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Functional integral approach to the bound-state problem in atomic physics

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Zusammenfassung

In dieser Dissertation wurde ein alternativer mathematischer Formalismus für die Untersuchung von Strahlungskorrekturen in der Atomphysik entwickelt. In diesem Zusammenhang werden hochgeladene Ionen (HCIs) untersucht, bei denen die Auswirkungen solcher QED-Korrekturen sehr deutlich werden und Präzisionsexperimente ermöglichen. Die Coulomb-Wechselwirkung zwischen Elektron und Kern führt zu gebundenen Zuständen, die von Natur aus nichtstörungstheoretisch sind. Dies erfordert die Einbeziehung des lokalisierenden Kernpotentials in die Dirac-Gleichung nullter Ordnung. Dies wird durch die Konstruktion der Propagatoren von QED-Prozessen in einem starken Coulomb-Feld unter Verwendung von Funktionsintegralen erreicht. Die freien Propagatoren und die Dirac-Coulomb Green's function, die zentrale Einheit der QED im gebundenen Zustand, werden in geschlossenen analytischen Formen abgeleitet. Die geschlossenen Formen werden dann verwendet, um die formale Theorie der Lamb-Verschiebung auf der Ein-Schleifen-Ebene unter Verwendung der Schwinger-Dyson-Gleichungen zu konstruieren. Die Vakuum-Polarisationskorrektur der Energieniveaus der gebundenen Zustände wird mit Hilfe von Störungspfadintegralen untersucht, wobei das Uehling-Potential als lokales Störungspotential behandelt wird. Nach demselben mathematischen Schema wird der Propagator der gebundenen Elektronen mit korrigierter Eigenenergie bestimmt. Die Verschiebungen der Energieniveaus werden dann durch analytische Methoden der komplexen Konturintegration ermittelt und numerisch mit endlichen Basissätzen berechnet. Anhand der numerischen Ergebnisse identifizieren wir eine Reihe von Ionen, die neuartige Beobachtung von QED-Effekten mittels Präzisionsmassenspektrometrie ermöglichen.

Abstract

In this Thesis, an alternate mathematical formalism for the study of radiative corrections in atomic physics has been developed. In this context, highly charged ions (HCIs) are studied, where the effect of such QED corrections become very evident and allow for precision experiments. The Coulomb interaction between electron and nucleus leads to bound states that are innately non-perturbative and requires the inclusion of the localizing nuclear potential in the zeroth order of the Dirac equation. This is implemented by constructing the propagators of QED processes in a strong Coulomb field using functional integrals. The free propagators and the Dirac-Coulomb Green's function (DCGF), the central entity of bound-state QED, are derived in closed analytical forms. The closed forms are then used to construct the formal theory of the Lamb shift at the one-loop level using Schwinger-Dyson equations. Vacuum-polarization correction to the bound-state energy levels is studied using perturbative path integrals, where the Uehling potential is treated as a local perturbing potential. Within the same framework, the self-energy corrected bound-electron propagator is determined. The energy-level shifts are then obtained through methods of complex contour integration and computed numerically using finite basis sets. From the numerical results we identify a range of ions enabling the novel observation of QED effects via precision mass spectrometry.

Within the framework of this thesis, the following articles have been submitted to refereed journals:

- Path integral formalism for the free Dirac propagator in spherical coordinates
  Sreya Banerjee, Zoltán Harman
  arXiv:2309.13688 (Ref. [1])

- Vacuum polarization correction to atomic energy levels in the path integral formalism
  Sreya Banerjee, Zoltán Harman
  arXiv:2309.13739 (Ref. [2])

- Self-energy correction to energy levels of highly charged ions in a path integral formalism
  Sreya Banerjee, Zoltán Harman
  arXiv:2309.15590 (Ref. [3])

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Introduction

Quantum electrodynamics (QED), the theory of interactions between charged particles and the electromagnetic field, or as Feynman called it, "the strange theory of light and matter" [4], can be considered to be the first successful interpretation of a quantum field theoretic model. In the words of Weinberg, this quantization of the electromagnetic field is "still the paradigmatic example of a successful quantum field theory" [5]. QED, an abelian gauge field theory with U(1) symmetry, could be considered to be a quantum extension of the classical theory of electromagnetism and forms one of the pillars of the standard model (SM).

Quantum field theory (QFT) was conceived in the late 1920s as a replacement of quantum mechanics (QM) to describe 'relativistic' particle dynamics. The idea was to combine the concepts of quantum mechanics with relativistic invariance and extend the theory from a discrete particle treatment and generalise it to a field treatment. Dirac is accredited with the inception of QFT through his pioneering 1927 work "The quantum theory of the emission and absorption of radiation" [6], which incidentally was QED. QED effects have since been experimentally observed and studied and the development of the theory gained traction after one such experimental observation, the Lamb shift [7–11]. The splitting of the $2p_{1/2} - 2s_{1/2}$ states in the hydrogen spectra, which was observed by Lamb and Retherford using radio frequency spectroscopy to be 1050 MHz, could not be explained using the Dirac equation, according to which these states were degenerate. It was Hans Bethe, who theoretically predicted the origin of this shift to be due to the electron interacting with its own electromagnetic field [12]. Though his work completely overlooked the inclusion of electron spin and treated the electron as a non-relativistic particle, he laid the groundwork for the further development of QED. This, along with the experimental discovery of the anomalous magnetic moment of the electron, necessitated a revaluation of the theory and led to the birth of modern QED in the hands of Richard P. Feynman, Freeman Dyson, Sin-Itiro Tomonoga and Julian Schwinger in the 1940s [13–15]. The theoretical development of QED and the subsequent taming of the infininties, that arose at higher orders of perturbation theory, based on renormalization theory made it the language of choice to describe the dynamics of atomic and subatomic particles, and their interactions. This prompted a successful extension of the renormalization theory to other field theoretic models. The accuracy with which the theoretical predictions of QED matched the experimental observations has made it the most relevant field theorectic model for the study of elementary particle physics.

Since its conception, field theory in general has been studied using canonical quantization as the mathematical tool of choice. It was used by Dirac in his 1927 work [6] that introduced field theory in the form of QED. Based on the operator formalism, it derives its name from the Hamiltonian formalism of classical mechanics. The dynamical variables of the field are represented as operators, obeying canonical commutation relations, that act on particles which are interpreted by their eigenstates in the Hilbert space defined by these states. The eigenvalues, thus obtained, quantify the particle dynamics.

There is, however, an alternate method to approach the problem of field quantization. This alternate approach to the quantization of fields was proposed by Feynman himself in his doctoral work, which was later presented through the seminal paper "*Space-Time Approach to Non-Relativistic Quantum Mechanics*" [16], is the path integral formulation.

Unlike canonical quantization, which uses operators to describe the dynamical field variables, the 'path integral' or the 'functional integral' method employs an action-based approach. The dynamics of the system is derived from the very classical concept of the 'least action principle', according to which a classical particle while travelling between an initial and a final point, chooses the path that requires it to spend the least amount of energy, or in other words, has the least action associated with it. This path of least action then describes the dynamics of the particle through the Euler-Lagrange equations. When we talk about atomic and subatomic physics, our particles are no longer classical and their paths can no longer be defined by sharp trajectories. To accommodate this simple classical formalism into the definition of quantum mechanics, the path followed by the particle is so chosen that it is a superposition of all the infinite number of paths that the particle can take and the transition amplitude is given as a function of a complex Boltzmann factor which depends on the action of the path created by the constructive interference of all the superimposing paths [17]. The two different methods of field quantization, one based on the canonical quantization and the other on the path integral formalism, serve the same purpose and ultimately yield the same results, however they are distinctive at the fundamental level. While the canonical quantization method relies heavily on the operator formalism and the corresponding commutation relations, the path integral formalism is much more intuitive, preserves all symmetries of the system while manifestly preserving Lorentz invariance, since it is fundamentally based on the Lagrangian formalism. It is more of a general theory that can be applied to any gauge field, in fact, it is a very common tool used to describe non-abelian gauge theories. Quoting a part of Feynman's Nobel acceptance speech, "*It always seems odd to me that the fundamental laws of physics, when discovered, can appear in so many different forms that are not apparently identical at first, but, with a little mathematical fiddling you can show the relationship. An example of that is the Schrödinger equation and the Heisenberg formulation of quantum mechanics. I don't know why this is – it remains a mystery, but it was something I learned from experience. There is always another way to say the same thing that doesn't look at all like the way you said it before. I don't know what the reason for this is. I think it is somehow a representation of the simplicity of nature. A thing like the inverse square law is just right to be represented by the solution*

of Poisson's equation, which, therefore, is a very different way to say the same thing that doesn't look at all like the way you said it before. I don't know what it means, that nature chooses these curious forms, but maybe that is a way of defining simplicity. Perhaps a thing is simple if you can describe it fully in several different ways without immediately knowing that you are describing the same thing...Theories of the known, which are described by different physical ideas, may be equivalent in all their predictions and hence scientifically indistinguishable. However, they are not psychologically identical when trying to move from that base into the unknown. For different views suggest different kinds of modifications which might be made and hence are not equivalent in the hypotheses one generates from them in one's attempt to understand what is not yet understood. I, therefore, think that a good theoretical physicist today might find it useful to have a wide range of physical viewpoints and mathematical expressions of the same theory (for example, of quantum electrodynamics) available to him."

The path integral formalism, or functional integrals in the context of field theory, enters quantum mechanics very organically through the Young's double-slit experiment. If the electron were to be considered classical particle, one expects the formation of two distinct lines where the particle hits the detector, instead, in the double-slit experiment we have the formation of an interference pattern which is counterintuitive if the electron were a classical particle. The formation of the interfernce pattern thus establishes that, the electron is a quantum particle with wave-like properties, through the superposition principle. The interference pattern is formed since the electron, being a quantum particle, can take any possible path to reach the detector once it has passed through the two slits, and the probability amplitude of its detection at any point on the detector is then given by the superposition of the amplitudes of the particle passing through both the slits. But what happens if the two slits are replaced by more number of slits? To answer this, Feynman put forward a revolutionary idea where he argued that if the number of slits on the screen were increased infinitely such that the screen did not exist anymore, and also the number of screens between the source and the detector were increased infintely such that it could essentially be considered as empty space, the transition amplitude of the particle between the source and the detector would still be given by the sum of all the transition amplitudes for the particle to go through all the infinite slits on infinite screens. Thus, Feynman established that even in empty space, the transition amplitude of a particle between an initial and a final point is given by the sum over the transition amplitudes of all the possible paths that the particle can take – the path integral formalism.

The classical action principle states that among all the classical paths, the system 'chooses' the path that is associated with the least action. This is the classical least action principle. From the calculus of variations, this path that minimizes the action, satisfies the Euler-Lagrange equation and gives us the dynamics of the system. In the quantum limit, if the extremum of some action $\mathcal{S}$ is varied with respect to some variable x, it can be expressed in a way that corresponds to the classical equations of motion. The quantum-mechanical probability amplitude, K, for any given transition between

two points a and b, which corresponds to the action $\mathcal{S}$, can then be given by,

$$K(b,a) = \int_a^b e^{\frac{i}{\hbar}\mathcal{S}[b,a]}\, dx\,(t)\ . \tag{1}$$

This is the basic approach to the path integral formulation.

Feynman's approach to quantization of QED was based on this integral over paths which he introduced into the theory through the Feynman diagrams, which visualize the fundamental processes in terms of space-time trajectories of particles [18]. The initial success with non-relativistic quantum theory however did not prompt its extension to relativistic theory, especially the establishment of QED starting from a classical particle theory. This was largely due to the lack of sufficient mathematical tools required to quantize the electron spin in the classical regime; another setback was that the concept of antiparticles, as had been established by Dirac's theory, could not be classically justified. This complication was addressed by Berezin through the formulation of fermionic path integrals using Grassmann algebra [19, 20], where the anticommuting Grassmann variables form a classical representation of the fermion and antifermion fields, which allow for the quantization of the fermionic spin. In the definition of fermions in the relativistic regime, Berezin drew inspiration from various works on supersymmetry, and used a Grassmann algebra space with five generators denoted by the Grassmannian η, comprising of a four axial vector, $\eta_a = (\eta_0, \eta_k); k \in \{1,2,3\}$, and a pseudoscalar η_5, which upon quantization led to Clifford algebra with five generators corresponding to the Dirac matrices $\boldsymbol{\alpha}$ and β [19]. This led to a classical-mechanical description of a relativistic quantum particle and a convincing classical Lagrangian could now be constructed for the theory. A series of works on this classical treatment of spinning particles was then carried out using anticommuting Grassmann numbers [20–24]. Using such a pseudoclassical system, where the system was reduced to the classical regime using a Lagrangian, which was named the Barducci-Casalbuoni-Lusanna Lagrangian [25], equations of motion were extracted from its variation, and one could construct a functional integral, not in the context of field theory, but by a reduction of the system from a quantum to a classical regime [26].

In the more modern representation of field theory and its quantization using path integrals, we no longer concern ourselves with the reduction of the system to a classical one, instead a generating functional, for the propagators of the field, is constructed in terms of the classical action which contains the classical Lagrangian for the system, and 'sources', which include the field-theoretic description of the system. These sources are the generators for the fields that are associated with the particles and the correlation functions or the propagators are obtained as derivatives with respect to these source terms. This can be interpreted as introducing small perturbations to the system by introducing small variations to the source, which in turn alters the associated particle fields, which is what we evaluate using the correlation functions. Since the propagators are defined in terms of the sources, which are Grassmannians, they encapsulate all information about the particles, including their spin dynamics and the quantization of the system reduces to a very lucid definition: a derivative of the generating functional with

respect to the source terms. This method is thus not only elegant but also mathematically simplistic.

The quantization of the system using functional integrals is rooted in the Lagrangian formalism which is intrinsically Lorentz invariant owing to the action being relativistically invariant. Since we sum over all of space-time, path integrals take into account the global landscape of the gauge fields which makes it a very efficient tool for the quantization of both abelian and non-abelian gauge fields and in particular, constrained systems. Extension of Feynman's path integral formalism in the non-abelian theory is made through the Fadeev-Popov path integrals and it provides a very successful quantization of the theory. The biggest advantage of this formalism is that it preserves the non-perturbative information that the system holds through identification of the stationary configurations of the action and hence provides for a self-consistent methodology for a complete understanding of the physics of complex quantum systems [27]. Besides its application to quantum mechanics and field theory, path integrals are a powerful mathematical tool that is very commonly used in the fields of statistical mechanics, polymer physics, cosmology, neural networks, and also used as an efficient optimization tool in quantitative finance [28–38].

In this Thesis, we exploit the non-perturbative information that is provided by the functional integral formalism and apply it to atomic physics, particularly to study the field theory of electromagnetic interactions of elementary charged particles, QED, in the bound state.

Strong-field QED provides an excellent test for the standard model and fundamental physics and also to explore physics beyond the standard model. We study in this Thesis, strong-field phenomena in the context of highly charged ions (HCIs) [39–41]. HCIs are atomic systems that have been stripped off of most of their electrons, thereby subjecting the remaining one or few electrons to the strong background field of the nucleus. The stronger Coulomb field of the nuclei in HCIs result in a larger effective overlap between the nucleus and the bound states which in turn causes the QED effects to be much more pronounced. The strong internal electric field of the nucleus, of the order of 10^{16} V cm^{-1} in the heaviest systems, e.g., H-like $^{238}U^{91+}$ [42–45], warrants lower sensitivity to external effects, thus rendering these ions as perfect candidates for QED precision tests [46], highly stable HCI clocks [47, 48] as well as for quantum information processing [49, 50]. Strong-field QED effects with HCIs have been studied, for more than two decades, at various facilities which include GSI Helmholtz Center for Heavy Ion Research, Darmstadt where such studies have been carried out using x-ray and laser spectroscopy at the SIS/ESR facility [51, 52] where masses of stored ions are measured precisely and precision studies are carried out [43–45, 53, 54]. The electron beam ion traps (EBIT) located at e.g. the Max Planck Institute for Nuclear Physics (MPIK) in Heidelberg, Germany, at the National Institute of Standards and Technology (NIST) at Gaithersburg, USA, and at the Lawrence Livermore National Laboratory (LLNL) also enable the production and investigation of HCI [55–61]. The Mainz Penning trap [62, 63] and the ALPHATRAP Penning-trap setup at the MPIK performs high-precision bound-electron g-factor experiments [64–67], partially with ions extracted

from an EBIT [55]. With the recent developments in experimental techniques and the availability of stronger fields in terms of intense lasers [68]; experiments with HCI channeling in crystals, thus subjected to strong periodic electric fields [69, 70], and also the possibility to have improved experiments, e.g., LUXE (Laser Und XFEL Experiment) a new experiment proposed at DESY and the European XFEL [71], where the electric fields approach the Sauter-Schwinger limit, will make it possible to study QED non-perturbatively and also investigate physics beyond the standard model.

The experimental motivation behind this Thesis is one such precision measurement in HCIs at the PENTATRAP setup at MPIK [72], where measurement of electronic binding energies via mass spectrometry on the sub-eV level is possible through electromagnetic confinement of heavy HCIs in a Penning trap. Masses of ions can be precisely determined by the measurement of the cyclotron frequency. Mass differences, e.g. the binding energy of an electron, can be extracted from the frequency ratio for two ions [73–75]. Theoretically, for HCIs with high atomic number, Z, even though we are still in the weak coupling regime, the coupling parameter $Z\alpha$ is quite large, almost of the order of one, and the background nuclear field can no longer be treated as a perturbation but has to be taken into account non-perturbatively. Such systems are best described by the Furry picture [76] where instead of considering free particle states, the particle states are defined by including the background nuclear field in the Dirac equation i.e., in zeroth order, to produce bound states. This formalism of treating QED in the Furry picture ensures an exact non-perturbative treatment of the nuclear background field, resulting in better theoretical accuracy for high-Z elements. The QED effects such as self-energy and vacuum polarization are treated perturbatively as a power series in terms of the fine-structure constant α, i.e. the number of loops appearing in the diagrams.

The aim of this work is to apply the functional integral formalism to arrive at the bound-state propagators, and evaluate the effect of radiative corrections to the electronic energy levels in HCIs to match the experimental precision. To this effect, we derive the free and bound Dirac propagators using the path integral formalism. These propagators are then used to construct the vacuum-polarization (VP) and self-energy corrected bound-electron Green's functions, using Schwinger-Dyson equations derived using the functional integral formalism. The radiative shifts to bound-electron energy levels are then derived from the poles of the Green's functions and numerical evaluations are performed using finite basis sets as outlined in more detail in the subsequent Section.

Structure of the thesis

We divide this Thesis into a set pattern of chapters, such that the physical implications of the path integral formulation in atomic physics calculations flow naturally from the mathematical details. We preserved the intuitive nature of the path integral formalism by taking a very lucid and not-so-equation-heavy approach in the construction of the theory while also highlighting the finer details.

In Chapter 1, an introduction to the path integral formalism as proposed by Feynman is given in the context of quantum mechanics. This is then extended to the theory of

quantum fields as the functional integral formalism. In Chapter 2, the mathematical and numerical tools used in the Thesis have been introduced.

We revisit the derivation of the free photon and electron propagators in Chapter 3 using the field-theoretical functional integral approach.

In Chapter 4, we take a detour from field theory and treat the electron analogous to a relativistic particle to derive the propagator for the free Dirac particle in spherical coordinates. A second-order Dirac equation is constructed to establish a correspondence with the Schrödinger equation. The Hamiltonian for this second-order equation is reduced in Biedenharn's basis [77, 78] which reduces it from the relativistic to a form analogous to the non-relativistic Hamiltonian. The effective action obtained from this reduced Hamiltonian now bears semblance to the action of an isotropic harmonic oscillator and the radial path integral takes a simple Gaussian form. This is then solved to arrive at the free propagator which lays the foundation for the derivation of the dressed, self-energy corrected electron propagator in Chapter 6.

In Chapter 5, the Dirac propagator in the presence of the Coulomb field is rederived using the eigenfunction expansion method following the work of Wong and Yeh [79]. This is then contrasted against the path integral method of Kayed and Inomata [80], where, the Dirac particle in the presence of the static nuclear field is treated in the non-relativistic limit through a basis transformation which reduces the radial Hamiltonian of the second-order Dirac equation for the relativistic problem to that of the non-relativistic hydrogen atom through the introduction of the Martin-Glauber operator [81]. The radial path integral that is constructed from the resulting reduced action is then converted from the Coulomb type to that of an isotropic harmonic oscillator through coordinate transformation and local time rescaling [80] to obtain the Dirac-Coulomb Green's function or the propagator for the bound electron in the Furry picture.

In Chapter 6, we utilise the tools developed in the preceeding Chapters to now evaluate QED effects that can be experimentally observed. We study Lamb shift at the one-loop level starting with the polarization of the vacuum, where the electron interacts with the nucleus through the exchange of a photon that in turn propagates with the creation and annihilation of a lepton-antilepton pair. This virtual pair production and annihilation process results in a weakening of the background nuclear field, and thus produces a correction to the binding energies of the electronic states. At the leading order, the vacuum polarization correction is approximated by the Uehling correction or the photon self-energy, and we study this using the Schwinger-Dyson equation for the photon propagator using functional integrals following Ref. [82]. The Green's function or the corrected strong-field propagator is obtained using perturbative methods for path integrals and the energy shift is calculated from the poles of the spectral representation of the Green's function through complex contour integration. Numerical results are presented for different charge states of heavy HCIs.

In Chapter 7, we continue the Lamb shift derivations through the determination of the shift induced by the electron self-energy, which is the dominant radiative correction in comparison to the Uehling correction to the bound energy levels. The self-energy corrected fermion propagator is mathematically evaluated using the Schwinger-Dyson

equation derived using functional integrals. As done in the case of the Uehling correction, the self-energy corrected Green's function is obtained using perturbative methods for path integrals and the divergences are addressed following the method of expansion of the Dirac-Coulomb Green's function in terms of zero-, one-, and many-potential terms as presented in Ref. [83, 84], and the energy shift is obtained from the poles of the Green's function in its spectral representation. Numerical results are shown for H-like systems using B-spline codes [85–87]. We identify a range of elements and ionic charge states enabling the observation of QED effects via precision mass spectrometry with Penning traps.

This Thesis is concluded by summarising the functional integral formalism in the context of QED effects at the one-loop level followed by an outlook which elaborates on the future research possibilities and applications of this mathematical tool to problems in atomic physics and precision spectroscopy.

Chapters 4, 6, and 7 have been adopted directly or with slight modifications from Refs. [1–3] on arXiv, respectively.

Notation scheme

The units for the entire Thesis are chosen following the convention of natural system of units, where $\hbar = c = \varepsilon_0 = 1$; $\hbar$ is the reduced Planck constant, c is the speed of light in vacuum, and ε_0 is the electric permittivity of free space. The fine structure constant in this notation scheme is given as

$$\alpha = \frac{e^2}{4\pi} \,.$$

The metric tensor $g_{\mu\nu}$ follows the same convention for relativistic metric and can be represented in a diagonal matrix format

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \,.$$

Repeated indices are implicitly summed over as per the Einstein summation convention. The metric convention for the 4-vectors follows the book of Bjorken and Drell [88], where the Lorentz indices are denoted by $\mu, \nu \in \{0, 1, 2, 3\}$ to represent the four space-time dimensions. We also follow the notation of Peskin-Schröder [89] and denote four-vectors in light italic font, e.g., a; their components are denoted in light italic font with a Lorentz index, as a superscipt in the covariant notation, e.g., a^μ; three-vectors are denoted by bold upright font, e.g., $\mathbf{a}$, and its magnitude is denoted by light upright font, e.g., a. To denote operators, a hat is used, e.g., $\hat{A}$. We will also use the Feynman slash notation wherever necessary, e.g., $\not{a} = \gamma^\mu a_\mu$. We also redefine all notations, and any deviation of notations from the standard definitions, used in every Chapter.

1. Preface to the path integral formulation

1.1 Path integrals in quantum mechanics

The path integral formalism was developed in the context of quantum mechanics as a special case of the classical theory. We do not go into the details of the formulation and only mention the basics in this Section.

The dynamics of a quantum system is defined by its trasition amplitude or the probability of the system to transition from an initial space-time point $(\mathbf{x}', 0)$ to a final point $(\mathbf{x}, t)$. In the Schrödinger picture of non-relativistic quantum mechanics, this transition amplitude is given in terms of the *unitary time evolution operator*, $\hat{U}$,

$$\hat{U}(t,0) = \mathrm{T} e^{-i\int_0^t dt'\, \hat{H}(t')}\,, \tag{1.1}$$

where T is the time ordering operator, and $\hat{H}$ is the Hamiltonian of the system.

The time-ordered solution to the Schrödinger equation for a time-independent Hamiltonian in terms of this time evolution operator becomes

$$\begin{aligned} |\psi(t)\rangle &= e^{-i\hat{H}t}\,|\psi(0)\rangle \\ &= \hat{U}(t,0)\,|\psi(0)\rangle\ . \end{aligned} \tag{1.2}$$

Eq. (1.2) shows that the system evolves in time from the initial state $|\psi(0)\rangle$ to the final state $|\psi(t)\rangle$, i.e., the particle state at the space-time point $(\mathbf{x}', 0)$ transitions to the final point $(\mathbf{x}, t)$ when acted upon by the time evolution operator. The position dependence is brought in by a coordinate-space representation of Eq. (1.2)

$$\langle \mathbf{x}|\psi(t)\rangle = \int d^3\mathbf{x}'\, \langle \mathbf{x}|\, e^{-i\hat{H}t}\, |\mathbf{x}'\rangle\, \langle \mathbf{x}'|\psi(0)\rangle\ , \tag{1.3}$$

or simply

$$\psi(\mathbf{x}, t) = \int d^3\mathbf{x}' K(\mathbf{x}, t; \mathbf{x}', 0)\psi(\mathbf{x}', 0)\,, \tag{1.4}$$

where $K(\mathbf{x}, t; \mathbf{x}', 0)$ is the transition amplitude or the kernel that represents the propagator. Establishing the equivalence between Eq. (1.3) and Eq. (1.4), the transition

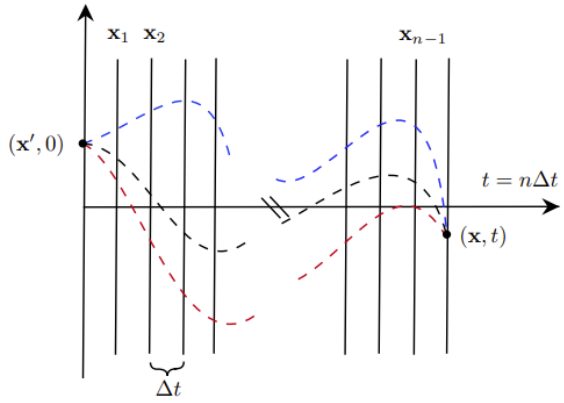

Figure 1.1: Diagrammatic representation of sliced-time trajectories.

amplitude or the propagator is

$$K(\mathbf{x}, t; \mathbf{x}', 0) = \langle \mathbf{x} | \, e^{-i\hat{H}t} \, | \mathbf{x}' \rangle = \langle \mathbf{x} | \, \hat{U}(t, 0) \, | \mathbf{x}' \rangle \ . \tag{1.5}$$

If we now introduce an intermediate space-time point $(\mathbf{y}, t_y)$, such that the system transitions between the initial and the final states while traversing through this intermediate state and the transition amplitude for the entire process is given due to the superposition principle as a summation of the transition amplitude from the inintial to the intermediate state and the transition amplitude from the intermediate to the final state. Eq. (1.4) thus becomes

$$\psi(\mathbf{x}, t) = \int d^3\mathbf{x}' \int d^3\mathbf{y} \, K(\mathbf{x}, t; \mathbf{y}, t_y) K(\mathbf{y}, t_y; \mathbf{x}', 0) \psi(\mathbf{x}', 0) \, . \tag{1.6}$$

The transition amplitude now simply becomes

$$K(\mathbf{x}, t; \mathbf{x}', 0) = \int d^3\mathbf{y} \, K(\mathbf{x}, t; \mathbf{y}, t_y) K(\mathbf{y}, t_y; \mathbf{x}', 0) \, . \tag{1.7}$$

This process can be repeated for infinite insertions of these intermediate points and leads us to the next part where we derive this transition amplitude using path integrals. As Feynman argued [90], a quantum particle transitioning between an initial point and a final point, as in the Young's double-slit experiment example, can pass through an infinite number of intermediate points and the final transition amplitude would be the summation of all the transition amplitudes for all these intermediate points where short time evolutions are calculated by considering consecutive points as initial and final points. This time-sliced approach involves the division of the entire time interval over which the time evolution occurs into infinitesimal time intervals, $\Delta t = t/n$, $n \to \infty$, as seen in Fig. 1.1. Following the Trotter product formula for two operators that may or may not be commutating, $\exp\Big(\hat{A} + \hat{B}\Big) = \lim_{N\to\infty}(\exp\Big(\hat{A}/N\Big) \exp\Big(\hat{B}/N\Big))^N$, we

can write the time evolution operator in terms of short time evolution operators for each of the infinitesimal time intervals. Thus, we have

$$\exp\Big(-i(\hat{T}+\hat{V})t\Big) = \lim_{n\to\infty}\left(\exp\Big(-i(\hat{T}+\hat{V})\Delta t\Big)\right)^n , \tag{1.8}$$

where the Hamiltonian in the exponent has been decomposed into the kinetic and potential part. The R.H.S. of Eq. (1.8) gives us the short-time-evolution operators. Since the two operators for the kinetic and potential energy are non-commutating, we employ the Zassenhaus formula [91] to expand the short-time-evolution operators, and obtain

$$e^{(-i(\hat{T}+\hat{V})\Delta t)} = e^{(-i\hat{T}\Delta t - i\hat{V}\Delta t + (\Delta t)^2[\hat{T},\hat{V}]+\dots)} . \tag{1.9}$$

Since we consider $n \to \infty$, our time intervals $\Delta t \to 0$, and thus we can neglect all higher-order terms as well as the contribution from the $(\Delta t)^2$ term. Eq. (1.8) then becomes

$$\exp\Big(-i(\hat{T}+\hat{V})t\Big) = \lim_{n\to\infty}\left(e^{(-i\hat{T}\Delta t - i\hat{V}\Delta t)}\right)^n = \lim_{n\to\infty}\left(e^{-i\hat{H}\Delta t}\right)^n . \tag{1.10}$$

The transition amplitude in Eq. (1.7) can now be written using Eq. (1.5), in terms of this time-evolution operator for infinitesimal time intervals becomes

$$\begin{aligned} K(\mathbf{x},t;\mathbf{x}',0) &= \lim_{n\to\infty}\int d^3\mathbf{x}_1 \dots d^3\mathbf{x}_{n-1} \left\langle \mathbf{x}\right| e^{-i\hat{H}\Delta t}\left|\mathbf{x}_{n-1}\right\rangle \dots \\ &\qquad\qquad \times \left\langle \mathbf{x}_1\right| e^{-i\hat{H}\Delta t}\left|\mathbf{x}'\right\rangle , \\ &= \lim_{n\to\infty}\int_{-\infty}^{\infty}\left(\prod_{j=1}^{n-1} d^3\mathbf{x}_j\right)\left\langle \mathbf{x}\right| e^{-i\hat{H}\Delta t}\left|\mathbf{x}_{n-1}\right\rangle \dots \\ &\qquad\qquad \times \left\langle \mathbf{x}_1\right| e^{-i\hat{H}\Delta t}\left|\mathbf{x}'\right\rangle . \end{aligned} \tag{1.11}$$

Considering now the simplest example of a particle in three dimensions whose dynamics is given by the Hamiltonian

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + \hat{V}(\mathbf{x}) , \tag{1.12}$$

each bra-ket factor on the R.H.S. of Eq. (1.11) becomes

$$\left\langle \mathbf{x}_{j+1}\right| e^{-i(\hat{H}\Delta t)}\left|\mathbf{x}_j\right\rangle = \left\langle \mathbf{x}_{j+1}\right| e^{-i\hat{T}\Delta t}\left|\mathbf{x}_j\right\rangle e^{-i\hat{V}(\mathbf{x}_j)\Delta t} . \tag{1.13}$$

The first term on the R.H.S. has been obtained in Ref. [17], and we directly use the result to arrive at the expression for the individual transition amplitudes

$$\left\langle \mathbf{x}_{j+1}\right| e^{-i(\hat{H}\Delta t)}\left|\mathbf{x}_j\right\rangle = \left(\sqrt{\frac{m}{2\pi i\Delta t}}\right)^3 \exp\left[i\left(\frac{m}{2}\frac{(\mathbf{x}_{j+1}-\mathbf{x}_j)}{\Delta t} - \hat{V}(\mathbf{x}_j)\Delta t\right)\right] . \tag{1.14}$$

Combining these individual factors, the expression for the complete transition amplitude for the particle in three dimentions is obtained as

$$K(\mathbf{x},t;\mathbf{x}',0) = \lim_{n\to\infty}\left(\sqrt{\frac{m}{2\pi i\Delta t}}\right)^{3n}\int_{-\infty}^{\infty}\prod_{j=1}^{n-1}d^3\mathbf{x}_j \\ \times\exp\left[i\sum_{j=0}^{n-1}\left(\frac{m}{2}\frac{(\mathbf{x}_{j+1}-\mathbf{x}_j)}{\Delta t}-\hat{V}(\mathbf{x}_j)\right)\Delta t\right]. \tag{1.15}$$

where, from the limits of the summation in the exponential on the R.H.S., $\mathbf{x}_0 = \mathbf{x}'$ and $\mathbf{x}_n = \mathbf{x}$.

The Lagrangian is explicitly defined in Eq. (1.15), and is obtained as (here we have dropped the operator notation)

$$L = \frac{m}{2}\dot{\mathbf{x}}^2 - V(\mathbf{x})\,, \tag{1.16}$$

where $\dot{\mathbf{x}} = \frac{(\mathbf{x}_{j+1}-\mathbf{x}_j)}{\Delta t}$. This leads us to the action term which appears as the summation term in the exponent in Eq. (1.15)

$$\mathcal{S}[\mathbf{x}] = \int_0^t dt'\left(\frac{m}{2}\dot{\mathbf{x}}^2 - V(\mathbf{x})\right). \tag{1.17}$$

Eq. (1.15) can thus be written in a more intuitive form, in terms of the discretized classical action pertaining to all paths satisfying the boundary condition $\mathbf{x}_0 = \mathbf{x}(0) = \mathbf{x}'$ and $\mathbf{x}_n = \mathbf{x}(t) = \mathbf{x}$, as

$$K(\mathbf{x},t;\mathbf{x}',0) = \mathcal{N}\int\mathcal{D}\mathbf{x}\,e^{i\mathcal{S}[\mathbf{x}(t')]}\,, \tag{1.18}$$

where the integration measure $\mathcal{D}\mathbf{x}$ is given as

$$\mathcal{D}\mathbf{x} = \lim_{n\to\infty}\prod_{j=1}^{n-1}d^3\mathbf{x}_j\,, \tag{1.19}$$

and the normalization constant is

$$\mathcal{N} = \lim_{n\to\infty}\left(\sqrt{\frac{m}{2\pi i\Delta t}}\right)^{3n}. \tag{1.20}$$

With this, we arrive at the path integral formulation of quantum mechanics, where the quantum mechanical transition amplitude is determined in terms of the discretized classical action for each transition path, each path differing from the other by a phase $e^{i\mathcal{S}[\mathbf{x}(t')]}$.

1.2 Extending to field theory

In quantum field theory, the quantum mechanical transition amplitude has an analogous form, the Green's functions. These encode all the relevant information about the system's dynamics, from scattering amplitudes to transition widths and decay rates, and hence play a pivotal role in the study of field theoretic processes. In field theory, the Green's functions are represented as vacuum expectation values of time-ordered field operators [89]. We ease into the functional integral representation of the Green's function by first deriving its quantum mechanical counterpart.

Rewriting the quantum mechanical transition amplitude in Eq. (1.5) in the Heisenberg picture

$$K(\mathbf{x},t;\mathbf{x}',0) = \langle \mathbf{x}|\, e^{-i\hat{H}t}\, |\mathbf{x}'\rangle = \langle \mathbf{x},t|\mathbf{x}',0\rangle \ . \tag{1.21}$$

We are interested in deriving the two-point correlation function for field theory. For this purpose, we first look at a similar quantity in qunatum mechanical terms. The analogous quantity in quantum mechanics is given as

$$\langle \mathbf{x},t|\, \mathrm{T}\hat{\mathbf{x}}(t_1)\hat{\mathbf{x}}(t_2)\, |\mathbf{x}',0\rangle \ , \tag{1.22}$$

with T being the usual time-ordering operator, and it represents the Eq. (1.6) with the insertion of two intermediate points at times t_1 and t_2, where $\hat{\mathbf{x}}$ is the position operator in the Heisenberg picture. Considering $t_1 > t_2$, we can write Eq. (1.22) in terms of complete set of states [89],

$$\begin{aligned}\langle \mathbf{x},t|\, \mathrm{T}\hat{\mathbf{x}}(t_1)\hat{\mathbf{x}}(t_2)\, |\mathbf{x}',0\rangle &= \langle \mathbf{x},t|\, \hat{\mathbf{x}}(t_1)\hat{\mathbf{x}}(t_2)\, |\mathbf{x}',0\rangle \\ &= \langle \mathbf{x}|\, e^{-i\hat{H}(t-t_1)}\hat{\mathbf{x}}_s e^{-i\hat{H}(t_1-t_2)}\hat{\mathbf{x}}_s e^{-i\hat{H}t_2}\, |\mathbf{x}'\rangle \ ,\end{aligned} \tag{1.23}$$

where $\hat{\mathbf{x}}_s$ is the position operator in the Schrödinger picture; the equivalence between the Heisenberg and the Schrödinger representation given is by $\hat{\mathbf{x}}(t) = e^{i\hat{H}t}\hat{\mathbf{x}}_s e^{-i\hat{H}t}$.

Using now the completeness relation for a continuous basis $\int d^3\mathbf{x}\ |\mathbf{x}\rangle\langle\mathbf{x}| = \mathbf{1}$ and $\hat{\mathbf{x}}\,|\mathbf{x}\rangle = \mathbf{x}\,|\mathbf{x}\rangle$, the expression in Eq. (1.23) becomes

$$\begin{aligned}\langle \mathbf{x},t|\, \mathrm{T}\hat{\mathbf{x}}(t_1)\hat{\mathbf{x}}(t_2)\, |\mathbf{x}',0\rangle = \int d^3\mathbf{x}_1 d^3\mathbf{x}_2\, \mathbf{x}_1\mathbf{x}_2\ &\langle \mathbf{x}|\, e^{-i\hat{H}(t-t_1)}\, |\mathbf{x}_1\rangle \\ &\times \langle \mathbf{x}_1|\, e^{-i\hat{H}(t_1-t_2)}\, |\mathbf{x}_2\rangle\, \langle \mathbf{x}_2|\, e^{-i\hat{H}t_2}\, |\mathbf{x}'\rangle \ .\end{aligned} \tag{1.24}$$

The resemblance of the R.H.S. of Eq. (1.6) to the R.H.S. of the above equation already establishes the functional integral formulation of the two-point function implicitly. We now try to explicate this. As seen in Eq. (1.24), each bra-ket factor of the integrand on the R.H.S. are individual transition amplitudes of the form of Eq. (1.5). Thus, Eq. (1.24) can be written, by implementing Eq. (1.18), in terms of path integrals as

$$\begin{aligned}\langle \mathbf{x},t|\, \mathrm{T}\hat{\mathbf{x}}(t_1)\hat{\mathbf{x}}(t_2)\, |\mathbf{x}',0\rangle = \int d^3\mathbf{x}_1 d^3\mathbf{x}_2\, \mathbf{x}_1\mathbf{x}_2 \int_{\mathbf{x}_1,t_1}^{\mathbf{x},t} \mathcal{D}\mathbf{x}\, e^{i\mathcal{S}[\mathbf{x}]} \\ \times \int_{\mathbf{x}_2,t_2}^{\mathbf{x}_1,t_1} \mathcal{D}\mathbf{x}\, e^{i\mathcal{S}[\mathbf{x}]} \int_{\mathbf{x}',0}^{\mathbf{x}_2,t_2} \mathcal{D}\mathbf{x}\, e^{i\mathcal{S}[\mathbf{x}]} \ .\end{aligned} \tag{1.25}$$

The R.H.S. of Eq. (1.25) thus gives the amplitude of transition from the initial space-time point $(\mathbf{x}', 0)$ to the final point $(\mathbf{x}, t)$ while traversing through the two intermediate points at $(\mathbf{x}_2, t_2)$ and $(\mathbf{x}_1, t_1)$ over all possible paths. We now combine these three individual amplitudes into one single integral over all paths and for all times, and obtain the two-point function in the funtional integral form

$$\langle \mathbf{x}, t | \, \mathrm{T}\hat{\mathbf{x}}(t_1)\hat{\mathbf{x}}(t_2) \, |\mathbf{x}', 0\rangle = \int \mathcal{D}\mathbf{x} \, \mathbf{x}(t_1)\mathbf{x}(t_2) \, e^{i\mathcal{S}[\mathbf{x}]} \, . \tag{1.26}$$

We now make a generalization to fields by replacing the position operators by field operators in the two-point correlation function. Following the work of Peskin and Schröder [89], we derive the correlation function in terms of functional integrals, going in a backward fashion starting from Eq. (1.26); however, we first work with the free theory where the vacuum state denoted by $|0\rangle$, unlike [89] where the interacting theory has been used. Since we transition to field theory, we make use of relativistic notations of four vectors $x^\mu = (x^0, \mathbf{x})$, x^0 denoting the time coordinate, which we write in the usual notation t in this Section.

The two-point correlation function for a field ϕ, in functional integral form, in analogy to the R.H.S. of Eq. (1.26), can be written as

$$\int \mathcal{D}\phi(x) \, \phi(x_1)\phi(x_2) \, e^{i\mathcal{S}[\phi]} = \int \mathcal{D}\phi(x) \, \phi(x_1)\phi(x_2) \, \exp\biggl(i \int_{t_i}^{t_f} d^4x \, \mathcal{L}(\phi) \biggr) \, , \tag{1.27}$$

where the system is evolving under the Lagrangian density $\mathcal{L}$, from the field point $\phi(t_i, \mathbf{x}) = \phi_i(\mathbf{x})$ to $\phi(t_f, \mathbf{x}) = \phi_f(\mathbf{x})$.

As in Eq. (1.25), we can represent the integration measure on the R.H.S. of the above equation with the insertion of intermediate field points and constrain the path at two additional times t_1 and t_2. Since we are treating the time coordinate separately and integrating over the field configurations, $\phi_1(\mathbf{x})$ and $\phi_2(\mathbf{x})$, at these time points, the fields $\phi(x_1)$ and $\phi(x_2)$ can be written simply in terms of the space coordinates $\phi_1(\mathbf{x}_1)$ and $\phi_2(\mathbf{x}_2)$ at the intermediate times t_1 and t_2. We also decompose the main integral into individual transition amplitudes $\langle \phi_f(\mathbf{x}) | \, e^{-i\hat{H}(t_f - t_i)} \, |\phi_i(\mathbf{x})\rangle = \int \mathcal{D}\phi \, \exp\bigl(i \int_{t_i}^{t_f} d^4x \, \mathcal{L} \bigr)$ [89] to obtain in analogy with Eq. (1.24), for $t_1 > t_2$

$$\begin{aligned} \int \mathcal{D}\phi_1(\mathbf{x}) \int \mathcal{D}\phi_2(\mathbf{x}) \, \phi_1(\mathbf{x}_1)\phi_2(\mathbf{x}_2) \\ \times \langle \phi_f | \, e^{-i\hat{H}(t_f - t_1)} \, |\phi_1\rangle \, \langle \phi_1 | \, e^{-i\hat{H}(t_1 - t_2)} \, |\phi_2\rangle \, \langle \phi_2 | \, e^{-i\hat{H}(t_2 - t_i)} \, |\phi_i\rangle \end{aligned} \tag{1.28}$$

Now, making use of the completeness relation and inserting complete sets by converting the fields into Schrödinger-picture operator using $\hat{\phi}_s(\mathbf{x}) \, |\phi\rangle = \phi(\mathbf{x}) \, |\phi\rangle$ [89], we arrive at the expression

$$\langle \phi_f | \, e^{-i\hat{H}(t_f - t_1)} \hat{\phi_s}(\mathbf{x}_1) e^{-i\hat{H}(t_1 - t_2)} \hat{\phi}_s(\mathbf{x}_2) e^{-i\hat{H}(t_2 - t_i)} \, |\phi_i\rangle \, , \tag{1.29}$$

which is analogous to Eq. (1.23). We can now simply replace the Schrödinger operators by the corresponding operators in the Heisenberg picture and Eq. (1.27) becomes [89]

$$\int \mathcal{D}\phi(x)\,\phi(x_1)\phi(x_2)\,\exp\left(i\int_{t_i}^{t_f} d^4x\,\mathcal{L}(\phi)\right) = \langle\phi_f|\,e^{-i\hat{H}t_f}\mathrm{T}\{\hat{\phi}(x_1)\hat{\phi}(x_2)\}e^{i\hat{H}t_i}\,|\phi_i\rangle \tag{1.30}$$

To obtain the exact correlation function, we now decouple the states $|\phi_i\rangle$ and $|\phi_f\rangle$ from the vacuum state $|0\rangle$ by taking the limit $t_{f,i} \to \pm\infty(1-i\varepsilon)$ [89], which ensures that the vacuum state decays the slowest. This simple manipulation of the real time variable by sending it in a "slightly imaginary direction" [89] introduces the Feynman $+i\varepsilon$ prescription into the momentum space propagators to ensure causality. There are also other methodologies to introduce the Feynman prescription, e.g., by taking the limit $t \to \infty$, followed by the use of the Riemann-Lebesgue lemma [92] according to which the oscillatory terms vanish at infinty. The former formalism was used by Peskin and Schröder and since we follow their work, we use the same formalism. With this we arrive at the expression for the two-point correlation function given as

$$\langle 0|\,\mathrm{T}\hat{\phi}(x_1)\hat{\phi}(x_2)\,|0\rangle = \lim_{t_{f,i}\to\pm\infty(1-i\varepsilon)} \frac{\int \mathcal{D}\phi\,\phi(x_1)\phi(x_2)\,\exp\left(i\int_{t_i}^{t_f} d^4x\,\mathcal{L}(\phi)\right)}{\int \mathcal{D}\phi\,\exp\left(i\int_{t_i}^{t_f} d^4x\,\mathcal{L}(\phi)\right)}\,, \tag{1.31}$$

where the term in the denominator is introduced to eliminate the phase and overlap factors that arise due to the overlap of the vacuum state with the states $|\phi_i\rangle$ and $|\phi_f\rangle$ [89].

Eq. (1.31) is thus the functional integral representation of the correlation function or the two-point Green's function. This is a general formula and can be used to derive correlation functions for various field theoretic models. In case of non-interacting theories, the integrals are just simple Gaussian integrals that can be calculated albeit the fact that they involve derivatives of fields and Fourier transforms [89] which can be cumbersome to evaluate for higher-order correlation functions. In order to further generalize and simplify this formalism, we introduce *generating functionals* of the fields into the theory.

The generating functional is defined as

$$Z[J] = \int \mathcal{D}\phi\,\exp(i\mathcal{S}[\phi] + i\mathcal{S}_E)\,, \tag{1.32}$$

where, $\mathcal{S}[\phi] = \int d^4x\,\mathcal{L}$ is the action defined in terms of the Lagrangian density $\mathcal{L}$, and $\mathcal{S}_E = \int d^4x\,\phi(x)J(x)$, denotes the action due to the external source field, $J(x)$. The source field, according to Schwinger's formulation, acts as a background field which when coupled to the original field, leads to the creation and annihilation of particles.

As a general property of *functional derivatives*, a derivative of the source action w.r.t. the source field $J(x)$ produces the original field $\phi(x)$ [89],

$$\frac{\delta}{\delta J(x)}\mathcal{S}_E = \frac{\delta}{\delta J(x)}\int d^4y\,\phi(y)J(y) = \int d^4(y)\,\delta^4(x-y)\phi(y) = \phi(x)\,, \tag{1.33}$$

where $\delta^4(x-y)$ is a four-dimensional Dirac delta function. This leaves the action term in the exponent of the generating functional unchanged. Following this very simple property, the two-point correlation function can now be obtained by taking a functional derivative of the generating functional in Eq. (1.32), twice [89]

$$\frac{-i\delta}{\delta J(x_1)}\frac{-i\delta}{\delta J(x_2)}Z[J] = \int \mathcal{D}\phi\, \phi(x_1)\phi(x_2)\, \exp(i\mathcal{S}[\phi] + i\mathcal{S}_E)\,. \tag{1.34}$$

The R.H.S. of Eq. (1.34) is the numerator of Eq. (1.31) without the source term. In order to obtain the two-point correlation function, we set the source term $J(x)$ to zero and after normalization obtain,

$$\langle 0|\, \mathrm{T}\hat{\phi}(x_1)\hat{\phi}(x_2)\,|0\rangle = \frac{1}{Z_0}\left[\frac{-i\delta}{\delta J(x_1)}\frac{-i\delta}{\delta J(x_2)}Z[J]\right]\Bigg|_{J=0}, \tag{1.35}$$

where $Z_0 = Z[J=0]$. In order to calculate n-point correlation functions, we insert n functional derivatives, such that the n-point Green's function looks like

$$\langle 0|\, \mathrm{T}\hat{\phi}(x_1)\ldots\hat{\phi}(x_n)\,|0\rangle = \frac{1}{Z_0}\left[\frac{(-i)^n\delta^n Z[J]}{\delta J(x_1)\ldots\delta J(x_n)}\right]\Bigg|_{J=0}. \tag{1.36}$$

The normalization constant is chosen such that $Z_0 = Z[J=0] = \langle 0|0\rangle = 1$. This gives us the n-point Green's function in the form

$$G^n(x_1\ldots x_n) = \frac{(-i)^n\delta^n Z[J]}{\delta J(x_1)\ldots\delta J(x_n)}\Bigg|_{J=0}. \tag{1.37}$$

This expression brings us to the functional integral representation of the most important entity of a field-theoretic model, the Green's function. We can now exploit Eq. (1.37) to derive the propagators for Feynman diagrams by simply defining a proper expression for the generating functional from the Lagrangian density of the system. The functional integral formalism thus gives us a very simple yet elegant mathematical pathway to extract the physical information stored in a system, and we further develop this formalism to study QED in the bound state.

2. Mathematical and numerical tools

2.1 A primer on Grassmann techniques for fermion fields

In the language of second (canonical) quantization, the fields are treated as field operators. In this treatment, the fermionic field operators, unlike their bosonic counterparts, obey the property of anti-commutation. As such, creation and annihilation of fermionic and antifermionic states are described by the creation and annihilation operators, which too obey anti-commutation relations in order to satisfy spin statistics. This comes directly as a requirement of the Pauli exclusion principle. Naturally, to define such anticommuting field operators it would be useful to represent them in terms of anti-commuting numbers. This brings us to the concept of Grassmann variables which are simple classical numbers but satisfy anti-commutation relations [5].

Spin is a well-defined entity in the canonical quantization formalism, but when it comes to the 'classical' functional integral method, 'quantum' spin is an alien quantity. Grassmann numbers serve as a mathematical tool that enables the successful inclusion of spin in the functional integral formalism, as a classical limit of the fermionic fields. The physical interpretation of Grassmann numbers would be as classical numbers that are analogous to the fermionic creation and annihilation operators, which encode the information of the fermion spins and anti-commute with each other as well as all other fermionic operators [5].

This Section gives a brief overview on Grassmann numbers and a few techniques of Grassmann algebra, required for the quantization of the Dirac field, as described in [89].

We define two anti-commuting Grassmann numbers, η and $\bar{\eta}$, such that

$$\eta\bar{\eta} = -\bar{\eta}\eta\,. \tag{2.1}$$

Since a Grassmann number also anti-commutes with itself, we have

$$\eta^2 = 0\,. \tag{2.2}$$

Grassmann numbers behave like ordinary numbers and addition of two Grassmann numbers or a scalar multiplication involving Grassmann numbers have the same properties as of these operations on an ordinary vector space [89]. An analytical function of Grassmann numbers, $f(\eta)$, like ordinary complex numbers, can be Taylor expanded

$$f(\eta) = f_0 + f_1\eta + f_2\eta^2 + \dots\,, \tag{2.3}$$

however, owing to Eq. (2.2), the series terminates after the second term which makes Eq. (2.3) a linear function. This smiplifies single-variable Grassmann algebra, particulary integrals over functions of single Grassmann variables. The application of functional integral methods to field theory requires translational invariance of the integrals. This was established by F. A. Berezin [20, 93] through the introduction of *Berezin integrals*. Berezin integrals have the following properties :

- the integral over a total derivative is zero

$$\int d\eta \, \frac{d}{d\eta} f(\eta) = 0 \,, \tag{2.4}$$

- the integral is invariant under a shift $\eta \to \eta + \phi$ [89], i.e.,

$$\begin{aligned} \int d\eta \, f(\eta + \phi) &= \int d\eta \, f(\eta) \\ &= \int d\eta \, f_0 + f_1 \eta + f_1 \phi \\ &= \int d\eta \, f(\eta) + f_1 \phi \int d\eta \,, \end{aligned} \tag{2.5}$$

  for the property of invariance to hold the second term on the R.H.S. of the above equation should vanish,

- thus, this brings us to another important property of Berezin integrals

$$\int d\eta = 0 \,. \tag{2.6}$$

- Owing to the above property, we have

$$\begin{aligned} \int d\eta \, f(\eta + \phi) &= \int d\eta (f_0 + f_1 \eta) \\ &= f_0 \int d\eta + f_1 \int d\eta \, \eta \,, \end{aligned} \tag{2.7}$$

  following Berezin's convention, $\int d\eta \, \eta = 1$.

- Finally, we define the Berezin integral as

$$\int d\eta (f_0 + f_1 \eta) = f_1 \,. \tag{2.8}$$

We now generalize the theory of Grassmann variables, to complex Grassmann numbers, to accommodate the fermion field [89]. For Grassmann algebra with complex generators, we can define the usual complex conjugates as

$$(\eta\bar{\eta})^* \equiv \bar{\eta}^* \eta^* = -\eta^* \bar{\eta}^* \,, \tag{2.9}$$

also, the Grassmann number η and its complex conjugate η^* act as individual generators for the algebra, and we can define a relation similar to Eq. (2.1)

$$\eta\eta^* = -\eta^*\eta = 0\,, \tag{2.10}$$

which leads to the relation [89]

$$\int d\eta^* d\eta(\eta\eta^*) = 1\,. \tag{2.11}$$

Since we are interested in functional integrals in the context of bound-state QED, where we mostly encounter spherical potentials, the functional integrals usually have a Gaussian form. Thus, we introduce the property of Gaussian integrals over fermionic Grassmann numbers according to [89]

$$\int d\boldsymbol{\eta}^* \int d\boldsymbol{\eta}\, \exp(-\boldsymbol{\eta}^* A\boldsymbol{\eta}) = \det(A)\,, \tag{2.12}$$

where, $\boldsymbol{\eta}^* A\boldsymbol{\eta} = \sum_{i,j=1}^{n} \eta_i^* A_{ij}\eta_j$ and $d\boldsymbol{\eta}^* d\boldsymbol{\eta} \equiv d\eta_1^* d\eta_1 \ldots d\eta_n^* d\eta_n \equiv \prod_{i=1}^{n} d\eta_i^* d\eta_i$. A is a $n \times n$ Hermitian matrix.

We now try to establish the property of Grassmann Gaussian integrals given in Eq. (2.12). Let us consider the simplest case of $n = 1$ such that A is a simple classical number. Expanding the exponential in a power series we obtain for the integral in Eq. (2.12) in the form

$$\int d\eta^* \int d\eta\, \exp(-\eta^* A\eta) = \int d\eta^* \int d\eta\, (1 + A\eta\eta^*)\,. \tag{2.13}$$

Owing to the relation (2.11) and the property (2.6), we can rewrite Eq. (2.13) as

$$\int d\eta^* \int d\eta\, \exp(-\eta^* A\eta) = A\,. \tag{2.14}$$

Considering now $n = 2$, such that A is now a 2×2 matrix, the exponential in the integrand of Eq. (2.12) is expanded as

$$\exp(-\boldsymbol{\eta}^* A\boldsymbol{\eta}) = 1 - \boldsymbol{\eta}^* A\boldsymbol{\eta} + \frac{1}{2!}(\boldsymbol{\eta}^* A\boldsymbol{\eta})^2\,, \tag{2.15}$$

where the the third term on the R.H.S. can be expanded as

$$\frac{1}{2!}(\boldsymbol{\eta}^* A\boldsymbol{\eta})^2 = \frac{1}{2!} A_{ij}A_{kl}\eta_i^*\eta_j\eta_k^*\eta_l = -\frac{1}{2!} A_{ij}A_{kl}\eta_j\eta_l\eta_i^*\eta_k^*\,. \tag{2.16}$$

Since Grassmann numbers are actually the basis elements of a vector space, we can deduce that [20]

$$\eta_j\eta_l = \epsilon_{jl}\eta_1\eta_2\,, \quad \text{and} \quad \eta_i^*\eta_k^* = \epsilon_{ik}\eta_1^*\eta_2^*\,, \tag{2.17}$$

where ϵ_{jl} and ϵ_{ik} are Levi-Civita symbols in two dimensions. We can therefore write Eq. 2.12 for $n = 2$, using Eq. (2.11), as

$$\int d\boldsymbol{\eta}^* \int d\boldsymbol{\eta} \, \exp(-\boldsymbol{\eta}^* A \boldsymbol{\eta}) = \frac{1}{2!} A_{ij} A_{kl} \epsilon_{jl} \epsilon_{ik} \, . \tag{2.18}$$

Considering the product of two Levi-Civita tensors $\epsilon_{jl}\epsilon_{ik} = \delta_{ji}\delta_{lk} - \delta_{jk}\delta_{li}$, the term on the R.H.S. simply becomes

$$\begin{aligned} \frac{1}{2!} A_{ij} A_{kl} \epsilon_{jl} \epsilon_{ik} &= \frac{1}{2} A_{11} A_{22} - \frac{1}{2} A_{12} A_{21} - \frac{1}{2} A_{21} A_{12} + \frac{1}{2} A_{22} A_{11} \\ &= A_{11} A_{22} - A_{12} A_{21} \\ &= \det(A) \, . \end{aligned} \tag{2.19}$$

Thus, the property holds for two sets of independent Grassmann numbers.

Now, if we introduce n independent Grassmann variables η, and their complex conjugates as another independent set, and expand the exponential in the integrand of Eq. (2.12), we obtain

$$\begin{aligned} &1 + \cdots + \frac{1}{n!} (\sum_{i,j=1}^{n} -\eta_i^* A_{ij} \eta_j)^n = \frac{1}{n!} (\sum_{i,j=1}^{n} -\eta_i^* A_{ij} \eta_j)^n \qquad (2.20) \\ &= \frac{(-1)^n}{n!} A_{i_1 j_1} A_{i_2 j_2} \ldots A_{i_n j_n} A_{i_n j_n} \eta_{i_1}^* \eta_{j_1} \eta_{i_2}^* \eta_{j_2} \ldots \eta_{i_n}^* \eta_{j_n} \\ &= \frac{(-1)^n}{n!} A_{i_1 j_1} A_{i_2 j_2} \ldots A_{i_n j_n} A_{i_n j_n} (-1)^{n(n+1)/2} \eta_{j_1} \ldots \eta_{j_n} \eta_{i_1}^* \ldots \eta_{i_n}^* \, . \end{aligned}$$

Implementing again the concept of $n-$dimensional Levi-Civita symbol for Grassmann numbers, we obtain

$$\eta_{j_1} \ldots \eta_{j_n} = \epsilon_{j_1, \ldots, j_n} \eta_1 \ldots \eta_n \, , \tag{2.21}$$

and for their complex conjugates

$$\eta_{i_1}^* \ldots \eta_{i_n}^* = (-1)^{n(n-1)/2} \epsilon_{j_1, \ldots, j_n} \eta_n^* \ldots \eta_1^* \, . \tag{2.22}$$

Using Eq. (2.21) and Eq. (2.22), and following the same procedure as in case the of $n = 2$, we finally obtain

$$\begin{aligned} \int d\boldsymbol{\eta}^* \int d\boldsymbol{\eta} \, \exp(-\boldsymbol{\eta}^* A \boldsymbol{\eta}) &= \frac{1}{n!} A_{i_1 j_1} A_{i_2 j_2} \ldots A_{i_n j_n} A_{i_n j_n} \epsilon_{j_1, \ldots, j_n} \epsilon_{j_1, \ldots, j_n} \\ &= \det(A) \, . \end{aligned} \tag{2.23}$$

This result could also be achieved by a basis change of the Grassmann variables, by unitary transformation, to diagonalize the matrix A and by proving that the integral remains invariant under a unitary transformation as shown in [89].

2.2 Faddeev-Popov Gauge-fixing technique

The requirement for fixing of a particular gauge orbit, which is a path along the gauge field with equivalent field configurations under a transformation, for field quantization comes from a particular Maxwell's law for classical electromagnetism, $\mathbf{B} = \boldsymbol{\nabla} \times \mathbf{A}$, where $\mathbf{A}$ is the magnetic vector potential. The requirement that $\mathbf{B}$ remains unchanged by a shift in the vector potential, called *gauge transformation*, $\mathbf{A}' = \mathbf{A} + \frac{1}{e}\boldsymbol{\nabla}\alpha$, imposes certain *gauge freedom*. A similar argument applies to the electric field as well, wherein a shift in the electric potential, or a gauge transformation, $V' = V - \frac{1}{e}\frac{\partial \alpha}{\partial t}$, leaves the field unaffected and ensures gauge freedom. [94].

The QED Lagrangian, without the presence of any sources, is defined by the free electromagnetic field

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \,, \tag{2.24}$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the field strength tensor, given in terms of the photon gauge field or the four-potential A_μ. As in the case of classical electromagnetism, *gauge freedom* applies to the photon field as well under the local gauge transformation

$$A^\alpha_\mu(x) = A_\mu(x) + \frac{1}{e}\partial_\mu \alpha(x) \,, \tag{2.25}$$

where $\alpha(x)$ is an arbitrary scalar field. This local gauge invariance results in an infinite choice of gauge fields for which the Eq. (2.25) holds. A direct consequence of this is that for every field configuration that we choose, there can be an infinite number of gauge fields with the same configuration. This will result in the generating functional in Eq. (1.32) to diverge because of the integration measure $\int \mathcal{D}A$, as we go over infinitely many equivalent configurations of A^α_μ. The Faddeev-Popov gauge-fixing technique, as the name suggests, tries to fix the gauge such that this overcounting of similar field configurations can be avoided and in turn regularize the functional integral. This technique is, however, used in the context of non-abelian fields and was implemented for the quantization of the Yang-Mills field. It can be extended to successfully describe abelian field theories, of which QED is an example.

We follow [95] and [96] and lay down the fundamentals of the Faddeev-Popov gauge-fixing method.
The usual generating functional is given as

$$Z = \int \mathcal{D}A \exp(i\mathcal{S}[A]) \,. \tag{2.26}$$

For a fixed gauge orbit where all field configurations are denoted by Eq. (2.25), we want to restrict the integral to a single unique field, A_μ, over each gauge orbit. Since the volume of the orbit is proportional to the integral [95] on the R.H.S. of Eq. (2.26), we can write [96]

$$Z = \int \mathcal{D}A^\alpha_\mu \exp\big(i\mathcal{S}[A^\alpha_\mu]\big) \sim \int \mathcal{D}A_\mu \exp(i\mathcal{S}[A_\mu]) \int \mathcal{D}\alpha \,, \tag{2.27}$$

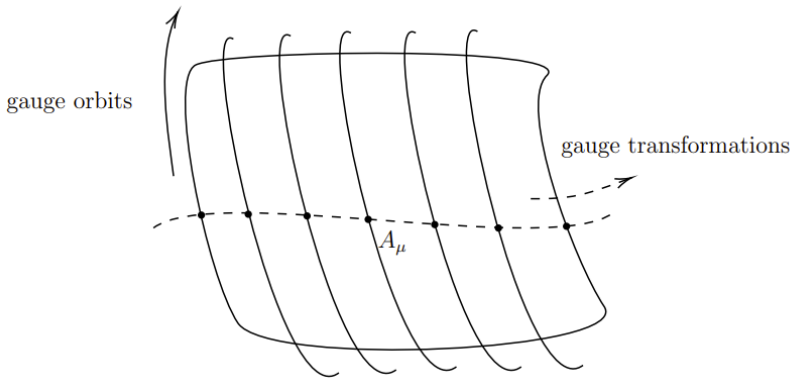

Figure 2.1: Diagrammatic representation of the gauge-fixing procedure. Gauge orbits represent the lines of similar field configurations under a gauge transformation. We pick out unique representative points along each such gauge orbit to fix the gauge.

where the integral over all gauge fields $\int \mathcal{D}A^\alpha_\mu$ is separated into a unique component and the component that introduces invariance through the scalar field α. To fix the gauge, we set up the condition that $F[A^\alpha_\mu] = 0$. If we apply the Lorenz gauge condition of QED, $\partial^\mu A^\alpha_\mu = 0$, the functional $F[A^\alpha_\mu]$ is given as $F = \partial^\mu A^\alpha_\mu$ [96]. We, however, work in a general gauge called the Feynman-'t Hooft-Landau gauge for which the gauge-fixing parameter, $\xi = 1$. The functional in this gauge is given as [96]

$$F = \partial^\mu A^\alpha_\mu + C(x)\,, \tag{2.28}$$

where $C(x)$ is any arbitrary functional, and the gauge-fixing condition becomes

$$F = \partial^\mu A^\alpha_\mu + C(x) = 0\,. \tag{2.29}$$

Employing now the Faddeev-Popov method of regularizing the integral in Eq. (2.27) by resolving it into an integral over the gauge orbits and a transverse plane [95], we enforce the condition from multivaribale calculus for an integral over a delta-function [95, 96]

$$\Delta_F[A^\alpha_\mu] \int \mathcal{D}\alpha\, \delta(F[A^\alpha_\mu]) = 1\,, \tag{2.30}$$

where $\Delta_F[A]$ is the Faddeev-Popov determinant which is defined by [96]

$$\Delta_F[A^\alpha_\mu] = \det\left(\frac{\delta F[A^\alpha_\mu]}{\delta\alpha}\right) \equiv \det(M)\,, \tag{2.31}$$

M being the Faddeev-Popov operator.

The generating functional in Eq. (2.27), in terms of the identity relation in Eq. (2.30), can now be written as

$$Z = \int \mathcal{D}A^\alpha_\mu\, \Delta_F[A^\alpha_\mu] \int \mathcal{D}\alpha\, \delta(F[A^\alpha_\mu]) e^{i\mathcal{S}[A^\alpha_\mu]}\,. \tag{2.32}$$

Now, we consider the gauge invariance of the action, the integration measure and the Faddeev-Popov determinant, and make the following replacements: $\mathcal{S}[A^{\alpha}_{\mu}] \rightarrow \mathcal{S}[A_{\mu}]$; $\int \mathcal{D}A^{\alpha}_{\mu} \rightarrow \int \mathcal{D}A_{\mu}$; $\Delta_F[A^{\alpha}_{\mu}] \rightarrow \Delta_F[A_{\mu}]$. We also consider the fact that with these replacements, the integrand no longer depends on the scalar field $\alpha(x)$, and the integration over $\alpha(x)$ yields a constant that is absorbed into the normalization factor. The Eq. (2.32) can thus be written as

$$Z = \int \mathcal{D}A_{\mu} \Delta_F[A_{\mu}]\, \delta(F[A_{\mu}]) e^{i\mathcal{S}[A_{\mu}]}\,. \tag{2.33}$$

We now evaluate the Faddeev-Popov determinant in terms of the gauge condition in Eq. (2.29). This gives

$$\Delta_F[A_{\mu}] = \det\left(\frac{\delta F[A^{\alpha}_{\mu}]}{\delta\alpha}\right) = \frac{1}{e}\Box\,, \tag{2.34}$$

where, $\Box = \partial^{\mu}\partial_{\mu}$ is the d'Alembertian. This makes the determinant independent of both A_{μ} and $\alpha(x)$, and we can pull it out of the integral. The functional now depends solely on the physically unique field configurations A_{μ} over every gauge orbit. As done in [96], $\Delta_F[A_{\mu}]$ can also be expressed in terms of the ghost fields. To implement this, we invoke the property of Gaussian integrals over Grassmann numbers given in Eq. (2.12), and simply replace the complex conjugates with Hermitian conjugates (since now we are working with fields). We thus have, by making the change $M \rightarrow iM$ [96],

$$\det(iM) = \int \mathcal{D}c^{\dagger}\, \mathcal{D}c \exp\left(-i \int c^{\dagger} M c\, d^4x\right), \tag{2.35}$$

where, c and $c^{\dagger}$ are the Faddeev Popov ghost fields (two anti-commuting Grassmannians), which represent unphysical particles and are only introduced for the purpose of gauge-fixing. In the case of QED, these fields decouple from the original gauge field and have no contribution.

We now want to introduce the gauge-fixing parameter into our generating functional and because the Faddeev-Popov determinant is independent of the function $C(x)$, which is again independent of A_{μ}, the generating functional does not depend on $C(x)$ and we can multiply it with any arbitrary factor which ultimately gets absorbed into the normalization constant [96]. To that effect our generating functional becomes

$$Z = \mathcal{N} \int \mathcal{D}A_{\mu} \mathcal{D}c^{\dagger}\, \mathcal{D}c\, e^{(-i\int c^{\dagger} M c\, d^4x)}\, \delta(\partial^{\mu}A_{\mu} + C(x))\, e^{(i\int \mathcal{L}\, d^4x)}\,. \tag{2.36}$$

We now multiply it with a factor [96]

$$\exp\left(-\frac{i}{2\xi}\int C^2(x)\, d^4x\right), \tag{2.37}$$

and impose the gauge-fixing condition which allows us to remove the delta function in the integrand on the R.H.S. of Eq. (2.36). We now have as the generating functional

$$Z = \mathcal{N} \int \mathcal{D}A_\mu \mathcal{D}c^\dagger \, \mathcal{D}c \, \exp\left\{ i \int \left(\mathcal{L} - \frac{1}{2\xi} C^2(x) - c^\dagger M c \right) d^4x \right\} \tag{2.38}$$
$$= \mathcal{N} \int \mathcal{D}A_\mu \mathcal{D}c^\dagger \, \mathcal{D}c \, \exp\left\{ i \int \left(\mathcal{L} - \frac{1}{2\xi} (\partial^\mu A_\mu)^2 - c^\dagger M c \right) d^4x \right\}.$$

Since the ghost fields decouple in QED, the final gauge-fixed QED generating functional is

$$Z = \int \mathcal{D}A \exp\left\{ i \int \left(\mathcal{L} - \frac{1}{2\xi} (\partial^\mu A_\mu)^2 \right) d^4x \right\}, \tag{2.39}$$

where $\int \mathcal{D}A$ gives the integration over all unique gauge fields A_μ over all gauge orbits. The gauge-fixed QED Lagrangian is thus,

$$\begin{aligned} \mathcal{L}_{\rm QED}^{\rm GF} &= \mathcal{L} - \mathcal{L}^{\rm GF} \\ &= \mathcal{L} - \frac{1}{2\xi} (\partial^\mu A_\mu)^2 \,, \end{aligned} \tag{2.40}$$

where $\mathcal{L}$ is the usual QED Lagrangian [89].

The generating functional in Eq. (2.38) is a general expression and can be used to quantize both abelian and non-abelian field theories. The ghost terms appear only in the case of non-abelian fields since they couple with the gauge fields of non-abelian theories, which are considered to be 'charged'.

2.3 B-splines

The entire theory of quantum electrodynamics in particular, and atomic theory in general, is based on the solution of the Dirac equation in the presence of a static nuclear field. Calculations in relativistic atomic theory, as we will see in the succeeding Chapters, require the construction of numerical wave functions to evaluate infinite sums over the entire spectrum consisting of both bound states and continuum states, that comprise of negative- and positive-energy states. For a single-particle system, in the lowest order of perturbation theory, in the non-relativistic case, such single sums over intermediate states could, in principle, be analytically obtained by using techniques of differential equations [97]; but even in such cases, as we move to the evaluation of higher-order terms, multiple sums over intermediate states are encountered which become relatively difficult to solve using partial differential equations, even numerically [97, 98]. In the relativistic case of QED, the presence of the negative-energy continuum, besides the positive-energy continuum and bound states complicate the problem further since the direct approach invariably leads to remainders which need to be extrapolated and result in numerical inaccuracies [99].

In order to increase the computational efficiency and accuracy of the evaluation of such sums, a numerical approximation of the radial wavefunction, obtained as the solution of the stationary Dirac equation, is given in terms of a basis set of spline functions. The basis set construction is performed by containing the system in a spherical cavity of radius $R_{\rm cav}$ with appropriate boundary conditions, given by the MIT *bag model* [100]. The confinement in the cavity, the size of which is so chosen that it is large but finite, modifies the original spectrum by discretizing the continuum states into two infinite but discrete spectra of negative and positive energies. This modified spectrum is then approximated by the implementation of a finite basis set [97]. A static, spherically symmetric potential is chosen to reduce the limitations that the choice of potential might inflict on the overall accuracy of the B-spline algorithm.

For the solution of the Dirac equation in the presence of an external central potential, $V(\mathrm{r})$, a separation ansatz is proposed [101]

$$\psi(\mathbf{r}) = \frac{1}{\mathrm{r}} \begin{pmatrix} g(\mathrm{r})\chi_\kappa^\mu(\hat{\mathbf{r}}) \\ \\ if(\mathrm{r})\chi_{-\kappa}^\mu(\hat{\mathbf{r}}) \end{pmatrix} , \tag{2.41}$$

where we represent the magnetic quantum number as μ and $\kappa = (-1)^{j+l+\frac{1}{2}}(j+1/2)$, l being the orbital angular momentum quantum number and $j = l \pm 1/2$ the total angular momentum quantum number, is the eigenvalue of the Dirac operator $\hat{K} = \beta(\hat{\boldsymbol{\Sigma}} \cdot \hat{\boldsymbol{L}} + 1)$, and $\hat{\mathbf{r}} = \mathbf{r}/\mathrm{r}$. The angular wave functions χ_κ^μ are the two-component spherical spinors given as [101, 102]

$$\chi_\kappa^\mu = \sum_{\mu'=\pm\frac{1}{2}} C\left(l\,, \frac{1}{2}\,, j; \mu-\mu'\,, \mu'\,, \mu\right) Y_l^{\mu-\mu'}(\theta,\phi)\chi_{\frac{1}{2}}^{\mu'}\,.$$

Here the $Y_l^{\mu-\mu'}$ are the spherical harmonics and the two-component spinors $\chi_{\frac{1}{2}}^{\mu'}$ have the form

$$\chi_{\frac{1}{2}}^{\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \quad \chi_{\frac{1}{2}}^{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} ,$$

and all other quantities and functions have their usual meaning. For a detailed derivation of Eq. (2.41) and definition of all other related functions we refer to [101].

Using the definitions

$$G = \mathrm{r}g \quad \text{and} \quad F = \mathrm{r}f\,,$$

we obtain a set of ordinary differential equations [101]

$$G'(\mathrm{r}) + \frac{\kappa}{\mathrm{r}}G(\mathrm{r}) - [\epsilon + m - V(\mathrm{r})]F(\mathrm{r}) = 0\,, \tag{2.42}$$

$$F'(\mathrm{r}) - \frac{\kappa}{\mathrm{r}}F(\mathrm{r}) + [\epsilon - m - V(\mathrm{r})]G(\mathrm{r}) = 0\,, \tag{2.43}$$

m being the mass of the elementary Dirac particle, which in our case is the electron, and ϵ is the energy eigenvalue.

The radial Dirac equation can be written in terms of the radial wave functions $G(\mathrm{r})$ and $F(\mathrm{r})$ in matrix format as

$$\begin{pmatrix} V(\mathrm{r}) + m & \frac{\kappa}{\mathrm{r}} - \frac{d}{d\mathrm{r}} \\ \frac{\kappa}{\mathrm{r}} + \frac{d}{d\mathrm{r}} & V(\mathrm{r}) - m \end{pmatrix} \begin{pmatrix} G(\mathrm{r}) \\ F(\mathrm{r}) \end{pmatrix} = \epsilon \begin{pmatrix} G(\mathrm{r}) \\ F(\mathrm{r}) \end{pmatrix} . \tag{2.44}$$

The spectrum that is obtained by solving Eq. (2.44) contains bound states that have discrete eigenvalues for $0 < \epsilon < m$, and the continuum states with energy eigenvalues in the regions $\epsilon < -m$ and $\epsilon > m$. The solution for the discrete bound states is represented as

$$\psi_{n\kappa\mu}(\mathbf{r}) = \frac{1}{\mathrm{r}} \begin{pmatrix} G_{n\kappa}(\mathrm{r})\chi^{\mu}_{\kappa}(\hat{\mathbf{r}}) \\ iF_{n\kappa}(\mathrm{r})\chi^{\mu}_{-\kappa}(\hat{\mathbf{r}}) \end{pmatrix} , \tag{2.45}$$

the additional label n being the principal quantum number of the state. The continuum states take real-valued energy eigenvalues.

For a point-like nucleus with charge number Z, the potential given in terms of the fine-structure constant α is, $V(\mathrm{r}) = -\frac{\alpha Z}{\mathrm{r}}$. For such a system the radial Dirac Eq. (2.44) can be solved analytically [101], and the energy spectrum is given as

$$\epsilon_{pt}(n\kappa) = m \left[1 + \frac{(\alpha Z)^2}{\left(n - |\kappa| + \sqrt{\kappa^2 - (\alpha Z)^2} \right)^2} \right] . \tag{2.46}$$

However, for precise practical calculations, the finite size of the nucleus needs to be taken into consideration. For such an extended nuclear model, numerical techniques are required to solve the radial Dirac equation and this is where the method of B-splines becomes applicable.

Following Ref. [85] we now proceed with the construction of the basis set that approximates our wave function. The radial Dirac Eq. (2.44) can be written in the form

$$H_{\kappa}\phi = \epsilon\phi \, , \tag{2.47}$$

where

$$\phi = \begin{pmatrix} G(\mathrm{r}) \\ F(\mathrm{r}) \end{pmatrix} , \tag{2.48}$$

is the two-component vector of the radial wave functions. This function ϕ is expanded in a basis set of $2N$ basis functions over the defined cavity and an approximation of the modified spectrum is obtained. This expansion is given as

$$\phi(\mathrm{r}) = \sum_{i=1}^{2N} c_i \, u_i(\mathrm{r}) \, . \tag{2.49}$$

For the construction of the basis set comprising of the radial wave functions, $G(\mathrm{r})$ and $F(\mathrm{r})$, B-spline functions are used. An efficient choice for the approximation scheme of the modified spectrum of the Dirac equation was the use of piecewise polynomials to construct the splines [97, 103]. The basis set is constructed systematically in terms of these spline functions of order k, each of which are piecewise polynomials of degree $k-1$, by dividing the cavity, defined in the interval $[0, R_{\mathrm{cav}}]$, into subsegments. Each of these subsegments have endpoints given by a *knot sequence*, t_i, $i = 1, 2, \ldots, N+k$, N being the number of B-splines defined in each subsegment. On this *knot sequence*, a spline function is defined recursively as [97, 103]

$$B_{i,1}(\mathrm{r}) = \begin{cases} 1, & \text{if } \; t_i \leq \mathrm{r} < t_{i+1} \\ 0, & \text{otherwise} \end{cases} \tag{2.50}$$

and

$$B_{i,k}(\mathrm{r}) = \frac{\mathrm{r} - t_i}{t_{i+k-1} - t_i} B_{i,k-1}(\mathrm{r}) + \frac{t_{i+k} - \mathrm{r}}{t_{i+k} - t_{i+1}} B_{i+1,k-1}(\mathrm{r}) \,, \tag{2.51}$$

where the function $B_{i,k}(\mathrm{r})$ exists only inside the interval $t_i \leq \mathrm{r} < t_{i+1}$ and outside this interval $B_{i,k}(\mathrm{r}) = 0$. At the endpoints of these intervals on which each single B-spline function is defined, the 'knots' have a given multiplicity, and at the endpoints, 0 and R_{cav}, of the main interval defining the cavity, these knots have k-fold multiplicity, k being the order of the B-splines. Thus, $t_1 = t_2 = \cdots = t_k = 0$ and $t_{N+1} = t_{N+2} = \cdots = t_{N+k} = R_{cav}$. These endpoints, or in general any endpoint, where the multiplicity of the knots is greater than 1, a limiting form of the recursion relations in Eqs. (2.50) and (2.51) is used [97, 103]. This set of B-splines in each of the subsegments, spanned by the *knot sequence* t_i, forms a complete set of basis functions that are then used to construct our basis functions u_i, as

$$u_i(\mathrm{r}) = \begin{pmatrix} B_{i,k}(\mathrm{r}) \\ 0 \end{pmatrix} \,, \; i = 1, \ldots, N \,, \tag{2.52}$$

$$u_i(\mathrm{r}) = \begin{pmatrix} 0 \\ B_{i-N,k}(\mathrm{r}) \end{pmatrix} \,, \; i = N+1, \ldots, 2N \,. \tag{2.53}$$

Provided that the basis functions u_i obey proper boundary conditions, we can construct an action term to represent the radial Dirac Eq. (2.47)

$$\mathcal{S} = \langle \phi | \, H_\kappa \, | \phi \rangle - \epsilon \, \langle \phi | \phi \rangle \,, \tag{2.54}$$

and a variation of this action reduces the radial Dirac equation from a differential one to a linear algebraic one, given by a $2N \times 2N$ symmetric generalized eigenvalue equation [85, 97, 99]

$$\boldsymbol{A} \cdot \boldsymbol{c} = \epsilon \boldsymbol{B} \cdot \boldsymbol{c} \,, \tag{2.55}$$

where $\boldsymbol{A}$ and $\boldsymbol{B}$ are $2N \times 2N$ symmetric matrices given by [85]

$$A_{ij} = \frac{\langle u_i | \, H_\kappa \, | u_j \rangle + \langle u_j | \, H_\kappa \, | u_i \rangle}{2} \,, \qquad B_{ij} = \langle u_i | u_j \rangle \,. \tag{2.56}$$

The eigenvalue Eq. (2.55) can now be solved for a given value of κ to obtain $2N$ energy eigenvalues $\epsilon_{n\kappa}$, the n denotes the index of intermediate states over which the summations are carried out, and it runs over the entire modified spectrum, i.e., $n = 1, \ldots, 2N$. Of the $2N$ energy eigenvalues that are obtained, the first N eigenvalues approximate the negative-energy eigenstates and the eigenvalues from $N+1$ to $2N$ represent the positive-energy eigenstates comprising of both the bound states and the positive continuum. We also obtain the vector $\boldsymbol{c}$ as a set of $2N$ coefficients, $\boldsymbol{c} = \{c_1, \ldots, c_N; c_{N+1}, \ldots, c_{2N}\}$. It was also observed that the implementation of B-splines to approximate the radial wave functions in the basis defined by Eqs. (2.52) and (2.53) leads to rapidly oscillating spurious states which, although do not affect the numerical procedures, disturb the spectrum and may lead to convergence issues [85]. This was addressed in the referenced paper by the introduction of the dual-kinetically-balanced basis set [85]. In this approach, the basis functions are represented as

$$u_i(\mathrm{r}) = \begin{pmatrix} B_{i,k}(\mathrm{r}) \\ \\ \frac{1}{2m}\left(\frac{d}{d\mathrm{r}} + \frac{\kappa}{\mathrm{r}}\right) B_{i,k}(\mathrm{r}) \end{pmatrix} , \; i = 1, \ldots, N \, , \tag{2.57}$$

$$u_i(\mathrm{r}) = \begin{pmatrix} \frac{1}{2m}\left(\frac{d}{d\mathrm{r}} - \frac{\kappa}{\mathrm{r}}\right) B_{i-N,k}(\mathrm{r}) \\ \\ B_{i-N,k}(\mathrm{r}) \end{pmatrix} , \; i = N+1, \ldots, 2N \, . \tag{2.58}$$

With this definition of the basis set in terms of the spline functions, any numerical calculation with the radial wave functions $G(\mathrm{r})$ and $F(\mathrm{r})$ can be simply relegated to calculations involving the basis functions $u_i(\mathrm{r})$ and the wave functions being represented by the coefficient vector $\boldsymbol{c}$.

All numerical evaluations in this Thesis are carried out following this algorithm of approximating the radial wave functions by B-spline basis set implemented in the dual-kinetic-balance approach. The numerics have been developed by Halil Cakir [87] and have been employed for the involved computations of the radiative corrections.

We now have the essential tools for constructing a well-defined and self-consistent functional integral method for the derivation of propagators, both free and bound, for the quantization of field theory in general, and QED in the scope of this Thesis. We visit in the next Chapter, the derivation of the free photon and electron propagator obtained using the tools developed in this Chapter.

3. The photon and the electron propagator

3.1 The photon propagator

To arrive at the photon propagator, we make use of the Faddeev-Popov gauge-fixing procedure that we summarized in Chapter 2. We begin this Section by showing why we need to gauge-fix the generating functional for the derivation of the photon propagator following Ref. [96].

We start with the QED Lagrangian density without the presence of any sources for just the free electromagnetic field

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \,, \tag{3.1}$$

where the usual electromagnetic field strength tensor is given as

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \,. \tag{3.2}$$

We now vary the Lagrangian in Eq. (3.1) w.r.t. the gauge field A^ν [96] to obtain Euler-Lagrange equations of motion, which gives us

$$\partial^\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial^\mu A^\nu)} \right) = \partial^\mu F_{\mu\nu} = \partial^\mu (\partial_\mu A_\nu - \partial_\nu A_\mu) = 0 \,, \tag{3.3}$$

$$(g^{\mu\nu}\partial^2 - \partial^\mu \partial^\nu) A_\mu = 0 \,. \tag{3.4}$$

The Eq. (3.4) is the inhomogeneous Maxwell's equation of the second kind. We can define a Green's function for this equation, which will be our photon propagator [96]

$$(g_{\mu\nu}\partial^2 - \partial_\mu \partial_\nu) D^{\nu\lambda}(x - y) = i\delta^\lambda_\mu \delta^4(x - y) \,, \tag{3.5}$$

where δ^λ_μ is the Kronecker delta and $\delta^4(x-y)$ is a four-dimensional Dirac delta function. Now, if we consider the fact that our gauge field is invariant under the transformation given in Eq. (2.25), the operator $(g_{\mu\nu}\partial^2 - \partial_\mu \partial_\nu)$, acting on acting on the gradient of the arbitrary scalar field $\alpha(x)$ of the four-potential, gives a zero value, i.e.,

$$(g_{\mu\nu}\partial^2 - \partial_\mu \partial_\nu)(\partial^\mu \alpha(x)) = (\partial_\nu \partial^2 - \partial^2 \partial_\nu)\alpha(x) = 0 \,. \tag{3.6}$$

This would mean that under the gauge transformation, $A^\mu(x) \to A^\mu(x) + \partial\alpha(x)$, the action of the operator would produce the same results for both field configurations, leaving us with no unique solution for the gauge field. Also, if we compare Eq. (3.6) to an eigenvalue equation, we see that the operator has zero eigenvalue which is only true when the operator has no inverse [96].

From Eq. (3.5), however, we see that the inverse of the operator $(g_{\mu\nu}\partial^2 - \partial_\mu\partial_\nu)$ is the photon propagator $D^{\nu\lambda}$, but from the argument that we obtain above, the inverse of the operator cannot physically exist and what we have is an unphysical result for the photon propagator. This is a direct consequence of gauge invariance and we can address this problem by fixing the gauge.

To this extent, we implement the gauge-fixing technique developed in the previous Chapter and we can now start from the gauge-fixed Lagrangian

$$\begin{aligned}\mathcal{L}^{\mathrm{GF}} &= \mathcal{L} - \frac{1}{2\xi}(\partial^\mu A_\mu)^2 \\ &= -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \frac{1}{2\xi}(\partial^\mu A_\mu)^2 \qquad (3.7)\\ &= \frac{1}{2}A_\mu\left[g^{\mu\nu}\partial^2 - \left(\frac{1}{\xi} - 1\right)\partial^\mu\partial^\nu\right]A_\nu \qquad (3.8)\end{aligned}$$

We can now redefine Eq. (3.5) for the Green's function

$$\left[g^{\mu\nu}\partial^2 - \left(\frac{1}{\xi} - 1\right)\partial^\mu\partial^\nu\right]D^{\nu\lambda}(x-y) = i\delta^\lambda_\mu\delta^4(x-y)\,, \qquad (3.9)$$

and represent the above equation in momentum space [96],

$$\left[-g^{\mu\nu}k^2 - \left(\frac{1}{\xi} - 1\right)k^\mu k^\nu\right]D^{\nu\lambda}(k) = i\delta^\lambda_\mu\mathbb{1}\,. \qquad (3.10)$$

The photon propagator is thus the inverse of the operator on the L.H.S of Eq. (3.10) and is given as [96]

$$D^{\mu\nu}(k) = -\frac{i}{k^2 + i\varepsilon}\left(g^{\mu\nu} + (\xi - 1)\frac{k^\mu k^\nu}{k^2}\right)\,, \qquad (3.11)$$

where the $i\varepsilon$ term in the denominator arises from the *Feynman prescription* of causal propagators, and the positive ε converges to zero from above in the final result [89].

The Eq. (3.11) thus gives us the photon propagator derived using techniques of functional differentiation. The gauge-fixing parameter ξ takes finite values and is equal to 0 for the Landau gauge and 1 for the Feynman gauge.

3.2 The electron propagator

The quantization of QED is based on the foundation of the free Dirac propagator. All the QED processes that we study in this Thesis and the processes that have been studied

in the illustrious history of QED, have as their building block the free propagator for the Dirac field. To derive this propagator, we simply begin with the free Lagrangian density of the Dirac field and proceed with the construction of the generating functional, whose functional derivative leads us to the desired propagator for Dirac fermions. We follow closely the work of Lewis H. Ryder [96] as we have done in the previous Section. We also exploit the formalism of Grassmann numbers developed in Section 2.1 to construct the generating functional.

The Lagrangian for the free Dirac field is written in the form

$$\mathcal{L} = \bar{\psi}(x)(i\gamma^\mu \partial_\mu - m)\psi(x)\,, \tag{3.12}$$

where we drop the a^* notation used in the context of Grassmann numbers to denote complex conjugates and replace them by $\bar{a}$, a being any arbitrary vector, such that $\bar{\psi} = \psi^\dagger\gamma^0$, $\psi^\dagger$ being the Hermitian conjugate of ψ. γ^μ are the Dirac gamma matrices. ψ and $\bar{\psi}$ are the Dirac fields representing the electron and the positron and are independent of each other dynamically which allows us to assign Grassmann-valued sources for each of these fields.

The Lagrangian now in terms of the source terms is given as

$$\mathcal{L} = \bar{\psi}(x)(i\gamma^\mu \partial_\mu - m)\psi(x) + \bar{\eta}(x)\psi(x) + \eta(x)\bar{\psi}(x)\,. \tag{3.13}$$

η represents the source term for the field $\bar{\psi}$ and $\bar{\eta}$ is the source term for the field ψ.

The generating funtional, written in terms of the Lagrangian defined in Eq. (3.13), is given as

$$Z[\eta,\bar{\eta}] = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \exp\left\{ i\int d^4x[\bar{\psi}(x)(i\gamma^\mu\partial_\mu - m)\psi(x) + \bar{\eta}(x)\psi(x) + \eta(x)\bar{\psi}(x)]\right\}. \tag{3.14}$$

The generating functional without the source terms is given as

$$Z_0[\eta,\bar{\eta}] = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \exp\left\{ i\int d^4x[\bar{\psi}(x)(i\gamma^\mu\partial_\mu - m)\psi(x)]\right\}. \tag{3.15}$$

We now define an operator [96]

$$S^{-1} = \delta^4(x-y)(i\gamma^\mu\partial_\mu - m)\,. \tag{3.16}$$

In terms of this operator, we rewrite the generating functional as [96]

$$Z[\eta,\bar{\eta}] = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \exp\left\{ i\int d^4x[\bar{\psi}(x)S^{-1}\psi(x) + \bar{\eta}(x)\psi(x) + \eta(x)\bar{\psi}(x)]\right\}. \tag{3.17}$$

The term in the exponential of the integrand in the above equation now has the form of the Lagrangian given in terms of the newly defined operator in Eq. (3.16). We can write down this new Lagrangian density as [96]

$$\mathcal{Q} = \bar{\psi}S^{-1}\psi + \bar{\eta}\psi + \eta\bar{\psi}\,. \tag{3.18}$$

We adopt the least action principle and minimise this Lagrangian w.r.t. the fields ψ and $\bar{\psi}$ [96],

$$\frac{\partial \mathcal{Q}}{\partial \psi} = \bar{\psi} S^{-1} + \bar{\eta} = 0\,, \quad \text{and} \quad \frac{\partial \mathcal{Q}}{\partial \bar{\psi}} = \psi S^{-1} + \eta = 0\,. \tag{3.19}$$

The fields for which the minimum of the Lagrangian is obtained are now given as [96]

$$\psi_{\min} = -S\eta\,, \quad \text{and} \quad \bar{\psi}_{\min} = -\bar{\eta} S\,. \tag{3.20}$$

The minimised Lagrangian in terms of these fields is given as [96]

$$\mathcal{Q} = (\bar{\psi} - \bar{\psi}_{\min}) S^{-1} (\psi - \psi_{\min}) - \bar{\eta} S \eta\,. \tag{3.21}$$

Rewriting the generating functional in terms of this Lagrangian, we have

$$\begin{aligned} Z[\eta, \bar{\eta}] = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \Bigg[\exp\left\{ -i \int d^4x d^4y [\bar{\eta}(x) S(x-y) \eta(y)] \right\} \\ \times \exp\left\{ i \int d^4x [(\bar{\psi} - \bar{\psi}_{\min}) S^{-1} (\psi - \psi_{\min})] \right\} \Bigg]\,. \end{aligned} \tag{3.22}$$

We can pull the first exponential term on the R.H.S. of Eq. (3.22) out of the integral since it is depends only on the sources and is a constant in the fields, while the integral over the second exponential term is a Berezin integral whose value, from Eq. (2.23), can be given simply by the determinant of the operator iS^{-1} [96]. The generating functional, with these modifications, becomes

$$Z[\eta, \bar{\eta}] = \exp\left\{ -i \int d^4x d^4y [\bar{\eta}(x) S(x-y) \eta(y)] \right\} \det\left(iS^{-1}\right)\,. \tag{3.23}$$

The two-point Green's function or the propagator is now given in terms of the functional derivative of the generating functional, as defined by Eq. (1.35), and has the form

$$\begin{aligned} &\frac{1}{Z_0} \frac{-i\delta^2}{\delta\eta(x)\delta\bar{\eta}(y)} \exp\left\{ -i \int d^4x d^4y [\bar{\eta}(x) S(x-y) \eta(y)] \right\} \det\left(iS^{-1}\right) \\ &\quad = \frac{\det(iS^{-1})}{Z_0} \frac{-i\delta^2}{\delta\eta(x)\delta\bar{\eta}(y)} \exp\left\{ -i \int d^4x d^4y [\bar{\eta}(x) S(x-y) \eta(y)] \right\}\,, \end{aligned} \tag{3.24}$$

where, since $\det(iS^{-1})$ is independent of the source terms, it is treated as a constant in the above derivative.

The functional $Z_0 = Z[\eta = \bar{\eta} = 0]$, which is the generating functional without the presence of any source terms, following the same argument of the Berezin integral, has the form

$$\begin{aligned} Z_0 &= \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \exp\left\{ i \int d^4x [(\bar{\psi} - \bar{\psi}_{min}) S^{-1} (\psi - \psi_{min})] \right\} \\ &= \det\left(iS^{-1}\right)\,. \end{aligned} \tag{3.25}$$

We thus have as the Green's function for the Dirac field

$$\begin{aligned}\langle 0|\,\mathrm{T}\bar{\psi}(x)\psi(y)\,|0\rangle &= \frac{-i\delta^2}{\delta\eta(x)\delta\bar{\eta}(y)}\exp\left\{-i\int d^4xd^4y[\bar{\eta}(x)S(x-y)\eta(y)]\right\} \\ &= \frac{-i\delta^2}{\delta\eta(x)\delta\bar{\eta}(y)}\exp\left\{-i\int d^4xd^4y[\bar{\eta}(x)(\delta^4(x-y)(i\gamma^\mu\partial_\mu - m))^{-1}\eta(y)]\right\}.\end{aligned} \tag{3.26}$$

The fermionic propagator or the two-point correlation function can now be obtained through the functional differentiation of the integrand, and from Eq. (3.16) is seen to be

$$S(x-y) = [\delta^4(x-y)(i\gamma^\mu\partial_\mu - m)]^{-1}\,. \tag{3.27}$$

In the momentum representation this is given as [89]

$$S(x-y) = \int \frac{d^4k}{(2\pi)^4}\frac{\not{p}+m}{k^2-m^2+i\varepsilon}e^{-ip(x-y)}\,, \tag{3.28}$$

where we have introduced the Feynman slashed notation $\not{p} = \gamma^\mu p_\mu$ and the $i\varepsilon$ has been introduced as in the Section on the photon propagator, following the Feynman prescription for the causal propagation for electrons and positrons [89].
Thus, we have arrived at the Green's function or the propagator of the free Dirac field using the functional integral formalism.

4. The free Dirac propagator in spherical coordinates

Green's function of the Dirac equation has been used in different areas of atomic physics: in the calculation of radiative corrections in atoms and highly charged ions [83, 104–112], tested by various state-of-the-art experimental methods (see e.g., [62, 113–117]); in describing relativistic atomic processes [118, 119], multiphoton interactions [120], x-ray scattering [121, 122], atoms in external fields [123], and the weak decay in muonic atoms [124], to name a few examples.

In this Chapter, we derive the free Dirac Green's function using the path integral formalism of Feynman. However, we take a slight detour from the field-theoretic approach taken in the last Chapter, and arrive at the propagator, in the particle representation, by reducing the relativistic quantum mechanical system to the form of a non-relativistic particle. For this purpose, the Green's function is reduced in Biedenharn's basis [77] into a radial path integral, the effective action of which is similar to that of a non-relativistic particle. In order to express the energy-dependent Green's function in a closed form, we convert the radial path integral to the path integral of an isotropic harmonic oscillator through a coordinate transformation along with local time rescaling. This approach is analogous to earlier works of Inomata and collaborators on the hydrogen atom [80, 125]. The final result agrees with the solution of the inhomogeneous Dirac equation in previous works, e.g. in Refs. [104, 126].

4.1 First- and second-order Dirac equation

The time-independent Dirac equation is customarily expressed, in natural units ($c = 1$, $\hbar = 1$), as

$$(E - \boldsymbol{\alpha} \cdot \hat{\mathbf{p}} - \beta m)\psi = 0\,. \tag{4.1}$$

Here, E is the energy, m is the mass of a particle, and $\hat{\boldsymbol{p}}$ is the operator of 3-momentum. The $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β are the usual 4×4 Dirac matrices, and ψ is the bispinor wave function. The Green's function $G(\mathbf{r}_2, \mathbf{r}_1; E)$ depends on the two positions $\mathbf{r}_1$, $\mathbf{r}_2$ and the energy, and it satisfies the inhomogeneous Dirac equation

$$(m - \hat{M})G(\mathbf{r}_2, \mathbf{r}_1; E) = \delta(\mathbf{r}_2 - \mathbf{r}_1)\,, \tag{4.2}$$

where $\hat{M} = -\beta\boldsymbol{\alpha}\cdot\hat{\mathbf{p}} + \beta E$. This Green's function can be expressed as [127]

$$G(\mathbf{r}_2, \mathbf{r}_1; E) = (m + \hat{M})g(\mathbf{r}_2, \mathbf{r}_1; E)\,, \tag{4.3}$$

where $g(\mathbf{r}_2, \mathbf{r}_1; E)$ is the solution of the second-order – or iterated – inhomogeneous Dirac equation

$$(E - \boldsymbol{\alpha}\cdot\hat{\mathbf{p}} - \beta m)(E - \boldsymbol{\alpha}\cdot\hat{\mathbf{p}} + \beta m)\Psi = 0\,,$$

where Ψ is the solution of the iterated Dirac equation. The Green's function for this equation, which we denote as $g(\boldsymbol{r}_2, \boldsymbol{r}_1; E)$ following Ref. [80], also follows the inhomogeneous iterated Dirac equation

$$(m^2 - \hat{M}^2)g(\mathbf{r}_2, \mathbf{r}_1; E) = \delta(\mathbf{r}_2 - \mathbf{r}_1)\,, \tag{4.4}$$

where the above equation directly follows from the definition of the operator $\hat{M}$ and the Dirac Eq. (4.1).

The second-order Dirac equation resembles the Schrödinger equation, and its solution has a simpler form than the usual first-order equation [77].

We use spherical coordinates to find explicit expressions for these Green's functions. Generally, operators of interest can be rewritten using the Dirac operator

$$\hat{K} = \beta(\hat{\boldsymbol{\Sigma}}\cdot\hat{\boldsymbol{L}} + 1)\,. \tag{4.5}$$

The radial momentum operator is

$$\hat{p}_{\mathrm{r}} = \frac{1}{\mathrm{r}}(\mathbf{r}\cdot\hat{\mathbf{p}} - i)\,, \tag{4.6}$$

and

$$\alpha_{\mathrm{r}} = \frac{\boldsymbol{\alpha}\cdot\mathbf{r}}{\mathrm{r}}\,, \tag{4.7}$$

which is the component of the Dirac matrix $\boldsymbol{\alpha}$ in the direction $\mathbf{r}$. Here, the operator $\hat{\boldsymbol{\Sigma}}(= \mathbf{1}\otimes\boldsymbol{\sigma})$, $\boldsymbol{\sigma}$ being the vector of the Pauli matrices, defines the Dirac spin operator $\hat{\boldsymbol{S}}_D = \frac{\hat{\boldsymbol{\Sigma}}}{2}$ and its components are $\hat{\Sigma}_j = -i\alpha_k\alpha_l$ [101, 128], and $\hat{\boldsymbol{L}}$ is the operator of orbital angular momentum.

The operator $\hat{K}$ commutes with the first-order Dirac Hamiltonian and with α_r. The Dirac operator is related to the total angular momentum operator [102] $\hat{\boldsymbol{J}}$ via $\hat{K}^2 = \hat{\boldsymbol{J}}^2 + \frac{1}{4}$. The operator $\hat{\boldsymbol{J}}^2$ has the eigenvalues $j(j+1)$, with j being half-integer, and thus the eigenvalues of $\hat{K}^2$ are $(j+\frac{1}{2})^2$. The eigenvalues of $\hat{K}$ are

$$\kappa = \pm\left(j + \frac{1}{2}\right). \tag{4.8}$$

4.2 Path integral form of the Green's function

We seek the solution to equation (4.4) using the quantum mechanical functional integral representation, as follows from Eq. (1.11)

$$g(\mathbf{r}_2, \mathbf{r}_1; E) \equiv \langle \mathbf{r}_2 | \, \hat{g} \, | \mathbf{r}_1 \rangle = \frac{i}{2m} \int_0^\infty \langle \mathbf{r}_2 | \, e^{i\hat{H}u} \, | \mathbf{r}_1 \rangle \, du \, . \tag{4.9}$$

In the above equation, the integration is done with respect to the time-like parameter u, and the integrand $\langle \mathbf{r}_2 | \, e^{i\hat{H}u} \, | \mathbf{r}_1 \rangle$ can be interpreted as a propagator that describes a system evolving with the parameter u from $\mathbf{r}_1$ to $\mathbf{r}_2$, and has an effective Hamiltonian, $\hat{H}$. As stated by Feynman, propagators can be written in the form of path integrals [17]. Here, we express the integral in Eq. (4.9) in terms of a path integral. Finally, we evaluate the Green's function for the iterated Dirac equation by using Eq. (4.4).

The effective Hamiltonian for Eq. (4.4) can be written as

$$\hat{H} = \frac{1}{2m}(m^2 - \hat{M}^2) \, . \tag{4.10}$$

With the operators introduced above, following Biedenharn [78], $\hat{M}$ can be written as

$$\hat{M} = -\beta(\alpha_{\rm r}\hat{p}_{\rm r}) + i\frac{\alpha_r \hat{K}}{\rm r} + \beta E \, . \tag{4.11}$$

In terms of this operator, the effective Hamiltonian (4.10) can now be cast in the form

$$\hat{H} = \frac{1}{2m}\left(\hat{p}_{\rm r}^2 + \frac{\hat{K}(\hat{K} - \beta)}{\rm r^2} - E^2 + m^2 \right) \, . \tag{4.12}$$

In Eq. (4.12), the coefficient of the $1/\mathrm{r}^2$ term in the Hamiltonian is analogous to the term containing the orbital angular momentum term in the Hamiltonian of the Schrödinger equation. To establish this correspondence, we use a specific case of the Martin-Glauber operator [81]

$$\hat{\mathscr{L}} = -\beta \hat{K} \, , \tag{4.13}$$

for which the following holds: $\hat{\mathscr{L}}^2 = \hat{K}^2$. The eigenvalue of $\hat{\mathscr{L}}$, γ, is given as

$$\gamma = \pm \left(j + \frac{1}{2} \right) \, . \tag{4.14}$$

We define λ as a function of γ, $\lambda \equiv |\gamma| + \frac{1}{2}(\mathrm{sign}\gamma - 1)$, such that the eigenvalue equation [81]

$$\hat{\mathscr{L}} \left(\hat{\mathscr{L}} + 1 \right) |\lambda\rangle = \lambda(\lambda + 1) \, |\lambda\rangle \, . \tag{4.15}$$

is fulfilled. The angular wave functions $\langle \theta\phi | \lambda \rangle = \left\langle \theta\phi \middle| j, \mu, \kappa, \tilde{\beta} \right\rangle$ are the simultaneous eigenstates of the operators $\hat{\mathscr{L}}(\hat{\mathscr{L}}+1)$, $\hat{\boldsymbol{J}}^2$, $\hat{J}_z$, $\hat{K}$ and the β matrix, with the eigenvalues

$\lambda(\lambda+1)$, $j(j+1)$, μ, κ and $\tilde{\beta}=\pm 1$, respectively. They can be written in the explicit bispinor form as [77, 80]

$$\left\langle \theta\phi \middle| j,\mu,\kappa,\tilde{\beta}=-1 \right\rangle = \begin{pmatrix} 0 \\ \chi^{\mu}_{\kappa} \end{pmatrix},$$
$$\left\langle \theta\phi \middle| j,\mu,\kappa,\tilde{\beta}=1 \right\rangle = \begin{pmatrix} \chi^{\mu}_{-\kappa} \\ 0 \end{pmatrix}, \tag{4.16}$$

where the χ^{μ}_{κ} are the well-known spherical spinors [102]

$$\chi^{\mu}_{\kappa} = \sum_{\mu'=\pm\frac{1}{2}} C\left(l\,,\frac{1}{2}\,,j;\mu-\mu'\,,\mu'\,,\mu\right) Y_{l}^{\mu-\mu'}(\theta,\phi)\chi^{\mu'}_{\frac{1}{2}}\,, \tag{4.17}$$

expressed in terms of the Clebsch-Gordan coefficients $C(\dots)$, the spherical harmonics $Y_{l}^{\mu-\mu'}$, and the unit spinors

$$\chi^{\frac{1}{2}}_{\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi^{-\frac{1}{2}}_{\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{4.18}$$

The Hamiltonian of Eq. (4.12) is now represented in this basis as

$$\hat{H}_{\lambda} = \frac{\hat{p}_{\mathrm{r}}^{2}}{2m} + \frac{\lambda(\lambda+1)}{2m\mathrm{r}^{2}} - \frac{k^{2}}{2m}\,, \tag{4.19}$$

where $k^{2}=E^{2}-m^{2}$.

Having defined the radial Hamiltonian, the Green's function for the second-order Dirac equation can be expressed as a partial wave expansion

$$\langle \mathbf{r}_2|\,\hat{g}\,|\mathbf{r}_1\rangle = \sum_{\lambda} \langle\theta_2\phi_2|\lambda\rangle\,\langle \mathrm{r}_2|\,\hat{g}_{\lambda}\,|\mathrm{r}_1\rangle\,\langle\lambda|\theta_1\phi_1\rangle\,. \tag{4.20}$$

Here, the radial Green's function is

$$\langle \mathrm{r}_2|\,\hat{g}_{\lambda}\,|\mathrm{r}_1\rangle = \frac{i}{2m}\int \langle \mathrm{r}_2|\,e^{-i\hat{H}_{\lambda}u}\,|\mathrm{r}_1\rangle\,du\,, \tag{4.21}$$

where the operator $\hat{H}_{\lambda}$ is defined in Eq. (4.19). This radial Hamiltonian undergoes an evolution in u, and it is very similar in form to the radial propagator of the non-relativistic hydrogen atom, as introduced by Inomata [125].

The Green's function given in Eq. (4.20) can now be reduced using Eqs. (4.19-4.21), yielding

$$\langle \mathbf{r}_2|\,\hat{g}\,|\mathbf{r}_1\rangle = \sum_{j,\kappa} \langle \mathrm{r}_2|\,\hat{g}_{\lambda}\,|\mathrm{r}_1\rangle\,\Omega^{j}_{\kappa,\kappa'}(\theta_2\phi_2|\theta_1\phi_1)\beta^{2}\,, \tag{4.22}$$

where

$$\Omega^{j}_{\kappa,\kappa'}(\theta_2\phi_2|\theta_1\phi_1) = \sum_{\mu} \chi^{\mu}_{\kappa}(\theta_2,\phi_2)\chi^{\mu\dagger}_{\kappa'}(\theta_1,\phi_1)\,. \tag{4.23}$$

In order to proceed with the construction of the path integral in spherical coordinates, we establish the partial action term for a very short time interval $t_j = u_j - u_{j-1}$. This partial action can be approximated as $S(\mathrm{r}_j, \mathrm{r}_{j-1}) \approx t_j L(\Delta \mathrm{r}_j/t_j, \mathrm{r}_j)$, where $\Delta \mathrm{r}_j = \mathrm{r}_j - \mathrm{r}_{j-1}$.The total path is divided into N intervals by time slicing such that $\mathrm{r}_0 = \mathrm{r}_1$, $\mathrm{r}_N = \mathrm{r}_2$, and $u = \sum t_j$. The radial action term for the Hamiltonian in Eq. (4.19) is given as

$$S(t_j) = \frac{m(\Delta \mathrm{r}_j)^2}{2t_j} - \frac{\lambda(\lambda+1)t_j}{2m\mathrm{r}_j\mathrm{r}_{j-1}} + \frac{(E^2-m^2)t_j}{2m}\,. \tag{4.24}$$

Since angular motion has rotational symmetry, we concern ourselves with only the radial motion associated with this action. As such, the corresponding radial function is

$$\begin{aligned} R_\lambda(\mathrm{r}_j, \mathrm{r}_{j-1}) &= \frac{it_j}{2m\mathrm{r}_j\mathrm{r}_{j-1}} \\ &\times \exp\left\{\frac{im(\Delta \mathrm{r}_j)^2}{2t_j} - \frac{it_j\lambda(\lambda+1)}{2m\mathrm{r}_j\mathrm{r}_{j-1}} + \frac{ik^2t_j}{2m}\right\}\,. \end{aligned} \tag{4.25}$$

Summing over all the time intervals, the radial propagator kernel for the radial function in Eq. (4.25), is obtained as

$$\begin{aligned} &K_\lambda(\mathrm{r}_2, \mathrm{r}_1; u) = \\ &\lim_{N\to\infty} \int \prod_{j=1}^{N} \{R_\lambda(\mathrm{r}_j, \mathrm{r}_{j-1})\} \prod_{j=1}^{N} \left[\frac{m}{2\pi i t_j}\right]^{\frac{3}{2}} \prod_{j=1}^{N-1} (\mathrm{r}\, d\mathrm{r})\,. \end{aligned} \tag{4.26}$$

This expression for the radial propagator kernel can be represented as [80, 125]

$$\begin{aligned} &K_\lambda(\mathrm{r}_2, \mathrm{r}_1; u) = \langle \mathrm{r}_2 |\, e^{-i\hat{H}_\lambda u}\, | \mathrm{r}_1 \rangle = (\mathrm{r}_1\mathrm{r}_2)^{-1} \\ &\times \lim_{N\to\infty} \int \exp\left[i\sum_{j=1}^{N} S(t_j)\right] \prod_{j=1}^{N} \left[\frac{m}{2\pi i t_j}\right]^{\frac{1}{2}} \prod_{j=1}^{N-1} d\mathrm{r}_j\,. \end{aligned} \tag{4.27}$$

In order to solve the path integral in Eq. (4.26), we simplify the radial function in Eq. (4.25). Taking all contributions in t_j up to the first order into consideration, for small t_j, we can apply the approximation formula for modified Bessel functions of the first kind [92, 129]

$$\begin{aligned} &I_\nu\left(\frac{n}{t_j}\right) = \\ &\left(\frac{2\pi n}{t_j}\right)^{-\frac{1}{2}} \exp\left\{\frac{n}{t_j} - \frac{1}{2}\left[\left(\nu^2 - \frac{1}{4}\right)\frac{t_j}{n} + \mathscr{O}(t_j^2)\right]\right\}\,, \end{aligned} \tag{4.28}$$

here our $n = -im\mathrm{r}_j\mathrm{r}_{j-1}$, and $\nu = \lambda + \frac{1}{2}$. Applying this approximation, the radial function, in terms of the modified Bessel fuction, can be written in the form

$$\begin{aligned} R_\lambda(\mathrm{r}_j, \mathrm{r}_{j-1}) &= \left(\frac{i\pi t_j}{2m\mathrm{r}_j\mathrm{r}_{j-1}}\right)^{\frac{1}{2}} \\ &\times \exp\left[\frac{im(\mathrm{r}_j^2 + \mathrm{r}_{j-1}^2)}{2t_j} + \frac{ik^2t_j}{2m}\right] I_{\lambda+\frac{1}{2}}\left(\frac{m\mathrm{r}_j\mathrm{r}_{j-1}}{it_j}\right)\,, \end{aligned} \tag{4.29}$$

Substituting this expression into Eq. (4.26) and performing the full integral, we obtain the radial propagator kernel as

$$K_\lambda(\mathrm{r}_2,\mathrm{r}_1;u) = (\mathrm{r}_1\mathrm{r}_2)^{-\frac{1}{2}}\left(\frac{-im}{u}\right) \times \exp\left\{\frac{ik^2u}{2m}\right\}\exp\left\{\frac{1}{2}\frac{im(\mathrm{r}_1^2+\mathrm{r}_2^2)}{u}\right\} I_{\lambda+\frac{1}{2}}\left(\frac{m\mathrm{r}_2\mathrm{r}_1}{iu}\right). \tag{4.30}$$

Eq. (4.30) gives the radial propagator for the radial Hamiltonian, and when substituted into Eq. (4.21) yields the radial Green's function in the form

$$\langle \mathrm{r}_2|\, g_\lambda\, |\mathrm{r}_1\rangle = (\mathrm{r}_1\mathrm{r}_2)^{-\frac{1}{2}}\int\left(\frac{-im}{u}\right) \times \exp\left\{\frac{ik^2u}{2m}\right\}\exp\left\{\frac{1}{2}\frac{im(\mathrm{r}_1^2+\mathrm{r}_2^2)}{u}\right\} I_{\lambda+\frac{1}{2}}\left(\frac{m\mathrm{r}_2\mathrm{r}_1}{iu}\right) du\,. \tag{4.31}$$

However, the integration on the R.H.S. of Eq. (4.31) does not have a known closed-form solution. Thus, to enable the calculation process, and to bring the integral in Eq. (4.31) to a reducible form, following Ref. [125], we modify the radial action in Eq. (4.24), such that it represents the action of a three-dimensional isotropic harmonic oscillator. This can be achieved by replacing the radial variable r_j by $\rho_j = \sqrt{r_j}$ and the local time-slicing parameter t_j by $\sigma_j = t_j/4\bar{r}_j$, where the geometric mean is $\bar{r}_j = \sqrt{r_j r_{j-1}} = \rho_j\rho_{j-1} = \bar{\rho}_j^2$. For small values of t_j, the geometric mean, $\bar{r}_j$, gives the mid-point value which is well-defined for a classical path. The action term can now be represented as

$$S(\tau_j) = \frac{m(\Delta\rho_j)^2}{2\sigma_j} + \frac{m(\Delta\rho_j)^4}{8\sigma_j\bar{\rho_j}^2} - \frac{2\lambda(\lambda+1)\sigma_j}{m\bar{\rho}_j^2} - \frac{1}{2}m\omega^2\bar{\rho_j}^2\sigma_j\,, \tag{4.32}$$

with $\omega = \frac{2ik}{m}$. The measure of the integrand in the Eq. (4.27) also changes according to the transformed variables, and it can be expressed as

$$\prod_{j=1}^{N}\left[\frac{m}{2\pi i t_j}\right]^{\frac{1}{2}}\prod_{j=1}^{N-1}d\mathrm{r}_j = \frac{1}{\sqrt{4\rho_1\rho_2}}\prod_{j=1}^{N}\left[\frac{m}{2\pi i\sigma_j}\right]^{\frac{1}{2}}\prod_{j=1}^{N-1}d\rho_j\,.$$

Despite these modifications, we encounter a different problem that makes the integration of Eq. (4.27) difficult; the second term in the modified radial action expression contains ρ_j raised to its fourth power, which causes the integral to diverge. Rewriting Eq. (4.27) after making the necessary substitutions, we obtain

$$\langle \mathrm{r}_2|\, e^{-i\hat{H}_\lambda u}\,|\mathrm{r}_1\rangle = (\rho_1\rho_2)^{-2}\lim_{N\to\infty}\int\exp\left[i\sum_{j=1}^{N}\frac{m(\Delta\rho_j)^2}{2\sigma_j} + \frac{m(\Delta\rho_j)^4}{8\sigma_j(\bar{\rho}_j)^2} - \frac{2\lambda(\lambda+1)\sigma_j}{m(\bar{\rho}_j)^2} - \frac{1}{2}m(\omega)^2(\bar{\rho}_j)^2\sigma_j\right] \times(4\rho_1\rho_2)^{-\frac{1}{2}}\prod_{j=1}^{N}\left[\frac{m}{2\pi i\sigma_j}\right]^{\frac{1}{2}}\prod_{j=1}^{N-1}d\rho_j\,. \tag{4.33}$$

In order to overcome the problem posed by ρ_j^4, we use the integral formula [92, 125] that is valid for large A and integer n:

$$\int x^{2n} \exp\left[-Ax^2 + Bx^4 + \mathscr{O}(x^6)\right] dx = \int x^{2n} \exp\left[-Ax^2 + \frac{3}{4}BA^{-2} + \mathscr{O}(A^{-3})\right] dx \,. \tag{4.34}$$

This allows the fourth-order term to be represented by a replacement term given by $-3\sigma_j/(8m\bar{\rho}_j^2)$, yielding

$$\begin{aligned} &\langle \mathrm{r}_2 |\, e^{-i\hat{H}_\lambda u} \,| \mathrm{r}_1 \rangle = \\ &(\rho_1\rho_2)^{-2} \lim_{N\to\infty} \int \exp\left[i \sum_{j=1}^{N} \frac{m(\Delta\rho_j)^2}{2\sigma_j} + \frac{3\sigma_j}{8m(\bar{\rho}_j)^2} \right. \\ &\left. - \frac{2\lambda(\lambda+1)\sigma_j}{m(\bar{\rho}_j)^2} - \frac{1}{2}m(\omega)^2(\bar{\rho}_j)^2\sigma_j \right] \\ &\times (4\rho_1\rho_2)^{-\frac{1}{2}} \prod_{j=1}^{N} \left[\frac{m}{2\pi i\sigma_j}\right]^{\frac{1}{2}} \prod_{j=1}^{N-1} d\rho_j \,. \end{aligned} \tag{4.35}$$

We express this equation in a compact form as

$$\langle \mathrm{r}_2 |\, e^{-i\hat{H}_\lambda u} \,| \mathrm{r}_1 \rangle = \frac{1}{2}(\rho_1\rho_2)^{-\frac{3}{2}} \tilde{K}_\lambda(\rho_2, \rho_1; \sigma) \,, \tag{4.36}$$

where the propagator $\tilde{K}$ of the σ evolution is defined as

$$\begin{aligned} &\tilde{K}_\lambda(\rho_2, \rho_1; \sigma) = (\rho_1\rho_2)^{-1} \\ &\times \lim_{N\to\infty} \int \exp\left[i \sum_{j=1}^{N} \tilde{S}(\sigma_j) \right] \prod_{j=1}^{N} \left[\frac{m}{2\pi i\sigma_j}\right]^{\frac{1}{2}} \prod_{j=1}^{N-1} d\rho_j \,, \end{aligned} \tag{4.37}$$

and the modified action term is now given as

$$\tilde{S}(\sigma_j) = \frac{m(\Delta\rho_j)^2}{2\sigma_j} - \frac{\lambda'(\lambda'+1)\sigma_j}{2m(\bar{\rho}_j)^2} - \frac{1}{2}m\omega^2(\bar{\rho}_j)^2\sigma_j \,, \tag{4.38}$$

where $\lambda' = 2\lambda + \frac{1}{2}$.

This effective action term is analogous to the radial action term of a three-dimensional harmonic oscillator. Thus, the propagator in Eq. (4.21), evolving with u, has also been reduced to the propagator of a harmonic oscillator, and can be evaluated by following the procedure introduced by Inomata and Peak [130]. Thus, we obtain the radial propagator kernel, in terms of the modified Bessel function $I_\nu(x)$ with $\nu = \lambda' + \frac{1}{2}$, as

$$\begin{aligned} &\tilde{K}_\lambda(\rho_2, \rho_1; \sigma) = -i(\rho_1\rho_2)^{-\frac{1}{2}}(m\omega)\csc(\omega\sigma) \\ &\exp\left[\frac{1}{2}im\omega\left((\rho_1^2+\rho_2^2)\cot(\omega\sigma)\right]\right. I_{\lambda'+\frac{1}{2}}\left(\frac{m}{i}\omega\rho_1\rho_2\csc(\omega\sigma)\right) \,. \end{aligned} \tag{4.39}$$

It is to be noted that in the limit that ω vanishes, the propagator in Eq. (4.39) reduces to that defined in Eq. (4.30), which is the propagator for a free particle in three dimensions. However, since we are concerned with determining the energy-dependent Green's function in a closed form, we proceed with a finite-valued ω.

Substituting the radial propagator from the above equation into Eq. (4.36) yields

$$\begin{aligned}\langle \mathrm{r}_2|\, e^{-i\hat{H}_\lambda u}\,|\mathrm{r}_1\rangle &= \frac{1}{2}(\mathrm{r}_1\mathrm{r}_2)^{-1}(2k) \\ &\times \csc\left(\frac{ikt}{m(\mathrm{r}_1\mathrm{r}_2)^{\frac{1}{2}}}\right)\exp\left[-k(\mathrm{r}_1+\mathrm{r}_2)\cot\left(\frac{ikt}{m(\mathrm{r}_1\mathrm{r}_2)^{\frac{1}{2}}}\right)\right] \\ &\times I_{2\lambda+1}\left(2k(\mathrm{r}_1\mathrm{r}_2)^{\frac{1}{2}}\csc\left(\frac{ikt}{m(\mathrm{r}_1\mathrm{r}_2)^{\frac{1}{2}}}\right)\right)\,.\end{aligned} \tag{4.40}$$

Using this result for the integrand in Eq. (4.21) we obtain

$$\begin{aligned}\langle \mathrm{r}_2|\,\hat{g}_\lambda\,|\mathrm{r}_1\rangle &= (\mathrm{r}_1\mathrm{r}_2)^{-\frac{1}{2}}\int \exp[ik(\mathrm{r}_1+\mathrm{r}_2)\coth q] \\ &\times\ I_{2\lambda+1}\left(-2ik(\mathrm{r}_1\mathrm{r}_2)^{\frac{1}{2}}\operatorname{csch} q\right)\operatorname{csch} q\,dq\,,\end{aligned} \tag{4.41}$$

where

$$q = \frac{kt}{(4\mathrm{r}_1\mathrm{r}_2m^2)^{\frac{1}{2}}}\,.$$

The type of integral in Eq. (4.41) has a closed solution [92]:

$$\begin{aligned}&\int \exp[ik(\mathrm{r}_1+\mathrm{r}_2)\coth q]I_{2\lambda+1}\left(-2ik(\mathrm{r}_1\mathrm{r}_2)^{\frac{1}{2}}\operatorname{csch} q\right)\operatorname{csch} q\,dq = \\ &\qquad\frac{\Gamma(\lambda+1)}{2ik(\mathrm{r}_1\mathrm{r}_2)^{\frac{1}{2}}\Gamma(2\lambda+2)}M_{0,\lambda+\frac{1}{2}}(-2ik\mathrm{r}_2)W_{0,\lambda+\frac{1}{2}}(-2ik\mathrm{r}_1)\,,\end{aligned} \tag{4.42}$$

where Γ is the gamma function, and M and W are the Whittaker functions. They can be expressed in terms of the modified Bessel functions [131]:

$$\begin{aligned}M_{0,\nu}(2z) &= 2^{2\nu+\frac{1}{2}}\Gamma(1+\nu)\sqrt{z}I_\nu(z)\,, \\ W_{0,\nu}(2z) &= \sqrt{\frac{2z}{\pi}}K_\nu(z)\,.\end{aligned}$$

Substituting these into Eq. (4.42), we obtain

$$\begin{aligned}\langle \mathrm{r}_2|\,\hat{g}_\lambda\,|\mathrm{r}_1\rangle &= \frac{\Gamma(\lambda+1)}{2ik\mathrm{r}_1\mathrm{r}_2\Gamma(2\lambda+2)}2^{2\lambda+\frac{3}{2}} \\ &\times\Gamma\left(\lambda+\frac{3}{2}\right)\sqrt{-ik\mathrm{r}_2}I_{\lambda+\frac{1}{2}}(-ik\mathrm{r}_2)\sqrt{\frac{-2ik\mathrm{r}_1}{\pi}}K_{\lambda+\frac{1}{2}}(-ik\mathrm{r}_1)\,.\end{aligned} \tag{4.43}$$

Using this expression for the radial part in the expression for the total Green's function of the iterated Dirac equation yields

$$\langle \mathbf{r}_2 | \, \hat{g} \, | \mathbf{r}_1 \rangle = \sum_{j,\kappa} \frac{\Gamma(\lambda+1)}{2ik\mathrm{r}_1\mathrm{r}_2\Gamma(2\lambda+2)} 2^{2\lambda+\frac{3}{2}} \tag{4.44}$$
$$\times\Gamma\left(\lambda+\frac{3}{2}\right)\sqrt{-ik\mathrm{r}_2}I_{\lambda+\frac{1}{2}}(-ik\mathrm{r}_2)\sqrt{\frac{-2ik\mathrm{r}_1}{\pi}}K_{\lambda+\frac{1}{2}}(-ik\mathrm{r}_1)\Omega^{j}_{\kappa,\kappa'}(\theta_2\phi_2|\theta_1\phi_1)\beta^2\,.$$

The modified Bessel functions of the first and second kind can be expressed in terms of spherical functions [131], and so we obtain

$$\langle \mathbf{r}_2 | \, \hat{g} \, | \mathbf{r}_1 \rangle = \sum_{j,\kappa} \frac{\Gamma(\lambda+1)}{2ik\mathrm{r}_1\mathrm{r}_2\Gamma(2\lambda+2)} 2^{2\lambda+\frac{3}{2}} \tag{4.45}$$
$$\times\Gamma\left(\lambda+\frac{3}{2}\right)\sqrt{-ik\mathrm{r}_2}(i)^{-\left(\lambda+\frac{1}{2}\right)}\sqrt{\frac{2ik\mathrm{r}_2}{\pi}}j_\lambda(ik\mathrm{r}_2)$$
$$\times\sqrt{\frac{-2ik\mathrm{r}_1}{\pi}}\frac{\pi}{2}(i)^{\lambda+\frac{3}{2}}\sqrt{\frac{2ik\mathrm{r}_1}{\pi}}h_\lambda(ik\mathrm{r}_1)\Omega^{j}_{\kappa,\kappa'}(\theta_2\phi_2|\theta_1\phi_1)\beta^2\,,$$

where j_λ and h_λ are the spherical Bessel and Hankel functions, respectively. The operator $\hat{M}$, when acting on a state with a given κ, takes the form

$$i\beta\alpha_{\mathrm{r}}\left[\frac{\partial}{\partial \mathrm{r}}+\frac{1-\gamma\beta}{\mathrm{r}}\right]+\frac{\kappa E}{\gamma}\beta\,. \tag{4.46}$$

We can turn to deriving the free Dirac Green's function from Eq. (4.3):

$$\langle \mathbf{r}_2 | \, \hat{G} \, | \mathbf{r}_1 \rangle = \sum_{j,\kappa} \frac{\Gamma(\lambda+1)}{2ik\mathrm{r}_1\mathrm{r}_2\Gamma(2\lambda+2)} 2^{2\lambda+\frac{3}{2}} \tag{4.47}$$
$$\times\Gamma\left(\lambda+\frac{3}{2}\right)\sqrt{-ik\mathrm{r}_2}(i)^{-\left(\lambda+\frac{1}{2}\right)}\sqrt{\frac{2ik\mathrm{r}_2}{\pi}}$$
$$\times\sqrt{\frac{-2ik\mathrm{r}_1}{\pi}}\frac{\pi}{2}(i)^{\lambda+\frac{3}{2}}\sqrt{\frac{2ik\mathrm{r}_1}{\pi}}h_\lambda(ik\mathrm{r}_1)$$
$$\times\left(m+i\beta\alpha_{\mathrm{r}}\left[\frac{\partial}{\partial \mathrm{r}}+\frac{1-\gamma\beta}{\mathrm{r}}\right]+\frac{\kappa E}{\gamma}\beta\right)j_\lambda(ik\mathrm{r}_2)$$
$$\times\Omega^{j}_{\kappa,\kappa'}(\theta_2\phi_2|\theta_1\phi_1)\beta^2\,.$$

Using the relation for the derivative of spherical Bessel functions [131] one obtains

$$\begin{aligned}\langle \mathbf{r}_2|\,\hat{G}\,|\mathbf{r}_1\rangle &= \sum_{j,\kappa} k(2\lambda+2) i h_\lambda(ik\mathrm{r}_1) \\ &\times\Bigg\{\left(m+\frac{\kappa E}{\gamma}\beta\right) j_\lambda(ik\mathrm{r}_2)\Omega^j_{\kappa,\kappa'}(\theta_2\phi_2|\theta_1\phi_1)\beta^2 \\ &\quad +i\left[k\left\{\frac{\lambda}{ik\mathrm{r}_2}j_\lambda(ik\mathrm{r}_2)-j_{\lambda+1}(ik\mathrm{r}_2)\right\}+\frac{(1\pm\gamma)}{\mathrm{r}_2}j_\lambda(ik\mathrm{r}_2)\right] \\ &\qquad\qquad \times\Omega^j_{\kappa,\kappa'}(\theta_2\phi_2|\theta_1\phi_1)\beta^2\alpha_\mathrm{r}\Bigg\}\,. \end{aligned} \tag{4.48}$$

On account of the relations

$$\begin{aligned}\alpha_\mathrm{r} &= i\sigma_\mathrm{r}\beta\gamma^1\gamma^2\gamma^3\,, \\ \gamma^i &= \beta\alpha_i\,, \quad \text{with } i\in\{1,2,3\}\,, \\ \sigma_\mathrm{r}\Omega^j_{\kappa,\kappa'} &= -\Omega^j_{\kappa,-\kappa'}\,. \end{aligned}$$

the Green's function of the first-order free Dirac equation can be finally written as

$$\begin{aligned}&\langle \mathbf{r}_2|\,\hat{G}\,|\mathbf{r}_1\rangle = \sum_{j,\kappa} ik(2\lambda+2) h_\lambda(ik\mathrm{r}_1) \\ &\times\Bigg\{\left(m+\frac{\kappa E}{\gamma}\beta\right) j_\lambda(ik\mathrm{r}_2)\Omega^j_{\kappa,\kappa'}(\theta_2\phi_2|\theta_1\phi_1)\beta^2 \\ &-\tilde{\beta}\left[k\left(\frac{\lambda}{ik\mathrm{r}_2}j_\lambda(ik\mathrm{r}_2)-j_{\lambda+1}(ik\mathrm{r}_2)\right)+\frac{(1\pm\gamma)}{\mathrm{r}_2}j_\lambda(ik\mathrm{r}_2)\right] \\ &\times\Omega^j_{\kappa,-\kappa}(\theta_2\phi_2|\theta_1\phi_1)\alpha_1\alpha_2\alpha_3\Bigg\}\,. \end{aligned} \tag{4.49}$$

This formula is equivalent to the free Green's function derived by different methods [83, 104, 126] and in this Chapter, the free Dirac Green's function has been derived from first principles within the path integral formalism. Spherical coordinates were used, in order to arrive to a form applicable in atomic physics calculations. The Green's function has been transformed in Biedenharn's basis [77] into a radial path integral, with an effective action resembling the action of the Schrödinger equation. The radial path integral has been converted through coordinate transformation and with a time rescaling to that of a classical isotropic harmonic oscillator, which reduces the problem to an exactly solvable form. The final result is expressed with spherical Bessel functions and spherical spinors in Eq. (4.49) and we will implement this form in our derivations of the first-order Lamb shift in the following chapters.

5. The Coulomb-Dirac Propagator – the path integral method

We have seen in the previous Chapters the derivation of the free Dirac propagator using the functional integral formalism in the context of field theory and also the free Dirac propagator in spherical coordinates by reducing it to a form analogous to that of the non-relativistic Hydrogen atom problem.

In this Chapter, we proceed with the derivation of the Green's function of a Dirac particle in the presence of the nuclear Coulomb field, i.e., the Dirac-Coulomb Green's function. The DCGF or the Dirac-Coulomb Green's function is essential in the formulation of QED of an electron bound by the Coulomb potential of the nucleus.

In Section 5.1, a simplified solution for the wave functions satisfying the homogeneous Dirac-Coulomb equation has been obtained in accordance with the method devised by Wong and Yeh[79]. The solution they obtain involves a change of basis using the Biedenharn transformation and with this they show that the radial wave functions, $g(\mathrm{r})$ and $f(\mathrm{r})$, of the Dirac equation, which originally are represented as sums of two different hypergeometric functions each [101, 132] can be reduced to each component containing one term of a hypergeometric function only [79]. Their solution is also applicable to both bound and continuum states. We introduce this simplified solution of the Dirac equation since the mathematical formulation used in the derivation is in keeping with the formalism used in the derivation of the free propagator in spherical co-ordinates, in Chapter 4, and is also further used in the path integral derivation of the DCGF.

In Section 5.2, using the simplified solution, the Green's function is derived by the usual eigenfunction expansion method; the Green's function that is obtained by Wong and Yeh [122] is in good agreement with the solution provided by Wichmann and Kroll[105], and Schaefer and Brown[133]. However, owing to the simplified radial wavefunctions introduced in Section 5.1, the corresponding Green's function that is constructed is simpler than that obtained by Wichmann and Kroll or Schaefer and Brown in that the radial component of the Green's function, each component contains only one term instead of four [122]. The Green's function thus obtained can also be easily reduced to the non-relativistic limit owing to the basis transformation introduced in Section 5.1.

In Section 5.3, the DCGF is derived using the path integral formalism.

5.1 The simplified solution of the Dirac-Coulomb Equation

The stationary Dirac equation with a Coulomb potential is represented as per [79]

$$(E - (\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m - V))\psi = 0\,, \tag{5.1}$$

where the unusual positive sign in front of the mass term is introduced for later convenience. The $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and β matrices are the 4×4 Dirac matrices,

$$\alpha_i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix}\,, \qquad \beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}\,, \tag{5.2}$$

where σ_i are the 2×2 Pauli matrices, $i = 1, 2, 3$ and $\mathbb{1}$ is the 2×2 identity matrix. The α_i and β matrices are related to the Dirac gamma matrices as

$$\alpha_i = \gamma^0 \gamma^i\,,$$
$$\beta = \gamma^0\,.$$

Eq. (5.1) can also be written as [77, 78]

$$\left[\rho_2 \hat{\boldsymbol{\Sigma}} \cdot \hat{\boldsymbol{\nabla}} - \rho_3 \left(E + \frac{Ze^2}{\mathrm{r}}\right) - m\right]\psi = 0\,, \tag{5.3}$$

where $\hat{\boldsymbol{\Sigma}}$ has been defined in Section (4.1) as

$$\hat{\boldsymbol{\Sigma}} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix}\,,$$

and

$$\rho_i \rho_j = -\rho_j \rho_i = i\rho_k\,.$$

In matrix format they are reperesented as,

$$\rho_1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}\,, \rho_2 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}\,, \rho_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}\,. \tag{5.4}$$

Now we consider the Dirac equation in the second-order given by

$$[\rho_2 \hat{\boldsymbol{\Sigma}} \cdot \hat{\boldsymbol{\nabla}} - \rho_3(E + Ze^2/\mathrm{r}) - m][\rho_2 \hat{\boldsymbol{\Sigma}} \cdot \boldsymbol{\nabla} - \rho_3(E + Ze^2/\mathrm{r}) + m]\Psi = 0\,. \tag{5.5}$$

We can rewrite the above equation by considering the r-dependent derivative as

$$\left[\frac{1}{\mathrm{r}^2}\frac{\partial}{\partial \mathrm{r}}\mathrm{r}^2\frac{\partial}{\partial \mathrm{r}} - \frac{\hat{K}^2 - Z^2e^4}{\mathrm{r}^2} + \frac{2Z^2E}{\mathrm{r}} + \frac{\rho_3 \hat{K} + iZe^2\rho_1 \hat{\boldsymbol{\Sigma}} \cdot \hat{\mathrm{r}}}{\mathrm{r}^2} + E^2 - m^2\right]\Psi = 0\,, \tag{5.6}$$

To solve this iterated Dirac equation, we invoke an operator introduced in [81]

$$\hat{\mathscr{L}} = -\hat{K}\beta - Ze^2\alpha_{\rm r}\,, \tag{5.7}$$

and called the Martin-Glauber operator, where,

$$\hat{K} = \beta(\hat{\boldsymbol{\Sigma}}\cdot\hat{\boldsymbol{L}} + 1)\,, \tag{5.8}$$

$$\alpha_{\rm r} = \frac{\boldsymbol{\alpha}\cdot\mathbf{r}}{\rm r}\,, \tag{5.9}$$

$\hat{\boldsymbol{L}}$ being the orbital angular momentum operator. The eigenvalue of $\hat{\mathscr{L}}$ is given by $\gamma = \pm|\gamma| = \pm[\kappa^2 - (Ze^2)^2]^{1/2}$, where, $\kappa = \pm(j+1/2)$ is the eigenvalue of the Dirac operator $\hat{K}$. From Eq. (5.6) and Eq. (5.7), we can infer that $\rho_3 = \beta$, which is also what we get from Eq. (5.4). We rewrite the Martin-Glauber operator in an alternate form using the relation $\rho_1\hat{\boldsymbol{\Sigma}} = \boldsymbol{\alpha}$

$$\hat{\mathscr{L}} = -(\rho_3\hat{K} + iZe^2\rho_1\hat{\boldsymbol{\Sigma}}\cdot\hat{\rm r})\,, \tag{5.10}$$

The iterated Dirac Eq. (5.6) can now be represented in terms of the Martin-Glauber operator as

$$\left[\frac{1}{\rm r^2}\frac{\partial}{\partial \rm r}{\rm r}^2\frac{\partial}{\partial \rm r} - \frac{\hat{\mathscr{L}}(\hat{\mathscr{L}}+1)}{\rm r^2} + \frac{2Z^2E}{\rm r} + E^2 - m^2\right]\Psi = 0\,. \tag{5.11}$$

Eq. (5.11) is the generalized iterated Dirac equation which can be solved for the continuum case [77] as well as the bound state [79]. For the bound state case where $m^2 - E^2 > 0$, Eq. (5.11) can be rewritten as

$$\left[\frac{1}{\zeta^2}\frac{\partial}{\partial\zeta}\zeta^2\frac{\partial}{\partial\zeta} - \frac{\hat{\mathscr{L}}(\hat{\mathscr{L}}+1)}{\zeta^2} + \frac{\omega}{4\zeta} - \frac{1}{4}\right]\Psi(\zeta) = 0\,, \tag{5.12}$$

where we have considered the following Ref. [81]

$$\begin{aligned}
\zeta &= 2m'{\rm r} = 2(m^2 - E^2)^{1/2}{\rm r}\,,\\
m' &= (m^2 - E^2)^{1/2}\,,\\
\frac{\omega}{4} &= \frac{Ze^2E}{m'}\,.
\end{aligned}$$

With the above transformations, Eq. (5.12) is now analogous to the Schrödinger equation of the form [134]

$$\left[\frac{1}{\zeta^2}\frac{\partial}{\partial\zeta}\zeta^2\frac{\partial}{\partial\zeta} - \frac{l(l+1)}{\zeta^2} + \frac{\lambda}{4\zeta} - \frac{1}{4}\right]R = 0\,. \tag{5.13}$$

The eigenvalues of the operators $\hat{K}$ and $\hat{\mathscr{L}}$ are, as before, given by

$$\kappa = \pm(j + \frac{1}{2}) \,, \tag{5.14}$$

and

$$\begin{aligned} \gamma &= \pm[\kappa^2 - (Ze^2)^2]^{1/2} \\ &= \pm[(j + 1/2)^2 - (Ze^2)^2]^{1/2} \,. \end{aligned} \tag{5.15}$$

For the sake of brevity, we define the signs of the eigenvalues κ and γ, by $\tilde{\omega}$ and $\tilde{\gamma}$ respectively, as

$$\begin{aligned} \tilde{\omega} &= \text{sign}[\kappa] \,, \\ \tilde{\gamma} &= \text{sign}[\gamma] \,. \end{aligned}$$

In order to solve the modified second-order Dirac Eq. (5.12), we introduce λ as a function of γ [79]

$$\lambda(\gamma) = |\gamma| + \frac{1}{2}(\tilde{\gamma} - 1) \,. \tag{5.16}$$

In terms of this function, the solution is obtained as

$$\Psi_{\lambda(\gamma)}(\zeta) = C_{\lambda(\gamma)} \zeta^{\lambda(\gamma)} e^{-\zeta/2} 1F1(-\frac{\omega}{4} + \lambda(\gamma) + 1;\, 2\lambda(\gamma) + 2;\, \zeta) \,, \tag{5.17}$$

where the coeffcient is given as

$$C_{\lambda(\gamma)} = \frac{[\Gamma(\frac{\omega}{4} + \lambda(\gamma) + 1)\Gamma(\frac{\omega}{4} - \lambda(\gamma) + 1)]^{1/2}}{\Gamma(2\lambda(\gamma) + 2)} \,, \tag{5.18}$$

and $1F1$ represents a confluent hypergeometric series [92, 135]. For this series to converge, we must have

$$\frac{\omega}{4} = \lambda + 1 + n' \,, \tag{5.19}$$

where n' is any non-negative integer. Substituting the values for ω and λ in Eq. (5.19) leads us to the energy eigenvalues for the Dirac-Coulomb equation

$$\frac{Ze^2 E}{(m^2 - E^2)^{1/2}} = |\gamma| + \frac{1}{2}\tilde{\gamma} + \frac{1}{2} + n' \,, \tag{5.20}$$

or

$$E = \frac{m}{[1 + (Ze^2)^2/(|\gamma| + \frac{1}{2}\tilde{\gamma} + \frac{1}{2} + n')^2]^{1/2}} \,, \tag{5.21}$$

$$= \frac{m}{\left[1 + (\alpha Z)^2 / \left\{(\kappa^2 - (\alpha Z)^2)^{1/2} + \frac{\tilde{\gamma}}{2} + \frac{1}{2} + n'\right\}^2\right]^{1/2}} \,. \tag{5.22}$$

Eq. (5.22) agrees with the energy spectrum given by Eq. 2.46, and reproduces the standard energy eigenvalue relation [101].

We now proceed to find the solution of the Dirac-Coulomb Eq. (5.3) in the first order. We choose sharp eigenvalues for the operators $\hat{K}$ and $\hat{\mathscr{L}}$ and for ρ_3. This is done by choosing the following representation for these operators

$$\rho_3 = -1\,, \tag{5.23}$$

$$\kappa = \tilde{\omega}(j + \frac{1}{2})\,, \tag{5.24}$$

$$\gamma = \tilde{\gamma}[(j+1/2)^2 - (Ze^2)^2]^{1/2}\,, \tag{5.25}$$

$$\tilde{\omega} = \tilde{\gamma}\,. \tag{5.26}$$

When the Coulomb potential is switched off i.e., $Z = 0$, we have $\hat{\mathscr{L}} = -\rho_3\hat{K}$, and solving the iterated Dirac equation yields the free propagator, as was seen in the last Chapter. Now, if we choose ρ_3 to have a value -1, then we must have as a direct consequence of this, $\tilde{\omega} = \tilde{\gamma}$. Owing to the above operator representations, it is seen that the spinors χ^{μ}_{κ} satisfy the eigenvalue problem

$$(\hat{\boldsymbol{\Sigma}} \cdot \hat{\boldsymbol{L}} + 1)\chi^{\mu}_{\kappa} = -\kappa\chi^{\mu}_{\kappa}\,, \tag{5.27}$$

and has the solution

$$\chi^{\mu}_{\kappa} = \sum_{\mu'} \left(\begin{array}{ccc|c} l & & \frac{1}{2} & j \\ \mu-\mu' & & \mu' & \mu \end{array}\right) Y_l^{\mu-\mu'}(\theta,\phi)\chi^{\mu'}_{\frac{1}{2}}\,. \tag{5.28}$$

This can also be written as

$$\chi^{\mu}_{-\kappa} = \sum_{\mu'} \left(\begin{array}{ccc|c} l & & \frac{1}{2} & j \\ \mu-\mu' & & \mu' & \mu \end{array}\right) Y_{l'}^{\mu-\mu'}(\theta,\phi)\chi^{\mu'}_{\frac{1}{2}}\,, \tag{5.29}$$

where l and $l^{'}$ take the values

$$l = j + \frac{1}{2}\tilde{\omega} \quad \text{and} \quad l^{'} = j - \frac{1}{2}\tilde{\omega}\,. \tag{5.30}$$

With the definitions of Eq. (5.30), it is evident that the spinor components in Eqs. (5.28) and (5.29) are actually bispinors, corresponding to the cases $\tilde{\omega} = \pm 1$.

We have also obtained angular wavefunctions as a solution of the eigenvalue equation [81] in Section 4.2.

$$\hat{\mathscr{L}}\left(\hat{\mathscr{L}} + 1\right)|\lambda\rangle = \lambda(\lambda+1)\,|\lambda\rangle\ .$$

We reintroduce the relevant expressions here as done in Section 4.2. The angular wave functions $\langle\theta\phi|\lambda\rangle = \left\langle\theta\phi\middle|j,\mu,\kappa,\tilde{\beta}\right\rangle$ are the simultaneous eigenstates of the operators

$\hat{\mathscr{L}}(\hat{\mathscr{L}}+1)$, $\hat{\boldsymbol{J}}^2$, $\hat{J}_z$, $\hat{K}$ and the β matrix, with the eigenvalues $\lambda(\lambda+1)$, $j(j+1)$, μ, κ and $\tilde{\beta}=\pm 1$, respectively. They can be written in the explicit bispinor form as [77, 80]

$$\left\langle \theta\phi \middle| j,\mu,\kappa,\tilde{\beta}=-1 \right\rangle = \begin{pmatrix} 0 \\ \chi^{\mu}_{\kappa} \end{pmatrix},$$

$$\left\langle \theta\phi \middle| j,\mu,\kappa,\tilde{\beta}=1 \right\rangle = \begin{pmatrix} \chi^{\mu}_{-\kappa} \\ 0 \end{pmatrix},$$

where the χ^{μ}_{κ} are the well-known spherical spinors [102]

$$\chi^{\mu}_{\kappa} = \sum_{\mu'=\pm\frac{1}{2}} C\left(l,\frac{1}{2},j;\mu-\mu',\mu',\mu\right) Y_l^{\mu-\mu'}(\theta,\phi)\chi^{\mu'}_{\frac{1}{2}},$$

expressed in terms of the Clebsch-Gordan coefficients $C(\dots)$, the spherical harmonics $Y_l^{\mu-\mu'}$, and the unit spinors

$$\chi^{\frac{1}{2}}_{\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi^{-\frac{1}{2}}_{\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Now, we can obtain the solution to the first order Dirac-Coulomb Eq. (5.3). Keeping in mind that we have chosen the eigenvalue of the operator ρ_3 to be -1, we can write the eigenfunction for the Eq. (5.5) as

$$\Psi_{\rho_3=-1} = \Psi_- = \begin{bmatrix} 0 \\ \Psi_{\lambda(\gamma)}(\zeta)\chi^{\mu}_{\kappa} \end{bmatrix}. \tag{5.31}$$

To solve the iterated Dirac Eq. (5.6), we had introduced the Martin-Glauber operator, and in Eq. (5.25), we choose sharp eigenvalues for it. This is facilitated by the diagonalization of the operator $\hat{\mathscr{L}}$ in a new basis, which is given by the canonical transformation,

$$S = \exp\left\{ -\frac{1}{2}\rho_2 \hat{\boldsymbol{\Sigma}}\cdot\hat{\mathrm{r}}\tanh^{-1}\left(\frac{Ze^2}{\hat{K}}\right)\right\}, \tag{5.32}$$

called the Biedenharn transformation [78]. The diagonalization gives us

$$S\hat{\mathscr{L}}S^{-1} = -\rho_3\hat{K}\left|\left[1-\left(\frac{Ze^2}{K^2}\right)^2\right]^{1/2}\right|. \tag{5.33}$$

We can thus obtain a solution for the first-order Dirac-Coulomb Eq. (5.3), using this transformation as

$$\psi = S\hat{O}_+S^{-1}\Psi_-, \tag{5.34}$$

where the operator $\hat{O}_+$ is defined in Eq. (5.5) as,

$$\hat{O}_+ = \left[\rho_2\hat{\boldsymbol{\Sigma}}\cdot\boldsymbol{\nabla} - \rho_3(E+Ze^2/\mathrm{r})+m\right].$$

Under the similarity transformation we find [79]

$$S\hat{O}_+S^{-1} = \rho_2\hat{\mathbf{\Sigma}}\cdot\hat{\mathrm{r}}\left[\frac{\partial}{\partial \mathrm{r}} + \frac{1-\gamma\rho_3}{\mathrm{r}} + \rho_3\frac{EZe^2}{\gamma}\right] - \rho_3\frac{E\kappa}{\gamma} + m\,. \tag{5.35}$$

The operator $S\hat{O}_+S^{-1}$ can be represented in matrix format (in ρ space) as

$$S\hat{O}_+S^{-1} = \begin{bmatrix} -\frac{E\kappa}{\gamma} + m & -i\hat{\mathbf{\Sigma}}\cdot\hat{\mathrm{r}}\left[\frac{\partial}{\partial \mathrm{r}} + \frac{1+\gamma}{\mathrm{r}} + \frac{EZe^2}{\gamma}\right] \\ i\hat{\mathbf{\Sigma}}\cdot\hat{\mathrm{r}}\left[\frac{\partial}{\partial} + \frac{1-\gamma}{\mathrm{r}} + \frac{EZe^2}{\gamma}\right] & \frac{E\kappa}{\gamma} + m \end{bmatrix}. \tag{5.36}$$

A recurrence relation is established between $\Psi_{\lambda(\gamma)}$ and $\Psi_{\lambda(-\gamma)}$ which are the two distinct solutions of the iterated Dirac equation for the two different values of γ given in Eq. (5.15) [79]

$$\begin{aligned}\left[\frac{\partial}{\partial \mathrm{r}} + \frac{1+\gamma}{\mathrm{r}} + \frac{EZe^2}{\gamma}\right]\Psi_{\lambda(\gamma)} &= \mu\tilde{\gamma}\left[\left[\frac{EZe^2}{\mu\gamma}\right]^2 - 1\right]^{1/2}\Psi_{\lambda(-\gamma)} \\ &= i\tilde{\gamma}\left[m^2 - \left[\frac{\kappa E}{\gamma}\right]^2\right]^{1/2}\Psi_{\lambda(-\gamma)}\,. \end{aligned}\tag{5.37}$$

Finally, applying Eq. (5.36) to Eq. (5.34) and using the recurrence relation above, we obtain as a solution of the first order Dirac equation

$$\psi = N(\gamma)\begin{bmatrix}\left[m - \frac{\kappa E}{\gamma}\right]^{1/2}\Psi_{\lambda(-\gamma)}\chi^{\mu}_{-\kappa} \\ \tilde{\omega}\left[m + \frac{\kappa E}{\gamma}\right]^{1/2}\Psi_{\lambda(\gamma)}\chi^{\mu}_{\kappa}\end{bmatrix}. \tag{5.38}$$

The normalization constant is evaluated as follows

$$N^2(\gamma)\int_0^\infty \mathrm{r}^2 d\mathrm{r}\left[\left[m - \frac{\kappa E}{\gamma}\right]^{1/2}\Psi^2_{\lambda(-\gamma)} + \left[m + \frac{\kappa E}{\gamma}\right]^{1/2}\Psi^2_{\lambda(\gamma)}\right] = 1\,. \tag{5.39}$$

Since the iterated Dirac wave functions are already normalized, we can obtain the normalization constant from the above equation straightforwardly as

$$\begin{aligned} N(\gamma) = &\left[\frac{16\mu^3}{\omega}\right]\left[\left(\frac{\omega}{4} - \gamma\right)!\left(\frac{\omega}{4} - \gamma - 1\right)!\right]^{-1/2} \\ &\times \quad \left[\left(\frac{\omega}{4} - \gamma\right)\left(\frac{\omega}{4} - \gamma + 1\right)\left(m - \tilde{\omega}\frac{\kappa E}{\gamma}\right) + \left(m + \tilde{\omega}\frac{\kappa E}{\gamma}\right)\right]^{-1/2}. \end{aligned}\tag{5.40}$$

We now justify here the choice of the positive sign in front of the mass term in Eq. (5.1). We have inferred in this Chapter that $\rho_3 = \beta$ and we also have the eigenvalue of the β matrix as $\tilde{\beta} = \pm 1$. In the operator representation laid out in the beginning

of the derivation, we have considered that the eigenvalue of the ρ_3 matrix to be -1 so that we have $\tilde{\beta} = -1$, this then establishes our choice of the positive sign in Eq. (5.1). With this choice, we have $\tilde{\gamma} = \tilde{\omega}$, and in Eq. (5.38) the lower component is the "large" component; in case we considered $\rho_3 = +1$, the first-order Dirac Eq. (5.1) would have the usual negative sign in front of the mass term, since $\tilde{\beta} = 1$ and the wave function in Eq. (5.38) would have the usual solution with the upper component being the "large" component.

The Eq. (5.38) gives us a simplified solution of the Dirac-Coulomb equation and we see that each of the upper and lower component of the eigenfunction is defined by only a single confluent hypergeometric function as defined in Eq. (5.17).

5.2 The Dirac-Coulomb Green's function

The DCGF in the coordinate space has been explicitly defined in the work of Wichmann and Kroll[105], and has also been obtained in the later works by Mohr[126], Gyulassy[106], and Hylton[136]. Its general form has been obtained by Brown and Schaefer[133]. In the solution obtained by Wichmann and Kroll, each component of the DCGF contains four terms since the radial solution, derived using the conventional method devised by Bethe and Salpeter[137] contains two terms for each component. We have, however, obtained in the previous Section a simplified solution of the first-order Dirac-Coulomb equation following the methodology of Wong and Yeh [79]. Using this wave function, the DCGF obtained by eigenfunction expansion method is seen to contain a single term instead of four [122].

We adopt the works of Wong and Yeh [79, 122] in this Thesis since their work not only provides a simple yet elegant form of the solutions, but in the limit that the Coulomb potential is turned off, they produce the usual plane-wave solution of the Dirac equation, can be easily extended to the continuum case and also reduces both the wave function and the Green's function to much simpler forms. They also show that it is possible to obtain the momentum-space representation of the Green's function using their methods, however, since we are interested in the coordinate-space representation of the energy-dependent Green's function, we only present the key points related to it, from their work [122].

We consider that the DCGF, say $G(\mathbf{r}_2, \mathbf{r}_1; E)$, satisfies the inhomogeneous Dirac equation

$$[\mathcal{H}(\mathbf{r}_2) - E]G(\mathbf{r}_2, \mathbf{r}_1, ; E) = \delta^3(\mathbf{r}_2 - \mathbf{r}_1)\,, \tag{5.41}$$

where

$$\mathcal{H}(\mathbf{r}) = SH(\mathbf{r})S^{-1}\,. \tag{5.42}$$

S being the similarity transformation in Eq. (5.32), and

$$H(\mathbf{r}) = \boldsymbol{\alpha} \cdot \mathbf{p} - \beta m + V\,. \tag{5.43}$$

We use the same sign conventions as used in the Section (5.1). Expanding the Green's function in the basis introduced in the last Section, in terms of the angular eigenfunctions

[105, 138] χ^{μ}_{κ} of the Dirac operator $\hat{K}$,having eigenvalues given by $\kappa = \tilde{\omega}(j + \frac{1}{2})$, and $\hat{J}_z$, having eigenvalue μ, we obtain

$$G(\mathbf{r}_2, \mathbf{r}_1; E) = \sum_{\kappa\mu} \begin{pmatrix} G^{1\,1}_{\kappa}(\mathrm{r}_2, \mathrm{r}_1; E) S_2 \chi^{\mu}_{-\kappa}(\hat{\mathrm{r}}_2) \chi^{\mu+}_{-\kappa}(\hat{\mathrm{r}}_1) S_1 & -iG^{1\,2}_{\kappa}(\mathrm{r}_2, \mathrm{r}_1; E) S_2 \chi^{\mu}_{-\kappa}(\hat{\mathrm{r}}_2) \chi^{\mu+}_{\kappa}(\hat{\mathrm{r}}_1) S_1 \\ iG^{2\,1}_{\kappa}(\mathrm{r}_2, \mathrm{r}_1; E) S_2 \chi^{\mu}_{\kappa}(\hat{\mathrm{r}}_2) \chi^{\mu+}_{-\kappa}(\hat{\mathrm{r}}_1) S_1 & G^{2\,2}_{\kappa}(\mathrm{r}_2, \mathrm{r}_1; E) S_2 \chi^{\mu}_{\kappa}(\hat{\mathrm{r}}_2) \chi^{\mu+}_{\kappa}(\hat{\mathrm{r}}_1) S_1 \end{pmatrix}, \tag{5.44}$$

where, the index $i, j = 1, 2$, is used to define the matrix elements and the transformations S_k , $k = 1, 2$, have the same definition as Eq. (5.32) but for different $\hat{\mathrm{r}}_k$. Also, each $G^{ij}_{\kappa}(\mathrm{r}_2, \mathrm{r}_1; E)$ represents the radial components of the full Green's function. The summation over the magnetic angular quantum number or the angular momentum projection μ states yields

$$\Omega_{\kappa,\kappa'}(\theta_2, \phi_2 | \theta_1, \phi_1) = \sum_{\mu} \chi^{\mu}_{\kappa}(\theta_2, \phi_2) \chi^{\mu^{\dagger}}_{\kappa'}(\theta_1, \phi_1)\,. \tag{5.45}$$

χ^{μ}_{κ} represents the angular eigenfunctions that is defined in Eq. (4.17). The expression for the Green's function can now be written as a summation of terms over κ only

$$G(\mathbf{r}_2, \mathbf{r}_1; E) = \sum_{\kappa} \begin{pmatrix} G^{1\,1}_{\kappa}(\mathrm{r}_2, \mathrm{r}_1; E) S_2 \Omega_{-\kappa}(\hat{\mathrm{r}}_2\,, \hat{\mathrm{r}}_1) S_1 & G^{1\,2}_{\kappa}(\mathrm{r}_2, \mathrm{r}_1; E) S_2 i\hat{\boldsymbol{\Sigma}} \cdot \hat{\mathrm{r}}_2 \Omega_{\kappa}(\hat{\mathrm{r}}_2\,, \hat{\mathrm{r}}_1) S_1 \\ -G^{2\,1}_{\kappa}(\mathrm{r}_2, \mathrm{r}_1; E) S_2 i\hat{\boldsymbol{\Sigma}} \cdot \hat{\mathrm{r}}_2 \Omega_{-\kappa}(\hat{\mathrm{r}}_2\,, \hat{\mathrm{r}}_1) S_1 & G^{2\,2}_{\kappa}(\mathrm{r}_2, \mathrm{r}_1; E) S_2 \Omega_{\kappa}(\hat{\mathrm{r}}_2\,, \hat{\mathrm{r}}_1) S_1 \end{pmatrix}. \tag{5.46}$$

We now insert Eq. (5.46) to obtain an inhomogeneous differential equation which is satisfied by $G^{ij}_{\kappa}(\mathrm{r}_2, \mathrm{r}_1; E)$.

$$\begin{bmatrix} \frac{\kappa z}{\gamma} + m & \left[\frac{d}{d\mathrm{r}_2} + \frac{1+\gamma}{\mathrm{r}_2} + \frac{EZe^2}{\gamma}\right] \\ \left[\frac{d}{d\mathrm{r}_2} + \frac{1-\gamma}{\mathrm{r}_2} + \frac{EZe^2}{\gamma}\right] & m - \frac{\kappa z}{\gamma} \end{bmatrix} \begin{bmatrix} G^{11}_{\kappa}(\mathrm{r}_2, \mathrm{r}_1; E) & G^{12}_{\kappa}(\mathrm{r}_2, \mathrm{r}_1; E) \\ G^{21}_{\kappa}(\mathrm{r}_2, \mathrm{r}_1; E) & G^{22}_{\kappa}(\mathrm{r}_2, \mathrm{r}_1; E) \end{bmatrix} = \frac{\delta(\mathrm{r}_2 - \mathrm{r}_1)}{\mathrm{r}_1\,\mathrm{r}_2}\,, \tag{5.47}$$

where, the above form of the Hamiltonian has been obtained in Eq. (5.36).

We now obtain a solution to the radial Green's function through the eigenfunction expansion method. In the Section (5.1), the expression for the bound state wave functions in Eq. (5.38), was obtained as

$$\psi(\tilde{\omega}) = \left(\frac{\kappa E}{\gamma} + m\right)^{1/2} N'(\tilde{\omega}) \zeta^{\lambda(\tilde{\omega})} e^{-\zeta/2} \times 1F1(-n_{\mathrm{r}}, 2\lambda(\tilde{\omega}) + 2, \zeta)\,, \tag{5.48}$$

$$\psi(-\tilde{\omega}) = i\tilde{\omega}\left(\frac{\kappa E}{\gamma} - m\right)^{1/2} N'(-\tilde{\omega})\rho^{\lambda(-\tilde{\omega})}e^{-\zeta/2} \times 1F1(-n_{\rm r}, 2\lambda(\tilde{-\omega}) + 2, \zeta)\,. \tag{5.49}$$

where n_r is defined by Eq. (5.19). The equivalence of these wave functions with the solutions obtained from the Schrödinger equation simply by replacing $\lambda(\pm\tilde{\omega})$ with $l(\pm\tilde{\omega})$ prompts that we can reduce the above wave functions in terms of the normalized Schrödinger wave function R, obtained as a solution of Eq. (5.13) [134], and can write Eq. (5.48) and similarly Eq. (5.49), in a simplified form as [122]

$$\begin{aligned}\psi(\tilde{\omega}) = &\left(\frac{\kappa E}{\gamma} + m\right)^{1/2}\left(\frac{\gamma}{2\kappa E}\right)^{1/2}2^{3/2}m'^{2} \\ &\times \left[\frac{\Gamma(n+\lambda+1)}{2Ze^2E\,\Gamma(n-\lambda)}\right]^{1/2}\frac{1}{\Gamma(2\lambda+2)} \\ &\times \zeta^{\lambda(\tilde{\omega})}e^{-\rho/2}1F1(-n_r, 2\lambda(\tilde{\omega}) + 2, \zeta)\,,\end{aligned} \tag{5.50}$$

where $n = \frac{\omega}{4}$ and all related terms have been defined in Section (5.1).

We also need to take into consideration the continuum wave functions of the homogeneous Dirac-Coulomb equation in order to determine the Green's function over the full spectrum. We have from Ref. [79], the expressions for the continuum wave functions as

$$\psi^{\hat{\zeta}}(\tilde{\omega}) = \left(\frac{\kappa E}{\gamma} + m\right)^{1/2}\phi^{\hat{\zeta}}(k'\mathrm{r})\,, \tag{5.51}$$

$$\psi^{\hat{\zeta}}(\tilde{-\omega}) = i\tilde{\omega}\left(\frac{\kappa E}{\gamma} - m\right)^{1/2}\phi^{\hat{\zeta}}(k'\mathrm{r})\,, \tag{5.52}$$

$$\begin{aligned}\phi^{\hat{\zeta}}(k'\mathrm{r}) = &\frac{\sqrt{2}mk'}{E^{3/2}}\left(\frac{\gamma}{2\pi\kappa}\right)^{1/2}\Gamma(\lambda+1+i\eta)e^{i\sigma} \\ &\times e^{\epsilon_{\hat{\zeta}}\pi\eta/2}(-2ik'\mathrm{r}\epsilon_{\hat{\zeta}})^{-1}M_{i\eta,\lambda+1/2}(-2ik'\mathrm{r}\epsilon_{\hat{\zeta}})\,,\end{aligned} \tag{5.53}$$

where, for the continuum case we have $\frac{\omega}{4} = i\eta = -iZe^2E/k$, where $k' = (E'^2 - m^2)^{1/2}$, the wave function $\phi^{\hat{\zeta}}(k\mathrm{r})$ is normalized in the scale k'. The $e^{i\sigma}$ term arises from the normalized Schrödinger wave function, and

$$\epsilon_{\hat{\zeta}} = \begin{cases} 1 & \text{for} \quad \hat{\zeta} = 1\,, \\ -1 & \text{for} \quad \hat{\zeta} = 2\,. \end{cases} \tag{5.54}$$

The choice of $\epsilon_{\hat{\zeta}}$ determines the "large" and "small" component of the eigenfunction; as was the choice of notation in Section (5.1), -1 denotes the "large" component while

1 denotes the "small" component [122]. Here, a new function M called the Whittaker function [135], has been introduced [122], and is defined as

$$M_{i\eta,\lambda+1/2}(E') = E^{\lambda+1}\frac{e^{\mp z/2}}{\Gamma(2\lambda+2)}1F1(\lambda+1\mp i\eta, 2\lambda(\tilde{\omega})+2, \pm E)\,. \tag{5.55}$$

Along with the Whittaker function M, we also establish the second Whittaker function in terms of M

$$W_{i\eta,\lambda+1/2}(E') = \frac{\pi}{\sin\pi(2\lambda+1)}\left\{\frac{-M_{i\eta,\lambda+1/2}(E')}{\Gamma(-\lambda-i\eta)} + \frac{M_{i\eta,-\lambda-1/2}(E')}{\Gamma(\lambda+1-i\eta)}\right\}. \tag{5.56}$$

The Green's function that is obtained by the eigenfunction expansion method is given by

$$G_\kappa(\mathrm{r}_1,\mathrm{r}_2;E) = \sum_{\hat{\zeta}=1}^{2}\epsilon_{\hat{\zeta}}\int_0^\infty dk'\frac{\psi^{\hat{\zeta}}(k'\mathrm{r}_2)\bar{\psi}^{\hat{\zeta}}(k'\mathrm{r}_1)}{E-\epsilon_{\hat{\zeta}}E'} + \sum_{n_\mathrm{r}}\frac{\psi_{n_\mathrm{r},\kappa}(\mathrm{r}_2)\bar{\psi}_{n_\mathrm{r},\kappa}(\mathrm{r}_1)}{E-E_{n,\kappa}}\,. \tag{5.57}$$

Here, E' represents the continuum energy, and $E_{n,\kappa}$ denotes the bound-state energy spectrum. The Green's function is calculated by integrating over the continuous spectrum. In this context, we define a function J, following the work of Hostler [139] who derived the Green's function for the Klein-Gordon equation, as

$$J_\kappa = \sum_{\hat{\zeta}=1}^{2}\epsilon_{\hat{\zeta}}\int_0^\infty dk'\frac{\phi^{\hat{\zeta}}(k'\mathrm{r}_2)\bar{\phi}^{\hat{\zeta}}(k'\mathrm{r}_1)}{E-\epsilon_{\hat{\zeta}}E'}\,. \tag{5.58}$$

Using the Whittaker-function identity

$$M_{i\eta,\lambda+1/2}(z) = \frac{e^{\pm\pi i k'}\,W_{-i\eta,\lambda+1/2}(Ee^{\pm i\pi})}{\Gamma(\lambda+1-i\eta)} + \frac{e^{\pm i\pi(i\eta-\lambda-1)}\,W_{i\eta,\lambda+1/2}(E)}{\Gamma(\lambda+1+i\eta)}\,, \tag{5.59}$$

one obtains

$$\begin{aligned}
J_\kappa = {}& \frac{m^2}{4\pi\mathrm{r}_1\mathrm{r}_2}\frac{\gamma}{\kappa} \\
&\times\Bigg[\int_0^\infty\frac{dk'}{E'^3}\frac{\Gamma(1+\lambda-i\eta)W_{i\eta,\lambda+\frac{1}{2}}(-2ik'\mathrm{r}_2)e^{-i\pi(\lambda+1)}M_{-i\eta,\lambda+\frac{1}{2}}(2ik'\mathrm{r}_1)}{E-E'} \\
&\quad+\int_0^\infty\frac{dk'}{E'^3}\Gamma(1+\lambda+i\eta)\frac{W_{-i\eta,\lambda+\frac{1}{2}}(2ikr_2)M_{-i\eta,\lambda+\frac{1}{2}}(2ik'\mathrm{r}_1)}{E-E'} \\
&\quad-\int_0^\infty\frac{dk'}{E'^3}\Gamma(1+\lambda+i\eta)\frac{W_{-i\eta,\lambda+\frac{1}{2}}(-2ik'\mathrm{r}_2)M_{-i\eta,\lambda+\frac{1}{2}}(-2ik'\mathrm{r}_1)}{E+E'} \\
&\quad-\int_0^\infty\frac{dk'}{E'^3}\Gamma(1+\lambda-i\eta)\frac{W_{i\eta,\lambda+\frac{1}{2}}(2ik'\mathrm{r}_2)e^{i\pi(\lambda+1)}M_{-i\eta,\lambda+\frac{1}{2}}(-2ik'\mathrm{r}_1)}{E+E'}\Bigg]\,.
\end{aligned} \tag{5.60}$$

Changing the integral variable from k' to $E' = (k'^2+m^2)^{\frac{1}{2}}$ for the integrals with positive sign in Eq. (5.60), and to $E' = -(k'^2+m^2)^{\frac{1}{2}}$ for the negatively-signed integrals we have

$$\begin{aligned} J_\kappa = \frac{m^2}{4\pi \mathrm{r}_1\mathrm{r}_2}\frac{\gamma}{\kappa}\Bigg[& \int_\infty^m \frac{dE'}{k'E'^2}\frac{\Gamma(1+\lambda-i\eta)W_{i\eta,\lambda+\frac{1}{2}}(-2ik'\mathrm{r}_2)M_{i\eta,\lambda+\frac{1}{2}}(-2ik'\mathrm{r}_1)}{E'-E} \\ & - \int_m^\infty \frac{dE'}{k'E'^2}\frac{\Gamma(1+\lambda+i\eta)W_{-i\eta,\lambda+\frac{1}{2}}(2ik'\mathrm{r}_2)M_{-i\eta,\lambda+\frac{1}{2}}(2ik'\mathrm{r}_1)}{E'-E} \\ & + \int_{-\infty}^{-m} \frac{dE'}{k'E'^2}\frac{\Gamma(1+\lambda-i\eta)W_{i\eta,\lambda+\frac{1}{2}}(-2ik'\mathrm{r}_2)M_{i\eta,\lambda+\frac{1}{2}}(-2ik'\mathrm{r}_1)}{E'-E} \\ & - \int_{-m}^{-\infty} \frac{dE'}{k'E'^2}\frac{\Gamma(1+\lambda+i\eta)W_{-i\eta,\lambda+\frac{1}{2}}(2ik'\mathrm{r}_2)e^{i\pi(\lambda+1)}M_{-i\eta,\lambda+\frac{1}{2}}(2ik'\mathrm{r}_1)}{E'-E}\Bigg] . \end{aligned} \tag{5.61}$$

From Eq. (5.61), we see that in the complex plane, E' has two branch cuts lying between $-\infty < E' \leq -m$ and $m \leq E' < \infty$. We define k', in the complex plane, for the general values of E' and $\mathrm{Im}\, k' > 0$ for all E' on this cut plane [122]. The integrands in the definition for J_κ can thus be collapsed into one single function when evaluating above the positive energy branch cut or below the negative energy branch cut, and is given as,

$$\frac{m^2}{4\pi \mathrm{r}_1\mathrm{r}_2}\frac{\gamma}{\kappa}\frac{\Gamma(1+\lambda-i\eta)W_{i\eta,\lambda+\frac{1}{2}}(-2ik'\mathrm{r}_2)M_{i\eta,\lambda+\frac{1}{2}}(-2ik'\mathrm{r}_1)}{k'E'^2(E'-E)} . \tag{5.62}$$

This can be interpreted as a contour integral of the above function, the contour consisting of two disconnected parts that run along the branch cuts in the positive and negative halves of the complex plane such that they encircle the branchpoints $E' = \pm m$ in the counterclockwise direction. The asymptotic behaviour of the Whittaker functions, M, regular at the origin, and W, which shows regularity at infinity, allows one to evaluate the asymptotic behaviour of the integrand given by Eq. (5.62) of the contour integral as $|E'| \to \infty$. We find that as long as $\mathrm{r}_2 > \mathrm{r}_1$, we can close the contour on the 'upper' and 'lower' halves of the complex plane, by a semicircle, for both the halves, "at infinity" [122]. This requires the condition $\mathrm{Re}(k') > 0$ to be satisfied. The expression for the function J_κ can thus be given as

$$J_\kappa = \frac{m^2\gamma}{4\pi\kappa}\oint \frac{dE'}{\mathrm{r}_1\mathrm{r}_2}\frac{\Gamma(1+\lambda-i\eta)W_{i\eta,\lambda+\frac{1}{2}}(-2ik'\mathrm{r}_2)M_{i\eta,\lambda+\frac{1}{2}}(-2ik'\mathrm{r}_1)}{k'E'^2(E'-E)} , \tag{5.63}$$

$$\text{for} \quad \mathrm{r}_2 > \mathrm{r}_1 .$$

Finally evaluating the residue at the poles of the gamma function, which occur at the bound-state energy levels, and a double pole that arises at $E' = 0$, it was seen that this term exactly cancels the bound-state wave function term on the R.H.S. of Eq. (5.57), and we arrive at the standard form [105] of the Green's function for the first-order

Dirac-Coulomb equation in the coordinate space as

$$G_{\kappa}^{ij}(\mathrm{r}_2,\mathrm{r}_1;E) = f(i\,j)\frac{m^2\gamma}{2i\kappa}\frac{1}{\mathrm{r}_1\mathrm{r}_2(E^2-m^2)^{1/2}E^2}\Gamma(1+\lambda-i\eta) \\ \times W_{i\eta,\lambda+1/2}(-2ik\mathrm{r}_2)M_{i\eta,\lambda+1/2}(-2ik\mathrm{r}_1)\,, \qquad (5.64)$$

$$\text{for } \mathrm{r}_2 > \mathrm{r}_1,\ \ \eta = \frac{Ze^2E}{k},\ \ k = (E^2-m^2)^{1/2},\ \ \mathrm{Im}(k) > 0\,.$$

Here,

$$f(i\,j) \simeq \begin{cases} \left(\frac{\kappa E}{\gamma}+m\right)^{\frac{1}{2}}\,, & \text{for} \quad i,j=2\,, \\ i\tilde{\omega}\left(\frac{\kappa E}{\gamma}-m\right)^{\frac{1}{2}}\,, & \text{for} \quad i,j=1\,, \end{cases} \qquad (5.65)$$

and λ in the Green's function is a function of $\tilde{\omega}$; for $i,j=2$, $\lambda=\lambda(\tilde{\omega})$ and for $i,j=1$, $\lambda=\lambda(-\tilde{\omega})$, denoting the "large" and "small" component of the eigenfunction of the Dirac-Coulomb Hamiltonian.

This closed form solution of the DCGF is obtained for the point-like nucleus. For extended nuclear models, the derivation becomes quite complicated and numerical evaluation of the bound and continuum wave functions is required to construct the Green's function.

Having arrived at the analytical form of the DCGF in Eq. (5.64), we now try to reconstruct this in the framework of path integrals.

5.3 Path Integral representation of the DCGF

The Feynman path integral approach to the various quantum mechanical problems seemed to be severly limited in the scope of its application owing to the lack of solutions for the Hydrogen atom and the spin problem until Duru and Kleinert [140] provided a complete and exact solution to the Hydrogen atom problem, in three dimensions in the non-relativistic regime, that involved the reparametrization of the paths by local time rescaling and a change of the integration variables through the Kustaanheimo-Stiefel transformations [141].

We follow in this Section the work of Inomata and Kayed [80] exactly, where they take into account the methodology by Duru and Kleinert [140] and proceed with the path integral representation of a Dirac particle in a Coulomb potential. The derivation of the DCGF closely follows the works of Martin and Glauber [81] and Biedenharn [77, 78] where they use the iterated or second-order Dirac-Coulomb equation and reduce the associated iterated Green's function, through a canonical basis transformation called the Biedenharn transformation, into a form analogous to the non-relativistic Schrödinger equation. This similarity is established by the introduction of a modified form of the Martin-Glauber operator. The reduced Green's function is then cast into the form of a radial path integral. The effective Hamiltonian, obtained following Ref. [122], as done in Section 5.2, is similar to the non-relativistic Hydrogen atom Hamiltonian. Following

Duru and Kleinert, the radial path integral is converted from Coulomb to that of an isotropic harmonic oscillator through coordinate transformation along with local time rescaling [80, 140]. An explicit path integral representation of the Dirac-Coulomb Green's function is obtained along with the energy spectrum of the Dirac-Coulomb system in the bound state. We have also used for reference further works of Inomata et al. [142][143].

The Dirac equation with a Coulomb potential is expressed as,

$$(E - \boldsymbol{\alpha} \cdot \hat{\mathbf{p}} - \beta m - V)\psi = 0\,. \tag{5.66}$$

It is to be noted that the above equation is different to the Dirac-Coulomb Eq. (5.1). Here, we use the conventional form unlike the one used in Section 5.1, which was constructed following Ref. [79]. The energy-dependent Green's function $G(\mathbf{r}_2, \mathbf{r}_1; E)$ satisfies the inhomogeneous Dirac-Coulomb equation,

$$(m - \hat{M})G(\mathbf{r}_2, \mathbf{r}_1; E) = \delta(\mathbf{r}_2 - \mathbf{r}_1)\,, \tag{5.67}$$

where, $\hat{M} = -\beta\boldsymbol{\alpha} \cdot \hat{\mathbf{p}} + \beta(E + Ze^2/\mathrm{r})$. A basis transformation is done following Biedenharn [78]

$$\hat{M}_s = S\hat{M}S^{-1}\,, \tag{5.68}$$

$$\psi_s = S\psi\,. \tag{5.69}$$

where S is given by Eq. (5.32). We can now write Eq. (5.66) in this new basis without altering its physical meaning. This gives us

$$(m - \hat{M}_s)\psi_s = 0\,. \tag{5.70}$$

Rewriting the Green's function in coordinate representation gives us

$$\langle \mathbf{r}_2 |\, \hat{G}\, | \mathbf{r}_1 \rangle = [m + \hat{M}_s]\, \langle \mathbf{r}_2 |\, \hat{g}\, | \mathbf{r}_1 \rangle\ , \tag{5.71}$$

where, the Green's function for the iterated Dirac-Coulomb Eq. (5.6), $g(\mathbf{r}_2, \mathbf{r}_1; E)$, is same in form to the one given in Eq. (4.4), but with the operator $\hat{M}$ being the one as defined above. Now, the Green's function for the second-order Dirac equation or the iterated Dirac equation is represented in integral form as

$$\langle \mathbf{r}_2 |\, \hat{g}\, | \mathbf{r}_1 \rangle = \frac{i}{2m} \int_0^\infty \langle \mathbf{r}_2 |\, e^{-i\hat{H}u}\, | \mathbf{r}_1 \rangle\, du\,. \tag{5.72}$$

In the above equation, the integration is done with respect to the time-like parameter u and the integrand can be interpreted as a propagator that describes a system that evolves with the parameter u and has an effective Hamiltonian, $\hat{H}$, which is defined as $\hat{H} = (m^2 - \hat{M}_s{}^2)/2m$. As done in Section 4.2, we try to express the integral in Eq. (5.72) in terms of a radial path integral.

We diagonalize the Hamiltonian in the integrand of Eq. (5.72) by using a similarity transformation defined by Biedenharden [78], as done in Section 5.2, using the radial

momentum operator $\hat{p}_r$, the component of the Dirac matrix $\boldsymbol{\alpha}$ in the direction $\mathbf{r}$, the Dirac operator $\hat{K}$, and the Martin-Glauber operator $\hat{\mathscr{L}}$

$$S\hat{H}S^{-1} = \frac{\hat{p}_{\mathrm{r}}^2}{2m} + \frac{\hat{\mathscr{L}}(\hat{\mathscr{L}}+1)}{2m\mathrm{r}^2} - \frac{Ze^2E}{m\mathrm{r}} - \frac{k^2}{2m}\,, \tag{5.73}$$

where,

$$k^2 = E^2 - m^2\,, \tag{5.74a}$$

$$\hat{p}_{\mathrm{r}} = \frac{\mathbf{r}\cdot\hat{\mathbf{p}} - i}{\mathrm{r}}\,, \tag{5.74b}$$

$$\hat{K} = \beta(\hat{\boldsymbol{\Sigma}}\cdot\hat{\mathbf{L}} + 1)\,, \tag{5.74c}$$

$$\hat{\mathscr{L}} = -(\beta\hat{K} + iZe^2\alpha_{\mathrm{r}}); \quad \text{for} \quad \alpha_{\mathrm{r}} = \frac{\boldsymbol{\alpha}\cdot\mathbf{r}}{\mathrm{r}}\,. \tag{5.74d}$$

The Eq. (5.73) bears semblance to the free Hamiltonian in Eq. (4.19), with only the addition of the Coulomb term.

In Eq. (5.33), we have seen that the Martin-Glauber operator $\hat{\mathscr{L}}$ has been diagonalised using Biedenharn's transformation[77, 78], S. The operator $\hat{\mathscr{L}}(\hat{\mathscr{L}}+1)$ can be diagonalised similarly using the similarity transformation S, such that the eigenvalue equation,

$$S\hat{\mathscr{L}}(\hat{\mathscr{L}}+1)S^{-1}\left|\lambda\right\rangle = \lambda(\lambda+1)\left|\lambda\right\rangle\,, \tag{5.75}$$

is fulfilled [81]. Here, λ is defined as a function of γ, given in Eq. (5.16), which is the eigenvalue of the operator $\hat{\mathscr{L}}$, and is given by the Eq. (5.15). The Green's function for the iterated Dirac equation, given in Eq. (5.72), can be expressed as a partial wave expansion, as shown below

$$\left\langle\mathbf{r}_2\right|\hat{g}\left|\mathbf{r}_1\right\rangle = \sum_{\lambda}\left\langle\theta_2\phi_2|\lambda\right\rangle\left\langle\mathrm{r}_2\right|\hat{g}_\lambda\left|\mathrm{r}_1\right\rangle\left\langle\lambda|\theta_1\phi_1\right\rangle\,. \tag{5.76}$$

The radial Green's function in the above equation can be expressed as

$$\left\langle\mathbf{r}_2\right|\hat{g}_\lambda\left|\mathbf{r}_1\right\rangle = \frac{i}{2m}\int\left\langle\mathrm{r}_2\right|e^{-i\hat{H}_\lambda u}\left|\mathrm{r}_1\right\rangle du\,, \tag{5.77}$$

where the operator $\hat{H}_\lambda$ is defined as

$$\hat{H}_\lambda = \frac{\hat{p}_{\mathrm{r}}^2}{2m} + \frac{\lambda(\lambda+1)}{2m\mathrm{r}^2} - \frac{Ze^2E}{m\mathrm{r}} - \frac{k^2}{2m}\,. \tag{5.78}$$

This radial propagator in Eq. (5.77), that is undergoing a u evolution, is very similar in form to the radial propagator for the non-relativistic Hydrogen atom [125] except for that fact that the constant term in Eq. (5.78) is missing in the Hamiltonian of the latter case. The angular wavefunctions have been discussed extensively in Eqs. (4.16)-(4.18) in Section 4.2, and in Eqs. (5.27)-(5.30) in Section 5.1, and we refer to them for the construction of Eq. (5.76), which can now be written by substituting the expression for

the Hamiltonian from Eq. (5.78) in the equation for the radial Green's function given by Eq. (5.77), and using the angular wave functions, to obtain the iterated Green's function as below

$$\langle \mathbf{r}_2|\, \hat{g}\, |\mathbf{r}_1\rangle = \sum_{\mu,\kappa} \langle \mathrm{r}_2|\, \hat{g}_\lambda\, |\mathrm{r}_1\rangle\, \chi^{\mu}_{\kappa}(\theta_2,\phi_2)\chi^{\mu\dagger}_{\kappa'}(\theta_1,\phi_1)\beta^2\,. \tag{5.79}$$

Summing over all angular momentum states, we can write the component spinor as

$$\sum_{\mu} \chi^{\mu}_{\kappa}(\theta_2,\phi_2)\chi^{\mu\dagger}_{\kappa'}(\theta_1,\phi_1) = \Omega^{j}_{\kappa,\kappa'}(\theta_2\phi_2|\theta_1\phi_1)\,. \tag{5.80}$$

Thus Eq. (5.79) can be written as

$$\langle \mathbf{r}_2|\, \hat{g}\, |\mathbf{r}_1\rangle = \sum_{j,\kappa} \langle \mathrm{r}_2|\, \hat{g}_\lambda\, |\mathrm{r}_1\rangle\, \Omega^{j}_{\kappa,\kappa'}(\theta_2\phi_2|\theta_1\phi_1)\beta^2\,. \tag{5.81}$$

This solution of the iterated Dirac equation is obtained following Biedenharn [77, 78].

We now proceed with deriving the first-order Green's function in the path integral formalism. We divide the entire integration interval of the radial propagator in Eq. (5.77) into smaller intervals of time and represent the integrand as

$$\langle \mathrm{r}_2|\, e^{-i\hat{H}_\lambda u}\, |\mathrm{r}_1\rangle = (\mathrm{r}_1\mathrm{r}_2)^{-1} \lim_{N\to\infty} \int \exp\left[i\sum_{j=1}^{N} S(t_j)\right] \prod_{j=1}^{N}\left[\frac{m}{2\pi i t_j}\right]^{1/2} \prod_{j=1}^{N-1} d\mathrm{r}_j\,. \tag{5.82}$$

In the above equation, the term $S(t_j)$ is the radial action term for a very short time interval $t_j = u_j - u_{j-1}$. Following Section 4.2, the total path is divided into N intervals such that $\mathrm{r}_0 = \mathrm{r}_1$ and $\mathrm{r}_N = \mathrm{r}_2$ and $u = \sum t_j$. The radial action term is given as

$$S(t_j) = \frac{m(\Delta \mathrm{r}_j)^2}{2t_j} - \frac{\lambda(\lambda+1)t_j}{2m\mathrm{r}_j\mathrm{r}_{j-1}} + \frac{Ze^2Et_j}{m\mathrm{r}_j} + \frac{(E^2-m^2)t_j}{2m}\,. \tag{5.83}$$

The presence of the Coulomb term in the action complicates the integration in Eq. (5.82), since there is no known closed form solution to this form of the integrand. We try to circumvent the problem posed by the Coulomb potential by replacing the radial variable r_j by $\rho_j = (r_j)^{1/2}$ and the local time slicing parameter t_j by $\sigma_j = t_j/4\bar{r_j}$, where $\bar{r_j} = (r_j r_{j-1})^{1/2} = \rho_j\rho_{j-1} = \rho_j^2$ following Ref. [80]. This is the coordinate transformation and local time rescaling operation suggested by Duru and Kleinert [140]. The action term can now be represented as

$$S(\tau_j) = \frac{m(\Delta\rho_j)^2}{2\sigma_j} + \frac{m(\Delta\rho_j)^4}{8\sigma_j{\bar{\rho}_j}^2} - \frac{2\lambda(\lambda+1)\sigma_j}{m{\bar{\rho}_j}^2} + 4\frac{Ze^2E}{m}\sigma_j - \frac{1}{2}m\omega^2{\bar{\rho}_j}^2\sigma_j\,, \tag{5.84}$$

$$\tag{5.85}$$

where $\omega = \frac{2ik}{m}$. The measure of the integrand in the Eq. (5.82) also changes according to the modified variables and is expressed as

$$\prod_{j=1}^{N}\left[\frac{m}{2\pi i t_j}\right]^{1/2} \prod_{j=1}^{N-1} d\mathrm{r}_j = (4\rho_1\rho_2)^{-1/2} \prod_{j=1}^{N}\left[\frac{m}{2\pi i\sigma_j}\right]^{1/2} \prod_{j=1}^{N-1} d\rho_j\,. \tag{5.86}$$

As seen in Section 4.2, the second term in the modified radial action expression contains ρ_j raised to its fourth power which causes the integral to blow up. Rewriting Eq. (5.82) in terms of the modified action (5.84) and using the integration measure from Eq. (5.86), we get

$$\begin{aligned}\langle \mathrm{r}_2|\, e^{-i\hat{H}_\lambda u}\,|\mathrm{r}_1\rangle = (\rho_1\rho_2)^{-2}\lim_{N\to\infty}\int \exp\Bigg[i\sum_{j=1}^{N}\frac{m(\Delta\rho_j)^2}{2\sigma_j}+\frac{m(\Delta\rho_j)^4}{8\sigma_j(\bar{\rho_j})^2}\\ -\frac{2\lambda(\lambda+1)\sigma_j}{m(\bar{\rho_j})^2}+4\frac{Ze^2E}{m}\sigma_j\\ -\frac{1}{2}m(\omega)^2(\bar{\rho_j})^2\sigma_j\Bigg](4\rho_1\rho_2)^{-1/2}\prod_{j=1}^{N}\left[\frac{m}{2\pi\iota\sigma_j}\right]^{1/2}\prod_{j=1}^{N-1}d\rho_j\,. \end{aligned}\tag{5.87}$$

We address the problem posed by ρ_j^4, by implementing integration techniques for higher-order transcendental functions [92, 131] as given in the equation below

$$\begin{aligned}\int x^{2n}\exp\big[-Ax^2+Bx^4+\mathscr{O}(x^6)\big]dx\\ =\int x^{2n}\exp\left[-Ax^2+\frac{3}{4}BA^{-2}+\mathscr{O}(A^{-3})\right]dx\,,\end{aligned}\tag{5.88}$$

where n takes integer values and Re $A>0$. This allows the fourth powered term to be represented by an equivalent term given by $-3\sigma_j/(8m\bar{\rho_j}^2)$ and we obtain the Eq. (5.87) in the form

$$\begin{aligned}\langle \mathrm{r}_2|\, e^{-i\hat{H}_\lambda u}\,|\mathrm{r}_1\rangle = (\rho_1\rho_2)^{-2}\lim_{N\to\infty}\int \exp\Bigg[i\sum_{j=1}^{N}\frac{m(\Delta\rho_j)^2}{2\sigma_j}-\frac{3\sigma_j}{8m(\bar{\rho_j})^2}\\ -\frac{2\lambda(\lambda+1)\sigma_j}{m(\bar{\rho_j})^2}+4\frac{Ze^2E}{m}\sigma_j\\ -\frac{1}{2}m(\omega)^2(\bar{\rho_j})^2\sigma_j\Bigg](4\rho_1\rho_2)^{-1/2}\prod_{j=1}^{N}\left[\frac{m}{2\pi\iota\sigma_j}\right]^{1/2}\prod_{j=1}^{N-1}d\rho_j\,.\end{aligned}\tag{5.89}$$

The above equation can be rewritten as

$$\begin{aligned}\langle \mathrm{r}_2|e^{-i\hat{H}_\lambda u}\,|\mathrm{r}_1\rangle = \frac{1}{2}(\rho_1\rho_2)^{-5/2}\exp\left[4i\frac{Ze^2E}{m}\sigma\right]\lim_{N\to\infty}\int\exp\Bigg[i\sum_{j=1}^{N}\frac{m(\Delta\rho_j)^2}{2\sigma_j}\\ -\frac{3\sigma_j}{8m(\bar{\rho_j})^2}-\frac{2\lambda(\lambda+1)\sigma_j{}^2}{m(\bar{\rho_j})^2}-\frac{1}{2}m(\omega)^2(\bar{\rho_j})^2\sigma_j\Bigg]\prod_{j=1}^{N}\left[\frac{m}{2\pi i\sigma_j}\right]^{1/2}\prod_{j=1}^{N-1}d\rho_j\,.\end{aligned}\tag{5.90}$$

Expressing this equation in a simpler form we obtain

$$\langle \mathrm{r}_2|\, e^{-i\hat{H}_\lambda u}\,|\mathrm{r}_1\rangle = \frac{1}{2}(\rho_1\rho_2)^{-3/2}\exp\left[4i\frac{Ze^2E}{m}\sigma\right]\tilde{K_\lambda}(\rho_2,\rho_1;\sigma)\,,\tag{5.91}$$

where the propagator with the σ evolution, $\tilde{K}$, is defined as

$$\tilde{K_\lambda}(\rho_2,\rho_1;\sigma) = (\rho_1\rho_2)^{-1}\lim_{N\to\infty}\int \exp\left[i\sum_{j=1}^{N}\tilde{S}(\sigma_j)\right]\prod_{j=1}^{N}\left[\frac{m}{2\pi\iota\sigma_j}\right]^{1/2}\prod_{j=1}^{N-1}d\rho_j\,, \quad (5.92)$$

and the modified action term is now given as

$$\tilde{S}(\sigma_j) = \frac{m(\Delta\rho_j)^2}{2\sigma_j} - \frac{\lambda^{'}(\lambda^{'}+1)\sigma_j}{2m(\bar{\rho_j})^2} - \frac{1}{2}m\omega^2(\bar{\rho_j})^2\sigma_j\,, \quad (5.93)$$

where $\lambda^{'} = 2\lambda + 1/2$. This effective-action term is now analogous to the radial-action term of a three-dimensional isotropic-harmonic oscillator [130]. Thus, the propagator in Eq. (5.77), which is evolving with u, has now been reduced to the propagator for an isotropic-harmonic oscillator in the above equation, and can be now be derived following Ref. [80], and thus we obtain the radial propagator as

$$\begin{aligned}\tilde{K_\lambda}(\rho_2,\rho_1;\sigma) &= -i(\rho_1\rho_2)^{-1/2}(m\omega)\csc(\omega\sigma)\\ &\times\exp\left[\frac{1}{2}im\omega(\rho_1^2+\rho_2^2)\cot(\omega\sigma)\right]I_{\lambda'+1/2}[-im\omega\rho_1\rho_2\csc(\omega\sigma)]\,. \quad (5.94)\end{aligned}$$

Substituting the value of the radial propagator from the above equation into Eq. (5.91) yields

$$\begin{aligned}\langle \mathrm{r}_2|e^{-i\hat{H}_\lambda u}|\mathrm{r}_1\rangle &= \frac{1}{2}(\rho_1\rho_2)^{-2}\exp\left(\frac{iZe^2Et}{m\rho_1\rho_2}\right)(2k)\csc\left(\frac{2ikt}{4m\rho_1\rho_2}\right)\\ &\times\exp\left[-k(\rho_1^2+\rho_2^2)\cot\left(\frac{2ikt}{4m\rho_1\rho_2}\right)\right]I_{\lambda'+1/2}\left[2k\rho_1\rho_2\csc\left(\frac{2ikt}{4m\rho_1\rho_2}\right)\right]\,. \quad (5.95)\end{aligned}$$

Using this value of the integrand in Eq. (5.77) gives us the radial component of the iterated Green's function as

$$\begin{aligned}\langle \mathrm{r}_2|\,\hat{g}_\lambda\,|\mathrm{r}_1\rangle &= (r_1r_2)^{-1/2}\int\exp(-2pq)\exp[ik(r_1+r_2)\coth q]\\ &\times I_{2\lambda+1}[-2\iota k(r_1r_2)^{1/2}\operatorname{csch} q]\operatorname{csch} q\,dq\,, \quad (5.96)\end{aligned}$$

where

$$\rho_1^2 = \mathrm{r}_1\,, \quad (5.97a)$$

$$\rho_2^2 = \mathrm{r}_2\,, \quad (5.97b)$$

$$m\omega = 2ik\,, \quad (5.97c)$$

$$\sigma = \frac{t}{4\rho_1\rho_2} = \frac{\tau}{4(\mathrm{r}_1\mathrm{r}_2)^{1/2}}\,, \quad (5.97d)$$

$$p = \frac{-imZe^2Ek}{m}\,, \quad (5.97e)$$

$$q = \frac{kt}{(4\mathrm{r}_1\mathrm{r}_2m^2)^{1/2}}\,. \quad (5.97f)$$

The type of integral equation in Eq. (5.96) has been solved in multiple works by Inomata [80, 125] and the solution can be readily obtained from [92, 131, 135] and has the form

$$\int \exp(-2pq)\exp[ik(\mathrm{r}_1+\mathrm{r}_2)\coth q]I_{2\lambda+1}[-2ik(\mathrm{r}_1\mathrm{r}_2)^{1/2}\operatorname{csch} q]\operatorname{csch} q\, dq = \frac{\Gamma(p+\lambda+1)}{2ik(\mathrm{r}_1\mathrm{r}_2)^{1/2}\Gamma(2\lambda+2)}M_{-p,\lambda+1/2}(-2ik\mathrm{r}_2)W_{-p,\lambda+1/2}(-2ik\mathrm{r}_1)\,. \quad (5.98)$$

We use this solution of the integral and substitute it in Eq. (5.96), which reduces the radial Green's function to a closed form and obtain the value of the radial propagator for the case $(r_1 > r_2)$ as

$$\langle \mathrm{r}_2|\,\hat{g}_\lambda\,|\mathrm{r}_1\rangle = \frac{\Gamma(p+\lambda+1)}{2ik\mathrm{r}_1\mathrm{r}_2\Gamma(2\lambda+2)}M_{-p,\lambda+1/2}(-2ik\mathrm{r}_2)W_{-p,\lambda+1/2}(-2ik\mathrm{r}_1)\,, \quad (5.99)$$

where M and W are the Whittaker functions [131]. The result obtained in the above equation is analogous to the result obtained by Hostler [139] in the Furry picture approximation.

The energy-dependent Green's function of the first-order Dirac equation, given by Eq. (5.67), can now be very simply obtained. We observe that, since we have used Biedenharden's transformation to diagonalize the Martin-Glauber operator $\hat{\mathscr{L}}$, this implicitly diagonalises $\hat{K}$. Thus the operator $\hat{M}_s$, when acting upon the eigenstates of $\hat{K}$, is represented as [80]

$$\hat{M}_s = i\beta\alpha_\mathrm{r}\left[\frac{\partial}{\partial \mathrm{r}}+\frac{1-\gamma\beta}{r}+\frac{Ze^2E}{\gamma}\beta\right]+\frac{\kappa E}{\gamma}\beta\,. \quad (5.100)$$

Furthermore, it is also observed that the Whittaker function $M_{\lambda(\gamma)}$ satisfies the recurrence relations given by [80]

$$D_\pm[\mathrm{r}^{-1}M_{\lambda(\pm\gamma)}] = \pm i\tilde{\gamma}\left[m^2-\left(\frac{\kappa E}{\gamma}\right)^2\right][\mathrm{r}^{-1}M_{\lambda(\mp\gamma)}]\,, \quad (5.101)$$

where

$$D_\pm = \frac{d}{d\mathrm{r}}+\frac{1\pm\gamma}{\mathrm{r}}\mp\frac{Ze^2E}{\gamma}\,. \quad (5.102)$$

Thus, substituting Eq. (5.99) into Eq. (5.81), we obtain

$$\langle \mathbf{r}_2|\,\hat{g}\,|\mathbf{r}_1\rangle = \sum_{j,\kappa}\frac{\Gamma(p+\lambda+1)}{2ik\mathrm{r}_1\mathrm{r}_2\Gamma(2\lambda+2)}M_{-p,\lambda+1/2}(-2ik\mathrm{r}_2)W_{-p,\lambda+1/2}(-2ik\mathrm{r}_1) \times\Omega^j_{\kappa,\kappa'}(\theta_2\phi_2|\theta_1\phi_1)\beta^2\,. \quad (5.103)$$

Finally the Dirac-Coulomb Green's function is obtained from the iterated Green's func-

tion using Eq. (5.71), and the relations given in Eqs. (5.100) and (5.101), as

$$\langle \mathbf{r}_2 | \hat{G} | \mathbf{r}_1 \rangle = \sum_{j,\kappa} \frac{\Gamma(p+\lambda+1)}{2ik\mathrm{r}_1\mathrm{r}_2\Gamma(2\lambda+2)} W_{-p,\lambda+1/2}(-2ik\mathrm{r}_1)$$
$$\times \Bigg\{ \left[m - \frac{\kappa E}{\gamma} \right] M_{-p,\lambda+1/2}(-2ik\mathrm{r}_2)\Omega^{j}_{\kappa,\kappa}(\theta_2\phi_2|\theta_1\phi_1)\beta^2$$
$$-k\,\tilde{\gamma} M_{-p,\bar{\lambda}+1/2}(-2ik\mathrm{r}_2)\Omega^{j}_{\kappa,-\kappa}(\theta_2\phi_2|\theta_1\phi_1)\alpha_1\alpha_2\alpha_3 \Bigg\} . \quad (5.104)$$

where $\lambda = \lambda(\gamma)$ and $\bar{\lambda} = \lambda(-\gamma)$. Thus, we have obtained the Dirac-Coulomb Green's function, as a solution of the first order Dirac equation, represented by the path integral formalism following Ref. [80].

The poles of the Γ function in Eq. (5.104) correspond directly to the bound state energy levels [122]. The poles arise in the Γ function when

$$p + \lambda + 1 = -n\,, \qquad n = 0, 1, 2, ... \quad (5.105)$$

where $p = -iZe^2E(E^2 - m^2)^{-1/2}$. From this relation, one obtains the standard energy spectrum [101] in the form

$$E_{nj} = m[1 + Z^2e^4(n+\lambda)^{-2}]^{-1/2}\,.$$

where $\lambda \equiv |\gamma| + \frac{1}{2}(\mathrm{sign}\gamma - 1)$, and $\gamma = \left[\left(j + \frac{1}{2}\right)^2 - (Ze^2)^2 \right]^{\frac{1}{2}}$.

We can thus obtain the energy-dependent expression for the DCGF using the path integral formulation and can also extract the bound-state spectrum. This expression of the DCGF in the closed form is then used in further derivations of the Lamb shift at the one loop level, as we will see in the following Chapters.

6. Radiative corrections at the one-loop level – Vacuum polarization

Vacuum polarization shift

The dominant radiative shift to the spectra of HCIs is made up of two contributions, the self-energy correction and the vacuum polarization correction, which together comprise the Lamb shift at the single-loop level. While the self-energy correction plays the most relevant role in defining radiative shifts in bound state energies, the inclusion of vacuum polarization correction provides for improved electron binding-energy values. At the lowest order, the vacuum polarization correction is given by the Uehling correction. In this Chapter, we study the effect of the Uehling potential as a perturbation to the electronic energy states in the Furry picture [76].

Bound states are innately non-perturbative in nature. The perturbative framework of quantum field theory overlooks the intricacies of the non-perturbative effects that show up in the study of bound states, especially for heavy HCIs, and is therefore not a good approximation to study bound states. We intend to overcome this existing disagreement between the intrinsically nonpertubative bound states and the perturbative nature of quantum electrodynamics (QED). We use Feynman's path integral formalism [144] in the relativistic regime [145–152], wherein, the time-sliced formulation of path integrals ensures that all the essentials of renormalized physics are preserved. To this effect, we treat the path integrals perturbatively and we proceed by summing the perturbative expansion to all orders [153, 154] in order to obtain non-perturbative results from this evidently perturbative formalism.

6.1 Schwinger-Dyson equations for photon self-energy

We begin this Section by deriving the complete expression for the vacuum polarization correction to the photon propagtor or the photon self-energy. This is done by defining the Schwinger-Dyson equation for the photon propagator using path integrals in analogy to Ref. [82].

The well-known guage-fixed QED Lagrangian is given as

$$\mathcal{L}_{\text{QED}}(x) = A_\mu(x)\left[g^{\mu\nu}\partial^2 + \left(\frac{1}{\xi} - 1\right)\partial^\mu\partial^\nu\right]A_\nu(x) + \bar{\psi}(x)(i\not{D} - m)\psi(x)\,. \tag{6.1}$$

where D_μ, being the covariant derivative, is given as $D_\mu(x) = \partial_\mu + ieA_\mu(x)$, $A_\mu(x)$ is the gauge field of the photon, ξ is the gauge-fixing parameter, m is the mass of the elementary particle, $g^{\mu\nu}$ is the metric tensor and ψ and $\bar{\psi}$ represent the fermion and anti-fermion fields.

The generating functional is now constructed using this Lagrangian and external sources, as done in 3.2

$$Z[\eta,\bar{\eta},J] = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi\mathcal{D}A\exp\left\{i\int d^4x[\mathcal{L}_{\text{QED}} + J_\mu(x)A^\mu(x) + \bar{\psi}(x)\eta(x) + \bar{\eta}(x)\psi(x)]\right\}. \tag{6.2}$$

To arrive at the Schwinger-Dyson equation, we make use of a fundamental theorem of calculus, and consider that the functional integral of a total derivative is zero,

$$\int \mathcal{D}[\phi]\frac{\delta}{\delta\phi} = 0\,,$$

where ϕ is any arbitrary field variable. For the derivation of the photon propagator, we apply the above theorem and take the derivative with respect to the gauge field $A_\mu(x)$.

$$\int \mathcal{D}[\bar{\psi}\psi A]\frac{\delta}{\delta A_\mu(x)}\exp\{i[S[\bar{\psi},\psi,A] + J_\mu(x)A^\mu(x) + \bar{\psi}(x)\eta(x) + \bar{\eta}(x)\psi(x)]\} = 0\,, \tag{6.3}$$

where $\mathcal{D}[\bar{\psi}\psi A]$ is just an abbreviated form for $\mathcal{D}\bar{\psi}\mathcal{D}\psi\mathcal{D}A$ and is adopted for the sake of simplicity. Eq. (6.3) can be written in terms of a differential equation in the generating functional Z

$$\left[\frac{\delta S}{\delta A_\mu(x)}\left(-i\frac{\delta}{\delta J_\mu}, i\frac{\delta}{\delta\eta}, -i\frac{\delta}{\delta\bar{\eta}}\right) + J^\mu(x)\right]Z[\eta,\bar{\eta},J] = 0\,, \tag{6.4}$$

where we have established a correspondence between fields and their source terms through functional derivatives

$$\psi(x) \leftrightarrow \frac{-i\delta}{\delta\bar{\eta}(x)}\,, \quad \bar{\psi}(x) \leftrightarrow \frac{i\delta}{\delta\eta(x)}\,, \quad A^\mu(x) \leftrightarrow \frac{-i\delta}{\delta J_\mu(x)}\,.$$

The first term on the L.H.S. of Eq. (6.4) is solved by implementing the Gateux derivative method [155, 156]:

$$\frac{\mathrm{d}S(\phi+\epsilon\tau)}{\mathrm{d}\epsilon}|_{\epsilon=0} = \int \mathrm{d}^4x\,\frac{\partial S}{\partial\phi}\tau\ , \tag{6.5}$$

which gives us

$$\frac{\delta S}{\delta A_\mu(x)} = \left\{ \left[g^{\mu\nu}\partial^2 + \left(\frac{1}{\xi} - 1\right)\partial^\mu\partial^\nu \right] A_\nu(x) - e\psi(x)\gamma^\mu\bar{\psi}(x) \right\} . \tag{6.6}$$

The differential Eq. (6.4) in terms of Eq. (6.6), written in terms of the source terms now becomes

$$\left\{ \left[g^{\mu\nu}\partial^2 + \left(\frac{1}{\xi} - 1\right)\partial^\mu\partial^\nu \right] \left(\frac{-i\delta}{\delta J^\nu(x)}\right) - e\frac{-i\delta}{\delta\bar{\eta}(x)}\gamma^\mu\frac{i\delta}{\delta\eta(x)} + J^\mu(x) \right\} Z[\eta,\bar{\eta},J] = 0 . \tag{6.7}$$

In terms of the generating functional W for connected Feynman diagrams defined by the Green's function $W[\eta,\bar{\eta},J] = \ln Z[\eta,\bar{\eta},J]$, Eq. (6.8) can be expressed as

$$\left\{ \left[g^{\mu\nu}\partial^2 + \left(\frac{1}{\xi} - 1\right)\partial^\mu\partial^\nu \right] \left(\frac{-i\delta}{\delta J^\nu(x)}\right) - e\frac{-i\delta}{\delta\bar{\eta}(x)}\gamma^\mu\frac{i\delta}{\delta\eta(x)} \right\} W - e\frac{-i\delta W}{\delta\bar{\eta}(x)}\gamma^\mu\frac{i\delta W}{\delta\eta(x)} = -J^\mu(x) . \tag{6.8}$$

We now introduce the effective action, defining the one-particle-irreducible (1PI) Green's functions, in terms of the generating functional W through a Legendre transformation [82, 157]

$$i\Gamma[\bar{\psi},\psi,A] = W[\eta,\bar{\eta},J] - i\int \mathrm{d}^4x\,(\bar{\psi}\eta + \psi\bar{\eta} + A^\mu J_\mu) . \tag{6.9}$$

Owing to the above transformation, we can define the field terms $(\bar{\psi},\psi,A_\mu)$ in terms of the source terms $(\eta,\bar{\eta},J_\mu)$ [82] given in (A.11)

$$A_\mu = -i\frac{\delta W[J]}{\partial J^\mu} , \quad \psi = -i\frac{\delta W[\eta]}{\delta\bar{\eta}} , \quad \bar{\psi} = i\frac{\delta W[\bar{\eta}]}{\delta\eta} .$$

$$J_\mu = -\frac{\delta\Gamma[A]}{\partial A^\mu} , \quad \eta = -\frac{\delta\Gamma[\bar{\psi}]}{\delta\psi} , \quad \bar{\eta} = \frac{\delta\Gamma[\psi]}{\delta\bar{\psi}} .$$

Setting the fermion sources to zero and using the above expressions, Eq. (6.8) then becomes

$$\frac{\delta\Gamma[A]}{\partial A_\mu(x)} = \left[g^{\mu\nu}\partial^2 + \left(\frac{1}{\xi} - 1\right)\partial^\mu\partial^\nu \right] A_\mu(x) - e\frac{-i\delta}{\delta\bar{\eta}(x)}\gamma^\mu\frac{i\delta}{\delta\eta(x)}W . \tag{6.10}$$

From the above expression, the connected two-point function or in this case, the electron propagator can be identified easily [157]

$$S(x,y) = -\frac{\delta^2 W[\eta,\bar{\eta},J]}{\delta\eta(y)\delta\bar{\eta}(x)}|_{\psi=\bar{\psi}=0} = i\left(\frac{\delta^2\Gamma}{\delta\psi(x)\delta\bar{\psi}(y)}\right)^{-1} . \tag{6.11}$$

Using the identity derived in [158]

$$\frac{-i\delta}{\delta\bar{\eta}(x)}\gamma^{\mu}\frac{i\delta W}{\delta\eta(y)} = \mathrm{Tr}\left\{\frac{-i\delta}{\delta\bar{\eta}(x)}\gamma^{\mu}\frac{i\delta}{\delta\eta(y)}W[\eta,\bar{\eta},J]\right\}$$
$$= -\,\mathrm{Tr}\{\gamma^{\mu}S(x,y)\}\,, \tag{6.12}$$

and Eq. (6.11), Eq. (6.10) reduces to

$$\frac{\delta\Gamma[A]}{\partial A_{\mu}(x)} = \left[g^{\mu\nu}\partial^2 + \left(\frac{1}{\xi}-1\right)\partial^{\mu}\partial^{\nu}\right]A_{\mu}(x) - e\,\mathrm{Tr}\{\gamma^{\mu}S(x,x)\}\,. \tag{6.13}$$

Since we want to determine the photon propagator, we take a second derivative of the effective action Γ with respect to $A_{\nu}(y)$, and as such the Eq. (6.13) becomes

$$\frac{\delta^2\Gamma[A]}{\partial A_{\mu}(x)\delta A_{\nu}(y)} = \left[g^{\mu\nu}\partial^2 + \left(\frac{1}{\xi}-1\right)\partial^{\mu}\partial^{\nu}\right]\delta(x-y)$$
$$-e\,\mathrm{Tr}\left\{\gamma^{\mu}\frac{\delta}{\delta A_{\nu}(y)}\left(\frac{\delta^2\Gamma}{\delta\psi(x)\delta\bar{\psi}(x)}\right)^{-1}\right\}. \tag{6.14}$$

The derivative of an inverse matrix is given as

$$\frac{\mathrm{d}B^{-1}}{\mathrm{d}t} = -B^{-1}\frac{\mathrm{d}B}{\mathrm{d}t}B^{-1}\,,$$

where

$$B = \frac{\delta^2\Gamma}{\delta\psi(x)\delta\bar{\psi}(x)}\,.$$

Applying this to the functional derivative in Eq. (6.14), referring to Eq. (6.11) and considering that similar to the fermionic case in Eq. (6.11) we can write the inverse of the photon propagator as,

$$\frac{\delta^2\Gamma[A]}{\partial A_{\mu}(x)\delta A_{\nu}(y)} = -iD^{-1}_{\mu\nu}(x-y)\,,$$

we obtain a modified version of Eq. (6.14)

$$D^{-1}_{\mu\nu}(x-y) = i\left[g_{\mu\nu}\partial^2 + \left(\frac{1}{\xi}-1\right)\partial_{\mu}\partial_{\nu}\right]\delta(x-y) \tag{6.15}$$
$$-ie\int \mathrm{d}^4x_1\,\mathrm{d}^4x_2\,\mathrm{Tr}\left\{\gamma_{\mu}\left(\frac{\delta^2\Gamma}{\delta\bar{\psi}(x)\delta\psi(x_1)}\right)^{-1}\right.$$
$$\left.\times\left(\frac{\delta^3\Gamma}{\delta A_{\nu}(y)\delta\bar{\psi}(x_1)\delta\psi(x_2)}\right)\left(\frac{\delta^2\Gamma}{\delta\psi(x)\delta\bar{\psi}(x_2)}\right)^{-1}\right\}.$$

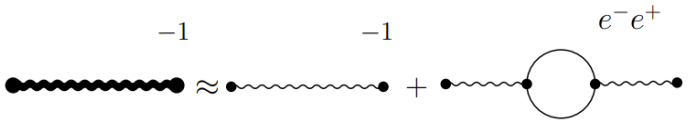

Figure 6.1: Pictorial representation of the photon Schwinger-Dyson equation in momentum space.

The third derivative of Γ gives us the connected three-point Green's function or the electron-photon vertex function (refer to appendix A)

$$\left(\frac{\delta^3\Gamma}{\delta A_\nu(y)\delta\psi(x_1)\delta\bar{\psi}(x_2)}\right) = e\Gamma^\nu(y;x_1,x_2)\,, \tag{6.16}$$

and using the expressions for the complete electron propgator from Eq. (6.11), we can write Eq. (6.15) as

$$\begin{aligned} D^{-1}_{\mu\nu}(x-y) &= i\left[g_{\mu\nu}\partial^2 + \left(\frac{1}{\xi}-1\right)\partial_\mu\partial_\nu\right]\delta(x-y) \\ &\quad -ie^2\int \mathrm{d}^4x_1\,\mathrm{d}^4x_2\,\mathrm{Tr}\Big\{S(x_1,x)\gamma_\mu S(x,x_2)\Gamma_\nu(x_2,x_1;x)\Big\}\,. \end{aligned} \tag{6.17}$$

The second term on the R.H.S. is the vacuum-polarization tensor in coordinate space

$$\begin{aligned} &\Pi_{\mu\nu}(x,y) \\ &= -ie^2\int \mathrm{d}^4x_1\,\mathrm{d}^4x_2\,\mathrm{Tr}\Big\{S(x_1,x)\gamma_\mu S(x,x_2)\Gamma_\nu(x_2,x_1;x)\Big\}\,. \end{aligned} \tag{6.18}$$

Fourier transforming into momentum space, we obtain [159]

$$\Pi_{\mu\nu}(k) = -ie^2\int\frac{\mathrm{d}^4p}{(2\pi)^4}\,\mathrm{Tr}\Big\{S(p)\gamma_\mu S(p-k)\Gamma_\nu(p,k;p-k)\Big\}\,. \tag{6.19}$$

The inverse photon propagator in momentum space thus becomes

$$D^{-1}_{\mu\nu}(k) = i\left[g_{\mu\nu}k^2 + \left(\frac{1}{\xi}-1\right)k_\mu k_\nu\right] + \Pi_{\mu\nu}(k)\,. \tag{6.20}$$

This gives us the Schwinger-Dyson equation for the unquenched (dressed) photon propagator in momentum space, where the second term on the R.H.S. gives us the photon propagator perturbed by the creation and annihilation of a virtual electron-positron pair.

Considering that the photon self-energy or the vacuum polarization is necessarily transverse [89, 160], we get for the full photon propagator as seen in Fig. 6.1

$$D_{\mu\nu}(k) = -i\left[\frac{g_{\mu\nu}}{k^2} - \frac{k_\mu k_\nu}{k^4}\right]\frac{1}{1+\Pi(k^2)} - i\xi\frac{k_\mu k_\nu}{k^4}\,, \tag{6.21}$$

where $\Pi_{\mu\nu}(k) = (-g_{\mu\nu}k^2 + k_\mu k_\nu)\Pi(k^2)$; ξ is the guage fixing parameter, $\xi = 0, 1$ for Landau and Feynman guage respectively. The photon propagator in lowest order perturbation theory is obtained by setting the scalar polarization, $\Pi(k^2) = 0$ and we arrive at the well-known expression for the photon propgator [159]

$$D'_{\mu\nu}(k) = -i\left[\frac{g_{\mu\nu}}{k^2} - \frac{k_\mu k_\nu}{k^4}\right] - i\xi\frac{k_\mu k_\nu}{k^4}\,. \tag{6.22}$$

6.2 The Uehling potential

In the book *Principles of Quantum Mechanics* and subsequently in the 1931 [161] and 1934 paper [162], Dirac introduces the theory of *positrons* in which he gives a detailed description of the existence of "negative energy states" that were almost nearly occupied. He states that "A hole, if there were one, would be a new kind of particle, unknown to experimental physics, having the same mass and opposite charge to an electron. We may call such a particle an anti-electron." [161]. After Dirac proposed his theory of positron, the study of the effect of polarization in positron theory was put forward by Uehling where he studied it's effect in impressed electrostatic fields. In his work on the polarization effects he states that "the electromagnetic field will, in general, induce a charge and current distribution due to the creation and annihilation of electron positron pairs." [163]. This conclusion by Uehling suggested the shift in the atomic energy levels due to the polarization of the vacuum, well-known as the Lamb shift. The correction to the nuclear potential due to vacuum polarization is often called the Uehling correction and is the lowest-order correction term that approximates the effect of vacuum polarization on two interacting charges.

We now proceed to evaluate the potential generated by an external charge density while taking into account the polarizability of the vacuum, namely the Uehling potential. This is done following Ref. [159].
We have derived in Section 6.1, the dressed-photon propagator in Eq. (6.21) in terms of the scalar polarization, and setting it to zero gives us the unperturbed photon propagator in Eq. (6.22). This propagator in the Feynman gauge ($\xi = 1$) becomes

$$D'_{\mu\nu}(k) = \frac{-i}{k^2 + i\varepsilon}g_{\mu\nu}\,. \tag{6.23}$$

Due to the polarization of vacuum, virtual electron-positron pairs are created which modify the photon propagator as we have seen in Figure 6.1. The dressed-photon propagator can now be written in terms of the unperturbed propagator and the vacuum polarization tensor given in Eq. (6.19)

$$iD_{\mu\nu}(k) = iD'_{\mu\nu}(k) + iD'_{\mu\lambda}(k)i\Pi^{\lambda\sigma}(k)iD'_{\sigma\nu}(k) + \ldots \tag{6.24}$$

In order to facilitate the perturbative path integral treatment of the vaccum-polarization correction to the bound-electron propagator, we now consider that the Uehling potential originates from an external charge density $j_\mu(x) = -Ze4\pi\delta^3(x)\delta_{\mu 0}$, as given by Greiner and Reinhardt [159] as,

$$A^{'}_{\mu}(x) = \int d^4y\, D_{\mu\nu}(x-y)\, j_\nu(y)\,. \tag{6.25}$$

In the momentum space this can rewritten as

$$A^{'}_{\mu}(x) = \int \frac{d^4k}{(2\pi)^4}\, e^{-ik\cdot x} D_{\mu\nu}(k)\, j^\nu(k)\,. \tag{6.26}$$

The above expressions take into consideration the full propagator and from the expression for the vaccum-polarization tensor in Eq. (6.19) it is clear that the integrand blows up (diverges) quadratically with k and needs to be *regularized*, which can be easily done keeping in mind the guage invariance of the polarization tensor, and the unquenched photon propagator, as obtained in Eq. (6.21), can be expressed in the momentum space in terms of the renormalized vacuum polarization tensor as [159]

$$D_{\mu\nu}(k) = \frac{-g_{\mu\nu}}{k^2}(1 + \Pi^R(k^2))\,, \tag{6.27}$$

where, $\Pi^R(k^2) \equiv \Pi(k^2) + \frac{e^2}{3\pi}\ln\frac{\Lambda^2}{m^2}$, Λ being an average cutoff momentum [159], stands for the renormalized vacuum polarization function that is obtained by the regularization of the scalar polarization function $\Pi(k^2)$ [159]. Using Eq. (6.27) and treating the external charge density as the generator of the unmodified potential, $A_\mu(k) = D_{\mu\nu}(k)j^\nu(k)$, the expression for the generated potential is obtained as [159]

$$A^{'}_{\mu}(x) = \int \frac{d^4k}{(2\pi)^4} e^{-ik\cdot x}(1 + \Pi^R(k^2))A_\mu(k)\,. \tag{6.28}$$

which can be then reduced to the form

$$\begin{aligned} A^{'}_{\mu}(\mathbf{x}) \quad &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}}(1 + \Pi^R(-\mathbf{k}^2))D_{\mu\nu}(0,\mathbf{k})j^\nu(\mathbf{k}) \\ &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}}(1 + \Pi^R(-\mathbf{k}^2))A_\mu(\mathbf{k})\,. \end{aligned} \tag{6.29}$$

This reduction can be made because we consider that the external charge density is stationary and hence independent of time (x^0), i.e.,

$$j^\nu(x) = j^\nu(\mathbf{x})\,. \tag{6.30}$$

In momentum space, the charge density thus becomes [159]

$$\begin{aligned} j^\nu(k) \quad &= \int d^4y\, e^{ik\cdot y} j^\nu(y) = \int dy^0\, e^{ik^0y^0} \int d^3\mathbf{y}\, e^{-i\mathbf{k}\cdot\mathbf{y}} j^\nu(\mathbf{y}) \\ &= 2\pi\delta(k^0) j^\nu(\mathbf{k})\,. \end{aligned} \tag{6.31}$$

If we now consider the stationary external charge density to be point-like, we have

$$j^{\nu}(\mathbf{k}) = \int d^3\mathbf{y}\, e^{-i\mathbf{k}\cdot\mathbf{y}} \left(-Ze4\pi\delta_{\nu 0}\delta^3(\mathbf{y})\right) = -Ze4\pi\delta_{\nu 0}\,. \tag{6.32}$$

We now substitute, in Eq. (6.29), the expression for the unperturbed photon propagator and the renormalized polarization tensor, which we use directly from [159]

$$A^{'}_{\mu}(\mathbf{x}) = -Ze4\pi \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} (1 + \Pi^R(-\mathbf{k}^2)) D_{\mu 0}(0,\mathbf{k})\,. \tag{6.33}$$

This expression for the potential can be expanded as

$$\begin{aligned} A^{'}_{0}(\mathbf{x}) \quad &= -Ze \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} \frac{1}{\mathbf{k}^2} \\ &\quad \times \left[1 + \frac{2\alpha}{\pi}\int_0^1 d\beta\, \beta(1-\beta) \ln\left(1 + \frac{\mathbf{k}^2}{m^2}\beta(1-\beta)\right)\right] \\ &= -Ze \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} \frac{4\pi}{\mathbf{k}^2} - Ze \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{x}} \frac{4\pi}{\mathbf{k}^2} \\ &\quad \times \frac{2\alpha}{\pi}\int_0^1 d\beta\, \beta(1-\beta) \ln\left(1 + \frac{\mathbf{k}^2}{m^2}\beta(1-\beta)\right)\,, \end{aligned} \tag{6.34}$$

where β is a scale transformation variable [159]. The first term in the above equation can be Fourier transformed and reduced to the conventional Coulomb potential term; similarly, in order to obtain a simplified version of the integral representation of the renormalized photon propagator which is given as

$$\begin{aligned} \Pi^R(-\mathbf{k}^2) \quad &= \frac{2\alpha}{\pi}\int_0^1 d\beta\, \beta(1-\beta) \ln\left(1 - \frac{\mathbf{k}^2}{m^2}\beta(1-\beta)\right) \\ &= -\frac{2\alpha}{\pi}\int_0^1 d\beta\, \left(\frac{1}{2}\beta^2 - \frac{1}{3}\beta^3\right) \frac{1}{1 - \frac{\mathbf{k}^2}{m^2}\beta(1-\beta)} \left[-\frac{\mathbf{k}^2}{m^2}(1-2\beta)\right]\,. \end{aligned} \tag{6.35}$$

The logarithmic term in Eq. (6.35) has been integrated out through integration by parts. The term in the denominator in the R.H.S. is reduced by introducing a new integration variable given by,

$$v = 2\beta - 1\,, \tag{6.36}$$

such that we have

$$\beta(1-\beta) = \frac{1}{4}(1 - v^2)\,. \tag{6.37}$$

Using this new integration variable we obtain a simplified expression for the renormalized photon polarization tensor given as

$$\Pi^R(-\mathbf{k}^2) = -\frac{\alpha}{\pi}\frac{\mathbf{k}^2}{4m^2}\int_0^1 dv \frac{v^2\left(1-\frac{1}{3}v^2\right)}{v^2+\frac{4m^2}{\mathbf{k}^2}-1}\,. \tag{6.38}$$

The potential in Eq. (6.34) can then be expressed by exchanging the order of integration and implementing the identity

$$\int \frac{d^3k}{(2\pi)^3}\frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{\mathbf{k}^2} = \frac{1}{4\pi \mathrm{r}}\,, \tag{6.39}$$

where, $\mathrm{r} = |\mathbf{x}|$. Thus the potential, $A_0^{'}(\mathbf{x})$, becomes

$$A_0^{'}(\mathbf{x}) = -Ze\left[\frac{1}{\mathrm{r}} + \frac{2\alpha}{\pi}\frac{4\pi}{8m^2}\int_0^1 dv\, v^2\left(1-\frac{1}{3}v^2\right)\int\frac{d^3\mathbf{k}}{(2\pi)^3}\frac{\exp(i\,\mathbf{k}\cdot\mathbf{x})}{1+\frac{\mathbf{k}^2}{4m^2}(1-v^2)}\right]. \tag{6.40}$$

The second integral on the R.H.S. of the above equation is solved using the theorem of residues, given by

$$\int \frac{d^3\mathbf{k}}{(2\pi)^3}\frac{\exp(i\,\mathbf{k}\cdot\mathbf{x})}{\mathbf{k}^2+a^2} = \frac{1}{4\pi}\frac{\exp(-a\mathrm{r})}{\mathrm{r}}\,. \tag{6.41}$$

where, r has already been defined as $\mathrm{r} = |\mathbf{x}|$. The simplified expression for the potential is then given as

$$A_0^{'}(\mathbf{x}) = -\frac{Ze}{\mathrm{r}}\left[1+\frac{\alpha}{\pi}\int_0^1 dv\,\frac{v^2\left(1-\frac{1}{3}v^2\right)}{(1-v^2)}\exp\left(-\frac{2m}{\sqrt{(1-v^2)}}\mathrm{r}\right)\right]. \tag{6.42}$$

We make another transformation to simplify the exponent in the expression for the potential in Eq. (6.42),

$$y = \frac{1}{\sqrt{(1-v^2)}}\,, \tag{6.43}$$

such that

$$v\,dv = \frac{1}{y^3}dy\,. \tag{6.44}$$

The simplified expression for the potential then becomes

$$\begin{aligned} A_0^{'}(\mathrm{r}) &= -\frac{Ze}{\mathrm{r}}\left[1+\frac{\alpha}{\pi}\int_1^\infty \frac{dy}{y^3}\frac{v}{3}(3-v^2)e^{-2my\mathrm{r}}\right] \\ &= -\frac{Ze}{\mathrm{r}}\left[1+\frac{2\alpha}{3\pi}\int_1^\infty dy\left(1+\frac{1}{2y^2}\right)\frac{\sqrt{y^2-1}}{y^2}e^{-2my\mathrm{r}}\right]. \end{aligned} \tag{6.45}$$

This equation gives the integral representation of the interaction potential, which gives the lowest order approximation of the effect of vacuum polarization between two interacting electric charges.

Uehling, in 1935, deduced this interaction potential between two charged particles that contained the effect of vacuum polarization as a correction term; Eq. (6.45) for the interaction potential can be written as a summation of two distinct terms,

$$A_0^{'}(\mathrm{r}) = -\frac{Ze}{\mathrm{r}}\left[1 + \frac{2\alpha}{3\pi}\int_1^\infty dy\left(1+\frac{1}{2y^2}\right)\frac{\sqrt{y^2-1}}{y^2}e^{-2my\mathrm{r}}\right] = -\frac{Ze}{\mathrm{r}} + U(\mathrm{r})\,. \quad (6.46)$$

this additional term in the above equation is the Uehling potential which originates from the lowest-order radiative correction to the photon propagator. In lighter atoms, non-zero Uehling potential is encountered only for atomic distances of the order of the Compton wavelength ($\Lambda_c = \frac{\hbar}{m_e c}$). We follow the work of Frolov and Wardlow [164] to obtain the closed analytical formula for the Uehling potential.
From Eq. (6.46), the expression for the Uehling potential can be written as

$$U(\mathrm{r}) = -\frac{2Ze\alpha}{3\pi r}\int_1^\infty dy\left(1+\frac{1}{2y^2}\right)\frac{\sqrt{y^2-1}}{y^2}e^{-2my\mathrm{r}}\,. \quad (6.47)$$

We consider the term in the integral and try to reduce it using modified Bessel functions [135],

$$I_U = \int_1^\infty dy\left(1+\frac{1}{2y^2}\right)\frac{\sqrt{y^2-1}}{y^2}e^{-2my\mathrm{r}}\,. \quad (6.48)$$

$$I_U(a) = \int_1^\infty dy\left(1+\frac{1}{2y^2}\right)\frac{\sqrt{y^2-1}}{y^2}e^{-ay}\,. \quad (6.49)$$

As is evident, the integral in the above equation is a function of the positive numerical parameter a.

In order to solve this integral, we take the help of modified zero order Bessel functions [135][92]; the ξ term in the integral is substituted by $y = \cosh(x)$ in order to reduce the term on the R.H.S. into a form that can be solved using modified Bessel function. Thus we get upon substituting

$$I_U(a) = \int_1^\infty dy\left(1+\frac{1}{2y^2}\right)\frac{\sqrt{y^2-1}}{y^2}e^{-ay}\,, \quad (6.50)$$

$$= \int_0^\infty dx\, e^{-a\cosh(x)}\left(1 - \frac{1}{2\cosh^2(x)} - \frac{1}{2\cosh^4(x)}\right)\,. \quad (6.51)$$

We now take recourse to modified Bessel functions in order to solve this integral; the modified Bessel functions I and K ,in the zeroth order, are given in the intgral representation as

$$I_0(z) = \frac{1}{\pi}\int_0^\pi \cosh(z\,cos\theta)d\theta\,, \quad (6.52)$$

$$K_0(z) = -\frac{1}{\pi}\int_0^\pi \exp(\pm\, z\,\cos(\theta))\{\gamma + \ln\big(2z\,\sin^2\theta\big)\}d\theta\,. \quad (6.53)$$

In the form of an ascending series [92, 135] these modified Bessel functions can be represented as

$$I_\nu(z) = \left(\frac{1}{2}z\right)^\nu \sum_{k=0}^{\infty} \frac{(\frac{1}{4}z^2)^k}{k!\Gamma(\nu+k+1)}\,, \tag{6.54}$$

$$\text{in zeroth-order i.e., for } \nu = 0,\ I_0(z) = \sum_{k=0}^{\infty} \frac{z^{2k}}{2^{2k}\,(k!)^2}, \qquad [\because \Gamma(k+1) = k!]\,. \tag{6.55}$$

Similarly,

$$K_n(z) = \frac{1}{2}\left(\frac{1}{2}z\right)^{-n} \sum_{k=0}^{n-1} \frac{(n-k-1)!}{k!}\left(-\frac{1}{4}z^2\right)^k + (-1)^{n+1}\ln\left(\frac{1}{2}z\right) I_n(z)$$
$$(-1)^n \frac{1}{2}\left(\frac{1}{2}z\right)^n \sum_{k=0}^{\infty} \{\psi(k+1) + \psi(k+n+1)\} \frac{(\frac{1}{4}z^2)^k}{k!(n+k)!}\,. \tag{6.56}$$

In zeroth-order this reduces to,

$$K_0(z) = \sum_{k=0}^{\infty} \{\psi(k+1) + \ln(2) - \ln(z)\} \frac{z^{2k}}{2^{2k}\,(k!)^2}\,, \tag{6.57}$$

where, the ψ in Eqs. (6.56) and (6.57) is the Euler *psi* function that is defined as

$$\psi(n) = -\gamma + \sum_{k=1}^{n-1} k^{-1}\,.$$

Using the Eqs. (6.52)-(6.57), the integral in Eq. (6.51) can be reduced to terms containing the modified Bessel function in zeroth order and the related recursive integrals as

$$I_U = \int_0^\infty dx\, e^{-a\cosh(x)} \left(1 - \frac{1}{2\cosh^2(x)} - \frac{1}{2\cosh^4(x)}\right)\,, \tag{6.58}$$
$$= K_0(a) - \frac{1}{2}Ki_2(a) - \frac{1}{2}Ki_4(a)\,, \tag{6.59}$$
$$\text{where,}\quad Ki_{\rm r}(z) = \int_0^\infty \frac{e^{-z\,\cosh(x)}}{\cosh^{\rm r} x} dx, \qquad r \geq 1\,. \tag{6.60}$$

Here the recursive integrals of $K_0(z) \equiv Ki_0(z)$ function are defined as per [135] as

$$Ki_{\rm r}(z) = \int_z^\infty Ki_{\rm r-1}(z) dz\,, \tag{6.61}$$

and can be written in expanded form as

$$rKi_{\rm r+1}(z) = -zKi_{\rm r}(z) + (r-1)Ki_{\rm r-1}(z) + zKi_{\rm r-2}(z)\,. \tag{6.62}$$

Rewriting the expression in Eq. (6.59), by expanding each of the three terms, using the above expansion, we obtain

$$\begin{aligned} I_U &= K_0(z) - \frac{1}{2}\left[-z2Ki_1(z)\right] - \frac{1}{6}\left[-zKi_3(z) + 2Ki_2(z) + zKi_1(z)\right] \\ &= K_0(z) + \frac{1}{3}zKi_1(z) - \frac{1}{6}zKi_1(z) + \frac{z}{12}[2Ki_3(z)] - \frac{1}{3}Ki_2(z) \\ &= \left(1 + \frac{z^2}{12}\right) K_0(z) + \frac{1}{3}zKi_1(z) + \frac{z}{12}Ki_1(z) - \frac{z^2}{12}Ki_2(z) - \frac{1}{3}Ki_2(z)\,. \end{aligned} \quad (6.63)$$

The term $\frac{1}{3}zKi_1(z)$ becomes $-\frac{1}{3}Ki_2(z)$ upon expansion using Eq. (6.62), and the term $\frac{z}{12}Ki_1(z)$ is expanded as

$$\frac{z}{12}Ki_1(z) = \left(\frac{1}{6} - \frac{1}{12}\right) zKi_1(z)\,. \quad (6.64)$$

Here again the first term is expanded using Eq. (6.62) to obtain $\frac{1}{6}zKi_1(z) = -\frac{1}{6}Ki_2(z)$. Using these relations in Eq. (6.63), we thus obtain,

$$\begin{aligned} I_U &= \left(1 + \frac{z^2}{12}\right) K_0(z) - \frac{1}{3}Ki_2(z) - \frac{z}{12}Ki_1(z) \\ &\qquad - \frac{z^2}{12}Ki_2(z) - \frac{1}{3}Ki_2(z) - \frac{1}{6}Ki_2(z) \\ &= \left(1 + \frac{z^2}{12}\right) K_0(z) - \frac{z}{12}Ki_1(z) - \left(\frac{5}{6} + \frac{z^2}{12}\right) Ki_2(z)\,. \end{aligned} \quad (6.65)$$

We can now replace the parameter z by the positive parameter a as defined in Eq. (6.49), and rewrite the expression for the interaction potential in the form defined by Uehling in his paper[163]

$$A_0^{'}(\mathrm{r}) = -\frac{Ze}{\mathrm{r}}\left[1 + \frac{2\alpha}{3\pi}\int_1^\infty e^{-2r/\lambda_0 y}\left(1 + \frac{1}{2y^2}\right)\frac{\sqrt{y^2-1}}{y^2}dy\right], \quad (6.66)$$

where,

$$\lambda_0 = \alpha a_0 \quad \text{and} \quad \mathrm{r}/a_0 = \mathrm{r}\,.$$

Thus, the above equation can be rewritten as

$$A_0^{'}(\mathrm{r}) = -\frac{Ze}{\mathrm{r}}\left[1 + \frac{2\alpha}{3\pi}\int_1^\infty e^{-2\alpha^{-1}\mathrm{r}y}\left(1 + \frac{1}{2y^2}\right)\frac{\sqrt{y^2-1}}{y^2}dy\right]. \quad (6.67)$$

Now, from Eq. (6.60) we have $a = z = 2\alpha^{-1}\mathrm{r}$, using the solution of the integral as obtained in Eq. (6.65), we have the expression for the Uehling potential which is written as

$$U(a) = -\frac{2Ze\alpha}{3\pi\mathrm{r}}\left[\left(1 + \frac{a^2}{12}\right)K_0(a) - \frac{a}{12}Ki_1(a) - \left(\frac{5}{6} + \frac{a^2}{12}\right)Ki_2(a)\right]. \quad (6.68)$$

Replacing a with the fine-structure constant α, and rewriting the expression for the interaction potential, we obtain,

$$A_0^{'}(\mathrm{r}) = -\frac{Ze}{\mathrm{r}}\left\{1+\frac{2\alpha}{3\pi}\left[\left(1+\frac{\mathrm{r}^2}{3\alpha^2}\right)K_0\left(\frac{2\mathrm{r}}{\alpha}\right)\right.\right.$$
$$\left.\left.-\frac{\mathrm{r}}{6\alpha}Ki_1\left(\frac{2\mathrm{r}}{\alpha}\right)-\left(\frac{5}{6}+\frac{\mathrm{r}^2}{3\alpha^2}\right)Ki_2\left(\frac{2\mathrm{r}}{\alpha}\right)\right]\right\}. \tag{6.69}$$

The above equation gives the expression for the interaction energy, in atomic units, and includes the lowest order correction to vacuum polarization, or the Uehling correction.

We work with the exact analytic expression for the Uehling potential, as has been worked out by Frolov and Wardlaw[164], to obtain the energy shift induced by the introduction of this perturbing potential using path integral formalism.

6.3 Path Integral formulation of the energy shift induced by the Uehling potential

In this Section, we deal with the problem of determining the energy dependent Green's function using perturbative methods for path integrals for the Uehling potential. The use of perturbative methods for path integrals was originally adressed by Feynman [17] and Devreese et al. [165] where they dealt with the Coulomb potential explicitly and derived all information on the discrete and continuous spectrum of the Coulomb potential using the path integral approach.

The Expansion

Briefly introducing the methodology developed by Feynman in his work [17] where he introduced perturbative path integrals in the non-relativistic picture, we start by considering the motion of the particle in a potential $V(x,t)$ in one dimension. The Feynman kernel, giving the transition amplitude between points a and b, is

$$K_V(a,b) = \int_a^b \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}\left(\frac{m}{2}\dot{x}^2 - V(x,t)\right)dt\right\}\mathscr{D}x(t)\,. \tag{6.70}$$

the integral in the exponential being the action integral and the subscript V denoting that the particle is in moving under the influence of a potential, V. We keep the notations used by Feynman in his book and do not consider natural units for the non-relativistic derivations in this Section.

If we consider that the time integral of the potential along a path is smaller than $\hbar$, the term containing the exponential of the potential appearing in the integrand can be expanded according to the series expansion

$$e^x = \frac{x^n}{n!},$$

to obtain

$$\exp\left\{-\frac{i}{\hbar}\int_{t_a}^{t_b} V(x,t)\,dt\right\} = 1 - \frac{i}{\hbar}\int_{t_a}^{t_b} V(x,t)\,dt + \frac{1}{2!}\left(-\frac{i}{\hbar}\int_{t_a}^{t_b} V(x,t)\,d\right)^2 + \ldots \tag{6.71}$$

Using this expansion, Eq. (6.70) can be written as

$$K_V(a,b) = K_0(a,b) + K^{(1)}(a,b) + K^{(2)}(a,b) + \ldots \tag{6.72}$$

where each term of the kernel is defined by Eq. (6.71) as

$$\begin{aligned}
K_0(a,b) &= \int_a^b \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}\frac{m}{2}\dot{x}^2 dt\right\}\mathscr{D}x(t)\,,\\
K^{(1)}(a,b) &= -\frac{i}{\hbar}\int_a^b \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}\frac{m}{2}\dot{x}^2 dt\right\}\int_{t_a}^{t_b} V(x(s),s)\,ds\,\mathscr{D}x(t)\,,\\
K^{(2)}(a,b) &= -\frac{1}{\hbar^2}\int_a^b \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}\frac{m}{2}\dot{x}^2 dt\right\}\\
&\quad\times\int_{t_a}^{t_b} V(x(s),s)\,ds\int_{t_a}^{t_b} V(x(s'),s')\,ds'\mathscr{D}x(t)\,.
\end{aligned} \tag{6.73}$$

The first term in the above sequence of equations is the free particle propagator, the $K^{(1)}$ integral signifies the scattering of the free particle by a potential, V, and the third Feynman kernel gives the particle propagator having been scattered two or more times under the influence of the potential.

This can be better understood if we consider that in the time interval (t_a, t_b), the particle travels freely, which is represented by the kernel K_0. Next, we slice up the time interval into two halves, from (t_a, s) and from (s, t_b). We suggest that at the instant of time s, the particle is acted upon by a potential $V(x(s), s)$, and this is represented by the kernel $K^{(1)}$. We write down the path integral contained in the kernel $K^{(1)}$ and denote it as $F(s)$

$$K^{(1)}(a,b) = -\frac{i}{\hbar}\int_{t_a}^{t_b} F(s)\,ds\,, \tag{6.74}$$

where

$$F(s) = \int_a^b \exp\left\{\frac{i}{\hbar}\int_{t_a}^{t_b}\frac{m}{2}\dot{x}^2 dt\right\} V(x(s),s)\,\mathscr{D}x(t)\,. \tag{6.75}$$

The path integral $F(s)$ is defined as the sum of all possible trajectories that the particle traverses, given by the transition amplitude of the free particle, each trajectory being weighed by the potential $V(s)$, acting at the instant s. Sketching the paths taken by the particle in a postion vs. time graph would show that the particle traverses freely along all paths before and after the time $t = s$. As suggested earlier, we divide the time interval into two parts, one before time $t = s$, and one after. On the position axis, we

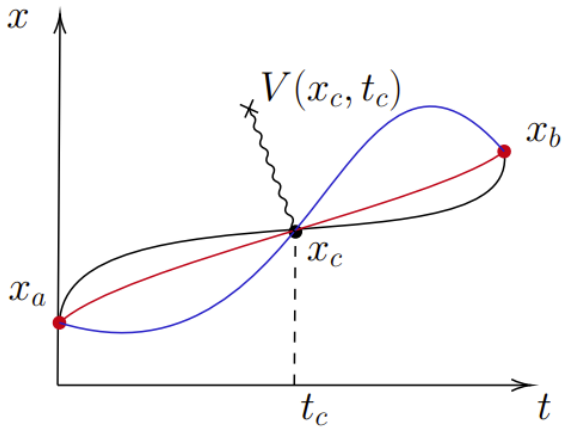

Figure 6.2: Diagrammatic representation of perturbative path integrals. The particle travels freely from x_a to x_c where it encounters an interaction before propagating freely again from x_c to x_b.

mark this as point x_c, the potential acting on the particle at time $s = t_c$. We assume that every path the particle takes goes through this point, and we integrate over all values of x_c. This is depicted in Fig. 6.2. As such the sum over all such paths can be written as $K_0(b,c)K_0(c,a)$ and the path integral is given as

$$F(s) = F(t_c) = \int_{-\infty}^{\infty} K_0(b,c)V(x_c,t_c)K_0(c,a)dx_c\,. \tag{6.76}$$

The limits on the integral over $x(t)$ is determined by the potential. Substituting this path integral in the kernel $K^{(1)}$ we get

$$K^{(1)}(a,b) = -\frac{i}{\hbar}\int_{t_a}^{t_b}\int_{-\infty}^{\infty} K_0(b,c)V(x_c,t_c)K_0(c,a)dx_c\,dt_c\,, \tag{6.77}$$

and we have the path integral calculated as an ordinary integral.
The interpretation of Eq. (6.77) is simple and straightforward, from right to left, the particle travels freely from the point a to point $c = (x_c, t_c)$, where it is acted upon by a *scattering potential*, $V(x_c, t_c)$, the amplitude for scattering being given by $-(i/\hbar)V$; after which it moves as a free particle again from point c to the final point b.

Using this scheme, the kernel $K^{(2)}$ can be easily defined as

$$K^{(2)}(a,b) = -\left(\frac{i}{\hbar}\right)^2\int\int K_0(b,c)V(x_c,t_c)K_0(c,d)V(x_d,t_d)K_0(d,a)\,d\tau_c\,d\tau_d\,, \tag{6.78}$$

where $d\tau = dx\,dt$. The kernel $K^{(2)}$ follows the same definition: the particle travels freely from the point a to point $d = (x_d, t_d)$, where it suffers a scattering by the potential $V(x_d, t_d)$; it then travels freely between the points d and c. At point c it once again undergoes a scattering by the potential $V(x_c, t_c)$; beyond this point, it travels as a

free particle till the final point b. In order to implement time ordering we assume that $K(a,b) = 0$ for $t_b < t_a$. This series expansion could be considered analogous to the *Born series*.

Mathematical formulation

What we saw in the preceeding text is essentially the *perturbative approach* to the path integral formalism and is a generalised mathematical framework that can be applied to both non-relativistic as well as relativistic problems [153, 154, 166]. To this effect, we proceed by summing the perturbative expansion to all orders in order to establish the non-perturbative results from this manifestly perturbative scheme, now in the relativistic regime.

We begin with the modification of the action integral, wherein the action is perturbed by a potential, and the perturbation expansion is summed to all orders.

$$S[\mathbf{r}(t)](\mathbf{r}_b, \mathbf{r}_a, t_b, t_a) = S^{(0)}[\mathbf{r}(t)](\mathbf{r}_b, \mathbf{r}_a, t_b, t_a) - \int_{t_a}^{t_b} \Delta V(\mathbf{r}(t), t)\, dt\,. \tag{6.79}$$

$S[\mathbf{r}(t)]$ is the classical action functional defined for the path $\mathbf{r}(t)$, connecting the starting point $\mathbf{r}_a = \mathbf{r}(t_a)$ to the end point $\mathbf{r}_b = \mathbf{r}(t_b)$, $V(\mathbf{r}(t), t)$ being the perturbing potential. To establish field definition invariance and to justify the "extra" terms arising from the stochastic nature of the Lagrangian path integrals, we proceed with the discretization of the time variable. The time interval $T = t_b - t_a$ is divided into N discrete intervals. The time lattice is divided into $N+1$ equidistant points denoted by u_j, such that

$$\begin{aligned} u_j &= t_a + j t_j\,, \quad \text{where,} \quad t_j = \frac{t_b - t_a}{N} = u_j - u_{j-1}\,, \\ u &= \sum t_j\,. \end{aligned}$$

With this discretization of the time interval, the lattice action reads as

$$\begin{aligned} S^{(N)}[\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}](\mathbf{r}_b, \mathbf{r}_a, t_b, t_a) & \\ &= S^{(0;N)}[\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}](\mathbf{r}_b, \mathbf{r}_a, t_b, t_a) \\ &\qquad + \Delta S^{(N)}[\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}](\mathbf{r}_b, \mathbf{r}_a, t_b, t_a)\,, \\ &= S^{(0;N)}[\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}](\mathbf{r}_b, \mathbf{r}_a, t_b, t_a) - t_j \sum_{j=0}^{N-1} \Delta V(\mathbf{r}_j, u_j)\,, \end{aligned} \tag{6.80}$$

where, $S^{(0;N)}$ is the unperturbed action in the time lattice definition. Using this time-lattice version of the action, if we construct the action integral for any arbitrary action perturbed by an arbitrary potential, we obtain

$$e^{\frac{i}{\hbar} S^{(N)}} = e^{\frac{i}{\hbar} S^{(0;N)}} + e^{\frac{i}{\hbar} \Delta S^{(N)}}\,. \tag{6.81}$$

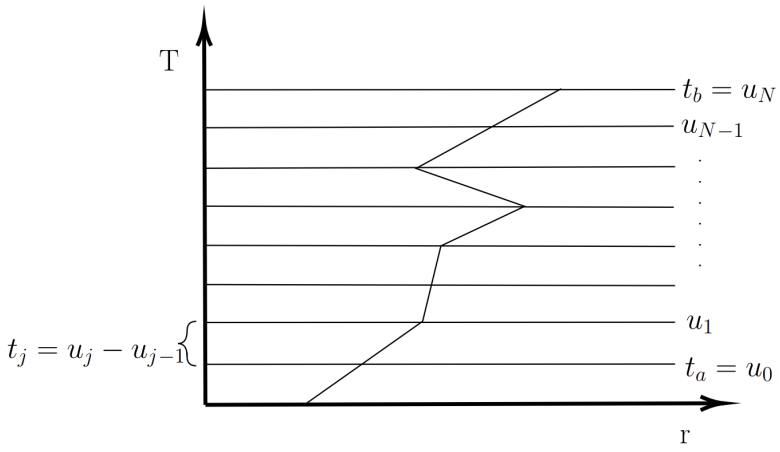

Figure 6.3: Time lattice division for a given path. The lattice is divided into $N+1$ equidistant points, the width given by t_j.

We expand the perturbation exponential upto all orders

$$\begin{aligned} e^{\frac{i}{\hbar}\Delta S^{(N)}} &= \sum_{n=0}^{\infty} \frac{t_j^n}{n!} \left[\sum_{j=0}^{N-1} \frac{\Delta V(\mathbf{r}_j, u_j)}{i\hbar} \right]^n \\ &= \sum_{n=0}^{\infty} \frac{t_j^n}{n!} \left[\sum_{j_n=0}^{N-1} \cdots \sum_{j_1=0}^{N-1} \frac{\Delta V(\mathbf{r}_{j_n}, u_{j_n})}{i\hbar} \cdots \frac{\Delta V(\mathbf{r}_{j_1}, u_{j_1})}{i\hbar} \right] \\ &= \sum_{n=0}^{\infty} t_j^n \left[\sum_{j_n=0}^{N-1} \cdots \sum_{j_1=0}^{N-1} \frac{\Delta V(\mathbf{r}_{j_n}, u_{j_n})}{i\hbar} \cdots \frac{\Delta V(\mathbf{r}_{j_1}, u_{j_1})}{i\hbar} \right] \left[1 + \mathscr{O}\left(\frac{1}{N}\right) \right] , \end{aligned} \tag{6.82}$$

where the correction terms of order $\mathscr{O}\left(\frac{1}{N}\right)$ are to take care of the repeated indices. In the limit $N \to \infty$ the Eq. (6.82) becomes

$$\begin{aligned} &\sum_{n=0}^{\infty} t_j^n \left[\sum_{j_n=0}^{N-1} \cdots \sum_{j_1=0}^{N-1} \frac{\Delta V(\mathbf{r}_{j_n}, u_{j_n})}{i\hbar} \cdots \frac{\Delta V(\mathbf{r}_{j_1}, u_{j_1})}{i\hbar} \right] \left[1 + \mathscr{O}\left(\frac{1}{N}\right) \right] \\ &\approx_{N\to\infty} \int_{t_a}^{t_b} du_n \int_{t_a}^{u_n} du_{n-1} \cdots \int_{t_a}^{u_2} du_1 \frac{\Delta V(\mathbf{r}_n, u_n)}{i\hbar} \cdots \frac{\Delta V(\mathbf{r}_1, u_1)}{i\hbar} . \end{aligned} \tag{6.83}$$

In order to simplify the notation in Eq. (6.82), in the context of perturbation theory, we redefine the time intervals as

$$\begin{aligned} u_{(0)} = u_0 = t_a , \qquad u_{(n+1)} = u_N = t_b , \\ u_{(k)} = u_{j_k} , \quad \mathbf{r}_{(k)} = \mathbf{r}_{j_k} , \qquad k = 1, \ldots, n \end{aligned} \tag{6.84}$$

At each order of perturbation n, the time interval $T = t_b - t_a$ is divided into $n+1$ subintervals. The subscript j defines the discretization of the time lattice into N discrete

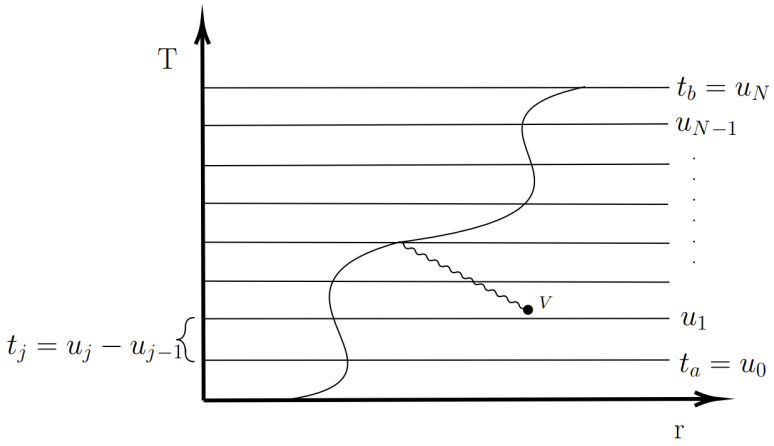

Figure 6.4: Time lattice division for first-order perturbation.

intervals, and the subscript k denotes the order of perturbation. Thus, we discretize time, and calculate the path integrals, for each order of perturbation theory. As such, the lattice unperturbed action at each order of perturbation is given as

$$\begin{aligned} &S^{(0;N)}[\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}](\mathbf{r}_b, \mathbf{r}_a, t_b, t_a) \\ &\qquad = \sum_{k=0}^{n} S^{(0;N)}[\mathbf{r}_1, \ldots, \mathbf{r}_{N-1}](\mathbf{r}_{(k+1)}, \mathbf{r}_{(k)}; u_{(k+1)}, u_{(k)}) \,. \end{aligned} \tag{6.85}$$

We can define the time-lattice division as per the following equation

$$T^N(t_b, t_a) = \{T^{(N_0)}(t_a, u_{(k)}); T^{(N_1)}(u_1, u_2); \ldots; T^{(N_n)}(u_n, t_b)\} \,, \tag{6.86}$$

where

$$T^{(N_k)}(u_{(k+1)}, u_{(k)}) = (u_{k,j_0} \equiv u_{(k)}, u_{k,j_1}, \ldots, u_{k,j_{N_{k-1}}} u_{k,j_{N_k}} \equiv u_{(k+1)}) \,. \tag{6.87}$$

the entire interval has been divided into $n+1$ subintervals and each of these subintervals, $[u_{(k+1)}, u_{(k)}]$ have been discretized into the usual N_k parts, at each order of perturbation theory. Owing to these time-lattice divisions, the integration measure for the path integrals can be given in terms of a partial measure for each order of perturbation

$$\int_{\mathbf{r}_a}^{\mathbf{r}_b} \mathscr{D}^N \mathbf{r}(\mathbf{u}) = \prod_{k=1}^{n} \left[\int d\mathbf{r}_k \right] \prod_{i=0}^{n} \left[\int_{\mathbf{r}_i}^{\mathbf{r}_{i+1}} \mathscr{D}^{(N_i)} \mathbf{r}(u) \right] \,. \tag{6.88}$$

We know that the Feynman path integral kernel has the form

$$K(\mathbf{r}_b, \mathbf{r}_a; t_b, t_a) = \lim_{N \to \infty} \int_{\mathbf{r}_a}^{\mathbf{r}_b} \mathscr{D}\mathbf{r}(t) \exp\left\{ \frac{i}{\hbar} S[\mathbf{r}(t)](\mathbf{r}_b, \mathbf{r}_a, t_b, t_a) \right\} \,. \tag{6.89}$$

Given the integration measure of Eq. (6.88), and with the help of Eq. (6.80) and Eq. (6.83), the Feynman kernel can be written as

$$K^{(n)}(\mathbf{r}_b, \mathbf{r}_a; t_b, t_a) = \int_{t_a}^{t_b} du_n \int_{t_a}^{u_n} du_{n-1} \cdots \int_{t_a}^{u_2} du_1 \times \prod_{k=1}^{n} \left[\int d\mathbf{r}_k \frac{\Delta V(\mathbf{r}_k, u_k)}{i\hbar} \right] \prod_{i=0}^{n} \left[K^{(0)}(\mathbf{r}_{i+1}, \mathbf{r}_i; u_{i+1}, u_i) \right] , \quad (6.90)$$

where the kernel $K^{(0)}$ is the propagator for the unperturbed action $S^{(N,0)}[\mathbf{r}(u)]$, defined in the limit $N \to \infty$. In case of systems with time-independent Hamiltonians, the Feynman kernel in Eq. (6.90) can be expressed as

$$K^{(n)}(\mathbf{r}_b, \mathbf{r}_a; T) = \prod_{k=1}^{n} \left[\int d\mathbf{r}_k \frac{\Delta V(\mathbf{r}_k)}{i\hbar} \right] \times \prod_{i=0}^{n} \left[\int_0^{\infty} dT_i \, K^{(0)}(\mathbf{r}_{i+1}, \mathbf{r}_i; T_i) \right] \delta \left(T - \sum_{\gamma=0}^{n} T_\gamma \right) . \quad (6.91)$$

Correspondingly, the n-th order energy-dependent Green's function is obtained by taking the Fourier transform of the propagator in the above equation, yielding

$$G^{(n)}(\mathbf{r}_b, \mathbf{r}_a; E) = \prod_{k=1}^{n} \left[\int_0^{\infty} d\mathbf{r}_k \, \Delta V(\mathbf{r}_k) \right] \prod_{i=1}^{n} \left[G^{(0)}(\mathbf{r}_{i+1}, \mathbf{r}_i; E) \right] . \quad (6.92)$$

6.4 Expanding to Vacuum Polarization

The infinte summation of a perturbation expansion using path integrals developed in the last Section is now implemented in the framework of QED to study the lowest order vacuum polarization correction to the binding energy of fermions in the Furry picture.

As in the Coulomb case, we start from the Dirac equation for a potential $\Delta V(\mathbf{r})$. The time-independent Dirac equation is customarily expressed, in natural units ($c = 1$, $\hbar = 1$), as

$$(E - \boldsymbol{\alpha} \cdot \hat{\boldsymbol{p}} - \beta m - \Delta V(\mathbf{r}))\Psi = 0 \, . \quad (6.93)$$

In order to calculate the contribution of the Uehling correction to the binding energy of the bound fermion, we treat the Uehling potential defined in Eq. (6.68) as the perturbation. As in Eq. (6.80), the lattice perturbed action is given as a sum of the unperturbed action and the action due to the perturbing potential. For our case, i.e., in the Furry picture, we consider the action due to the nuclear Coulomb potential as the unperturbed action $S^{(0)}$. Thus, we have from Eq. (5.83), for the bound fermion, the unperturbed action

$$S^{(0)}(t_j) = \frac{m(\Delta \mathrm{r}_j)^2}{2t_j} - \frac{\lambda(\lambda+1)t_j}{2m\mathrm{r}_j\mathrm{r}_{j-1}} + \frac{Ze^2Et_j}{m\mathrm{r}_j} + \frac{(E^2-m^2)t_j}{2m} \, . \quad (6.94)$$

Coupled with the perturbing potential this gives us the lattice perturbed action. From Eq. (6.80) we have

$$S[\mathbf{r}(t)](\mathbf{r}_b,\mathbf{r}_a,t_b,t_a) = \frac{m(\Delta \mathrm{r}_j)^2}{2t_j} - \frac{\lambda(\lambda+1)t_j}{2m\mathrm{r}_j\mathrm{r}_{j-1}} + \frac{Ze^2Et_j}{m\mathrm{r}_j} + \frac{(E^2-m^2)t_j}{2m} - \int_{t_a}^{t_b} \Delta V(\mathbf{r}(t))\,dt\,, \quad (6.95)$$

where

$$\Delta V(\mathbf{r}) = U_{VP}^{Ueh} = \quad (6.96)$$
$$-\frac{2\alpha Ze}{3\pi \mathrm{r}}\left[\left(1+\frac{\mathrm{r}^2}{3\alpha^2}\right)K_0\left(\frac{2\mathrm{r}}{\alpha}\right) - \frac{\mathrm{r}}{6\alpha}Ki_1\left(\frac{2\mathrm{r}}{\alpha}\right) - \left(\frac{5}{6}+\frac{\mathrm{r}^2}{3\alpha^2}\right)Ki_2\left(\frac{2\mathrm{r}}{\alpha}\right)\right].$$

is the perturbing Uehling potential.

The corresponding Feynman kernel can be obtained using Eq. (6.91) and eventually the energy-dependent Green's function is given by Eq. (6.92). Thus, the n-th order Green's function is obtained in terms of the Dirac-Coulomb propagator as,

$$\begin{aligned}
&G^{(n)}(\mathbf{r}_b,\mathbf{r}_a;E)\\
&= \prod_{k=1}^{n}\left[\int_0^\infty d\mathbf{r}_k\,\Delta V(\mathbf{r}_k)\right]\prod_{i=0}^{n}\left[G^{(0)}(\mathbf{r}_{i+1},\mathbf{r}_i;E)\right]\\
&= \prod_{k=1}^{n}\left[\int_0^\infty d\mathbf{r}_k\left\{-\frac{2\alpha Ze}{3\pi\mathrm{r}_k}\left[\left(1+\frac{\mathrm{r}_k^2}{3\alpha^2}\right)K_0 - \frac{\mathrm{r}_k}{6\alpha}Ki_1 - \left(\frac{5}{6}+\frac{\mathrm{r}_k^2}{3\alpha^2}\right)Ki_2\right]\right\}\right]\\
&\qquad\times\prod_{i=1}^{n}\left[\sum_{j,\kappa}\frac{\Gamma(p+\lambda+1)}{2ik\mathrm{r}_1\mathrm{r}_2\Gamma(2\lambda+2)}W_{-p,\lambda+1/2}(-2ik\mathrm{r}_1)\right.\\
&\qquad\qquad\times\left\{\left[m-\frac{\kappa E}{\gamma}\right]M_{-p,\lambda+1/2}(-2ik\mathrm{r}_2)\Omega^j_{\kappa,\kappa}(\theta_2\phi_2|\theta_1\phi_1)\beta^2\right.\\
&\qquad\qquad\left.\left.-k\,\tilde{\gamma}M_{-p,\bar{\lambda}+1/2}(-2ik\mathrm{r}_2)\Omega^j_{\kappa,-\kappa}(\theta_2\phi_2|\theta_1\phi_1)\alpha_1\alpha_2\alpha_3\right\}\right]. \quad (6.97)
\end{aligned}$$

The energy-dependent Green's function is then

$$G(\mathbf{r}_b,\mathbf{r}_a;E) = \sum_{n=0}^{\infty} G^{(n)}(\mathbf{r}_b,\mathbf{r}_a;E)\,. \quad (6.98)$$

Considering upto first-order the Green's function in Eq. (6.97) can be written as

$$G^{(1)}(\mathbf{r}_b,\mathbf{r}_a;E) = \left[\int_0^\infty d^3\mathbf{r}\,\Delta V(\mathbf{r})\right]\left[\prod_{i=0}^{1}G^{(0)}(\mathbf{r}_{i+1},\mathbf{r}_i;E)\right] \quad (6.99)$$

The bound state energy spectrum can be obtained from the poles of the spectral function in analogy to the relativistic H-atom problem [80], which is given as

$$G(E) = \int \langle \mathbf{r}| \, G \, |\mathbf{r}\rangle \; d\mathbf{r} \,, \tag{6.100}$$

$$= \sum_a \langle a| \, G \, |a\rangle + \text{non-singular part} \,. \tag{6.101}$$

$|a\rangle$ being the bound states with discrete energies E_a, and $\langle \mathbf{r}| \, G \, |\mathbf{r}\rangle$ being the Green's function in coordinate representation. The unperturbed bound state has a corresponding eigenenergy given by a sum $E_a^{(0)} = \epsilon_{a_1} + \cdots + \epsilon_{a_n}$, where each component is the conrtibution of non-interacting single-electron bound states.

The Green's function in Eq. (6.99) allows for the usual field-theoretic basis-state representation of the bound-state spectral function, in terms of the perturbed states ϕ_n and the corresponding eigenenergies E_n, which is given as

$$G(E) = \sum_n \frac{\phi_n(\mathbf{r}_b)\bar{\phi}_n(\mathbf{r}_a)}{E - E_n(1 - i\varepsilon)} \,. \tag{6.102}$$

Following Refs. [167–169], we introduce a function $G_a(E) = \langle a| \, G\gamma^0 \, |a\rangle$, which is the spectral function projected onto a single reference state $|a\rangle$, and contains the eigenenergies of the individual states. From the spectral representation of the function $G(E)$, we can write

$$G_a(E) = \frac{C_a}{E - E_a} + \text{non-singular part} \tag{6.103}$$

where the constant C_a is the residue term and has the known form

$$C_a = \int d^3\mathbf{r}_b \int d^3\mathbf{r}_a \, \psi_a^\dagger(\mathbf{r}_b)\phi_n(\mathbf{r}_b)\bar{\phi}_n(\mathbf{r}_a)\psi_a(\mathbf{r}_a) \,. \tag{6.104}$$

The energies are now determined using complex contour integration [167–169] by considering a small contour Γ which has an isolated pole at the perturbed bound-state energy E_a, we have

$$\frac{1}{2\pi i} \oint_\Gamma dE \, E \, G_a(E) = E_a C_a \tag{6.105}$$

and

$$\frac{1}{2\pi i} \oint_\Gamma dE \, G_a(E) = C_a \tag{6.106}$$

Thus, we have the energy level from the ratio of the above equations

$$E_a = \frac{\frac{1}{2\pi i} \oint_\Gamma dE \, E \, G_a(E)}{\frac{1}{2\pi i} \oint_\Gamma dE \, G_a(E)} \,. \tag{6.107}$$

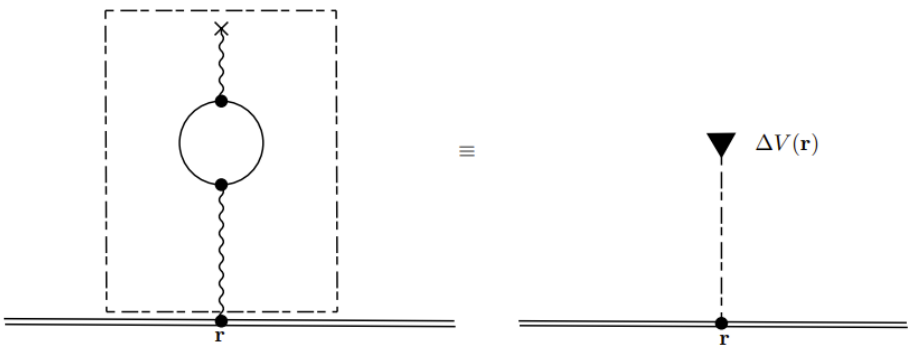

Figure 6.5: The bound-electron propagator corrected by the Uehling potential. The self-energy corrected photon propagator in the dashed box on the left-hand side figure is treated as an external perturbing potential as seen in Eq. (6.99)

It is much more convenient if we directly adopt the expression for the energy shift

$$\Delta E_a = \frac{\oint_\Gamma dE\, \Delta E\, \Delta G_a(E)}{2\pi i + \oint_\Gamma dE\, \Delta G_a(E)}\,. \tag{6.108}$$

where

$$\Delta E_a = \Delta E_a^{(1)} + \Delta E_a^{(2)} + \dots\,,$$
$$\Delta G_a = \Delta G_a^{(1)} + \Delta G_a^{(2)} + \dots\,,$$

have been expanded in terms of the fine-structure constant, α, in a perturbation series, and $\Delta G_a = G_a(E) - \Delta G_a^{(0)}$; $\Delta G_a^{(0)} = \frac{1}{E - E_a^{(0)}}$ being the zeroth-order contribution. We expand the Eq. (6.108) in a geometric series and obtain

$$\Delta E_a^{(1)} = \frac{1}{2\pi i} \oint_\Gamma dE\, \Delta E\, \Delta G_a^{(1)}(E)\,. \tag{6.109}$$

We can now deduce the energy shift very easily by first constructing the Green's function using Feynman rules For this, we consider the Uehling correction to the bound-electron propagator to be a simple correction due to a perturbing potential, as seen in Eq. (6.99). The above set of Eqs. (6.100)-(6.109) are applicable to many-electron systems, but we study a simple one-electron system having the bound-state eigenenergy ϵ_a. The Green's function has the form

$$G(\mathbf{r}_b, \mathbf{r}_a; E) = -2\pi i \gamma^0 \delta(E_b - E_a) \int d^3\mathbf{r} \frac{i}{2\pi} S(\mathbf{r}_b, \mathbf{r}; E_b) \Delta V(\mathbf{r}) \frac{i}{2\pi} S(\mathbf{r}, \mathbf{r}_a; E_a)\,. \tag{6.110}$$

The function G_a is written, in terms of the spectral representation of the bound propagator in Eq. (6.102), as

$$G_a(E) = \langle a|\, G(E)\gamma^0\, |a\rangle = \frac{i}{2\pi} \frac{\langle a|\, \Delta V\, |a\rangle}{(E - \epsilon_a)^2} \delta(E' - E)\,, \tag{6.111}$$

where we have replaced E_a with E and E_b with E' for notational purposes. Thus, using the above definitions, we have simply

$$\Delta G_a^{(1)}(E) \sim \frac{\langle a| \Delta V |a\rangle}{(E-\epsilon_a)^2} \,. \tag{6.112}$$

and from Eq. (6.109), we have

$$\Delta E_a^{(1)} = \langle a| \Delta V |a\rangle \;, \tag{6.113}$$

where $\Delta E = E - E_a^{(0)}$. In our calculations, the perturbing potential is the Uehling potential which we have denoted by U_{VP}^{Ueh}, and thus, the energy shift of the bound state $|a\rangle$ can be given as

$$\Delta E_a^{(1)} = \langle a| U_{VP}^{Ueh} |a\rangle \;. \tag{6.114}$$

The second-order energy shift can be obtained as a continuation of the geometric-series expansion of Eq. (6.108) as

$$\begin{aligned} \Delta E_a^{(2)} &= \frac{1}{2\pi i} \oint_\Gamma dE\, \Delta E\, \Delta G_a^{(2)}(E) \\ &- \left(\frac{1}{2\pi i} \oint_\Gamma dE\, \Delta E\, \Delta G_a^{(1)}(E) \right) \left(\frac{1}{2\pi i} \oint_\Gamma dE\, \Delta G_a^{(1)}(E) \right) \,. \end{aligned} \tag{6.115}$$

The first term in Eq. (6.115) is the irreducible (non-degenerate) part and the second term is the reducible (degenerate) part. For the irreducible part, we obtain

$$\begin{aligned} \frac{1}{2\pi i} \oint_\Gamma dE\, \Delta E\, \Delta G_a^{(2)}(E) = \\ \sum_{i\neq a} \frac{\langle a| U_{VP}^{Ueh} |i\rangle \langle i| U_{VP}^{Ueh} |a\rangle}{\epsilon_a - \epsilon_i} \,, \end{aligned} \tag{6.116}$$

and the reducible part is given as

$$\begin{aligned} &\left(\frac{1}{2\pi i} \oint_\Gamma dE\, \Delta E\, \Delta G_a^{(1)}(E) \right) \left(\frac{1}{2\pi i} \oint_\Gamma dE\, \Delta G_a^{(1)}(E) \right) \\ &\quad = \Delta\epsilon_a^{(1)} \left(\frac{1}{2\pi i} \oint_\Gamma dE\, \frac{\langle a| U_{VP}^{Ueh} |a\rangle}{(E-\epsilon_a)^2} \right) \\ &\quad = \langle a| U_{VP}^{Ueh} |a\rangle \langle a| (dU_{VP}^{Ueh}/dE)_{E=E_a} |a\rangle \;. \end{aligned} \tag{6.117}$$

The Uehling potential, as defined in Eq. (6.96), is independent of the bound-state energy and as such the derivative term in Eq. (6.117) vanishes and the second-order correction to the energy level is then given by the usual Rayleigh-Schrödinger perturbation expansion

$$\Delta E_a^{(2)} = \sum_{i\neq a} \frac{\langle a| U_{VP}^{Ueh} |i\rangle \langle i| U_{VP}^{Ueh} |a\rangle}{\epsilon_a - \epsilon_i} \,. \tag{6.118}$$

Z	Uehling correction [eV]					Ref.
	$1s$	$2s$	$3s$	$2p_{1/2}$	$2p_{3/2}$	
	H-like	Li-like	Na-like	B-like	N-like	
54	-7.3516	-1.0272	-0.306	-0.04931	-0.00555	
	-7.35163	-1.02717		-0.049313	-0.005545	[170]
82	-51.875	-8.4760	-2.466	-1.0938	-0.063801	
	-51.8751	-8.47600		-1.09378	-0.0638007	[170]
92	-97.996	-17.309	-4.878	-2.9954	-0.12653	
	-97.9960	-17.3092		-2.99533	-0.126532	[170]

Table 6.1: Uehling vacuum polarization corrections for certain H-like heavy ions, in units of eV.

6.5 Numerical results and summary

To confirm the validity of our approach, in Table 6.1, we present numerical results of first-order perturbative Uehling shifts [Eq. (6.113)] for heavy H-like ions and certain alkali ions, and compare them with earlier evaluations of this correction (see e.g. Ref. [170]. A good agreement can be stated. We assume for simplicity a point-like nuclear charge distribution.

Table 6.1 reiterates the well-known fact that with the increase in the atomic number, the VP effects become more and more pronounced; VP effects scale as $\sim (Z\alpha)^4$ to leading order. For most elements and charge states, the VP shift is experimentally discernible with modern Penning-trap mass spectrometric methods with experimental uncertainties on the 1-eV level or below [75, 171–173]. We thus identify ions which allow, for the first time, a test of QED via measuring the electronic binding energy of a valence electron by determining the mass difference of two ions, one with a single valence electron and one without. The values in the Table also show that it is not only H-like ions in the $1s$ ground state which feature VP effects well observable by these experimental methods, but also excited states possess observable radiative shifts. E.g. the VP shift given for the $2s$ state approximates the VP correction to the (negative of the) binding energy of a Li-like ion, which can be spectrometrically determined by measuring the mass difference of the Li- and the He-like ions in their ground states. In our approach presented here, we fully neglect many-electron (screening) effects, which, for the high-Z ions presented here, is a justified first approximation, as they contribute with a relative order of $\frac{1}{Z}$. Our path integral formalism however may be extended in future to many-electron systems, by allowing the exchange of photons between different electrons.

Similarly, the VP results given for the $3s$ state approximate the radiative shift of the binding energy of the valence electron in the Na-like charge state, and the values

given for the $2p_{1/2}$ and $2p_{3/2}$ orbitals give the first approximation for B- and N-like ions, respectively. Ions in these charge states are easier to produce experimentally, and Na- and B-like very heavy species feature observable VP contributions, enabling a proof-of-the-principle demonstration of QED tests via mass measurements.

We have calculated the VP correction to energy levels of HCIs employing a path integral formalism. First, the evaluation of the leptonic loop correction to the photon propagator by means of the Dyson-Schwinger equation is summarized. The effective potential describing the correction to the nuclear potential in the lowest order in $Z\alpha$, i.e. the Uehling potential, is used in an analytical form given by Frolov and Wardlow [164]. The contribution to the energy level of a H-like ion due to the perturbing Uehling potential is derived from the perturbed action using a relativistic path integral method. We show that the VP level shifts – or any energy shift induced by a local potential – can be extracted from the poles of the Green's function. The VP correction is given numerically for a range of heavy ions, concluding that in sufficiently highly charged ions, the VP effect is observable with state-of-the-art mass spectrometric methods.

7. Radiative corrections at the one-loop level – Self-energy

7.1 Self-energy correction

The corrections to energy levels of bound-electrons has been a focal point for theoretical and experimental studies on HCIs. Of utmost importance has been the evaluation of the radiative shift due to fermionic self-energy. Experimental advances in the production of HCIs and the corresponding determination of their properties with unprecedented accuracy [43, 45, 62, 65, 75, 113–115, 171, 173–175] dictate modern theoretical frameworks for the study of such systems.

From a theoretical standpoint, the calculations pertaining to radiative corrections in QED have been rigorously studied and developed by a multitude of authors [83, 104–107, 112, 126, 163, 176–180], to name a few. Historically, one of the first such study was done by Gell-Mann, Low and Sucher using the adiabatic S-matrix method[181, 182]. This method was followed by a plethora of alternate theoretical formalisms based on Green's functions [119, 169, 183–189].

In this Chapter, we arrive at the Green's function for the self-energy shifted fermion propagator in the Furry picture using the method of functional integrals, conceived by Feynman [90], and developed further by several authors, both in the non-relativistic and relativistic regime [17, 125, 130, 140, 142, 150, 153, 166, 190]. We put forward the functional integral formulation of the evaluation of self-energy correction to bound-electron energy levels at the one-loop level. We derive the dressed bound-electron propagator using Schwinger-Dyson equations in the framework of path integrals. The calculation of the energy shift induced by the interaction of the bound electron with its own electromagnetic field or the self-energy correction is done by separating the energy shift into zero- ,one- , and many-potential terms each of which are defined using perturbative path integrals. Numerical calculations have been extensively worked out in [83, 84], we follow these works and give only a brief overview of the methods implemented. The energy shifts due to these individual terms are calculated numerically using complex contour integrals through the implementation of B-spline codes [87].

We begin this Chapter by deriving the complete expression for the dressed bound-lepton propagtor. This is done by defining the Schwinger-Dyson equation for the leptonic propagator using path integrals, as done in the previous Chapter for the derivation of the photon propagator, in analogy to Ref. [82].

The gauge-fixed QED Lagrangian, as derived in Section 2.2, in the Furry picture [76] is given as

$$\mathcal{L}_{\text{QED}}(x) = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} - \frac{1}{2\xi}(\partial^\mu A_\mu)^2 + \bar{\psi}(x)(i\not{D} - m)\psi(x) - \bar{\psi}(x)e\gamma^\mu A_\mu(x)\psi(x)\,, \tag{7.1}$$

where

$$D_\mu(x) = \partial_\mu(x) + ie\mathcal{A}_\mu(x)\,,$$

$\mathcal{A}_\mu$ being the vector field of the nucleus; A_μ is the gauge field operator for the photon or the photon field, $\psi(x)$ is the field of the electron, m is its bare mass, e is the elementary charge. The first term in Eq. (7.1) stands for the free electromagnetic field Lagrangian density that has been gauge fixed, following the Faddeev-Popov gauge-fixing method as derived in Section 2.2, by the second term. The central term is the Dirac term in the presence of an external field and the last term gives the interaction of the Dirac field with the gauge field of the photon. We do not need to concern ourselves with fixing the gauge for the external field since we use the background field method [191], presented in Appendix B, according to which the effective action in the presence of a classical background field and in the absence of a background field is equivalent and hence the choice of gauge plays no role. Furthermore, we will see that we can also ignore the gauge-fixing term for the photon field since now we are interested in deriving the electron propagator in the presence of an external field, and we take derivatives w.r.t. the fermion fields, of which the gauge-fixing term is independent.

The generating functional is now constructed using this Lagrangian, and Grassmann-valued sources η and $\bar{\eta}$ of the fermionic fields, and the source J_μ for the gauge field

$$\begin{aligned} Z[\eta,\bar{\eta},J] = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi\mathcal{D}A \exp\Bigg\{ i\int \mathrm{d}^4x[\mathcal{L}_{\text{QED}} \\ + J_\mu(x)A^\mu(x) + \bar{\psi}(x)\eta(x) + \bar{\eta}(x)\psi(x)]\Bigg\}\,, \end{aligned} \tag{7.2}$$

where $\mathcal{D}$ represents the integral measure over all field configurations. To arrive at the Schwinger-Dyson equations, as in the last Chapter, we consider that the functional integral of a total derivative is zero, i.e.,

$$\int \mathcal{D}[\phi]\frac{\delta}{\delta\phi} = 0\,,$$

where $\frac{\delta}{\delta\phi}$ is the functional derivative w.r.t. ϕ, which is any arbitrary field variable. For the fermion propagator, the derivative is taken with respect to the classical fermion field $\bar{\psi}(x)$,

$$\begin{aligned} \int \mathcal{D}[\bar{\psi}\psi A]\frac{\delta}{\delta\bar{\psi}(x)}\exp\{i[\mathcal{S}[\bar{\psi},\psi,A] \\ + \int d^4x(J_\mu(x)A^\mu(x) + \bar{\psi}(x)\eta(x) + \bar{\eta}(x)\psi(x))]\} = 0\,, \end{aligned} \tag{7.3}$$

where $\mathcal{S} = \int \mathrm{d}^4x\, \mathcal{L}_{\text{QED}}$ is the QED action. Eq. (7.3) can be written in terms of a differential equation in the generating functional Z

$$\left[\frac{\delta \mathcal{S}}{\delta \bar{\psi}(x)}\left(i\frac{\delta}{\delta \eta}, -i\frac{\delta}{\delta \bar{\eta}}, -i\frac{\delta}{\delta J_\mu}\right) + \eta(x)\right] Z[\eta, \bar{\eta}, J] = 0\,, \tag{7.4}$$

where we have represented the action given in terms of the fields $\psi, \bar{\psi}$, and A^μ in corresponding functional derivative terms $\frac{-i\delta}{\delta \bar{\eta}}$, $\frac{i\delta}{\delta \eta}$, and $\frac{-i\delta}{\delta J_\mu}$.
We then take the functional derivative of the action $\mathcal{S}$, which is expressed in terms of the Lagrangian in Eq. (7.1) as

$$\mathcal{S} = \int d^4x \Bigg[-\frac{1}{4}F^{\mu\nu}F_{\mu\nu} - \frac{1}{2\xi}(\partial^\mu A_\mu)^2 + \bar{\psi}(x)(i\not{D} - m)\psi(x) \\ -\bar{\psi}(x)e\gamma^\mu A_\mu(x)\psi(x)\Bigg]\,, \tag{7.5}$$

by implementing the Gateux derivative method [155, 156] given by Eq. (6.5), and obtain

$$\frac{\delta \mathcal{S}}{\delta \bar{\psi}} = (i\not{D} - m)\psi(x) - e\gamma^\mu A_\mu(x)\psi(x)\,. \tag{7.6}$$

This yields the differential equation

$$\left[\left(i\not{\partial} - m - e\gamma^\mu \mathcal{A}_\mu - e\gamma^\mu(-i)\frac{\delta}{\delta J^\mu(x)}\right)(-i)\frac{\delta}{\delta \bar{\eta}(x)} + \eta(x)\right] Z[\eta, \bar{\eta}, J] = 0\,. \tag{7.7}$$

To obtain the two-point Green's function for the electron, we take another derivative with respect to the source field $\eta(y)$ (since the outgoing electron originates from this field point), which gives us

$$\delta(x-y)Z[\eta, \bar{\eta}, J] + \eta(x)\frac{\delta Z[\eta, \bar{\eta}, J]}{\delta \eta(y)} \tag{7.8}$$
$$+\left(i\not{\partial} - m - e\gamma^\mu \mathcal{A}_\mu - e\gamma^\mu(-i)\frac{\delta}{\delta J^\mu(x)}\right)(-i)\frac{\delta}{\delta \eta(y)}\frac{\delta}{\delta \bar{\eta}(x)}Z[\eta, \bar{\eta}, J] = 0\,.$$

We now set the leptonic source terms to zero and rewrite the Eq. (7.8) as

$$\delta(x-y)e^W + \tag{7.9}$$
$$+\left(i\not{\partial} - m - e\gamma^\mu \mathcal{A}_\mu - e\gamma^\mu(-i)\frac{\delta}{\delta J^\mu(x)}\right)(-i)\frac{\delta}{\delta \eta(y)}\frac{\delta}{\delta \bar{\eta}(x)}e^W = 0\,,$$

where we have represented the generating functional in terms of the functional for the connected Green's functions W ($Z = e^W$) [157]. Performing the functional derivative

and implementing the chain rule of derivatives, we obtain

$$e^{W[\eta,\bar{\eta},J]}\Bigg[\delta(x-y)-\Bigg(i\not{\partial}-m-e\gamma^{\mu}\mathcal{A}_{\mu} \\ -ie\gamma^{\mu}\frac{(-i)\delta W}{\delta J^{\mu}(x)}-ie\gamma^{\mu}(-i)\frac{\delta}{\delta J^{\mu}(x)}\Bigg)S(x,y)\Bigg]=0\,, \tag{7.10}$$

where $S(x,y)$ is the bound-electron propagator derived in Appendix A, Eq. (A.21). We rewrite Eq. (7.10) in terms of classical fields defined in Appendix A, Eq. (A.11), [2, 82, 157]

$$\delta(x-y)-\left(i\not{\partial}-m-e\gamma^{\mu}\mathcal{A}_{\mu}-ie\gamma^{\mu}A_{\mu}-ie\gamma^{\mu}(-i)\frac{\delta}{\delta J^{\mu}(x)}\right)S(x,y)=0\,. \tag{7.11}$$

We reintroduce the effective action, as done in the last Section [82]

$$i\Gamma[\bar{\psi},\psi,A]=W[\eta,\bar{\eta},J]-i\int \mathrm{d}^4x\,(\bar{\psi}\eta+\psi\bar{\eta}+A^{\mu}J_{\mu})\,, \tag{7.12}$$

and also define the field terms $(\bar{\psi},\psi,A_{\mu})$ in terms of the source terms $(\eta,\bar{\eta},J_{\mu})$ (for detailed derivations, refer to Appendix A) [82]

$$A_{\mu}=-i\frac{\delta W[J]}{\delta J^{\mu}}\,,\quad \psi=-i\frac{\delta W[\eta]}{\delta\bar{\eta}}\,,\quad \bar{\psi}=i\frac{\delta W[\bar{\eta}]}{\delta\eta}\,.$$

$$J_{\mu}=-\frac{\delta\Gamma[A]}{\delta A^{\mu}}\,,\quad \eta=-\frac{\delta\Gamma[\bar{\psi}]}{\delta\psi}\,,\quad \bar{\eta}=\frac{\delta\Gamma[\psi]}{\delta\bar{\psi}}\,.$$

We have

$$(-i)\frac{\delta S(x,y)}{\delta J^{\mu}(x)} \\ =-i\int d^4z\frac{\delta A_{\nu}(z)}{\delta J^{\mu}(x)}\frac{\delta}{\delta A_{\nu}(z)}\left(\frac{\delta^2\Gamma}{\delta\psi(x)\delta\bar{\psi}(y)}\right)^{-1}\,, \tag{7.13}$$

where we have defined $S(x,y)$ using Eq. (A.21). In analogy to Ref. [82] using the expressions for the complete bound electron propagator, photon propagator and the electron-photon vertex function, Γ^{ν}, we obtain

$$(-i)\frac{\delta S(x,y)}{\delta J^{\mu}(x)} \\ =-e\int d^4z\,d^4u\,d^4w D_{\mu\nu}(x-z)S(x,w)\Gamma^{\nu}(w,u;z)S(u,y)\,, \tag{7.14}$$

where, as in the case of the fermion propagator defined by Eq. (6.11), we have defined [157]

$$\frac{\delta A_{\nu}(z)}{\delta J^{\mu}(x)}=-i\frac{\delta^2W[J]}{\delta J^{\mu}(x)\delta J^{\nu}(z)}=iD_{\mu\nu}(x-z)\,,$$

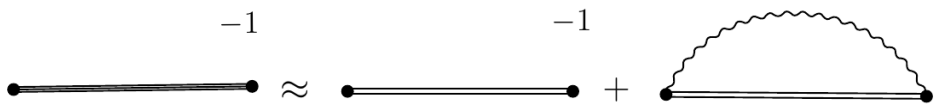

Figure 7.1: Diagrammatic representation of the Schwinger-Dyson equation for the bound dressed electron.

and

$$\begin{aligned}
&\frac{\delta}{\delta A_\nu(z)}\left(\frac{\delta^2\Gamma}{\delta\psi(x)\delta\bar{\psi}(y)}\right)^{-1} \\
&= -\left(\frac{\delta^2\Gamma}{\delta\psi(x)\delta\bar{\psi}(w)}\right)^{-1}\left(\frac{\delta^3\Gamma}{\delta A_\nu(z)\delta\psi(w)\delta\bar{\psi}(u)}\right)\left(\frac{\delta^2\Gamma}{\delta\psi(u)\delta\bar{\psi}(y)}\right)^{-1} \\
&= -iS(x,w)e\Gamma^\nu(w,u;z)(-i)S(u,y) \\
&= -eS(x,w)\Gamma^\nu(w,u;z)S(u,y)\,.
\end{aligned}$$

Using Eqs. (7.13) and (7.14), using the above two expressions, setting external source fields to zero, and considering that the nuclear field is static (all components other than $\mathcal{A}^0$ vanishes), Eq. (7.11) can be reduced to

$$\delta(x-y) = (i\partial\!\!\!/ - m - e\gamma^\mu\mathcal{A}^0)S(x,y) + \int d^4w\Sigma(x,u)S(u,y)\,, \tag{7.15}$$

where

$$\Sigma(x-y) = -ie^2\gamma^\mu\int d^4z\,d^4wD_{\mu\nu}(z-x)S(x,w)\Gamma^\nu(w,y;z)\,. \tag{7.16}$$

To obtain the SDE for the bound propagator in the coordinate space, we multiply Eq. (7.15) throughout with the inverse propagator and obtain

$$\begin{aligned}
S^{-1}(x,y) = (i\partial\!\!\!/ - m - e\gamma^\mu\mathcal{A}^0)\delta(x-y) \\
-ie^2\gamma^\mu\int d^4z\,d^4wD_{\mu\nu}(z-x)S(x,w)\Gamma^\nu(w,y;z)\,.
\end{aligned} \tag{7.17}$$

This is pictorially represented in Fig. (7.1)

7.2 Derivation of the self-energy shift

The second term on the R.H.S. of Eq. (7.17), given by Eq. (7.16) gives the self-energy-corrected bound propagator and is the well-known self-energy operator. Fourier transforming this with respect to the time variable only, and considering the electron-photon vertex operator in the lowest order, one obtains

$$\Sigma(\epsilon) = ie^2\int\frac{d\omega}{2\pi}\gamma^\mu S(\mathbf{x},\mathbf{w};\eta)D_{\mu\nu}(\mathbf{z}-\mathbf{x};\omega)\gamma^\nu\,, \tag{7.18}$$

where η and ω are the energies of the virtual electron and photon respectively.

To now derive the energy-level shift due to this self interaction of the electron, we imagine that the electron, travelling in the field of the nucleus, from an initial point to a final point, has a particular transition amplitude. In the event that the electron now interacts with its own electromagnetic field while moving between these two points, the final transition amplitude would be altered by this interaction. This correction to the transition amplitudes translates into a correction to the energy between the initial and the final state of the bound electron. Using the self-energy operator in Eq. (7.18) and using Feynman rules [89], we can construct the transition amplitude or the Green's function for the bound electron interacting with its own field. This has the form

$$\begin{aligned} G(\mathbf{x}_i, E_i; \mathbf{x}_f, E_f) = ie^2 \int d^3\mathbf{z}_1 \int d^3\mathbf{z}_2 \int d\eta \int d\omega \frac{i}{2\pi} S(\mathbf{x}_f, \mathbf{z}_2; E_f) \\ \times(-2\pi i) e\gamma^\mu \delta(E_f - \eta - \omega) \frac{i}{2\pi} S(\mathbf{z}_2, \mathbf{z}_1; \eta)(-2\pi i) e\gamma^\nu \delta(\eta + \omega - E_i) \\ \times \frac{i}{2\pi} S(\mathbf{z}_1, \mathbf{x}_i; E_i) \frac{i}{2\pi} D_{\mu\nu}(\mathbf{z}_1 - \mathbf{z}_2; \omega)\,, \end{aligned} \tag{7.19}$$

where $(\mathbf{x}_i, E_i)$ refers to the intial position and energy of the bound electron and $(\mathbf{x}_f, E_f)$ refers to the final position and energy. We integrate over the energy of the virtual electron η, which exists between the vertices $\mathbf{z}_1$ and $\mathbf{z}_2$ and obtain a simplified expression

$$\begin{aligned} G(\mathbf{x}_i, E_i; \mathbf{x}_f, E_f) \sim ie^2 \left(\frac{i}{2\pi}\right)^2 \int d^3\mathbf{z}_1 \int d^3\mathbf{z}_2 \int d\omega S(\mathbf{x}_f, \mathbf{z}_2; E_f) \\ \times e\gamma^\mu S(\mathbf{z}_2, \mathbf{z}_1; \eta) e\gamma^\nu S(\mathbf{z}_1, \mathbf{x}_i; E_i) D_{\mu\nu}(\mathbf{z}_1 - \mathbf{z}_2; \omega) \delta(E_f - E_i)\,. \end{aligned} \tag{7.20}$$

The bound-state energy spectrum is now obtained from the poles of the Green's function as done in Section 6.4. Using Eqs. (6.102)-(6.104) we introduce the spectral function

$$\langle a|\, G\, |a\rangle = \left(\frac{i}{2\pi}\right)^2 \frac{1}{(E - \epsilon_a)^2} \int d\omega \sum_n \frac{\langle an|\, I(\omega)\, |na\rangle}{E - \omega - \epsilon_n(1 - i\varepsilon)} \delta(E' - E)\,, \tag{7.21}$$

where we have introduced the photon-interaction operator $I(\mathbf{z}_1 - \mathbf{z}_2; \omega) = e^2 \alpha^\mu \alpha^\nu D_{\mu\nu}(\mathbf{z}_1 - \mathbf{z}_2; \omega)$ with $\alpha^\mu = \gamma^0\gamma^\mu$, and using the notation $|a\rangle$ for the reference state. We have also made the replacement $E_i = E$ and $E_f = E'$ in order to keep the notation clear. Using these notational modifications, we can now write using Eqs. (6.100)-(6.109),

$$\Delta G_a^{(1)}(E) = \frac{\langle a|\, \Sigma(E)\, |a\rangle}{(E - \epsilon_a)^2}\,, \tag{7.22}$$

where $\langle a|\, \Sigma(\epsilon_a)\, |b\rangle = \frac{i}{2\pi} \int d\omega \sum_n \frac{\langle an|I(\omega)|nb\rangle}{E - \omega - \epsilon_n(1 - i\varepsilon)}$; $|an\rangle$ denotes the tensor product of the single-electron states $|a\rangle$ and $|n\rangle$.

Thus we have the self-energy correction to the bound-state energy level from Eq. (6.109) as

$$\begin{aligned} \Delta E_a^{(1)} &= \frac{1}{2\pi i} \oint_\Gamma dE\, \Delta E\, \Delta G_a^{(1)}(E) \\ &= \langle a|\, \Sigma(\epsilon_a)\, |a\rangle\ . \end{aligned} \tag{7.23}$$

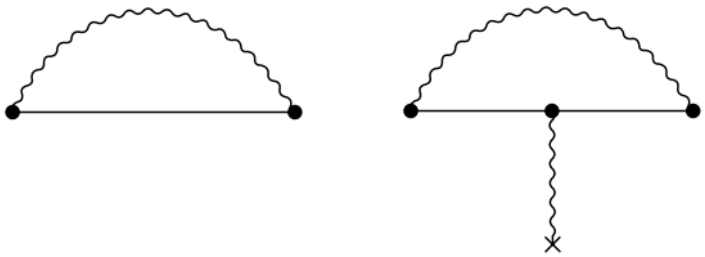

Figure 7.2: Diagrammatic representation of the zero- and one-potential terms of the self-energy function. On the left we have the zero-potential term with no interaction with the nuclear potential, while in the figure on the right, the electron propagator has exactly one interaction with the nuclear potential.

Here, we have considered the self-energy operator that has been renormalized using the usual on-shell renormalization scheme [89, 192, 193]. We can write down the mass counterterm, δm, explicitly and as such we have

$$\Delta E_a^{(1)} = \langle a| \Sigma(\epsilon_a) - \delta m \gamma^0 |a\rangle \ . \tag{7.24}$$

The expression, in Eq. (7.23), is however fraught with divergences and we follow [83, 84] and separate the self-energy shift into zero- , one- , and many-potential terms, respectively

$$\begin{aligned} \langle a| \Sigma(\epsilon_a) |a\rangle = \langle a| \Sigma^{(0)}(\epsilon_a) |a\rangle \\ + \langle a| \Sigma^{(1)}(\epsilon_a) |a\rangle + \langle a| \Sigma^{(2+)}(\epsilon_a) |a\rangle \ . \end{aligned} \tag{7.25}$$

The individual terms in Eq. (7.25) can be written in terms of the time-independent bound-electron Green's function[194], $G(\mathbf{r}_2, \mathbf{r}_1; E)$, $\bar{\psi} = \gamma^0 \psi^\dagger$ and the photon propagator using perturbative path integrals [2, 153, 154, 166], as discussed in the Section 6.3.

Using this approach, we write down the zero-, one- and many-potential terms separately, using Eq. (7.16) in Eq. (7.24). We overlook the renormalization term for the moment and address it in a subsequent Section on regularization.
The **zero-potential term** is

$$\begin{aligned} &\langle a| \Sigma^{(0)}(\epsilon_a) |a\rangle \\ &= 2i\alpha \int d\omega \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \psi_a^\dagger(\mathbf{r}_2) \alpha^\mu G^{(0)}(\mathbf{r}_2, \mathbf{r}_1; \epsilon_a - \omega) \\ &\qquad \times \alpha^\nu D_{\mu\nu}(\omega) \psi_a(\mathbf{r}_1) \ , \end{aligned} \tag{7.26}$$

where $G^{(0)}(\mathbf{r}_2, \mathbf{r}_1; \epsilon_a - \omega)$ is the free-electron Green's function given by Eq. (4.49) [1]. We will write later this term in the momentum space, since in that representation it can

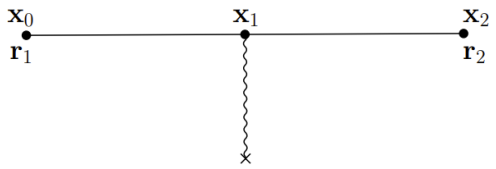

Figure 7.3: Diagrammatic representation of the one-potential Green's function

be traced back to the well-known regularized self-energy function.
Similarly, the **one-potential term** is given as

$$\begin{aligned} &\langle a|\,\Sigma^{(1)}(\epsilon_a)\,|a\rangle \\ &= 2i\alpha \int d\omega \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \psi_a^\dagger(\mathbf{r}_2)\alpha^\mu G^{(1)}(\mathbf{r}_2,\mathbf{r}_1;\epsilon_a-\omega) \\ &\qquad\qquad \times\alpha^\nu D_{\mu\nu}(\omega)\psi_a(\mathbf{r}_1)\,, \end{aligned} \tag{7.27}$$

where the Green's function for a single interaction of the electron with the nuclear potential V, as is shown in Fig. (7.3), in terms of the free Green's function is [2, 153, 154, 166]

$$\begin{aligned} &G^{(1)}(\mathbf{r}_2,\mathbf{r}_1;\epsilon_a-\omega) \\ &= \left[\int_0^\infty \mathrm{d}^3\mathbf{x_1}\, V(\mathbf{x_1})\right]\left[\prod_{i=0}^{1} G^{(0)}(\mathbf{x}_{i+1},\mathbf{x}_i;\epsilon_a-\omega)\right]\,. \end{aligned} \tag{7.28}$$

Also, as to be discussed later, this one-potential term will be evaluated in momentum space, as it can be expressed in terms of the known regularized vertex function.
Following the same formulation, the **many-potential term** is given as

$$\begin{aligned} &\langle a|\,\Sigma^{(2+)}(a)\,|\psi_a\rangle \\ &= 2i\alpha \int d\omega \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \psi_a^\dagger(\mathbf{r}_2)\alpha^\mu G^{(2+)}(\mathbf{r}_2,\mathbf{r}_1;\epsilon_a-\omega) \\ &\qquad\qquad \times\alpha^\nu D_{\mu\nu}(\omega)\psi_a(\mathbf{r}_1)\,. \end{aligned} \tag{7.29}$$

The Green's function for the many-potential term between the states $\mathbf{r}_3$ and $\mathbf{r}_4$, as seen in Fig. (7.4), with n insertions of the nuclear interaction where $n\to\infty$, can be given in terms of the free Green's function as

$$\begin{aligned} &G(\mathbf{r}_4,\mathbf{r}_3;\epsilon_a-\omega) \\ &= \sum_{n=0}^{\infty}\left\{\prod_{k=1}^{n}\left[\int_0^\infty \mathrm{d}^3\mathbf{x}_k\, V(\mathbf{x}_k)\right]\right. \\ &\qquad\qquad \left.\times\left[\prod_{i=0}^{n} G^{(0)}(\mathbf{x}_{n+1},\mathbf{x}_n;\epsilon_a-\omega)\right]\right\}\,. \end{aligned} \tag{7.30}$$

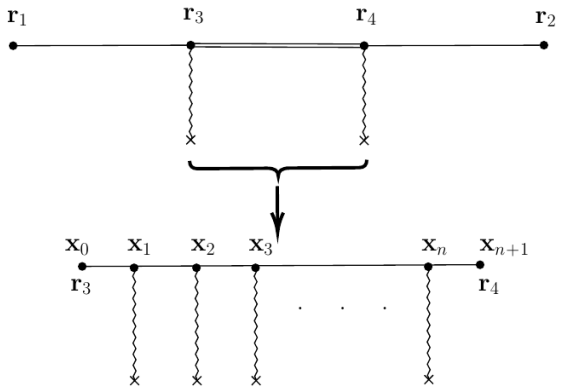

Figure 7.4: Diagrammatic representation of the many-potential Green's function.

This effectively gives us the exact Dirac-Coulomb Green's function[194]. The vector variable $\mathbf{x}_i$ has been introduced to maintain notational equivalence, in both Eqs. (7.28) and (7.30), to define the Green's functions with the nuclear interactions. It represents the position vectors denoting the intial and final points between which the free electron propagates before and after encountering an interaction.

The energy shift due to the many-potential contribution can thus be written as

$$\begin{aligned}
&\langle a|\,\Sigma^{(2+)}(\epsilon_a)\,|a\rangle \qquad (7.31)\\
&= 2i\alpha \int d\omega \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 d^3\mathbf{r}_3 d^3\mathbf{r}_4 \psi_a^\dagger(\mathbf{r}_2)\alpha^\mu\\
&\quad \times G^{(0)}(\mathbf{r}_2,\mathbf{r}_4;\epsilon_a-\omega)V(\mathbf{r}_4)G(\mathbf{r}_4,\mathbf{r}_3;\epsilon_a-\omega)\\
&\qquad \times V(\mathbf{r}_3)G^{(0)}(\mathbf{r}_3,\mathbf{r}_1;\epsilon_a-\omega)\alpha^\nu D_{\mu\nu}(\omega)\psi_a(\mathbf{r}_1)\,.
\end{aligned}$$

This term, due to the several Coulomb insertions in the Green's function, is finite and does not require regularization. Using the spectral representation for the free and bound-electron propagators [84], and in terms of the photon interaction operator $I(\omega)$ introduced earlier, the energy shift is given as

$$\begin{aligned}
&\langle a|\,\Sigma^{(2+)}(\epsilon_a)\,|a\rangle = \frac{i}{2\pi}\int d\omega \qquad (7.32)\\
&\times \sum_{\alpha,\beta,i} \frac{\langle i|\,V\,|\beta\rangle\,\langle a\beta|\,I(\omega)\,|\alpha a\rangle\,\langle\alpha|\,V\,|i\rangle}{(\epsilon_a-\omega-\epsilon_\alpha\varepsilon^+)(\epsilon_a-\omega-\epsilon_i\varepsilon^+)(\epsilon_a-\omega-\epsilon_\beta\varepsilon^+)}\,,
\end{aligned}$$

where $|a\rangle$ is the reference state, $|\alpha\rangle$ and $|\beta\rangle$ are the incoming and outgoing free-electron states and $|i\rangle$ represents the bound-electron state, and we use the notation $(1-i\varepsilon)=\varepsilon^+$.

Following Refs. [83, 84], we introduce frequency-dependent effective basis functions

$$\left|\phi_i^{(\pm)}(\omega)\right\rangle = \sum_\alpha \frac{\langle\alpha|\,V\,|i\rangle}{\omega-\epsilon_\alpha\varepsilon^\pm}\,|\alpha\rangle \qquad (7.33)$$

which simplifies Eq. (7.32) to the form

$$\langle a|\,\Sigma^{(2+)}(\epsilon_a)\,|a\rangle = \frac{i}{2\pi}\int d\omega \sum_i \frac{\left\langle a\phi_i^{(-)}\right|\,I(\omega)\,\left|\phi_i^{(+)}a\right\rangle}{\epsilon_a-\omega-\epsilon_i\varepsilon^+}\,. \tag{7.34}$$

As shown in [84], we can further simplify the Eq. (7.34), by expanding the numerator inside the integral on the R.H.S. in partial waves, such that the angular integrations can be performed analytically and only the radial integrals need to be computed numerically, which yields the many-potential term as [83]

$$\begin{aligned}&\langle a|\,\Sigma^{(2+)}(\epsilon_a)\,|a\rangle \\ &= \frac{i\alpha}{2\pi}\sum_{\kappa_i,n_i}\frac{(-1)^{j_i-j_a}}{2j_a+1}\int d\omega\sum_L(-1)^L\frac{R_L(\omega;a\phi_i^{(-)}\phi_i^{(+)}a)}{\epsilon_a-\omega-\epsilon_i\varepsilon^+}\end{aligned} \tag{7.35}$$

where κ_i are the Dirac quantum numbers of the effective basis states ϕ_i as introduced in Chapter 4. $j_i = |\kappa_i| - \frac{1}{2}$ is the total angular momentum quantum number of the basis states, $j_a = |\kappa_a| - \frac{1}{2}$ is the total angular momentum quantum number of the reference state, and the sum over L extends from $|j_i - j_a|$ to $j_i + j_a$. The generalized Slater integral R_L is defined in [84, 103].

Regularization

The zero- and one-potential terms are regularized following Refs. [83, 195]. We do not go into the mathematical details of the entire derivation as it has been already discussed in the aforementioned works and only present the most important results. In the following text, we represent integral measures over four vectors and their components as $\int \mathrm{d}a$ while integrals over scalar are denoted as $\int da$, also Fourier transformed functions are denoted as $\tilde{a}$, in order to increase comprehensibilty.

Zero-potential term:

We begin by expressing the zero-potential term given in Eq. (7.26) in the momentum representation

$$\langle a|\,\Sigma^{(0)}(\epsilon_a)\,|a\rangle = \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3}\tilde{\bar{\psi}}_a(\mathbf{p})\Sigma^0(p)\tilde{\psi}_a(\mathbf{p})\,, \tag{7.36}$$

where, $p = |\mathbf{p}|$, and the self-energy operator in the momentum space $\Sigma^0(p)$ can be obtained by Fourier transforming Eq. (7.16) and is given as

$$\Sigma^0(p) = -4\pi i\alpha\int\frac{\mathrm{d}^4k}{(2\pi)^4}\frac{1}{k^2+i\varepsilon}\gamma_\mu\frac{\not{p}-\not{k}+m_e}{(p-k)^2-m^2+i\varepsilon}\gamma^\mu\,. \tag{7.37}$$

The above expression, though infrared finite, is ultraviolet divergent and we use dimensional regularization to remove the divergence. We use the common formulation and set the space-time dimension as $D = 4 - 2d$, where d is a small number [83].

Eq. (7.37), after dimensional regularization, is written as

$$\Sigma^0(p) = \delta m - \frac{\alpha}{\pi}\frac{\Delta}{4}(\not{p} - m) + \Sigma^0_R(p)\,. \tag{7.38}$$

The first two terms in Eq. (7.38) are the divergent terms while the last term $\Sigma^0_R(p)$ is free of divergences. The first divergent term is given as [83]

$$\delta m = \frac{\alpha}{\pi}\left(\frac{3\Delta}{4} + 1\right) m\,, \tag{7.39}$$

and is cancelled by the mass counterterm in Eq. (7.24). The second divergent term is given as

$$\Delta = \frac{1}{d} - \gamma_E + \ln\left(\frac{4\pi}{m^2}\right), \tag{7.40}$$

where γ_E is called the Euler-Mascheroni constant. This term in Eq. (7.40) once again cancels out the ultraviolet divergent terms in the vertex operator of the one-potential correction term and the only contributing factor to the zero-potential term is the divergence-free term $\Sigma^0_R(p)$.

Thus the self-energy correction due to the zero-potential term now reduces to a finite expression and is given as [83]

$$\langle\psi_a|\,\Sigma^{(0)}(\epsilon_a)\,|\psi_a\rangle = \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3}\tilde{\bar{\psi}}_a(\mathbf{p})\Sigma^0_R(p)\tilde{\psi}_a(\mathbf{p})\,, \tag{7.41}$$

where the divergence-free remainder term is obtained as [83]

$$\Sigma^0_R(p) = \frac{\alpha(a(\vartheta) + \not{p}b(\vartheta))}{4\pi}\,, \tag{7.42}$$

where

$$a(\vartheta) = 2m\left(1 + \frac{2\vartheta}{1-\vartheta}\ln\vartheta\right), \tag{7.43}$$

$$b(\vartheta) = -\frac{2-\vartheta}{1-\vartheta}\left(1 + \frac{\vartheta}{1-\vartheta}\ln\vartheta\right), \tag{7.44}$$

$$\vartheta = \frac{m^2 - p^2}{m^2}\,. \tag{7.45}$$

A substitution of these terms in Eq. (7.41) gives us the expression for the contribution of the zero-potential term to the self-energy correction, and from [83] we write down the final result as

$$\begin{aligned}\langle\psi_a|\,\Sigma^{(0)}_{\mathrm{R}}(\epsilon_a)\,|\psi_a\rangle = \frac{\alpha}{4\pi}\frac{p^2}{(2\pi)^3}\int_0^\infty dp\Bigg\{ & a(\vartheta)\left[\tilde{G}^2_a(p) - \tilde{F}^2_a(p)\right] \\ & + b(\vartheta)\left[\epsilon_a\left(\tilde{G}^2_a(p) + \tilde{F}^2_a(p)\right) + 2p\tilde{G}_a(p)\tilde{F}_a(p)\right]\Bigg\}\,,\end{aligned} \tag{7.46}$$

where $\tilde{G}_{n\kappa}(p)$ and $\tilde{F}_{n\kappa}(p)$ are the radial Dirac wave functions that have been Fourier transformed into momentum space, and the integration variable $p = |\mathbf{p}|$ and is not to be confused with four momentum.

One-potential term:

Just like in the case of the zero-potential term, we start by representing Eq. (7.27) in the momentum space, using Eq. (7.16) to define the self-energy operator

$$\langle\psi_a|\,\Sigma^{(1)}(\epsilon_a)\,|\psi_a\rangle = \int \frac{\mathrm{d}^3\mathbf{p}'}{(2\pi)^3}\int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3}\tilde{\bar{\psi}}_a(\mathbf{p}')\Gamma^0(p',p)\tilde{V}(|\mathbf{p}'-\mathbf{p}|)\tilde{\psi}_a(\mathbf{p})\,, \tag{7.47}$$

where the free-electron vertex function, as given in Eq. (7.27), in momentum space is

$$\Gamma^\mu(p',p) = -4\pi i\alpha\int\frac{\mathrm{d}^4k}{(2\pi)^4}\frac{1}{k^2+i\varepsilon}\gamma_\nu\frac{\not{p}'-\not{k}+m}{(p'-k)^2+m^2-i\varepsilon}\gamma^\mu \times\frac{\not{p}-\not{k}+m}{(p-k)^2+m^2-i\varepsilon}\gamma^\nu\,, \tag{7.48}$$

and the Fourier transformed Coulomb potential is given as [83]

$$\tilde{V}(|\mathbf{p}'-\mathbf{p}|) = -4\pi\frac{\alpha Z}{(\mathbf{p}-\mathbf{p}')^2}\,. \tag{7.49}$$

To address the ultraviolet divergence, we once again take recourse to dimensional regularization and the vertex term is separated into a divergent part and a finite part. Following Ref. [83], this is given as

$$\Gamma^\mu(p',p) = \frac{\alpha}{4\pi}\Delta\gamma^\mu + \Gamma^\mu_R(p',p)\,. \tag{7.50}$$

We have defined the term Δ in Eq. (7.40). The first term in the above equation is once again divergent while the second term is divergence free. As discussed previously in the context of the regularization of the zero-potential term, the divergent term in Eq. (7.50) negates the second divergent term in Eq. (7.38) and only the divergence-free term $\Gamma^\mu_R(p',p)$ contributes to the evaluation of the one-potential self-energy correction. This finite part is given as [83]

$$\Gamma^\mu_R(p',p) = \frac{\alpha}{4\pi}[A\gamma^\mu + \not{p}'(B_1p'^\mu + B_2p^\mu) + \not{p}(C_1p'^\mu + C_2p^\mu) + D\not{p}'\gamma^\mu\not{p} + H_1p'^\mu + H_2p^\mu]\,, \tag{7.51}$$

$$A = C_{24} - 2 + p'^2C_{11} + p^2C_{12} + 4(p'\cdot p)(C_0 + C_{11} + C_{12}) + m^2(-2C_0 + C_{11} + C_{12})\,, \tag{7.52}$$

$$B_1 = -4(C_{11} + C_{21})\,, \tag{7.53}$$

$$B_2 = -4(C_0 + C_{11} + C_{12} + C_{23})\,, \tag{7.54}$$

$$C_1 = -4(C_0 + C_{11} + C_{12} + C_{23})\,, \tag{7.55}$$

$$C_2 = -4(C_{12} + C_{22})\,, \tag{7.56}$$

$$D = 2(C_0 + C_{11} + C_{12})\,, \tag{7.57}$$

$$H_1 = 4m(C_0 + 2C_{11})\,, \tag{7.58}$$

$$H_2 = 4m(C_0 + 2C_{12})\,, \tag{7.59}$$

where

$$C_0 = \int_0^1 \frac{dy}{(yp' + (1-y)p)^2}(-\ln X)\,, \tag{7.60}$$

$$\begin{pmatrix} C_{11} \\ C_{12} \end{pmatrix} = \int_0^1 \frac{dy}{(yp' + (1-y)p)^2} \begin{pmatrix} y \\ 1-y \end{pmatrix} (1 - Y \ln X)\,, \tag{7.61}$$

$$\begin{pmatrix} C_{21} \\ C_{22} \\ C_{23} \end{pmatrix} = \int_0^1 \frac{dy}{(yp' + (1-y)p)^2} \begin{pmatrix} y^2 \\ (1-y)^2 \\ y(1-y) \end{pmatrix} \times \left[Y(1 - Y \ln X) - \frac{1}{2} \right], \tag{7.62}$$

$$C_{24} = -\int_0^1 dy \ln\left(1 - y(1-y)\frac{(p'-p)^2}{m^2}\right), \tag{7.63}$$

$$Y = \frac{m^2 - yp'^2 - (1-y)p^2}{(yp' + (1-y)p)^2}\,, \tag{7.64}$$

$$X = 1 + \frac{1}{Y}\,. \tag{7.65}$$

The C_{ij} are evaluated numerically by integrating over the Feynman parameter y [83], and to this end the integrations are carried out using numerical quadrature routines [87].

The final expression for the self-energy shift due to the one-potential term is obtained by substituting all the above coefficients in the expression for the finite term in Eq. (7.51),

in terms of two functions $\mathcal{F}_1$ and $\mathcal{F}_2$ as defined in [83]

$$\langle a|\,\Sigma^{(1)}(\epsilon_a)\,|a\rangle = -\frac{\alpha}{4\pi(2\pi)^5}\int_0^\infty dp'\,p'\int_0^\infty dp\,p\int_{-1}^{1}d\xi\frac{\alpha Z}{q^2} \times[\mathcal{F}_1(p',p,\xi)P_l(\xi)+\mathcal{F}_2(p',p,\xi)P_l(\xi)]\,, \tag{7.66}$$

where $p=|\mathbf{p}|$ and $q=|\mathbf{p}'-\mathbf{p}|=\sqrt{p'^2+p^2-2p'p\xi}$, and $\xi=\frac{\mathbf{p}'\cdot\mathbf{p}}{p'p}$. $P_l(\xi)$ is a Legendre polynomial and it arises during the derivation of the $\tilde{\bar{\psi}}_a(\mathbf{p}')\Gamma^0(p',p)\tilde{\psi}_a(\mathbf{p})$ term in Eq. (7.47). This term is given as [83]

$$\tilde{\bar{\psi}}_a(\mathbf{p}')\Gamma^0(p',p)\tilde{\psi}_a(\mathbf{p}) = \frac{\alpha}{4\pi}[\mathcal{F}_1(p',p,\xi)\chi^{\mu_a\dagger}_{\kappa_a}(\hat{\mathbf{p}}')\chi^{\mu_a}_{\kappa_a}(\hat{\mathbf{p}}) +\mathcal{F}_2(p',p,\xi)\chi^{\mu_a\dagger}_{-\kappa_a}(\hat{\mathbf{p}}')\chi^{\mu_a}_{-\kappa_a}(\hat{\mathbf{p}})]\,, \tag{7.67}$$

where $\hat{\mathbf{p}}=\mathbf{p}/|\mathbf{p}|$, and the Legendre polynomial arises by the implementation of the summation rule [83]

$$\frac{4\pi}{2j+1}\sum_\mu \chi^{\mu\dagger}_\kappa(\hat{\mathbf{p}}')\chi^\mu_\kappa(\hat{\mathbf{p}}) = P_l(\xi)\,, \tag{7.68}$$

χ^μ_κ being the two-component spherical spinors of the Dirac wave function, or the angular components given by Eq. (4.17), $j=|\kappa|-1/2$, and $l=|\kappa+\frac{1}{2}|-\frac{1}{2}$.

$\mathcal{F}_1$ and $\mathcal{F}_2$ are given in terms of the Fourier transformed radial components of the Dirac wave function [83]

$$\begin{aligned}\mathcal{F}_1(p',p,\xi) = {}& A\tilde{G}'_a\tilde{G}_a+\epsilon_a(B_1+B_2)(\epsilon_a\tilde{G}'_a+p'\tilde{F}'_a)\tilde{G}_a \\ &+\epsilon_a(C_1+C_2)\tilde{G}'_a(\epsilon_a\tilde{G}_a+p\tilde{F}_a)+D(\epsilon_a\tilde{G}'_a+p'\tilde{F}'_a)(\epsilon_a\tilde{G}_a+p\tilde{F}_a) \\ &+\epsilon_a(H_1+H_2)\tilde{G}'_a\tilde{G}_a\,,\end{aligned} \tag{7.69}$$

and

$$\begin{aligned}\mathcal{F}_2(p',p,\xi) = {}& A\tilde{F}'_a\tilde{F}_a+\epsilon_a(B_1+B_2)(\epsilon_a\tilde{F}'_a+p'\tilde{G}'_a)\tilde{F}_a \\ &+\epsilon_a(C_1+C_2)\tilde{F}'_a(\epsilon_a\tilde{F}_a+p\tilde{G}_a)+D(\epsilon_a\tilde{F}'_a+p'\tilde{G}'_a)(\epsilon_a\tilde{F}_a+p\tilde{G}_a) \\ &-\epsilon_a(H_1+H_2)\tilde{F}'_a\tilde{F}_a\,.\end{aligned} \tag{7.70}$$

7.3 Numerical results and summary

The numerical computations of the wave functions and basis sets in the zero-,one-, and many-potential terms are done using B-splines [97, 99, 198], using codes developed by Halil Cakir [87], which implement the dual kinetic balance approach for basis-set construction [85].

The zero-potential contribution can be calculated numerically in a straightforward manner and involves only the evaluations of the upper and lower components of the

Ions	R (fm)	$1s$	$2s$	$2p_{1/2}$	$2p_{3/2}$	**Refs.**
Fe^{25+}	3.730	4.2749837(3)	0.57991(6)	-0.022611(9)	0.025216(4)	
	3.7377	4.281764	0.5881947(2)	-0.0146540(2)	0.029535	[170]
	0	4.282030	0.5882281(2)	-0.0146542(2)	0.029536	[170]
	0	4.2820304	0.5882281	-0.0146542	0.0295355	[196]
Hg^{79+}	5.475	206.08550(5)	35.3186(2)	3.155007(6)	4.530466(6)	
	5.475	206.1710(1)				[197]
	5.4648	206.1760(2)	35.3919(3)	3.23417(2)	4.602445	[170]
	0	207.181639	35.5677713(2)	3.243742	4.604478	[170]
	0	207.18170(6)	35.56777(1)	3.243747(2)	4.604480(2)	[196]
Pb^{81+}	5.505	226.2388(1)	39.2102(3)	3.82741(2)	5.093(2)	
	5.5012	226.33237(5)	39.28791(4)	3.91122(2)	5.168749	[170]
	0	227.611278	39.515805	3.924616	5.171412	[170]
	0	227.61127(5)	39.515797(6)	3.924620(4)	5.171414(2)	[196]
U^{91+}	5.863	354.938(2)	65.312(2)	9.4392(2)	8.853(3)	
	5.863		65.39(6)	9.52(6)		[84]
	5.8571	355.052(2)	65.4218(6)	9.55075(6)	8.89290(3)	[170]
	0	359.501961	66.295016	9.625267	8.901058	[170]
	0	359.50196(7)	66.295010(9)	9.62526(1)	8.9010555(3)	[196]

Table 7.1: Self-energy correction to the energy levels of H-like heavy ions. We use a homogenously-charged sphere as our nuclear model and compare our results to Refs. [84, 170, 197], and point-like nucleus results from Refs. [170, 196]. Results are given in eV. The numerical differences are due to the different nuclear models used.

Ions	$2p_{1/2} - 2s_{1/2}$	**Refs.**
Fe^{25+}	-0.60252(5) -0.6028823(2)	[170]
Hg^{79+}	-32.1633(2) -32.3240293(2)	[170]
Pb^{81+}	-35.3827(1) -35.591189	[170]
U^{91+}	-55.873(3) -55.87(1) -56.669749	[84] [170]

Table 7.2: Self-energy correction contribution to the Lamb shift in H-like heavy ions. Comparison with the point-like nuclear model result in Ref. [170] estimates the effect of nuclear-size correction. Results are given in eV.

Fourier transformed radial Dirac wave function. The wave functions are cast in the form of splines as discussed in Section (2.3) and the integration is performed numerically using QUADPACK routines [199].

For the evaluation of the one-potential contribution, we need to consider the choice of potential. Since we consider a finite homogeneously-charged spherical nucleus, modifications are made to the Fourier transformed potential in Eq. (7.49) to accommodate this finite-sized nucleus, and as such we have

$$\tilde{V}(|\mathbf{p}' - \mathbf{p}|) = -4\pi \frac{\alpha Z \tilde{\rho}(|\mathbf{p}' - \mathbf{p}|)}{(\mathbf{p} - \mathbf{p}')^2} \,. \tag{7.71}$$

where $\tilde{\rho}$ denotes the normalized nuclear charge density in momentum space. We follow the work of Blundell [84] and reduce the one-potential term in Eq. (7.66) to the form of a simple double integral which is evaluated again using QUADPACK routines [199].

Finally, the evaluation of the many-potential term depends on the frequency integration in Eq. (7.34). In order to avoid the poles arising from the bound states with $\epsilon_n < \epsilon_a$, and also to eliminate the possibility of strongly oscillating integrals, the integration contour is chosen according to [83], where the contour is divided into a low and a high energy part C_L and C_H. This allows the numerical algorithm to be applied to any arbitrary initial bound-state without the need to deduct the residues of the bound-state poles. The low-energy part of the contour, C_L, is given by two halves, each parameterized by

half an ellipse [83],

$$\omega = \frac{\epsilon_0}{2}\left(1 + \frac{\Delta e^{-i\varphi}}{\sqrt{\Delta^2 \cos^2\varphi + \sin^2\varphi}}\right). \tag{7.72}$$

The parameters for the numerics are chosen according to [83] as: $\epsilon_0 = \epsilon_a - 0.9\epsilon_{1s}$, ϵ_{1s} being the ground-state energy; $\Delta = \epsilon_a/5n^{1/3}$, where n is the principal quantum number of the initial state. This choice of parameters was seen to give optimum results while preserving numerical efficiency. The numerical implementation of the many-potential term now involves radial integrals over a partial-wave series in κ, that involves the creation of two separate basis sets for the free and bound electrons, using which the effective basis functions in Eq. (7.32) are constructed following Section 2.3. For each value of κ, a basis set is so chosen as to give maximum convergence. The theoretical uncertainties are then evaluated by considering for each value of RMS radii, a variation in the number of breakpoints, i.e., for a given value of R, we perform calculations for 50, 60, 70, 80, and 90 breakpoints; this is then repeated for $R \pm dR$. The integration over ω is done using QUADPACK routines [199]

We calculate the self-energy shift to the binding energy of H-like HCIs and results are shown in Table 7.1. The calculations are carried out for a finite homogenuously-charged spherical nucleus. The results obtained are compared to [84], where a Fermi distribution is chosen for the finite-sized nuclear model. We also compare our results to [170], where self-energy correction is presented for both point-like nucleus and a finite-sized nucleus. A comparison of the results for the finite-sized nuclear model used in [170], for a different nuclear radius, with our nuclear model is presented in Table 7.1. The nuclear-charge radius considered for our calculations have been taken from [197] and the numerical differences between our results and the results from [170] arise due to the difference in the RMS value of the radius used.
In Table 7.2, we present Lamb-shift results, for a homogeneously charged spherical nucleus, for H-like HCIs. A comparison of our result with the Lamb shift for the point-like nucleus from [170] gives us an estimate of the nuclear-size correction; in case of U (Z=92), we get a correction of 0.797 eV to the self-energy of the Lamb shift in Uranium, while Blundell [84] suggests a correction of 0.80(1) eV, Mohr and Soff [197] give a value of 0.8020(1) eV, and we conclude that our results are in good agreement. For the RMS radius of the finite-sized nuclei, used in our calculations, we refer to the values given in [197]. We also provide estimates for numerical uncertainties with each value. It can be easily inferred from Table 7.1, that with the increase in the atomic number, the QED effects become more and more pronounced and are experimentally observable with novel mass spectrometric methods with uncertainties on the 1-eV level or below [75, 171, 173]. With these results, we identify ions which allow, for the first time, the test of QED via measuring the mass of the ion – or the mass difference of the H-like ion and the bare nucleus, directly yielding the electronic binding energy, and by using the $E = mc^2$ equivalence relation.

Table 7.1 also shows that it is not only the $1s$ hydrogenic ground state which features QED effects well observable by these methods, but also excited states possess

observable radiative shifts. E.g. the Lamb shift given in the Table 7.1 for the $2s$ state approximates the self-energy correction to the binding energy of a Li-like ion, which could be spectrometrically determined by measuring the mass difference of the Li- and the He-like ions in their ground state. In our approach presented here, we fully neglect electron interaction effects, which, for HCIs, is a justified first approximation. Our path integral formalism however may be extended in future to many-electron systems, by allowing the exchange of photons between different electrons.

Similarly, the self-energy results given for the $2p_{1/2}$ state approximate the radiative shift of the binding energy of the valence electron in the B-like charge state, and the values given for the $2p_{3/2}$ orbital give the first approximation for a N-like ion. Ions in these charge states are easier to produce experimentally, yet, as we show, they feature observable QED corrections, enabling a proof-of-the-principle demonstration of QED tests via mass measurements.

In this Chapter and in Chapter 6, we have successfully developed an alternate formalism for the evaluation of the vacuum polarization correction and self-energy shift of the energy levels in bound electrons. The Green's function for the self-energy corrected photon and the bound electron is extracted from the Schwinger-Dyson equation derived using the functional integral technique. We completely avoid the operator formalism and present an elegant and intuitive framework that treats the system non-perturbatively in the nuclear Coulomb field, which is essential for the systems studied here.

Summary and outlook

In this Thesis, we have explored through the functional-integral formalism, a non-perturbative approach for the quantization of QED in the Furry picture. We exploit the fact that the QED Lagrangian is a fundamental entity of the theory and any quantization technique derived from the Lagrangian should, in principle, make the theory predictive for arbitrary energy scales.

The study of QED has a long and glorious history which spans almost an entire century since Dirac first postulated the wave equation, bringing quantum mechanics and special relativity under the same umbrella. Since then, in the hands of many stalwarts in the field, the theory has progressed immensely to the point that we can now study it with the greatest of detail and experiments can benchmark it with utmost precision. The development of the theory of quantized fields has seen many interesting breakthroughs. While the mathematics was clearly defined through the canonical quantization of fields in the early days, the formulation of perturbation theory in the coupling strength of interactions involved a lot of inconsistencies, the appearance of divergences being one. This was resolved through 'renormalization' which addressed the infinte corrections to the mass and charge of a particle by adjusting its 'original' mass so as to cancel out the infinities. The appearance of the 'Landau ghost' was another of the inconsistencies which predicts that at higher energies, the renormalized coupling constant, which scales with the energy and diverges at a certain energy range should render perturbative QED invalid–this led to a whole new field of lattice QED. Thus, though QED was an extremely effective and predictive field theory at low and intermediate energy scales, it was believed that at high energies the theory is inconsistent. However, whether or not we actually see the manifestations of Landau poles in QED, or if it is just a theoretical artefact is still an open question and addressing this theoretical issue is still a work in progress. Experimentally, since the energy scale ($\sim 10^{286}$ eV) of the Landau pole is way beyond the Planck scale in QED, it is safe to say that we are not at all likely to observe its effects on the theory. The gist of the whole argument is that, even without the existence of the Landau pole, the perturbation treatment of QED eventually breaks down and for higher orders, it becomes divergent (see for e.g., Dysons's famous paper [200]). This calls for a non-perturbative treatment of QED, especially in the treatment of bound states which are instrinsically non-perturbative in nature.

In Chapter 1, we explore the textbook concepts of the path integral formulation, both in quantum mechanics and in field theory. A general mathematical construct is provided which is applicable to both the non-relativistic as well as relativistic theories.

All processes involving free and interacting particles can be given by their transition amplitudes, represented by Green's functions or correlation functions in the context of field theory. This is what we derive using the path integral approach. While it is straightforward to establish a path integral formalism for quantum mechanical processes, the extension to field theory also involves time ordering of the operators in order to preserve causality. This, however, is an inherited property of the correlation functions, in field theory; the time-slicing operation used in the construction of the integral over paths ensures that time ordering comes naturally into the picture. We establish a generating functional, since in field theory we have particle states instead of well-defined particles, which are seen as excitations of the field, this generating functional acts as the generator of such fields. The derivative of the generating functional with respect to the 'sources' of these fields give us the propagators.

In Chapter 2, we discuss briefly about the numerical and mathematical tools required for a self-consistent theoretical framework based on the functional integral technique and its application to the study of QED effects in HCIs. We numerically evaluate spectral sums over the entire Dirac spectrum using the method of B-splines. To this extent, approximation of the radial wave functions staisfying the Dirac equation is obtained in terms of piecewise polynomial functions. These basis functions are then used to construct a finite basis set of $2N$ functions approximating the negative- and positive-energy eigenstates. A dual-kinetic-balance basis is chosen to eliminate unphysical states and improve convergence. In this Chapter we also discuss the essential elements of Grassmann algebra, where the anticommuting field operators are represented in the classical limit in terms of anticommuting Grassmann variables, thereby allowing for the inclusion of fermion spin in the quantization of field theory using the 'classical' functional integral formalism. The Faddeev-Popov gauge-fixing procedure has also been briefly introduced to allow for the fixing of a particular gauge orbit, in order to overcome a diverging functional integral due to overcounting of similar gauge configurations for a gauge field that is invariant under local transformations. This procedure, which is a common mathematical tool for fixing the gauge of non-abelian fields, has been generalized, in this Chapter, to gauge-fix the QED Lagrangian.

In Chapter 3, we make use of the mathematical tools developed in Chapter 2 to arrive at a generalized expression for the known free propagators of QED. For the photon propagator, we start with the Lagrangain for the electromagnetic field, and from the 'classical' concept of the least-action principle, obtain the equations of motion by varying the Lagrangian and derive the photon propagator from the gauge-fixed Lagrangian. A similar formulation is used for the derivation of the Dirac propagator. We begin with the Lagrangian for the free Dirac field and construct the generating functional in terms of these fields and their anticommuting Grassmann-valued 'sources'. A double derivative of this generating functional with respect to the source terms, as established in Chapter 1, then gives us the two-point Green's function for the free Dirac field.

In Chapter 4, we introduce an alternate formalism for deriving the free Dirac propagator in spherical coordinates, i.e., in a form applicable in atomic physics calculations,

by modifying slightly the work of Inomata and Kayed [80]. Instead of the usual field-theoretic functional integral approach of constructing a Lagrangian and reducing the generating functional to its classical limit by the introduction of 'source' terms as done in Chapter 3, we begin by reducing the relativistic Dirac equation to a form that is analogous to the non-relativistic Schrödinger equation. For this purpose, we make use of the second-order Dirac equation and the Green's function for the time-independent Dirac equation is obtained in terms of the Green's function for this second-order or iterated Dirac equation. The correspondence between the iterated Dirac equation and the Schrödinger equation is established through the introduction of a modified form of the Martin-Glauber operator, which brings the Hamiltonian of the iterated Dirac equation to the same mathematical form as that of the Schrödinger equation but without reducing it to the non-relativistic regime. Following a partial-wave expansion, the effective action (derived from the Hamiltonian) is used to construct a radial path integral and it becomes apparent that the integral has the same form as that of an isotropic harmonic oscillator, for which the solution is well-known. As a final step, the Green's function for the free Dirac propagator is obtained in terms of spherical spinors to suit our purpose of its application to atomic physics calculations.

In Chapter 5, we rederive an essential component of Furry-picture QED, the DCGF or the bound-electron propagator, in the framework of path integrals. This Chapter follows the works of Wong and Yeh [79, 122] to arrive at a simplified solution of the Dirac equation, where the radial wave functions, satisfying the radial Dirac equation, contain a single term of a hypergeometric function and the radial components of the full Green's function in turn, contain a single term instead of four. We follow this method since it introduces us to the Biedenharn basis transformation [77, 78] which diagonalizes the Martin-Glauber operator and is equivalent to the work of Inomata and Kayed [80] where a basis transformation is done to reduce the relativistic Dirac-Coulomb problem to a form analogous to the non-relativistic Schrödinger equation. The derivation is done exactly as in the free propagator case with the addition of the Coulomb term. However, a coordinate transformation followed by time rescaling addresses the problem posed by the Coulomb term and the radial path integral is reduced again to the isotropic harmonic oscillator form as in the free propagator case. The DCGF is then obtained in terms of Whittaker functions and spherical spinors.

We now assimilate all the mathematical formulations and the propagators, derived in Chapter 1 through to Chapter 5, in the derivation of the Lamb shift at the one-loop level, in Chapters 6 and 7. We first derive the self-energy corrected photon propagator using the Schwinger-Dyson equations in the framework of the functional-integral formalism. An analytical formula for the Uehling potential is then derived from this self-energy corrected photon propagator following the work of Frolov and Wardlow [164]. This derivation of the Uehling potential in a closed form now allows us to use perturbative path integrals [153, 166] where we treat the Uehling potential as the perturbing potential and arrive at the Green's function for the Uehling-corrected bound electron. The correction to the binding energy is obtained from the shift in the poles of the Green's function using complex contour integrals. Numerical evaluations are done by applying the B-spline

algorithm implemented by Halil Cakir [87]. Results are shown for different charge states of a few HCIs. We observe that for heavier ions, the Uehling correction has quite a significant contribution to the Lamb shift, and the energy-level shift decreases as we move from the $1s$ ground state to higher-lying orbitals, and are experimentally observable. For H-like $^{238}U^{91+}$ ($Z = 92$), this correction to the ground-state energy level is -97.996 eV, while for N-like $^{238}U^{85+}$, with the valence electron being in the $2p_{3/2}$ state, it reduces to -0.12653 eV.

In Chapter 7, we derive the self-energy corrected bound-electron propagator from the Schwinger-Dyson equations. The correction to the energy levels is once again obtained from the poles of this propagator through complex contour integration. The expression for the energy shift needs to be regularized in order to get rid of UV divergences that arise in the zero- and one-potential term, and this is achieved using dimensional regularization. Once we obtain the divergence free expression for the self-energy operator, the zero-, one-, and many-potential terms are numerically evaluated using B-spline codes. Results are presented for H-like heavy ions. As seen for the Uehling correction, the heavier ions tend to show a larger correction and are well above the threshold for experimental observation by means of Penning-trap precision mass spectrometry. H-like $^{238}U^{91+}$ ($Z = 92$) shows a self-energy correction of $354.938(2)$ eV to the $1s_{1/2}$ state while H-like $^{56}Fe^{25+}$ ($Z = 26$) shows a correction of 4.273 eV. We compare also the Lamb shift for our charged homogeneous-sphere model of the nucleus to that of the point-like nucleus to obtain an estimate of the correction due to the nuclear size, and for H-like $^{238}U^{91+}$ it is seen to be about 0.797 eV. The results obtained for both the vacuum-polarization correction and the self-energy correction to the electronic binding energies demonstrate that for sufficiently heavy HCIs, these effects are quite observable with state-of-the-art mass spectrometric methods

In this Thesis, starting with the derivation of the propagators both for the free and bound systems leading to a culmination in the final Chapters, where we combine all the different pieces of the mathematical puzzle to arrive at the full picture of the derivation of radiative corrections in atomic physics followed by their numerical evaluation, we establish that QED is a theory that is mathematically robust, and show that different mathematical tools used to quantize the theory lead us to the same results. We also draw inspiration from several techniques relevant in different fields of physics, namely, QCD and statistical mechanics, through the Faddeev-Popov gauge-fixing technique, the Schwinger-Dyson equations, most importantly, the generating functional itself, which bears semblance to the partition function in statistical mechanics, and show that the functional integral formalism is indeed a versatile mathematical tool that also acts as a common language between various fields of physics.

The successful application of the functional integral method in the derivation of one-loop QED effects in bound systems, developed in this Thesis, opens up a plethora of avenues for its application to other problems in bound-state atomic physics calculations. It can be extended, in principle, to study higher-order radiative corrections and energy shifts by, e.g. solving the coupled Schwinger-Dyson equations for the dressed propagators by numerical iteration, as achieved e.g. in QCD for the hadronic vacuum

polarization problem of the muon g factor [201]. The formalism can be extended to many-electron systems by also accounting for photon exchange between electrons, vastly improving the field of applicability in bound-state QED and precision atomic physics. A simple way of extending the theory to monovalent ions is to use a screening potential to approximately describe the effect of core electrons decreasing the nuclear Coulomb potential. This approach may find a timely application in the evaluation of QED corrections to binding energies of HCI, relevant for the determination of the neutrino mass via detecting the energy released in nuclear electron capture, i.e. the inverse of nuclear beta decay [202]. It is a task for precision atomic theory to deliver the binding energies of the mother and daugther atoms in the process, since Penning trap experiments can only determine the masses of HCI of these elements. At the sub-eV precision scale relevant for the neutrino mass, as we have evaluated, QED effects may also pay a role in certain ions. In a more sophisticated approach, the screening of QED effects is accounted for by the evaluation of diagrams which include photons exchanged between valence and core electrons besides the radiative loops.

Efforts can also be made to extend the formulation to non-perturbative calculations in the coupling constant α as in e.g. QCD, thereby establishing a complete non-perturbative definition of QED. Within our formalism, it should be straightforward to also include further classical external fields, such as a perturbative external magnetic field, or the magnetic dipole field of a nucleus with non-zero spin, to evaluate QED effects on the bound-electron g factor [62, 65] and the hyperfine splitting [203, 204], which can nowadays be experimentally investigated to high precision. The functional integral technique developed in this work provides a general mathematical construct that could potentially be extended to particles with any intrinsic angular momentum, e.g. gravitons, and would depend only on a proper definition of source terms for such particle fields. The functional methods derived in this Thesis also allow the derivation of interaction Hamiltonians from the propagators of hypothetical scalar, pseudoscalar, vector or axial vectors exchanged between an atomic electron and the nucleons or between two electrons. These accurate Hamiltonians can then be readily applied in atomic physics calculations to evaluate energy shifts due to these new bosons [41, 205–207], and by the comparision with experimental data one can extract or constrain parameters of such new interactions put forward to extend the standard model of particle physics.

A. Functional techniques for connected and 1PI diagrams

The n-point Green's function was evaluated in Eq. (1.37) in terms of the generating functional. The generating functional in terms of the n-point Green's function has the form [157]

$$Z[J] = \sum_{n=0}^{\infty} \frac{i^n}{n!} \int d^4x_1 \dots d^4x_n \, J(x_1) \dots J(x_n) G(x_1 \dots x_n) \,, \tag{A.1}$$

$$= \langle 0 | \, \mathrm{T} \exp\left[i \int d^4x \phi(x) J(x) \right] | 0 \rangle \ , \tag{A.2}$$

$$= \sum_{n=0}^{\infty} G^n(J) \,. \tag{A.3}$$

The generating functional itself represents vacuum diagrams of a theory with the Green's functions attached to sources. These Green's functions may contain *disconnected* parts and are represented by a plain blob.

We study QED, which is an interacting theory, and all QED processes are represented by *connected* diagrams. The generating functional for these diagrams is given by $W[J] = \ln Z[J]$ and can be expressed in the same way as Eq. (A.3)

$$W[J] = \sum_{n=1}^{\infty} G_c^n(J) \,, \tag{A.4}$$

$$= \sum_{n=1}^{\infty} \frac{i^n}{n!} \int d^4x_1 \dots d^4x_n \, J(x_1) \dots J(x_n) G_c(x_1 \dots x_n) \,, \tag{A.5}$$

where $G_c(x_1 \dots x_n)$ is the proper *connected* Green's function and $G_c^n(J)$ is its functional. It is also to be noted that $G_c^0(J) = 0$, which means that there are no *connected* vacuum diagrams, and the source $J = 0$.

Using Eq. (A.4) and the definition of $Z[J]$, we can now write

$$Z[J] = \exp\left(\sum_{n=1}^{\infty} G_c^n(J) \right) = \prod_{n=1}^{\infty} e^{G_c^n(J)} \,, \tag{A.6}$$

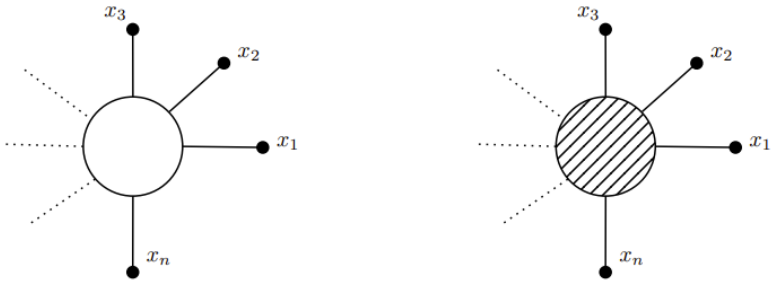

Figure A.1: Diagrammatic representation of n-point Green's functions. The left image describes a generic Green's function or the full propagator $G^n(x_1 \dots x_n)$, that may or may not contain disconnected parts, and the right image represents a connected Green's function $G_c^n(x_1 \dots x_n)$.

and this would give us the full n-point Green's function of Eq. (1.37) in terms of the generating functional for the connected Green's function, as

$$G^n(x_1 \dots x_n) = \frac{(-i)^n \delta^n \prod_{n=1}^{\infty} e^{G_c^n(J)}}{\delta J(x_1) \dots \delta J(x_n)}\bigg|_{J=0}, \tag{A.7}$$

or

$$G^n(x_1 \dots x_n) = \frac{(-i)^n \delta^n e^{W[J]}}{\delta J(x_1) \dots \delta J(x_n)}\bigg|_{J=0}. \tag{A.8}$$

From the product rule of differentiation, for any source, we obtain

$$\frac{-i\delta e^{W[J]}}{\delta J(x)} = -e^{W[J]} \frac{i\delta W[J]}{\delta J(x)}, \tag{A.9}$$

similarly

$$\frac{(-i)^2 \delta^2 e^{W[J]}}{\delta J(x_1)\delta J(x_2)} = e^{W[J]} \left[(-i)^2 \frac{\delta W[J]}{\delta J(x_1)} \frac{\delta W[J]}{\delta J(x_2)} + (-i)^2 \frac{\delta}{\delta J(x_1)} \frac{\delta}{\delta J(x_2)} W[J] \right], \tag{A.10}$$

and the series continues. The term $-\frac{i\delta W[J]}{\delta J(x)}$ gives us the effective fields [157] due to the sources. In case of QED, these effective fields are defined as

$$\psi = -\frac{i\delta W[J]}{\delta \bar{\eta}}, \quad \bar{\psi} = \frac{i\delta W[J]}{\delta \eta}, \quad A_\mu = -\frac{i\delta W[J]}{\delta J^\mu}, \tag{A.11}$$

where $\psi, \bar{\psi}$ and A_μ are the 'classical' fermionic and gauge fields respectively, and their sources are defined by $\bar{\eta}, \eta$ and J^μ. The Legendre transform of the generating functional $W[J]$ gives us the generating functional for proper vertices or the effective action, Γ [157],

$$i\Gamma[\phi_c(x)] = W[J] - i \int d^4x \, \phi_c(x) J(x), \tag{A.12}$$

where, $\phi_c(x) = \langle 0|\, \phi(x)\, |0\rangle = -\frac{i\delta W[J]}{\delta J(x)}$, is our effective field and is the conjugate Legendre variable of the source $J(x)$. Taking a derivative w.r.t. the effective field $\phi_c(x)$ yields [157]

$$i\frac{\delta\Gamma[\phi_c(x)]}{\delta\phi_c(x)} = \int d^4y\, \frac{\delta W[J]}{\delta J(y)}\frac{\delta J(y)}{\delta\phi_c(x)} - \int d^4y\, i\phi_c(y)\frac{\delta J(y)}{\delta\phi_c(x)} - iJ(x)\,. \tag{A.13}$$

Owing to the definition of $\phi_c(x)$, the first two terms in the above equation cancel out and we are left with the definition of the source in terms of the effective action

$$i\frac{\delta\Gamma[\phi_c(x)]}{\delta\phi_c(x)} = -iJ(x)\,. \tag{A.14}$$

In the absence of the source term, the above equation becomes

$$i\frac{\delta\Gamma[\phi_c(x)]}{\delta\phi_c(x)} = 0\,, \tag{A.15}$$

which makes $\Gamma[\phi_c(x)]$ a constant w.r.t. $\phi_c(x)$.

Using the Eq. (A.14) we can now define the QED source terms, in terms of the effective action

$$J_\mu = -\frac{\delta\Gamma[A]}{\delta A^\mu}\,, \quad \eta = -\frac{\delta\Gamma[\bar\psi]}{\delta\psi}\,, \quad \bar\eta = \frac{\delta\Gamma[\psi]}{\delta\bar\psi}\,. \tag{A.16}$$

We now want to define the effective action $\Gamma(\phi_c(x))$ as the generating functional for one-particle irreducible (1PI) Green's functions or proper vertex functions, and write it in the form of Eq. (A.1), which is the general form for all generating functionals [157]

$$\Gamma[\phi_c] = \sum\frac{1}{n!}\int d^4x_1\ldots d^4x_n\,\phi_c(x_1)\ldots\phi_c(x_n)\Gamma^n(x_1\ldots x_n)\,. \tag{A.17}$$

We now take the functional derivative of the effective field $\phi_c(x)$ w.r.t. $\phi_c(y)$, and this gives us

$$\frac{\delta\phi_c(x)}{\delta\phi_c(y)} = \frac{\delta}{\delta\phi_c(y)}\left[-\frac{i\delta W[J]}{\delta J(x)}\right], \tag{A.18}$$

$$\delta^4(x-y) = i\int d^4z\frac{\delta^2\Gamma[\phi_c]}{\delta\phi_c(z)\delta\phi_c(y)}\frac{\delta^2 W[J]}{\delta J(z)\delta J(x)}\,. \tag{A.19}$$

We thus have as functional inverses

$$\frac{\delta^2\Gamma[\phi_c]}{\delta\phi_c(y)\delta\phi_c(x)} = \left[i\frac{\delta^2 W[J]}{\delta J(y)\delta J(x)}\right]^{-1}. \tag{A.20}$$

Now, in the absence of a source, J, the effective field ϕ_c becomes zero and we obtain

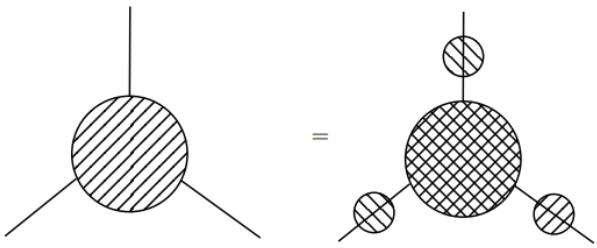

Figure A.2: Diagrammatic representation of Eq. (A.28). The connected 3-point function is represented in terms of the 1PI Green's function denoted by the cross-hatched circle, which is the *amputated* Green's function attached to connected Green's functions which have been pulled out of the connected 3-point function.

our usual two-point connected Green's function as the inverse of the second derivative of the effective action

$$G_c^2(y,x) = -\frac{\delta^2 W[J]}{\delta J(y)\delta J(x)} = i\left[\frac{\delta^2\Gamma[\phi_c]}{\delta\phi_c(y)\delta\phi_c(x)}\right]^{-1}. \tag{A.21}$$

Again, since we have $\phi_c(x) = -\frac{i\delta W[J]}{\delta J(x)}$, the two-point connected Green's function can also be written as

$$G_c^2(y,x) = -\frac{\delta^2 W[J]}{\delta J(y)\delta J(x)} = -i\frac{\delta\phi_c(x)}{\delta J(y)}\,. \tag{A.22}$$

From Eq. (A.15), we assume translational invariance of Γ^2 and we can write [157],

$$\int d^4z\Gamma^2(y-z)G_c^2(z-x) = i\delta^4(x-y)\,. \tag{A.23}$$

Further derivatives of Eq. (A.19) yields higher 1PI Green's functions. From Eq. (A.21), we can deduce the two-point connected Green's functions of QED as

$$S(x,z) = -\frac{\delta^2 W[J]}{\delta\eta(z)\delta\bar{\eta}(x)}\,, \tag{A.24}$$

which is the electron propagator. The photon propagator is given similarly

$$D_{\mu\nu}(x-z) = -\frac{\delta^2 W[J]}{\delta J^\mu(x)\delta J^\nu(z)}\,. \tag{A.25}$$

Since we want to establish correspondence between connected Green's functions and the 1PI Green's functions, with the effective action as their generating functional, we take higher-order functional derivatives of the connected Green's functions. To establish this, we write

$$\frac{\delta^3 W[J]}{\delta J(z)\delta J(y)\delta J(x)} = \int d^4w\frac{\delta\phi_c(w)}{\delta J(z)}\frac{\delta}{\delta\phi_c(w)}\frac{\delta^2 W[J]}{\delta J(y)\delta J(x)} \tag{A.26}$$

$$= -i\int d^4w\frac{\delta\phi_c(w)}{\delta J(z)}\frac{\delta}{\delta\phi_c(w)}\left[\frac{\delta^2\Gamma[\phi_c]}{\delta\phi_c(y)\delta\phi_c(x)}\right]^{-1}. \tag{A.27}$$

The derivative of an inverse functional is given as

$$\frac{\delta B^{-1}}{\delta t} = -B^{-1}\frac{\delta B}{\delta t}B^{-1}$$

Using this in Eq. (A.27), and the definitions in Eq. (A.21) and Eq. (A.22), we arrive at

$$\frac{\delta^3 W[J]}{\delta J(z)\delta J(y)\delta J(x)} = -i\int d^4w\, d^4u\, d^4v\, G_c^2(z,w)G_c^2(x,u)G_c^2(y,v)\frac{\delta^3\Gamma[\phi_c]}{\delta\phi_c(u)\delta\phi_c(v)\delta\phi_(w)}\,. \tag{A.28}$$

We thus have the proper 1PI Green's function in terms of the effective action , where

$$\frac{\delta^3 i\Gamma[\phi_c]}{\delta\phi_c(x)\delta\phi_c(y)\delta\phi_c(z)} = G^3_{\rm 1PI}(x,y,z) = \Gamma^3(x,y,z)\,. \tag{A.29}$$

In terms of the above equation, the QED proper vertex is given as

$$\left(\frac{\delta^3\Gamma}{\delta A_\nu(y)\delta\psi(x_1)\delta\bar{\psi}(x_2)}\right) = e\Gamma^\nu(y;x_1,x_2) \tag{A.30}$$

B. Background field method

The background field method [191, 208, 209] ensures the gauge invariance of the external field treated classically, which in the case of QED is the nuclear Coulomb field, while fixing the gauge for the gauge field of the photon, which is treated as a quantum fluctuation. This method also ensures that the effective action, which is the central entity for all functional derivations of field propagators, remain independent of the gauge of the external field.

We begin with the usual generating functional from Eq. (2.26),

$$Z[J] = \int \mathcal{D}A \exp\left(i\mathcal{S}[A] + i \int d^4x \, A_\mu J^\mu \right). \tag{B.1}$$

where the classical action is given in terms of the Lagrangian density $\mathcal{L}$, in the form $\mathcal{S} = \int d^4x \mathcal{L}$. The effective action, which acts as the generating functional for the proper vertices is given in terms of the generating functional for the connected diagrams in Eq. (A.12) as

$$i\Gamma[\bar{A}] = W[J] - i \int d^4x \, \bar{A}_\mu J^\mu \,, \tag{B.2}$$

where, $\bar{A}_\mu = \langle 0 | \, A_\mu \, | 0 \rangle = -\frac{i\delta W[J]}{\delta J^\mu}$ is our effective field, and is the conjugate Legendre variable of the source J. The generating functional $W[J]$ is given as $W[J] = \ln Z[J]$.

Introducing an external background field, the classical Lagrangian depends not only on the gauge field A but also on the background field $\mathcal{A}$. As such the generating functional depends on the source J of the gauge field, and also on the external field which acts as an alternate source [209], and is given as

$$\tilde{Z}[J, \mathcal{A}] = \int \mathcal{D}A \exp\left(i\mathcal{S}[A + \mathcal{A}] + i \int d^4x \, A_\mu J^\mu \right). \tag{B.3}$$

This modifies the generating functional for the connected diagrams which we write as $\tilde{W}[J, \mathcal{A}] = \ln \tilde{Z}[J, \mathcal{A}]$, and the effective action is given as

$$i\tilde{\Gamma}[\tilde{A}, \mathcal{A}] = \tilde{W}[J, \mathcal{A}] - i \int d^4x \, \tilde{A}_\mu J^\mu \,, \tag{B.4}$$

where $\tilde{A}_\mu = -\frac{i\delta \tilde{W}}{\delta J^\mu}$. To clarify the notations, following Ref. [191], we have used

$$\bar{A}_\mu = -\frac{i\delta W[J]}{\delta J^\mu} \,, \tag{B.5}$$

to denote the effective field for the plain gauge field without the application of the background, and

$$\tilde{A}_\mu = -\frac{i\delta\tilde{W}}{\delta J^\mu}\,, \tag{B.6}$$

to denote the inclusion of the background field in the modified generating functional $\tilde{W}[J, \mathcal{A}]$.

As done in the case of the photon field, where we apply a local gauge transformation given by Eq. (2.25), we apply a gauge transformation now in the presence of the classical background field. This is given by

$$A^\alpha_\mu = (A_\mu + \mathcal{A}_\mu) + \frac{1}{e}\partial_\mu\alpha\,, \tag{B.7}$$

where α is an arbitrary scalar field. We also choose the background gauge field condition as

$$F = \partial^\mu A^\alpha_\mu + e\mathcal{A}^\mu A_\mu = 0\,. \tag{B.8}$$

We now perform a field-shifting of the integration variable in Eq. (B.1), [191, 209] $A_\mu \to A_\mu - \mathcal{A}_\mu$. With this shifted field, we obtain that the generating functional with the inclusion of the background field is simply the generating functional for our simple gauge field that has undergone a phase shift

$$\tilde{Z}[J, \mathcal{A}] = Z[J]e^{-i\int d^4x\,\mathcal{A}_\mu J^\mu}\,, \tag{B.9}$$

and its logarithm gives us the modified generating functional for connected diagrams

$$\tilde{W}[J, \mathcal{A}] = W[J] - i\int d^4x\,\mathcal{A}_\mu J^\mu\,. \tag{B.10}$$

Functionally differentiating Eq. (B.10) w.r.t. the source J^μ we obtain [191, 209], from the definitions in Eqs. (B.5) and (B.6)

$$\tilde{A}_\mu = \bar{A}_\mu - \mathcal{A}_\mu\,. \tag{B.11}$$

This shows that a shift in the original gauge field also shifts the effective field. Using this deduction, and Eqs. (B.10) and (B.11), we now deduce the effective action term in Eq.(B.4), which becomes

$$\begin{aligned} i\tilde{\Gamma}[\tilde{A}, \mathcal{A}] &= \tilde{W}[J, \mathcal{A}] - i\int d^4x\,\tilde{A}_\mu J^\mu \\ &= W[J] - i\int d^4x\,\mathcal{A}_\mu J^\mu - i\int d^4x\,\tilde{A}_\mu J^\mu \\ &= W[J] - i\int d^4x\,\bar{A}_\mu J^\mu \\ &= i\Gamma[\bar{A}] \end{aligned} \tag{B.12}$$

This brings us to the required equality that the effective action in the presence of a background field is the same as that without the field and therefore represents the same one-particle irreducible Green's functions, and it is independent of the gauge of the background field.

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