Quantum Mechanics and Nonlinear Waves

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Preface

Quantum theory is like the proverbial little girl with the curl. When it is good, as in atomic theory, it is very, very good. When it is bad, as in systems with an infinite number of degrees of freedom, it is horrid. The central theme of this book is that the well-known deficiencies of quantum field theory are generally due to inattention to a basic characteristic of interacting quantum systems—the persistence of self-interactions. The sources of this lapse are twofold. In the strange world of microscopic physics, attempts to maintain continuity of ideas lead to choices of interactions which are familiar and valid in the macroscopic domain. Furthermore, a persistent self-interaction is already nonlinear at the classical level and, consequently, encounters profound difficulties in its analysis. However, in classical physics the field equations and their boundary conditions constitute the total theory, while in quantum theory the field equations are accompanied by a separate superposition principle for probability amplitudes. This principle is independent of the form (or existence!) of field equations. This enables us to find amplitudes accounting for the persistent interaction by a two-step process. Solution of the field equations for the intrinsically nonlinear, nonperturbative field operators, followed by construction of the amplitudes and superposition of the latter, comprise this process. Successful completion of this construction without the appearance of infinities then provides us with the freedom to allow experiment to suggest more general interactions. The result is quantum field theories with sensible interpretations free of artificial constraints. As expected, physics questions, posed specifically, are answered in a broad context. The generality of the ideas extends beyond the relativistic theories to applications in superconductivity, aperiodic systems such as liquids and others.

Any author quickly becomes aware of the confirmation of friendship. In this intensely active field, ideas, freely exchanged, have provided me with insights and understanding that I would not have obtained alone. My thanks to these friends and colleagues is but feebly expressed in this acknowledgement. Finally, the patience and love of Harriet, Elizabeth, Konni, Sydney and Timothy have made the burdens light and the way straight.

Philip B. Burt
Clemson, South Carolina

This work is dedicated to the memory of Louie Einsinger Burt, Sr., Louie Einsinger Burt, Jr. and Jesse Hoyle Clack . . . raphael

". . . And (the Lord) brought them to Adam to see what he would call them; and whatsoever Adam called every living creature, that was the name thereof . . . "

Genesis 2:19

" . . . The new creature calls it Niagara Falls—why I am sure I do not know—says it looks like Niagara Falls. That is not a reason, it is mere waywardness and imbecility . . . "

Adam's Diary, Mark Twain

Notation

$\check{k} = (k_0, \vec{k})$; this inverted caret is used for four-vectors throughout.

$\check{k}^2 = k_0^2 - \vec{k}^{\,2} = \check{k} \circ \check{k} = g_{\mu\nu} k^\mu k^\nu$

$g_{\mu\nu}$ = diagonal $(1, -1, -1, -1)$

γ_μ, Dirac matrix (Bjorken 64); $\gamma_\mu \gamma_\nu + \gamma_\nu \gamma_\mu = 2 g_{\mu\nu}$

$\not{p} = p^\mu \gamma_\mu$

summation convention; sum on repeated indicies

Contents

CHAPTER ONE

A Perspective on Quantum Theory

"...how is that past increased, which is now no longer..."
Augustine: Confessions, XI

1. Origins: Quantum Mechanics As An Analogy to Classical Mechanics

As the news of the revolution in physics based on quantum theory spread throughout the world, a jargon of scientific sounds became fashionable. One expression, "quantum jump", is now almost universally recognized as a synonym for a qualitative improvement or an abrupt, quantitative change. This pre-quantum mechanics notion—an artifact of the Bohr theory—actually has a remarkable counterpart, in a sense, in the original development of quantum mechanics. Although etymology is not the subject of this monograph, the statement of quantum mechanics, especially in the form presented by Schrödinger (Schrödinger 1926), provides an excellent illustration of the appropriateness of the term. In this first section the development of quantum mechanics in parallel to classical mechanics will be reviewed in order to emphasize the discontinuity in the ideas of theoretical physics leading to the former. A second purpose is to underline the analogical structure of quantum mechanics in comparison with classical mechanics.

The beginning point of Schrödinger's theory is the well known, completely classical Hamilton-Jacobi equation (in time independent form)

$$H(q_i, \partial S/\partial q_i) - E = 0\,, \tag{1-1-1}$$

where q_i are the coordinates of the system, E is the energy and S is Hamilton's characteristic function. Solution of this nonlinear partial differential equation is equivalent to solutions of the equations of motion of the system. After making the transformation of variable

$$S = K \ln(\psi) \qquad (1\text{-}1\text{-}2)$$

where K is a constant with dimensions of action, one finds, for the general mechanical system, that equation (1-1-1) has been replaced by a statement that a quadratic form of ψ and $\partial\psi/\partial q_i$ is zero, i.e.,

$$H(q_i, K(\partial\psi/\partial q_i)/\psi) - E = 0\,. \qquad (1\text{-}1\text{-}3)$$

This form is homogeneous in the dependent variable ψ.

The departure from classical mechanics, hence the quantum jump, consists of the assertion that the quadratic form is physically meaningful for nonzero values. The quadratic form is then used as the integrand of an integral such that, for arbitrary variations of ψ, the condition that the integral have an extremum is the statement of the new mechanics, namely, the (time independent) Schrödinger equation

$$H\psi = E\psi\,, \qquad (1\text{-}1\text{-}4)$$

where the familiar replacement

$$p_i\psi = (\hbar/i)\partial\psi/\partial q_i \qquad (1\text{-}1\text{-}5)$$

is made in the (now operator) Hamiltonian.

Nothing in classical physics supports the step in which the quadratic form appearing in equation (1-1-3) is extrapolated to nonvanishing values. In fact, Schrödinger quickly abandoned the details leading to equations (1-1-4)–(1-1-5), calling them unintelligible, and pursued the analogy between physical optics, its limit ray optics and the new wave equation and the Hamilton-Jacobi equation (Schrödinger 1926a). Simultaneously, a search for the time dependent form of the Schrödinger equation was begun. Even if it were not already clear that the above "derivation" is an artifice, the fact that it does not generalize to a development of the time dependent Schrödinger equation would make it so. Nonetheless, the grand step had been taken—a mechanical equation (for stationary states), from which the energy spectrum of hydrogen could be derived with some physically plausible assumptions, had been obtained. The equivalence of this theory and Heisenberg's matrix mechanics (Heisenberg 1925) was quickly demonstrated (Schrödinger 1926b).

The statement of quantum mechanics by Heisenberg and the subsequent abstraction and synthesis of Heisenberg and Schrödinger theory by Dirac (Dirac 1927, 1958) provide an especially clear illustration of the analogical relation of canonical quantum mechanics to canonical classical mechanics. The canonical classical system with n degrees of freedom is described by canonical coordinates $q_i(t)(i=1,2...n)$ and their conjugate momenta $p_i(t)$, where t is time. The Hamiltonian of the system is a function of p_i and q_i with the property, for any function $f(q_i,p_i;t)$,

$$\frac{\partial f}{\partial t} + [f, h]_{pb} = \frac{df}{dt} \tag{1-1-6}$$

where the Poisson bracket of the two functions f and g is defined as

$$[f,g]_{pb} = \sum_i \frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i} . \tag{1-1-7}$$

The fundamental Poisson brackets satisfy

$$[q_i,q_j]_{pb} = [p_i,p_j]_{pb} = 0 , \tag{1-1-8}$$

$$[q_i,p_j]_{pb} = \delta_{ij}(=1,i=j;0, i\neq j) . \tag{1-1-9}$$

Equation (1-1-6) expresses the fact that the Hamiltonian is the generator of time translations for the system. The canonical transformations of variables of the system—those transformations which leave the fundamental Poisson bracket relations unchanged—also generate the solutions of the equations of motion

$$[q_i,H]_{pb} = \frac{dq_i}{dt} , \tag{1-1-10}$$

$$[p_i,H]_{pb} = \frac{dp_i}{dt} . \tag{1-1-11}$$

The state of the canonical classical system may be described by specifying the solutions of equations (1-1-10)–(1-1-11) in terms of their values at some time t_o.

Using the definition of Poisson brackets, equation (1-1-7), the following results can be quickly established;

$$[f,g]_{pb} = - [g,f]_{pb} , \tag{1-1-12}$$

$$[f,a]_{pb} = 0 , \tag{1-1-13}$$

$$[f+g,h]_{pb} = [f,h]_{pb} + [g,h]_{pb} , \tag{1-1-14}$$

$$[fg,h]_{pb} = [f,h]_{pb}g + f[g,h]_{pb} , \tag{1-1-15}$$

$$[f,[g,h]_{pb}]_{pb} + [g,[h,f]_{pb}]_{pb} + [h,[f,g]_{pb}]_{pb} = 0 , \tag{1-1-16}$$

where f, g and h are arbitrary functions of p_i and q_i and a is an arbitrary constant. Equation (1-1-16) is the Jacobi identity. Throughout the entire discussion it has been assumed that all quantities are real.

Canonical quantum mechanics can now be constructed by assuming that Hermitian operators q_i and p_i exist which are analogous to the classical canonical variables in the following sense. There exists a bracket relation, the commutator, such that the fundamental commutators of the operators p_i and q_i have the values

$$[q_i,q_j] = q_iq_j - q_jq_i = 0\,, \tag{1-1-17}$$

$$[p_i,p_j] = p_ip_j - p_jp_i = 0\,, \tag{1-1-18}$$

$$[q_i,p_j] = q_ip_j - p_jq_i = i\hbar\delta_{ij}\,. \tag{1-1-19}$$

More generally, commutators of operator functions of q_i and p_j have values obtained by the correspondence

$$[f,g]_{pb} \rightarrow (i\hbar)^{-1}\,[f,g] \tag{1-1-20}$$

where the arrow means; calculate the Poisson bracket of f and g and replace the classical canonical variables in the result by the operators q_i and p_j to obtain $(i\hbar)^{-1}$ times the commutator. These results can be derived by assuming the existence and hermiticity of the commutator and by using the results of equations (1-1-12)–(1-1-16), assumed to be valid for the commutators (Dirac 1958). The only ambiguity encountered arises from ordering of products of p_i and q_i. This approach to quantization is, of course, equivalent to, but more general than, the Schrödinger theory. In this case, the "quantum jump" consists of the assumption that the canonical system is described by non commuting operators q_i and p_i.

The general statement of the canonical quantum mechanics of systems with a classical analogue is found in the fundamental commutators, equations (1-1-17)–(1-1-19), together with the equation of motion of the operators. The latter is found by using the correspondence expressed in equation (1-1-20),

$$[f,H]\,(i\hbar)^{-1} = \frac{df}{dt}\,, \tag{1-1-21}$$

where f is an arbitrary function of q_i and p_i with no explicit time dependence and H is the Hamiltonian of the system. The latter is obtained from the classical form by replacing canonical variables by their operator analogues. As usual, there may be an ambiguity in ordering of terms.

This describes the Heisenberg picture of quantum mechanics—perhaps the closest analogy to canonical classical mechanics. However, it also provides us with a basis for generalization to new systems possessing no classical analogues or systems for which no canonical variables exist. The basis for generalization is found in the fundamental commutator relations, where we see that variables representing independent degrees of freedom commute. This property is directly related to the uncertainty principle. By analogy, in some new system, a similar assumption can be taken to define the independent degrees of freedom. A further generalization is obtained by replacing the commutator by the anticommutator, for example. As is well known, this generalization enables us to describe systems which satisfy Fermi-Dirac statistics and the Pauli exclusion principle. Other generalizations of the basic commutation relations have been discussed which allow a description in terms of functions not expressible in a power series in the p_i and q_i (Weyl; Aharanov).

With the equations of motion for the operators of the canonical system in hand, the last step in the description of a system is the specification of its state. In this respect quantum theory is again qualitatively different from the classical description. The specification is made by assuming that the system can be described by a set of state vectors in an abstract vector space (Dirac 1958). These vectors are eigenvectors of a complete set of commuting operators representing the observables of the system, i.e.,

$$\zeta_j(q_i,p_k) \,|\zeta_j\rangle = z_j \,|\zeta_j\rangle \tag{1-1-22}$$

where $\{z_j\}$ is a set of numbers. The most important property of these state vectors is that they express the superposition principle of quantum theory—a linear superposition principle. An arbitrary state of the system, described by a state vector $|X\rangle$, can be written

$$|X\rangle = a_1 \,|\zeta_1\rangle + a_2 \,|\zeta_2\rangle + \ldots \tag{1-1-23}$$

where the a_i are complex numbers related to the probability that the system is found experimentally to be in one of the states $|\zeta_1\rangle$, $|\zeta_2\rangle$..., i.e., a measurement on the system produces the result ζ_1, ζ_2, ... a fraction of the time determined from the coefficients a_1, a_2, etc. The superposition principle, together with the uncertainty principle expressed by the noncommutativity of canonically conjugate variables, defines the general theoretical structure which we refer to as quantum theory.

In the Heisenberg picture discussed above the state vector is independent of time. Thus, all the dynamical evolution is found in the operators. Unitary transformations, which leave the fundamental commutators invariant, describe the time evolution of the system in terms of operators specified at some instant. These are analogous to the canonical transformations of classical mechanics.

2. The Analogy For Fields

The generalization of quantization to systems with an infinite number of degrees of freedom was initiated by Heisenberg and Pauli (Heisenberg 1929). The system is described classically by fields $\psi_j(\vec{x},t)$ and conjugate momentum fields $\pi_j(\vec{x},t)$, where j is a discrete index. The position vector $\vec{x}$ replaces the discrete index i for systems of point particles. This correspondence is exhibited most clearly by first dividing space into cells centered about a particular $\vec{x}$ and then passing to the limit in which the volume of the cell becomes infinitesimal (Goldstein; Wentzel). Rather than taking this approach we will describe the fields in terms of Fourier components.

The decomposition into Fourier components is accomplished by assuming that the system is periodic in a cell of volume V. Since the fields are real, the Fourier series can be written in terms of sines and cosines, where the wave vectors satisfy

$$\vec{k}_N = 2\pi V^{-1/3}(n_1\hat{e}_1 + n_2\hat{e}_2 + n_3\hat{e}_3) = 2\pi V^{-1/3}\vec{n} \qquad (1\text{-}2\text{-}1)$$

N denotes the triple of integers (n_1, n_2, n_3), $n_1 > 0$. Each Fourier sine or cosine mode, for each distinct wave vector, represents a distinct degree of freedom for the system. Consequently, writing (for j=1)

$$\psi = \sum_N \left(Q_{Ns}\sin(\vec{k}_N\cdot\vec{x}) + Q_{Nc}\cos(\vec{k}_N\cdot\vec{x})\right)(2/V)^{\frac{1}{2}} \qquad (1\text{-}2\text{-}2)$$

$$\pi = \sum_N \left(P_{Ns}\sin(\vec{k}_N\cdot\vec{x}) + P_{Nc}\cos(\vec{k}_N\cdot\vec{x})\right)(2/V)^{\frac{1}{2}} \qquad (1\text{-}2\text{-}3)$$

the canonical coordinates of the system can be chosen to be Q_{Ns} and Q_{Nc} while the canonical momenta are P_{Ns} and P_{Nc}. This treatment was originally introduced to describe the electromagnetic field (Heitler).

As in the case of discrete systems, the dynamics of the field can be discussed in terms of Poisson brackets. The only change to be made is to account for the two variables which occur for each $\vec{n}$. The Poisson bracket is redefined to be

$$[f,g]_{pb} = \sum_{N,r} \left(\frac{\partial f}{\partial Q_{Nr}} \frac{\partial g}{\partial P_{Nr}} - \frac{\partial f}{\partial P_{Nr}} \frac{\partial g}{\partial Q_{Nr}} \right) \tag{1-2-4}$$

where r ranges over s and c. The properties of the Poisson bracket given in section 1-1 follow immediately. The fundamental Poisson brackets are

$$[Q_{Nr},Q_{Mt}]_{pb} = [P_{mt},P_{Nr}]_{pb} = 0\,, \tag{1-2-5}$$

$$[Q_{Nr},P_{Mt}]_{pb} = \delta_{NM}\delta_{rt}\,, \tag{1-2-6}$$

while the time evolution of the system is still found from equation (1-1-6) written in terms of the new Poisson bracket.

The transition to the quantum theory of fields is made as in the mechanics of point particles. Assume that the canonical variables can be replaced by noncommuting, Hermitian operators P_{Nr} and Q_{Nr} with fundamental commutators

$$\left[Q_{Nr}, P_{Mt}\right] = i\hbar\delta_{NM}\delta_{rt}\,, \tag{1-2-7}$$

$$\left[Q_{Nr}, Q_{Mt}\right] = 0 = \left[P_{Nr},P_{Mt}\right]\,. \tag{1-2-8}$$

where, as before, the commutator of two operators a and b is defined as

$$[a,b] = ab - ba \tag{1-2-9}$$

The equation of motion for the operators describing the system is, in the Heisenberg picture,

$$\frac{\partial f}{\partial t} + [f,H]\,(i\hbar)^{-1} = \frac{df}{dt}\,, \tag{1-2-10}$$

where f is any function of P_{Nr} and Q_{Nr} and possibly t. The prescription for calculating general commutators follows the directions given in equation (1-1-20). The same ambiguities in order of factors arise.

Finally, to complete the quantum theory the state of the system is described by vectors in an abstract vector space (Dirac 1958). Once again, the basic assumption is that these vectors satisfy a linear superposition principle. The coefficients appearing in a superposition of vectors are related to the probability that a measurement on the system gives the eigenvalues of the operators for which the particular state vector is an eigenvector.

The end result of quantization of a field theory is that field strengths are quantized. Canonically conjugate functions of these field strengths satisfy the uncertainty relations. The state of the system is specified by giving the eigenvalues of some complete set of operator functions of the canonical variables. However, as we shall see in the next section, an important new property is present in the quantum field theory—an intrinsic particle property.

3. Quanta Of Fields: The Particle Aspect Of A Quantized Field

Classical field theories were originally developed to describe continuous systems, e.g., fluids, on the macroscopic level. No underlying particle structure of a fundamental nature was associated with the systems. However, as the atomic hypothesis became more plausible during the nineteenth century microscopic theories contemplating matter as intrinsically particulate in nature gained acceptance. The derivation of macroscopic continuum theories from particle theories soon followed. Only the electromagnetic field seemed to occupy a unique position among field theories. No medium such as the ether could be associated with the field in a nontrivial way. The only particle structure within electromagnetism consisted of wave packets, superpositions of waves of different frequencies and wave vectors. These were known to disperse, so nothing fundamental could be attributed to them. Thus, prior to the development of quantum theory at least one field theory existed which seemed to have no associated particle origins.

In the explanation of the photoelectric effect the idea of a photon is a central hypothesis. In the initial discussion of the quantum theory of radiation this idea, in its original form as the packet of energy of an oscillator, was combined with electromagnetism (Dirac 1927). Subsequently, quanta were associated with other field theories. These particles are qualitatively different from the classical conception of particles. They have momentum and energy, but localization in space is only an approximate characteristic.

In order to show how the particle aspect of a quantized field arises we will examine the spin zero field with the Klein Gordon equation as field equation. This is a relativistically invariant theory. While relativistic invariance is not essential, most of the applications in this monograph will employ such theories.

The Klein Gordon equation is constructed by analogy with the rules leading to the Schrödinger differential equation. With no interaction relativistic invariance is insured by assuming that the field $\phi(x)$ is a scalar with respect to Lorentz transformations and that the mass-