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国外物理名著系列 22

（影印版）

# Practical Quantum Mechanics

# 实用量子力学

S.Flügge

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# 国外物理名著系列序言

对于国内的物理学工作者和青年学生来讲，研读国外优秀的物理学著作是系统掌握物理学知识的一个重要手段。但是，在国内并不能及时、方便地买到国外的图书，且国外图书不菲的价格往往令国内的读者却步，因此，把国外的优秀物理原著引进到国内，让国内的读者能够方便地以较低的价格购买是一项意义深远的工作，将有助于国内物理学工作者和青年学生掌握国际物理学的前沿知识，进而推动我国物理学科研和教学的发展。

为了满足国内读者对国外优秀物理学著作的需求，科学出版社启动了引进国外优秀著作的工作，出版社的这一举措得到了国内物理学界的积极响应和支持，很快成立了专家委员会，开展了选题的推荐和筛选工作，在出版社初选的书单基础上确定了第一批引进的项目，这些图书几乎涉及了近代物理学的所有领域，既有阐述学科基本理论的经典名著，也有反映某一学科专题前沿的专著。在选择图书时，专家委员会遵循了以下原则：基础理论方面的图书强调“经典”，选择了那些经得起时间检验、对物理学的发展产生重要影响、现在还不“过时”的著作（如狄拉克的《量子力学原理》）。反映物理学某一领域进展的著作强调“前沿”和“热点”，根据国内物理学研究发展的实际情况，选择了能够体现相关学科最新进展，对有关方向的科研人员和研究生有重要参考价值的图书。这些图书都是最新版的，多数图书都是2000年以后出版的，还有相当一部分是当年出版的新书。因此，这套丛书具有权威性、前瞻性和应用性强的特点。由于国外出版社的要求，科学出版社对部分图书进行了少量的翻译和注释（主要是目录标题和练习题），但这并不会影响图书“原汁原味”的感觉，可能还会方便国内读者的阅读和理解。

“他山之石，可以攻玉”，希望这套丛书的出版能够为国内物理学工作者和青年学生的工作和学习提供参考，也希望国内更多专家参与到这一工作中来，推荐更多的好书。


杨国桢

中国科学院院士

中国物理学会理事长

# Preface

This work was first published in 1947 in German under the title "Rechenmethoden der Quantentheorie". It was meant to serve a double purpose: to help both, the student when first confronted with quantum mechanics and the experimental scientist, who has never before used it as a tool, to learn how to apply the general theory to practical problems of atomic physics. Since that early date, many excellent books have been written introducing into the general framework of the theory and thus indispensable to a deeper understanding. It seems, however, that the more practical side has been somewhat neglected, except, of course, for the flood of special monographs going into broad detail on rather restricted topics. In other words, an all-round introduction to the practical use of quantum mechanics seems, so far, not to exist and may still be helpful.

It was in the hope of filling this gap that the author has fallen in with the publishers' wish to bring the earlier German editions up to date and to make the work more useful to the worldwide community of science students and scientists by writing the new edition in English.

From the beginning there could be no doubt that the work had to be much enlarged. New approximation methods and other developments, especially in the field of scattering, had to be added. It seemed necessary to include relativistic quantum mechanics and to offer, at least, a glimpse of radiation theory as an example of wave field quantization. The choice of the problems, included in the old days in a somewhat happy-go-lucky way, had now to be carefully reconsidered.

Thus a total of about twice as many problems as in the last German edition has resulted. Not one of the original problems has been simply translated; not more than about fifty have only undergone reshaping from the earlier text; the bulk, however, is going to be presented here for the first time. Nevertheless, the general character has remained the same, with perhaps a slight tendency to arrive at even more applicable results and numerical values at the end of each problem.

The more elementary problems, such as square-well potentials, have not been omitted but somewhat abridged. The general introduction to the German edition, some twenty odd pages surveying the basic equations and their meaning, has been discarded. Any student using the problems will be sufficiently well acquainted with the general framework to justify that omission. On the other hand, the extensive use of special functions made throughout the work seemed to make a mathematical appendix useful in which such formulae as occur in the problems have been collected and, in part, derived.

With considerable hesitation but giving way to the publishers' practical arguments the author has consented to having this edition divided into two separate volumes, hoping that no serious damage has thus been done to the intrinsic structure and continuity of the work. To facilitate its use, the complete index for both parts has been printed twice and will appear at the end of each volume. The numbers, therefore, refer to the problems in question, not to pages.

Hinterzarten, March 1971

*The Author*

# Preface to the Paperback Edition

More than three years have elapsed, since this work appeared as a two-volume cloth edition. Author and publisher have been much gratified to learn how well it was received by scientists in many countries and how useful it proved to students of physics. To serve as a regular supplement to text books, however, it was hampered by its necessarily high price. Hence, the author has gratefully accepted the publisher's suggestion of a much less expensive one-volume Springer Study Edition; the more so, since it has always been his wish, as already expressed in the former edition's preface, to see the total work re-united in one volume. To save every conceivable additional cost, no corrections or alterations have been made; an errata sheet listing trivial errors, however, has been prepared, see p. XVI. Furthermore, the original pagination has been kept unchanged which, we trust, should cause very little inconvenience.

Author and publisher very much hope that a more widespread distribution of the book will thereby result and that it will meet especially the needs of the student.

Hinterzarten, September 1974

*The Author*

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# Contents Volume II

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# I. General Concepts

## Problem 1. Law of probability conservation

If the normalization relation

$$\int d^3x\,\psi^*\psi = 1 \tag{1.1}$$

is interpreted in the sense of probability theory, so that $d^3x\,\psi^*\psi$ is the probability of finding the particle under consideration in the volume element $d^3x$, then there must be a conservation law. This is to be derived. How may it be interpreted classically?

**Solution.** The conservation law sought must have the form of an equation of continuity,

$$\operatorname{div} s + \frac{\partial \rho}{\partial t} = 0 \tag{1.2}$$

with

$$\rho = \psi^*\psi \tag{1.3}$$

the probability density, and $s$ the probability current density. As $\rho$ is a bilinear form of $\psi$ and its complex conjugate, Eq. (1.2) can be constructed only by a combination of the two Schrödinger equations

$$H\psi = -\frac{\hbar}{i}\frac{\partial \psi}{\partial t}; \qquad H\psi^* = \frac{\hbar}{i}\frac{\partial \psi^*}{\partial t} \tag{1.4}$$

with the hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla^2 + V(r) \tag{1.5}$$

the same for both equations. Thus we find

$$\psi^* H\psi - \psi H\psi^* = -\frac{\hbar}{i}\frac{\partial \rho}{\partial t}.$$

According to (1.2) it ought to be possible to write the left-hand side in the form of a divergence. Indeed we have

$$\psi^* H\psi - \psi H\psi^* = -\frac{\hbar^2}{2m}(\psi^*\nabla^2\psi - \psi\nabla^2\psi^*) = -\frac{\hbar^2}{2m}\mathrm{div}(\psi^*\nabla\psi - \psi\nabla\psi^*)$$

so that we may identify

$$s = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*). \tag{1.6}$$

Classical interpretations may be arrived at as follows. If the quantities $\rho$ and $s$ are both multiplied by $m$, the mass of the particle, we obtain mass density $\rho_m$ and momentum density $\boldsymbol{g}$:

$$\rho_m = m\rho; \quad \boldsymbol{g} = m\,s, \tag{1.7}$$

and the equation of continuity may be interpreted as the law of mass conservation. In the same way, multiplication by the particle charge, $e$, yields charge density $\rho_e$ and electric current density $\boldsymbol{j}$:

$$\rho_e = e\rho; \quad \boldsymbol{j} = e\,s, \tag{1.8}$$

and (1.2) becomes the law of charge conservation.

It is remarkable that the conservation laws of both mass and charge are essentially identical. This derives from the fact that one particle by its convection current causes both.

The expression for the total momentum of the Schrödinger field, derived from (1.6) and (1.7),

$$\boldsymbol{p} = \int d^3x\,\boldsymbol{g} = \frac{\hbar}{2i}\int d^3x(\psi^*\nabla\psi - \psi\nabla\psi^*),$$

may by partial integration in the second term be reduced to

$$\boldsymbol{p} = \int d^3x\,\psi^*\left(\frac{\hbar}{i}\nabla\right)\psi \tag{1.9}$$

corresponding to its explanation as the expectation value of the momentum operator $(\hbar/i)\,\nabla$ in the quantum state $\psi$ (cf. Problem 3).

## Problem 2. Variational principle of Schrödinger

To replace the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\boldsymbol{r})\psi = E\psi \tag{2.1}$$

by a variational principle for the energy.

**Solution.** Since the constraint

$$\int d^3x\, \psi^* \psi = 1 \tag{2.2}$$

holds for any solution $\psi$ of the differential equation (2.1), the energy will be found by multiplying (2.1) with $\psi^*$ and integrating over the whole space:

$$E = \int d^3x\, \psi^* \left\{ -\frac{\hbar^2}{2m} \nabla^2 \psi + V(r)\psi \right\}. \tag{2.3}$$

A partial integration in the first term yields, according to Green's law,

$$\int d^3x\, \psi^* \nabla^2 \psi = \oint df \cdot \psi^* \nabla \psi - \int d^3x\, \nabla \psi^* \cdot \nabla \psi \,. \tag{2.4}$$

Now, the normalization integral (2.2) exists only if, at large distances $r$, the solution $\psi$ vanishes at least as

$$\psi \propto r^{-\frac{3}{2}-\varepsilon}; \qquad \varepsilon > 0 \,.$$

Under this condition, however, the surface integral in (2.4) vanishes when taken over an infinitely remote sphere so that (2.3) may be written

$$E = \int d^3x \left\{ \frac{\hbar^2}{2m} \nabla \psi^* \cdot \nabla \psi + \psi^* V(r) \psi \right\}. \tag{2.5}$$

This equation is completely symmetrical in the functions $\psi$ and $\psi^*$, as is the normalization (2.2), so that it might equally well have been derived from the complex conjugate of Eq. (2.1),

$$-\frac{\hbar^2}{2m} \nabla^2 \psi^* + V(r)\psi^* = E\psi^* \,. \tag{2.1*}$$

It would not be difficult to show that (2.1) and (2.1*) are the Euler equations of the variational problem to extremize the integral (2.5) with the constraint (2.2). We shall, however, make no use of the apparatus of variational theory and prefer a direct proof, instead.

Let $\psi_\lambda$ be a solution of (2.1) that belongs to its eigenvalue $E_\lambda$. It will give the integral (2.5) the value $E_\lambda$. Let us then replace $\psi_\lambda$ by a neighbouring function $\psi_\lambda + \delta\psi$ with $|\delta\psi|$ being small but arbitrary, except for (2.2) still to hold for $\psi_\lambda + \delta\psi$ as well as for $\psi_\lambda$:

$$\int d^3x (\psi_\lambda^* + \delta\psi^*)(\psi_\lambda + \delta\psi) = 1$$

and therefore

$$\int d^3x (\psi_\lambda \delta\psi^* + \psi_\lambda^* \delta\psi) + \int d^3x\, \delta\psi^* \delta\psi = 0 \,. \tag{2.6}$$