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Theoretical Molecular Biophysics

Second Edition

Springer

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ISSN 1618-7210 ISSN 2197-5647 (electronic)
Biological and Medical Physics, Biomedical Engineering
ISBN 978-3-662-55670-2 ISBN 978-3-662-55671-9 (eBook)
DOI 10.1007/978-3-662-55671-9

Library of Congress Control Number: 2017948199

Printed on acid-free paper

This Springer imprint is published by Springer Nature
The registered company is Springer-Verlag GmbH Germany
The registered company address is: Heidelberger Platz 3, 14197 Berlin, Germany

Preface to the Second Edition

The first edition of this book was based on a two-semester course at the physics department of TU München. Approximately, one-third of this edition is new. We tried to give a larger overview over the physical concepts which are applicable to biological systems including established models as well as more recent developments. The major changes are as follows:

The chapter on continuum solvent models contains a discussion of the time dependence of the reaction field after rapid excitation which is useful to understand ultrafast time-resolved experiments on Stokes shift and relaxation processes. The discussion of ion transport includes also models for cooperativity in ion channel kinetics. Here we concentrate on the famous MWC and KNF models for ligand-gated ion channels. In connection with electron transfer theory we present a simple model for the mutual interaction with the medium polarization and discuss the interplay between charge delocalization and self-trapping. Harmonic normal mode approximation and nonadiabatic interactions are discussed in more detail. A new chapter is devoted to intramolecular electronic transitions. The coupling to the radiation field is treated as well with the semiclassical as the quantum mechanical method and the Einstein coefficients for absorption and emission are derived. The chapter ends with an overview of radiationless processes. The chapter on crossing between states has been rewritten and extended. We begin with wavepacket motion for a free particle and a harmonic oscillator, and discuss the classical approximation of nuclear motion. We discuss the adiabatic to diabatic transformation and the definition of quasidiabatic states. The semiclassical approximation to one-dimensional curve crossing leads systematically to the famous Landau–Zener model. The chapter ends with an introduction to conical intersections and the linear vibronic coupling model as a simple example. Two new chapters were added about specific biological systems. First, we discuss charge transfer processes in DNA and describe the contributions of diffusive hopping and superexchange over bridge states. Second, we present rather new models on the photosynthetic reaction center and discuss the possible importance of heterogeneous superexchange and coupled proton motion. We would like to thank Dr. Wolfgang Dietz for his contributions to this chapter, which replaces a rather short one of the first edition. The molecular motor models include more recent ideas concerning ratchet models and localized reactions. Finally, we added two new chapters to the appendix on the classical approximation of quantum motion and on the complex cotangent function.

Garching, Germany
April 2017

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Preface to the First Edition

Biophysics deals with biological systems, such as proteins, which fulfill a variety of functions in establishing living systems. While the biologist uses mostly a phenomenological description, the physicist tries to find the general concepts to classify the materials and dynamics which underly specific processes. The phenomena span a wide range, from elementary processes, which can be induced by light excitation of a molecule, to the communication of living systems. Thus, different methods are appropriate to describe these phenomena. From the point of view of the physicist, this may be continuum mechanics to deal with membranes, hydrodynamics to deal with transport through vessels, bioinformatics to describe evolution, electrostatics to deal with aspects of binding, statistical mechanics to account for temperature and to learn about the role of the entropy, and last but not least quantum mechanics to understand the electronic structure of the molecular systems involved. As can be seen from the title, Molecular Biophysics, this book will focus on systems for which sufficient information on the molecular level is available. Compared to crystallized standard materials studied in solid-state physics, the biological systems are characterized by very big unit cells containing proteins with thousands of atoms. In addition, there is always a certain amount of disorder, so that the systems can be classified as complex. Surprisingly, the functions like a photocycle or the folding of a protein are highly reproducable indicating a paradox situation in relation to the concept of maximum entropy production. It may seem that a proper selection in view of the large diversity of phenomena is difficult, but exactly this is also the challenge taken up within this book. We try to provide basic concepts, applicable to biological systems or soft matter in general. These include entropic forces, phase separation, cooperativity, and transport in complex systems, like molecular motors. We also provide a detailed description for the understanding of elementary processes like electron, proton, and energy transfer, and show how nature is making use of them for instance in photosynthesis. Prerequisites for the reader are a basic understanding in the fields of mechanics, electrostatics, quantum mechanics, and statistics. This means the book is for graduate students, who want to specialize in the field of biophysics. As we try to derive all equations in detail, the book may also be useful to physicists or chemists who are interested in applications of statistical mechanics or quantum mhemistry to biological systems. The book is the outcome of a course presented by the authors as a basic element of the newly established graduation branch 'Biophysics' in the Physics Department of the Technische Universitaet Muenchen.

The authors would like to thank Dr. Florian Dufey and Dr. Robert Raupp–Kossmann for their contributions during the early stages of the evolving manuscript.

Garching, Germany
August 2009

Philipp O.J. Scherer
Sighart F. Fischer

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