

Chapter 1

Introduction

1.1 Standard Many-Body Perturbation Theory

The quantum-mechanical treatment of many-electron systems, based on the Schrödinger equation and the Coulomb interaction between the electrons, was developed shortly after the advent of quantum mechanics, particularly by John Slater in the late 1920s and early 1930s [230]. Self-consistent-field (SCF) schemes were early developed by Slater, Hartree, Fock and others.¹ Perturbative schemes for quantum-mechanical system, based on the Rayleigh–Schrödinger and Brillouin–Wigner schemes, were developed in the 1930s and 1940s, leading to the important *linked-diagram expansion*, introduced by Brueckner [40] and Goldstone [78] in the 1950s, primarily for nuclear applications. That scheme was in the 1960s and 1970s also applied to electronic systems [104] and extended to degenerate and quasi-degenerate energy levels (“multi-reference systems”) [34, 117]. The next step in this development was the introduction of “*all-order methods*” of *coupled-cluster* type, where certain effects are taken to all orders of the perturbation expansion (see [246]). This represents the last—and probably final—major step of the development of a non-relativistic many-body perturbation theory (MBPT).²

The first step towards a relativistic treatment of many-electron systems was taken in the early 1930s by Gregory Breit [35], extending works made somewhat earlier by J.A. Gaunt [73]. Physically, the Gaunt interaction represents the magnetic interaction between the electrons, which is a purely relativistic effect. Breit augmented this treatment by including the leading retardation effect, due to the fact that the Coulomb interaction is not instantaneous, which is an effect of the same order.

¹For a review of the SCF methods the reader is referred to the book by Ch. Froese-Fischer [71].

²By MBPT we understand here perturbative methods based upon the Rayleigh–Schrödinger perturbation scheme and the linked-diagram expansion. To that group we also include non-perturbative schemes, like the coupled-cluster approach (CCA), which are based upon the same formalism.

A proper relativistic theory should be *Lorentz covariant*, like the Dirac single-electron theory.³ The Dirac equation for the individual electrons together with the instantaneous Coulomb and Breit interactions between the electrons represent for a many-electron system all effects up to order α^2 H(artree atomic units) or $\alpha^4 m_e c^2$.⁴ This procedure, however, is NOT Lorentz covariant, and the instantaneous Breit interaction can only be treated to first-order in perturbation theory, unless projection operators are introduced to prevent the intermediate states from falling into the “Dirac sea” of negative-energy states, as discussed early by Brown and Ravenhall [39] and later by Joe Sucher [238]. The latter approach has been successfully employed for a long time in relativistic many-body calculations and is known as the *no-virtual-pair approximation* (NVPA).

A fully covariant relativistic many-body theory requires a field-theoretical approach, i.e., the use of *quantum electrodynamics* (QED). In principle, there is no sharp distinction between relativity and QED, but conventionally we shall refer to effects beyond the no-virtual-pair approximation as QED effects. This includes “*non-radiative*” effects (retardation and virtual electron-positron pairs) as well as “*radiative*” effects (self-energy, vacuum polarization, vertex correction). The systematic treatment of these effects requires a covariant approach, where the QED effects are included in the wave function and hence can be treated on the same footing as the electron-electron interaction. It is the main purpose of the present book to formulate the foundations of such a unified MBPT-QED procedure.

1.2 Quantum Electrodynamics

Already in the 1930s deviations were observed between the results of precision spectroscopy and the Dirac theory for simple atomic systems, primarily the hydrogen atom. Originally, this deviation was expected to be due to *vacuum polarization*, i.e., spontaneous creation of electron-positron pairs in the vacuum, but this effect turned out to be too small and even of the wrong sign. An alternative explanation was the *electron self-energy*, i.e., the emission and absorption of a virtual photon on the same electron—another effect that is not included in the Dirac theory. Early attempts to calculate this effect, however, were unsuccessful, due to singularities (infinities) in the mathematical expressions.

The first experimental observation of a clear-cut deviation from the Dirac theory was the detection in 1947 by Lamb and Retherford of the so-called *Lamb shift* [116],

³A physical quantity (scalar, vector, tensor) is said to be Lorentz covariant, if it transforms according to a representation of the Lorentz group. (Only a scalar is invariant under a that transformation.) An equation or a theory, like the theory of relativity or Maxwell’s theory of electromagnetism, is said to be Lorentz covariant, if it can be expressed entirely in terms of covariant quantities (see, for instance, the books of Bjorken and Drell [21, 22]).

⁴ α is the fine-structure constant $\approx 1/137$ and $m_e c^2$ is the electron rest energy (see Appendix K).

namely the shift between the $2s$ and $2p_{1/2}$ levels in atomic hydrogen, levels that are exactly degenerate in the Dirac theory [58, 59]. In the same year Hans Bethe was able to explain the shift by a non-relativistic calculation, eliminating the singularity of the self-energy by means of a *renormalization process* [19]. At about the same time Kusch and Foley observed that the magnetic g -factor of the free electron deviates slightly but significantly from the Dirac value -2 [110, 111]. These observations led to the development of the modern form of the quantum-electrodynamic theory by Feynman, Schwinger, Dyson, Tomanaga and others by which the deviations from the Dirac theory could be explained with good accuracy [63, 68, 69, 224, 244].⁵

The original theory of QED was applied to free electrons. During the last four to five decades several methods have been developed for numerical calculation of QED effects in *bound* electronic states. The scattering-matrix or *S-matrix formulation*, originally developed for dealing with the scattering of free particles, was made applicable also to bound states by Joe Sucher [236], and the numerical procedure was refined in the 1970s particularly by Peter Mohr [153]. During the last two decades the method has been extensively used in studies of highly charged ions in order to test the QED theory under extreme conditions, works that have been pioneered by Mohr and Soff (for a review, see [159]).

The *Green's function* is one of the most important tools in mathematical physics with applications in essentially all branches of physics.⁶ During the 1990s the method was adopted to bound-state QED problems by Shabaev et al. [226]. This procedure is referred to as the *two-time Green's function* and has recently been extensively applied to highly-charged ions by the St Petersburg group.

During the first decade of this century another procedure for numerical QED calculations was developed by the Gothenburg atomic theory group, first termed the *Covariant evolution-operator* method [130], which was applied to the fine structure and other energy-level separations of heliumlike ions. This can be combined with electron correlation to arbitrary order, and we then refer to this procedure as the *Green's-operator method*. This represents a step towards a fully covariant treatment of many-electron systems and formally equivalent to the *Bethe–Salpeter equation* (see below).

1.3 Bethe–Salpeter Equation

The first completely covariant treatment of a bound-state problem was presented in 1951 by Salpeter and Bethe [20, 213] and by Gell-Mann and Low [74]. The two-particle Bethe–Salpeter (BS) equation contains in principle the complete relativistic and interelectronic interaction, i.e., all kinds of electron-correlation and QED effects.

⁵For the history of the development of the QED theory the reader is referred to the authoritative review by Silvan Schweber [221].

⁶For a comprehensive account of the applications, particularly in condensed-matter physics, the reader is referred to the book by Gerald Mahan [140].

The BS equation is associated with several fundamental problems, which were discussed in the early days, particularly by Dyson [64], Goldstein [77], Wick [251] and Cutkosky [53]. Dyson found that the question of relativistic quantum mechanics is “*full of obscurities and unsolved problems*” and that “*the physical meaning of the 4-dimensional wave function is quite unclear*”. It seems that some of these problems still remain.

The BS equation is based upon field theory, and there is no direct connection to the Hamiltonian approach of quantum mechanics. The solution of the field-theoretical BS equation leads to a four-dimensional wave function with individual times for the two particles. This is not in accordance with the standard quantum-mechanical picture, which has a single time variable also for many-particle systems. The additional time variable leads sometimes to “*abnormal solutions*” with no counterparts in non-relativistic quantum mechanics, as discussed particularly by Nakanishi [172] and Namyslowski [173].

Much effort has been devoted to simplifying the BS equation by reducing it to a three-dimensional equation, in analogy with the standard quantum-mechanical equations (for reviews, see [32, 49]). Salpeter [212] derived early an “*instantaneous*” approximation, neglecting retardation, which led to a relativistically exact three-dimensional equation, similar to—but not exactly equal to—the Breit equation. More sophisticated is the so-called *quasi-potential approximation*, introduced by Todorov [242], frequently used in scattering problems. Here, a three-dimensional Schrödinger-type equation is derived with an **energy-dependent** potential, deduced from scattering theory. Sazdjian [216, 217] was able to separate the BS equation into a three-dimensional equation of Schrödinger type and one equation for the relative time of the two particles, serving as a perturbation—an approach that is claimed to be exactly equivalent to the original BS equation. This approach establishes a definitive link between the Hamiltonian relativistic quantum mechanics and field theory. Connell [49] further developed the quasi-potential approximation of Todorov by introducing series of corrections, a procedure that also is claimed to be formally equivalent to the original BS equation.

Caswell and Lepage [42] applied the quasi-potential method to evaluate the hyperfine structure of muonium and positronium to the order $\alpha^6 m_e c^2$ by combining analytical and perturbative approaches. Grotch and Yennie [32, 83] have applied the method to evaluate higher-order nuclear corrections to the energy levels of the hydrogen atom, and Adkins and Fell [3, 4] have applied it to positronium.

A vast literature on the Bethe–Salpeter equation, its fundamental problems and its applications, has been gathered over the years since the original equation appeared. Most applications are performed in the strong-coupling case (QCD), where the fundamental problems of the equation are more pronounced. The interested reader is here referred to some reviews of the field, where numerous references to original works can be found [82, 172, 173, 178, 217].

1.4 Helium Atom. Analytical Approach

An approach to solve the BS equation, known as the *external-potential approach*, was first developed by Sucher [235, 237] in order to evaluate the lowest-order QED contributions to the ground-state energy of the helium atom, and equivalent results were at the same time also derived by Araki [5]. The electrons are here assumed to move in the field of the (infinitely heavy) atomic nucleus. The relative time of the two electrons is eliminated by integrating over the corresponding energy of the Fourier transform, which leads to a Schrödinger-like equation, as in the quasi-potential-method. The solution of this equation is expanded in terms of a Brillouin–Wigner perturbation series. This work has been further developed and applied by Douglas and Kroll [60] and by Zhang and Drake [259, 263] by considering higher-order terms in the α and $Z\alpha$ expansions. This approach, which is reviewed in Chap. 11, can be used for light systems, such as light heliumlike ions, where the power expansions are sufficiently convergent. The QED effects are here evaluated by means of highly correlated wave functions of Hylleraas type, which implies that QED and electron-correlation effects are highly mixed. A related technique, referred to as the *effective Hamiltonian approach*, has been developed and applied to heliumlike systems by Pachucki and Sapirstein [179, 180, 181].

A problem that has been controversial for quite some time is the fine structure of the lowest P state of the neutral helium atom. The very accurate analytical results of Drake et al. and by Pachucki et al. give results close to the experimental results obtained by Gabrielse and others [258], but there have for quite some time been significant deviations—well outside the estimated limits of error. More recently, Pachucki and Yerokhin have by means of improved calculations shown that the controversy has been resolved [182, 183, 184, 185].

1.5 Field-Theoretical Approach to Many-Body Perturbation Theory

The methods mentioned for numerical QED calculations can for practical reasons be used only to evaluate one- and two-photon exchange in a complete way. This implies that the electron correlation can only be treated to lowest order. This might be sufficiently accurate for highly charged systems, where the QED effects dominate over the electron correlation, but is usually quite insufficient for lighter systems, where the situation is different.

In the numerical procedures for standard (relativistic) MBPT the electron correlation can be evaluated effectively to essentially all orders by techniques of coupled-cluster type. QED effects can here be included only as first-order energy corrections, a technique applied particularly by the Notre-Dame group [195]. To treat electron correlation, relativity and QED in a unified manner would require a field-theoretical many-body approach from the start.

The methods developed for QED calculations are all based upon field-theory. Of these methods, the covariant-evolution-operator method, has the advantage that it has a structure that is quite akin to that of standard MBPT. Contrary to the other methods it can be used to evaluate perturbations to the **wave function**—not only to the energy. Then it can serve as a basis for a unified field-theoretical many-body approach, where the dominating QED effects can be evaluated order for order together with the Coulomb interaction. This leads to a procedure for the combination of QED and electron correlation. This is the approach that will be described in the present book and represents the direction of research presently being pursued by the Gothenburg atomic theory group.

(It should be mentioned that a related idea was proposed by Leonard Rosenberg more than 20 years ago [203], namely of including Coulomb interactions in the QED Hamiltonian.)

The covariant evolution operator can be singular, as the standard evolution operator of non-relativistic quantum mechanics, but the singularities can be eliminated in a similar way as the corresponding singularities of the Green's function. The regular part of the covariant evolution operator is the *Green's operator*, which can be regarded as an extension of the Green's-function concept and shown to serve as a link between field theory and standard many-body perturbation theory. The perturbation used in this procedure represents the interaction between the electromagnetic field and the individual electrons. This implies that the equations operate in an extended *photonic Fock space* with variable number of photons.

The strategy is here to combine a single retarded photon with numerous Coulomb interactions. As long as no virtual pairs are involved, this can be performed iteratively. In this way the dominating QED effects can—for the first time—be treated in the same manner as standard many-body perturbations. For practical reasons only a single retarded photon can be included in each iteration at present time, but due to the iterations this corresponds to the most important (“reducible”) effects also in higher orders [132]. When extended to (“irreducible”) interactions of multi-photon type, this would lead for two-particle systems to the *Bethe–Salpeter equation*, and in the multi-reference case to an extension of this equation, referred to as the *Bethe–Salpeter–Bloch equation* [131].

In the first edition we dealt with the combination of electron correlation and **non-radiative** QED effects, mainly retardation and virtual electron-positron pairs, based upon the PhD thesis of Daniel Hedendahl in the Gothenburg group. In the meantime, similar calculations have been performed for **radiative** effects (electron self-energy and vertex correction) by Johan Holmberg in his thesis of the same group, and his main results are included in the present second edition.

In combining QED with electron correlation it has been found advantageous to work in the *Coulomb gauge*. In the Feynman gauge there are enormous cancellations between various QED effects, which is not the case in the Coulomb gauge, making the calculations in the latter gauge much more stable. This has the consequence, as is demonstrated in Chap. 9, that it is practically impossible to carry calculations involving radiative effects beyond second order using the Feynman gauge. With the Coulomb gauge, on the other hand, reliable results could here be obtained.

Furthermore, in this gauge one can, for instance, include the instantaneous Breit interaction, which in other gauges, like the Feynman gauge, would correspond to multiple transverse photons. Although this gauge is *non-covariant* in contrast to, for instance, the simpler Feynman gauge, it can be argued that the deviation from a fully covariant treatment will have negligible effect in practical applications when handled properly. This makes it possible to mix a larger number of Coulomb interactions with the retarded-photon interactions, which is expected to lead to the same ultimate result as a fully covariant approach but with faster convergence rate due to the dominating role of the Coulomb interaction.

The procedure can also be extended to systems with more than two electrons, and due to the complete compatibility between the standard and the extended procedures, the QED effects need only be included where they are expected to be most significant.

In principle, also the procedure outlined here leads to *individual times* for the particles involved, consistent with the full Bethe–Salpeter equation but not with the standard quantum-mechanical picture. We shall mainly work in the *equal-time approximation* here, and we shall not analyze effects beyond this approximation in any detail. It is expected that—if existing—any such effect would be extremely small for electronic systems.

1.6 Dynamical Processes

The first edition of the book dealt only with *static processes*, i.e., structure calculations. In recent time experiments on *dynamical processes* have become increasingly important in various parts of physics and chemistry. The standard theoretical procedure for dealing with such processes is the S-matrix formalism. In evaluating QED effects for such systems, where bound states are involved, intermediate model-space states will appear, which will lead to singularities that cannot be handled with the S-matrix formalism. However, these singularities are of the same kind as those appearing in structure calculations, which has the consequence that the methods developed for QED calculations for structure calculations, such as the covariant evolution operator method, work perfectly well also for dynamical processes. This is demonstrated in Part IV of the second edition for the case of transition rates and radiative recombination. Experiments are presently being performed to detect QED effects in such processes. These effects are presently on the verge of being detectable experimentally.

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