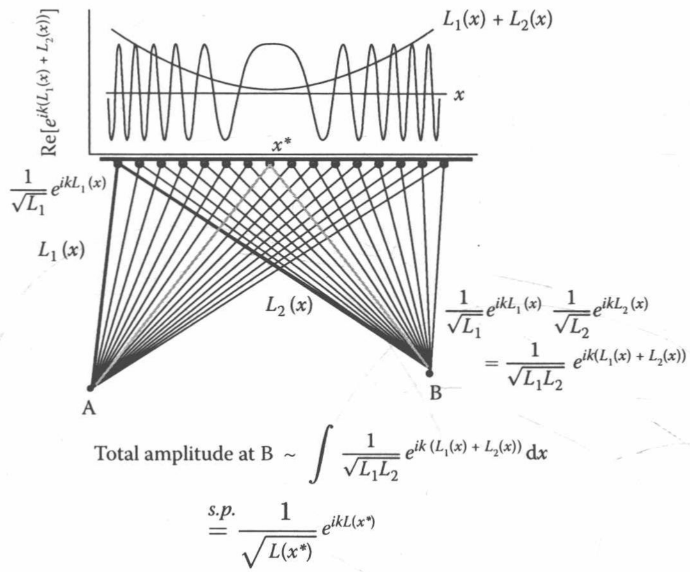

FIGURE 1.2 Schematic showing the construction of the amplitudes scattered from the point A to the point B by a mirror. The Kirchhoff construction supposes this amplitude to be decomposed in terms of waves arriving at various points along the mirror, and then from these points to a final position here the point B. The total amplitude at B is then obtained by adding up all the amplitudes along the mirror. Alternately, approximating the integral by stationary phase results in a compact formula involving only the specular path shown in gray.

of illumination of each point x is the expected form $\sim 1/\sqrt{L_1(x)}\ e^{ikL_1(x)}$ where L_1 is the distance from the source to the point at x, and k is the wavenumber. Illuminated by this amplitude, each point x radiates a spherical wave which reaches the point B, further attenuated by traveling a distance $L_2(x)$; the overall contribution at B for that impact point on the mirror is therefore $\sim 1/\sqrt{L_1}\ e^{ikL_1(x)} 1/\sqrt{L_2}\ e^{ikL_2(x)} = 1/\sqrt{L_1 L_2}\ e^{ik(L_1(x)+L_2(x))}$. Adding up all such impact points, we have the amplitude for scattering off the mirror from A to B as

$$a = \int \frac{1}{\sqrt{L_1 L_2}} e^{ik(L_1(x)+L_2(x))}\, dx = \frac{1}{\sqrt{L(x^*)}} e^{ikL(x^*)}, \tag{1.1}$$

where the integral is done by stationary phase over points x along the mirror. It is seen that the total path length from A to a point on the mirror at x and then on to B is a minimum at the specular scattering point. This should ring all sorts of bells (minimum action, etc.).

A straightforward stationary phase integration gives the right-hand side of Equation 1.1, where $L(x^*)$ is the total length of the classical, specular bounce off the mirror, and x^* is the specular, minimum action point. Thus, the Kirchhoff approximation gives exactly what we would have written down to begin with.

However, suppose now that the mirror is too short, or the points A and B are moved over, such that the would-be specular point is no longer on the mirror. According to what Miller would call the "primitive semiclassical approximation," a term pregnant with the possibility of doing better, meaning stationary phase for everything in sight, the amplitude for the indirect path from A to B is now zero. Stationary phase and the primitive semiclassical approximation always arrives at a classical path; since there is no classical path which bounces, the correct answer at this level is indeed zero.

The Kirchhoff approximation, the integral in Equation 1.1, is not necessarily intended to be evaluated by stationary phase. It is a perfectly good integral in its own right, and its exact evaluation

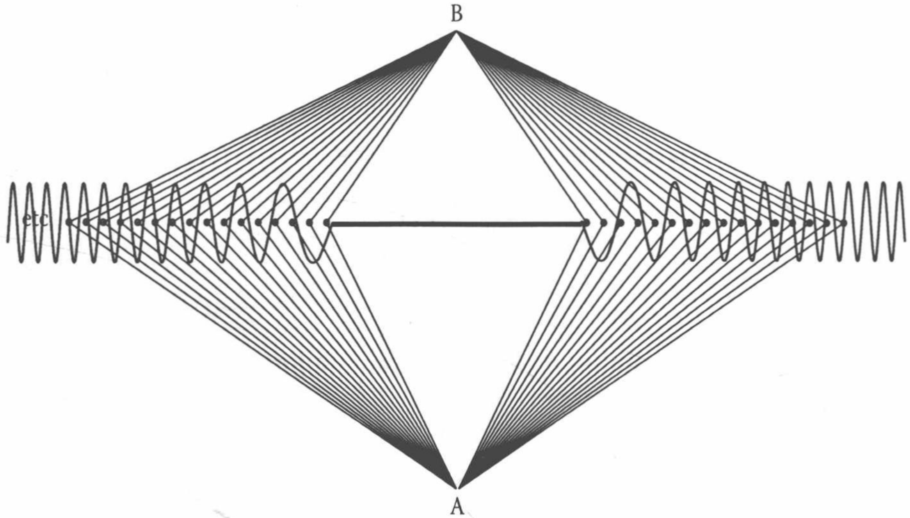

FIGURE 1.3 A construction similar to Figure 1.2, carried out for the shadow region.

would give a finite amplitude for scattering off the mirror from A to B. The resulting approximation is somehow semiclassical, but not primitive any longer; some would say this is a "uniform" approximation. The Kirchhoff integral in this case has a strong flavor of the more general initial value representations, a term and technique also introduced in the 1970s by Miller.

The Kirchhoff approximation to illumination in the shadow, the dark side of the barrier, can be handled in much the same way, using points x to either side of the mirror extending to infinity, and writing the amplitude in the shadow region as an integral over all the illuminated points not on the mirror but lying on a line which includes it (see Figure 1.3).

Books on the theory of the stationary phase approximation point out that the subleading contributions after the stationary phase points, if any, come from any sharp cutoff in the integrals. Our finite mirror gives precisely this type of cutoff. An end of the mirror may be thought of as a spherical source contributing a scattered amplitude of a magnitude which can be estimated by figuring the flux through a region about one wavelength long.

This example illustrates one of the paradigms for dynamical tunneling: stationary phase gives no contribution, since by definition there is no classical path connecting the regions in question. The amplitude is then written as a uniform integral, which is evaluated by direct means, not stationary phase. The result is a uniform semiclassical approximation, in some sense partly semiclassical and partly quantum mechanical. In any case, such uniform or initial value methods often give an accurate description of dynamical tunneling events.

1.2 ABOVE-BARRIER REFLECTION

Probably the most important paradigm for dynamical tunneling is above-barrier reflection, alluded to at the beginning of this chapter. The reason for the prominence of this paradigm is that many dynamical tunneling processes which appear to have nothing to do with the above barrier reflection can be recast as such by canonical transformations. Once the above-barrier reflection is understood, its characteristic signature can be seen in the phase space of quite different dynamical systems. The common denominator is a phase space separatrix, crossing it in a way which is classically forbidden, and quite analogous to barrier tunneling (Figure 1.4). In that figure, the dark gray path corresponds to "ordinary" barrier tunneling, that is, jumping across the barrier to an equivalent energy contour on