Quantum Mechanics

Selected Topics

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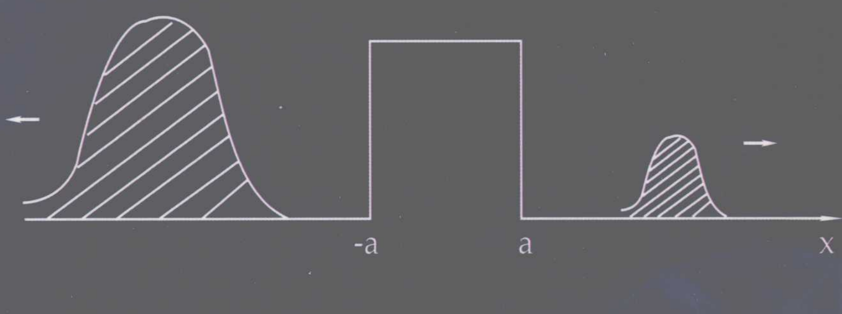

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QUANTUM MECHANICS — SELECTED TOPICS

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Preface

Just as a "demographic explosion" gives much trouble to sociologists and economists, the problem of an "information explosion" is in the face of scientists and teachers in all its magnitude.

The difference between both problems is in the fact that the birth-rate of the population can be limited much more easily than the birth-rate of articles.

Only the editors of scientific journals dream about the Golden Age when authors themselves would criticize their own works and reject all of them except brilliant ones.

The birth of an article which represents even a small step forward from the generally accepted level of knowledge gives a satisfaction and a pleasure which the author cannot overcome. In our opinion, one should not try to fight against the "information explosion", but rather try to direct its energy, i.e. efforts of the huge army of scientists, into a common channel.

What is important for chemistry and zoology is perhaps the classification of information and the mechanization of a search for materials concerning a given chemical compound or biological species.

As far as theoretical physics, we believe that overviews and monographs summarizing the results of some studies in the fields of today are of utmost importance. For an overview, one should select without a bias the most valuable results from a large number of works.

As a matter of fact, text-books in which the material is revised as science is developed, pursue the same goal. In the preface to the famouse Course of Theoretical Physics, L.D. Landau and E.M. Lifshitz state that learning of this Course provides the base which will be sufficient for understanding of original publications in journals.

One should note that in recent years there has been a certain gap between text-books and new original works. The present book aims to reduce this gap.

It is intended for to be intermediate between a course in quantum mechanics and a present-day study of a number of problems in atomic, nuclear physics and partly in physics of elementary particles.

This monograph is concerned with the following general physical problems.

1. **Systems with a low binding energy, namely the deuteron and the negatively charged hydrogen ion.**
2. **Systems with the Coulomb potential — the hydrogen atom.**
3. **Unstable systems, such as radioactive nuclei, and autoionization states.**
4. **The detailed theory of the harmonic oscillator and its application to oscillations of the electromagnetic field in laser systems.**

5. The ionization of bound states (a negative ion or an atom) by the field of a strong light wave (such as a laser light pulse focused by a lens).

The book also deals with some methods of theoretical physics which are discussed here in more detail than in most text-books. These are:

1. Analytic properties of the wave function and scattering matrix.

2. The Green function of the Schrödinger equation.

3. The quasiclassical approximation.

4. The inverse scattering problem.

5. Exact solutions of non-stationary problems.

It is not customary to point out in the preface of a book which problems are not touched upon, for the latter are difficult to limit, and besides this might prejudge to authors. Deviating from the tradition, we mention two problems which might be naturally expected to be included in a modern course of quantum mechanics, namely the Regge poles and the Feynman path integrals. Both questions are elucidated in the literature, and we consider it is reasonable to omit them.

The present monograph is a revised and extended version of a part of the book *Scattering, Reactions and Decays in Non-relativistic Quantum Mechanics* (Nauka: Moscow, 1971, in Russian) by A.I. Baz', A.M. Perelomov and Ya.B. Zel'dovich; namely of the part that was written by the second and the third authors. We recommend Chapters 8 to 11 of this book as an additional material.

Moscow, October 1987

A.M. Perelomov

Ya.B. Zel'dovich

Addendum

To my great regreat, I had to complete this book without the participation of my teacher and co-author, the remarkable scientist and human being, Academician Ya.B. Zel'dovich.

The author of these lines has been learned much from Ya.B. Zel'dovich and feels a great obligation towards him. His untimely decease interrupted our joint work on the book. However, the general scheme for compiling of it made by Ya.B. Zel'dovich and pages written by him are remained unchanged, although on technical reasons there is a considerable delay in the publication.

Zaragoza, April 1998

A.M. Perelomov

Contents

CHAPTER 1

DISCRETE SPECTRUM

1. Introduction

This Chapter concerns some properties of solutions of the Schrödinger equation belonging to the discrete spectrum. As it is well known, such solutions describe bound states. Three cases will be considered here: (a) states with a low binding energy; (b) bound states in the Coulomb field; (c) states of a three-dimensional harmonic oscillator.

States with the binding energy ε that is small compared to the depth U_0 of a potential well are of interest in some applications. The ground state of a deuteron is an example. The properties of these states are discussed in detail in Sec. 2 and Sec. 3 with a special attention to the case of $\varepsilon \to 0$, i.e. when the level just appears. In Sec. 4 the motion of particle in the field of several potential wells is considered. Also the important notation of pseudopotential is introduced and validated.

Cases (b) and (c) can be found almost in any textbook on quantum mechanics. By this reason, we pay attention here only to the existence of specific properties of states, when a degeneracy (usually called the "accidental" degeneracy) of states occurs with different values of the angular momentum l. Therefore superpositions of states with different values of l may be the stationary states, and the standard classification of levels can be supplemented by an alternative classification.

One should not understand literally the word "accidental" added to "degeneracy". Such a situation is not accidental. The existence of closed trajectories is a consequence of a particular property of classical mechanical systems. In quantum mechanics, the Schrödinger equation for such systems permits the separation of variables in several coordinate systems. However, a more important property is the existence of a transformation group that leaves the Schrödinger equation invariant. The other properties follow from the existence of this transformation group. These questions are considered in Sec. 5 for the Coulomb potential and in Sec. 6 for the oscillator. In this latter one the so-called "coherent" states are discussed. These non-stationary states have a number of interesting properties, for example the property of the closest similarity (in some sense of the word) to the properties of the classical oscillator.

Sec. 7 is devoted to the derivation of the so-called virial theorem and its generalization. The last Section of this Chapter concerns statistical properties of systems of identical particles.

Let us say now a few words how to read this book. In the first Section only basic notations are given. A reader who has recently studied a standard quantum mechanics course should not read this Section because he may get a wrong impression about whole book and put it aside before of reaching of topics that may be unknown and of interest for him.

Then we recall some of the main principles of quantum mechanics.

In non-relativistic quantum mechanics, the state of system is completely described by the wave function Ψ, the time-dependence of which is determined by the Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = H\Psi, \tag{1.1}$$

where H is the Hamiltonian of the system, and $\hbar$ is the Planck constant.

We shall mainly consider (except Sec. 4 of Ch. 6, and Ch. 7) the case when the Hamiltonian does not depend explicitly on time. In this case, there are stationary states, i.e. states for which the probability density $|\Psi|^2$ does not vary with time[1]

The wave function of such a state has the form

$$\Psi(t) = \psi \exp\left(-\frac{iEt}{\hbar}\right).$$

From this it follows that ψ is an eigenfunction of the Hamiltonian

$$H\psi = E\psi, \tag{1.2}$$

which describes a state with a definite real energy E.

In the case of one particle in a constant external field,

$$H = -\frac{\hbar^2}{2m}\Delta + U(\mathbf{r}),$$

[1] For the Hamiltonians depending on parameteres, after performing closed loops in the parameter space, we may obtain geometric phases. There has been a great interest in such questions after the work of M. Berry [Be 1984] (see the book [GPP 1989]).

$$\left(-\frac{\hbar^2}{2m}\Delta + U(\mathbf{r})\right)\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{1.3}$$

The wave function $\psi(\mathbf{r})$ must satisfy the usual conditions, i.e. it is single-valued and continuous everywhere in the space. The condition of single-valuedness of the wave function was considered in detail by W. Pauli [Pa 1933], [Pa 1939]. It leads to nontrivial effects such as the quantization of magnetic flux in a multi-connected superconductor [Lo 1950], [BY 1961] and the occurrence of quantized vortices in a liquid helium [On 1949], [Fe 1955]. It plays a significant role in the derivation of the Bohr–Sommerfeld quantization conditions in the multi-dimensional case (see Sec. 3 of Ch. 6).

In practice, the potential $U(\mathbf{r})$ often is spherically symmetric, i.e. depends only on $|\mathbf{r}|$. In such a field, the angular momentum operator $\mathbf{L}$ commutes with the Hamiltonian H (this corresponds to the conservation of the angular momentum in classical mechanics). Furthermore, the operator H commutes with the space inversion operator P (this property has not any analogue in classical mechanics [Wi 1964a]). Since the operators H, $\mathbf{L}^2$, L_z and P commute with one another, the eigenstates of H may be simultaneously the eigenstates of $\mathbf{L}^2$, L_z and P. In other words, a stationary state may be characterized by:

(i) a definite orbital angular momentum l with eigenvalue of $\mathbf{L}^2$ equal to $l(l+1)$ where l is an integer;

(ii) a definite projection m of the angular momentum L_z on an arbitrary axis z, m taking $2l+1$ values from $-l$ to $+l$;

(iii) a definite parity eigenvalue, $P = +1$ or $P = -1$.

In the one-particle problem, the parity is completely determined by the orbital angular momentum $P = (-1)^l$, i.e. P coincides the parity of l.

From the foregoing it follows that the Schrödinger equation has solutions of the form

$$\psi_{lm}(\mathbf{r}) = R_l(r)\, Y_{lm}(\theta, \varphi). \tag{1.4}$$

Here θ and φ are the polar and azimuthal angles of the vector $\mathbf{r}$, respectively; $Y_{lm}(\theta,\varphi)$ are spherical harmonics, and $R_l(r)$ is a function depending on r only. The substitution of Eq. (1.4) into Eq. (1.3) yields the following equation for R_l:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR_l}{dr}\right) + \left[\frac{2m}{\hbar^2}(E-U) - \frac{l(l+1)}{r^2}\right]R_l = 0. \tag{1.5}$$

Let us introduce now the new function

$$\chi_l(r) = r\,R_l(r), \tag{1.6}$$

which satisfies the equation

$$\chi_l'' + \left[k^2 - \left(V(r) + \frac{l(l+1)}{r^2}\right)\right]\chi_l = 0, \tag{1.7}$$

in which the first derivative does not enter. Here $k = \sqrt{2mE/\hbar^2}$, and $V = (2m/\hbar^2)U$.

In the case when we have not misunderstanding, we will refer to V also as the potential. The centrifugal potential $l(l+1)/r^2$ can be included in V. Then Eq. (1.7) takes the form

$$\chi_k'' + (k^2 - V(r))\chi_k = 0. \tag{1.8}$$

The properties of this equation are well known from quantum mechanics textbooks, first of all from *Quantum Mechanics* by L.D. Landau and E.M. Lifshitz [LL 1965]. Comprehensive courses [Ne 1982] and [Th 1981], [Th 1983] are also noteworthy. A detailed account of the history of the creation and development of quantum mechanical concepts is given in the book [Ja 1966] and in the collection of the original works on quantum mechanics [Wa 1967]. A mathematically rigorous investigation of a number of principal problems of quantum mechanics, for instance of the measurement process, can be found in the book [Ne 1932]. The modern interpretation of these questions is given in [Ja 1968]. Approximate methods in quantum mechanics are considered in the book [KM 1969].

In the case of non-singular potential, the function $\psi(\mathbf{r})$ is finite, thus leading to the following boundary conditions for χ_k :

$$\begin{aligned} \chi_k(r) &\to 0 \quad \text{at} \quad r \to 0, \\ \chi_k(r)/r \text{ is finite} &\quad \text{at} \quad r \neq 0,\ r \to \infty. \end{aligned} \tag{1.9}$$

Besides it is natural to require χ_k and χ_k' to be continuous for $r > 0$. This is consequence of the fact that Eq. (1.8) contains second-order derivatives. If χ_k' or χ_k is discontinuous, the right side of Eq. (1.8) is non-zero and contains $\delta-$ or a δ'-function.

In cases when $V(r)$ tends to a finite limit at $r \to \infty$, the origin of the energy scale is chosen so that $V(r)$ vanishes at infinity.

Almost all interactions between particles in the nature (except the Coulomb interaction and some other ones) are described by rapidly decreasing potentials, i.e. by potentials which decrease more rapidly than $1/r$ at large r. In many cases at r larger than some R, one may neglect by these interactions and suppose that $V(r) = 0$ at $r > R$. Let us call such potentials as short-range potentials. The introduction of the cut-off radius R considerably simplifies all formulae. This is the case we consider first. The centrifugal potential cannot be regarded as a short-range potential. In order not to complicate the problem, let us take the orbital momentum l to be zero.

Thus, we came to the problem: one needs to find all solutions $\chi_k(r)$ of equations

$$\begin{aligned} \chi_k'' + (k^2 - V(r))\chi_k = 0 \quad &\text{at } r < R, \\ \chi_k'' + k^2\chi_k = 0 \quad &\text{at } r \geq R, \end{aligned} \tag{1.10}$$

which satisfy conditions Eq. (1.9). In this case, the wave function has the form

$$\psi(\mathbf{r}) = R_{k0}(r)\, Y_{00}(\theta, \varphi) = \frac{1}{\sqrt{4\pi}} \frac{\chi_k(r)}{r}. \tag{1.11}$$

As can be seen from the second equation of Eq. (1.10), in the region of $r > R$ there exist two solutions

$$\chi_k^{(\pm)}(r) = \exp(\pm\, ikr). \tag{1.12}$$

For rapidly decreasing potentials, there are also two solutions, $\chi_k^{(\pm)}(r)$, which at large r behave like $\exp(\pm\, ikr)$.

These solutions are often denoted by $f(\pm k, r)$. Their properties were considered in detail in [Jo 1947]. In the case of the Coulomb-tail potentials, $U \approx \alpha/r$ at $r \to \infty$, the asymptotic form of the functions $\chi_k^{(\pm)}$ is $\exp[\pm\, i(kr - \eta \ln 2kr)]$, where $\eta = m\alpha/\hbar^2 k$. At $r < R$ there are also two solutions, but only one of them can be used because the another does not satisfy the boundary condition at $r = 0$.

Let us look for χ_k at $r \to 0$ in the form of a power function r^σ. From Eq. (1.10) we have

$$\sigma(\sigma - 1) \approx -r^2(k^2 - V(r)).$$

If $r^2 V(r) \to 0$ at $r \to 0$, then σ has two values: 0 and 1. (If this condition is not satisfied, the potential is called singular. New qualitative phenomena occurring in this case will be discussed in Appendix A). Accordingly, at $r \to 0$ the Schrödinger equation allows two solutions:

$$\psi_1(r) \to a, \qquad \psi_2(r) \to \frac{b}{r},$$

where a and b are constants. However, the solution ψ_2 must be rejected because

$$\Delta\, \frac{b}{r} = -\, 4\pi b\, \delta^3(\mathbf{r}).$$

Consequently, ψ_2 does not satisfy the Schrödinger equation at the point $r = 0$. Solutions of this type are used for describing of point interactions. Hence there remains only the solution ψ_1 corresponding to $\sigma = 1$.

The above reasoning may be viewed as the requirement of the boundary condition $\chi(r) \to 0$ at $r \to 0$. We write $\chi_k^{(0)}(r)$ for the solution satisfying this condition.

Now we proceed to the discussion of domains of positive and negative energies. The positive-energy case will be discussed in more detail in Ch. 2. Positive energies correspond to real values of k. In this case both solutions Eq. (1.12) remain finite at all values of $r \geq R$, i.e. both solutions are acceptable in this region. The general solution at $r > R$ may be written as

$$\chi_k(r) = A(k) \left(\chi_k^{(-)} - S(k)\,\chi_k^{(+)}\right). \tag{1.13}$$

At $r = R$ this solution is required to be continuously matched with the solution in the inner domain,

$$\begin{aligned} A(k) \left(\chi_k^{(-)} - S(k)\,\chi_k^{(+)}\right)\Big|_{r=R} &= \chi_k^{(0)}(R), \\ A(k) \left(\chi_k^{(-)\prime} - S(k)\,\chi_k^{(+)\prime}\right)\Big|_{r=R} &= \chi_k^{(0)\prime}(R). \end{aligned} \tag{1.14}$$

The matching can always be done by appropriate choosing of A and S. Indeed, regarding Eq. (1.14) as a system of equations for A and S, one can obtain

$$\begin{aligned} S(k) &= (\chi_k^{(-)\prime}\chi_k^{(0)} - \chi_k^{(-)}\chi_k^{(0)\prime})/(\chi_k^{(+)\prime}\chi_k^{(0)} - \chi_k^{(+)}\chi_k^{(0)\prime})\Big|_{r=R}, \\ A(k) &= (\chi_k^{(+)\prime}\chi_k^{(0)} - \chi_k^{(+)}\chi_k^{(0)\prime})/2ik\Big|_{r=R}. \end{aligned} \tag{1.15}$$

Thus, for each positive value of the energy there exists one and only one solution of the Schrödinger equation. The physical meaning of this solution will be discussed below.

At negative energies the situation changes essentially. Negative values of E correspond to imaginary $k = i\,|k|$. As usual, we consider k to be in the upper halfplane. If k is in the lower halfplane, the quantities $\chi^{(+)}$ and $\chi^{(-)}$ should be exchanged.

The solution $\chi_k^{(-)} = \exp(|k|r)$ increases exponentially at $r \to \infty$ and consequently does not satisfy the second condition in Eq. (1.9). Thus the most general solution at $r > R$ has the form

$$A(k)\,\chi_k^{(+)}(r), \tag{1.16}$$

and the matching condition for external and internal functions has the form

$$\left.\frac{\chi_k^{(+)\prime}}{\chi_k^{(+)}}\right|_{r=R} = \left.\frac{\chi_k^{(0)\prime}}{\chi_k^{(0)}}\right|_{r=R} = -|k|. \tag{1.17}$$

In fact, this condition is a transcendental equation for k, and therefore may be satisfied only at some discrete imaginary $k = k_n$ (or at discrete negative energies E_n, equivalently).

From Eq. (1.17) it follows that the logarithmic derivative of the function $\chi_k^{(0)}$ must be also negative.

As we will see later, this occurs if $V(r)$ is mainly negative (corresponding to the attraction) and its magnitude is sufficiently large. In this case, at $r > R$ the functions of the discrete spectrum have the form

$$\chi_{k_n}(r) = A(k_n)\,\chi_{k_n}^{(+)}(r) = A(k_n)\,\exp(-|k_n|r),$$

i.e. decrease exponentially to zero at large r. Note that in the case of rapidly decreasing potentials the function $\chi_{k_n}(r)$ behaves asymptotically like $\exp(-|k_n|r)$ at $r \to \infty$, and in the case of the Coulomb-tail potentials ($U(r) \sim \alpha/r$ at $r \to \infty$),

$$\chi_{k_n}(r) \sim r^{-\eta_n}\,\exp(-|k_n|r), \qquad \eta_n = m\alpha/\hbar^2|k_n|.$$

At $r < R$ the functions are finite, and therefore the integral

$$\int_0^\infty |\chi_{k_n}(r)|^2\,dr \tag{1.18}$$

converges. The function χ_{k_n} is usually normalized so that the above integral is equal to unity. Since χ_{k_n} decreases exponentially to zero at $r > R$, the solution characterizes a space-localized state. Such solutions correspond to the classical finite motion of a particle with the negative energy. In the usual case of non-singular potential, such states are called bound states. For a singular potential, the situation becomes more complicated (see Appendix A).

Thus, at positive energies the Schrödinger equation has a solution (satisfying the boundary conditions) at each positive value of E (i.e. at $k^2 > 0$), the value of l being arbitrary.

If the potential oscillates when $r \to \infty$ and does not decreases rapidly enough at infinity, then the positive energy bound states may occur (see Appendix A).

At negative energies and fixed l, solutions are possible (if at all possible) only at some discrete values $E = E_{nl}$. We may formulate the result as follows: the spectrum of positive energy eigenvalues is continuous, and one of the negative energy eigenvalues is discrete.

In the case of discrete spectrum, each level has a definite value of l. The levels with equal l but different m are degenerate. This is a consequence of the spherical symmetry of the potential.

However, at $l \neq 0$ the solutions are not spherically symmetric. Their angular dependence is determined by the angular part $Y_{lm}(\theta, \varphi)$ of the wave function. Note that the sum $\sum_{m=-l}^{l} |Y_{lm}(\theta, \varphi)|^2$ is independent on θ and φ. From this it follows that if at a given l the particle resides with the same probability in states with all possible values of m, then the probability density of finding of the particle at a given point of space possesses a spherical symmetry. The above property of the sum explains the fact that the charge density is spherically symmetric in the case of closed electron shells of an atom or of a nucleus.

Solutions with definite l also possess a definite parity P. The degeneracy corresponding to different m at the same l cannot change anything because all degenerate levels and any linear combination of them (that is a solution as well) possess the same P. The probability density $|\psi|^2$ (or the charge density for a charged particle) does not change under the parity transformation because ψ goes into ψ or $-\psi$.

In this way, it is proved that the charge distribution in a *spherically* symmetric potential needs to have a centre of symmetry, although it needs not necessary be spherically symmetric. Therefore, the electric dipole moment should be equal to zero.

In the special important case of the Coulomb potential, $U = -Ze^2/r$, a so-called accidental degeneracy occurs, namely the exact equality of energies of levels with different l. Here the conclusion about the zero dipole moment is violated. The particle may be in a state with a non-zero dipole moment. This phenomenon will be discussed in Sec. 5.

2. States with small binding energy

Let us consider the Schrödinger equation at $U(r) < 0$. One should note that in this case the difference between classical and quantum mechanics is as follows: in classical mechanics, any potential well, even the smallest one is sufficient to bind a particle. The particle may be at rest at the bottom of this well, i.e. there exists a solution with $E = U_{\min} < 0$.

It turns out that in three-dimensional problem of quantum mechanics, there are definite critical conditions for the existence of at least one discrete level. For this, a well must be sufficiently wide and deep. This result is qualitatively understandable from the viewpoint of the uncertainty principle: