

Chapter 2

The g -Factor - Exploring Atomic Structure and Fundamental Constants

Slightly more than 100 years ago Ernest Rutherford in 1911 and Niels Bohr in 1913 made the first fundamental steps to explain the atomic structure of nature [1, 2]. Since then, enormous efforts have been undertaken, such that the SM nowadays is able to predict properties of elementary particles up to the thirteens digit¹ [3–5]. In the following chapter I will illuminate the present understanding of the fundamental electromagnetic dynamics in atomic structure. The main focus will be set on the present workhorse of the underlying theory, the so-called bound-state quantum electrodynamics (BS-QED): the bound-electron g -factor.

In Sect. 2.1 the g -factor will be introduced and defined, followed by a summary of the most stringent test of QED in weak fields in Sect. 2.2, the g -factor calculations and measurements of the free electron. In Sect. 2.3 investigations of the bound-electron g -factor are motivated. Here, I will also report on the enormous progress of the theoretical calculations of the bound-electron g -factors and briefly summarize its various physical contributions. In Sect. 2.4 the fundamental measurement principle of the bound-electron g -factor is introduced and an overview on the last measurements is given in Sect. 2.5. The last two sections cover the specific theoretical backgrounds of the two physical topics of the present thesis: (1) The electron mass (Sect. 2.6) and (2) the g -factor isotope shift in the lithiumlike calcium ions $^{40}\text{Ca}^{17+}$ and $^{48}\text{Ca}^{17+}$ (Sect. 2.7).

¹Relative uncertainties of the g -factor of the free electron: $(\delta g/g)_{\text{theo}} = 0.8 \cdot 10^{-12}$ and $(\delta g/g)_{\text{exp}} = 0.3 \cdot 10^{-12}$, see also Sect. 2.2.

2.1 The g -Factor

In 1922, Otto Stern and Walther Gerlach performed their famous Stern-Gerlach experiment by sending a beam of silver atoms through an inhomogeneous magnetic field, observing a discrete splitting of the beam into two beams [6]. Not until 1925 Samuel A. Goudsmit and George E. Uhlenbeck interpreted the phenomena in the nowadays well-established model, proposing an intrinsic quantized property of the electron, the so-called spin $\vec{s}$, which generates an intrinsic magnetic moment $\vec{\mu}_s$ [7]. In an external magnetic field $\vec{B} = B \cdot \vec{e}_z$ ² the electron-spin has two discrete quantum states with the eigenvalues $s_z = m_s \hbar = \pm \frac{1}{2} \hbar$, where $\hbar = h/(2\pi)$ is the reduced Planck constant. The proportionality constant between the intrinsic magnetic moment and the spin in terms of the Bohr magneton μ_B is the g -factor:

$$\vec{\mu}_s = -g\mu_B \frac{\vec{s}}{\hbar}, \quad (2.1)$$

where $\mu_B \equiv \frac{e\hbar}{2m_e}$, e is the elementary electric charge and m_e the mass of the electron. The g -factor thus defines the strength of the interaction between the magnetic field and the spin of the electron, where the magnetic potential is given by $U_{\text{magn}} = -\vec{\mu} \cdot \vec{B}$. Assuming the spin as a classical angular momentum ($\vec{s} = \vec{r} \times \vec{p}$) and a classical magnetic moment ($\vec{\mu} = I \cdot A \cdot \vec{n}_A$) the g -factor would have a value of $g = 1$. Already in 1922 Alfred Landé proposed a phenomenological electron g -factor of $g = 2$ (also called Landé g -factor) to interpret the observed anomalous Zeeman effect, not yet knowing about the electron spin [8]. In 1928 finally Paul Dirac formulated his famous equation, combining quantum mechanics with special relativity. This theory unification entailed the electron as a spin-1/2 particle. As a direct consequence, the electron g -factor was $g = 2$. Almost 20 years later, in 1947, small deviations from Dirac's theory have been observed in different experiments: (1) in the energy levels of the hydrogen atom, nowadays called Lamb shift [9], and (2) in the electron g -factor [10–13]. Still in the same year Julian Schwinger managed to explain the deviation in the g -factor by considering the virtual coupling of the fields, more precisely the emission and subsequent absorption of photons. In that context, he performed first-order perturbation calculations within the especially developed framework of quantum electrodynamics (QED) [14]: $g = 2 \left(1 + \frac{\alpha}{2\pi}\right)$, where $\alpha \equiv \frac{1}{4\pi\epsilon_0} \frac{e^2}{\hbar c} \approx 1/137$ is the fine structure constant, which defines the coupling strength of QED. Furthermore, ϵ_0 is the electric constant (vacuum permittivity) and c is the speed of light in vacuum. This successful model flags the dawn of quantum electrodynamics, the mother of all quantum field theories.

²In the following a homogeneous magnetic field will always point in z -direction.

2.2 The g -Factor of the Free Electron

Since 1947 the electron g -factor is the key quantity for the most stringent test of QED and in that way of the SM. At present the anomalous magnetic momentum of the electron (g -factor anomaly): $a_e \equiv (g - 2)/2$ is calculated in a series expansion in terms of (α/π) up to the fifth order:

$$a_e = C_2(\alpha/\pi) + C_4(\alpha/\pi)^2 + C_6(\alpha/\pi)^3 + C_8(\alpha/\pi)^4 + C_{10}(\alpha/\pi)^5 + \dots \quad (2.2)$$

The Schwinger correction (vertex correction), which is a first-order correction ($C_2 = 1/2$), is represented in Fig. 2.1a as a one-loop Feynman diagram. The coefficients C_4 and C_6 have been also calculated analytically, whereas C_8 (891 Feynman diagrams) and C_{10} (12672 Feynman diagrams) have been numerically evaluated [3]. At the level of $C_{10}(\alpha/\pi)^5 = 6.2 \cdot 10^{-13}$ also contributions from hadronic vacuum-polarizations, $a_{\text{hadronic}} = 1.68(2) \cdot 10^{-12}$, become relevant. The most recent determination of the free electron g -factor has been performed in 2008 in the group of Gerald Gabrielse by David Hanneke [4]. Measuring directly the magnetic momentum anomaly of a single electron in a Penning trap, they determined the g -factor with a relative precision of $2.8 \cdot 10^{-13}$. In combination with the predicted series expansion in Eq. (2.2) the fine structure constant $\alpha^{-1} = 137.035\,999\,173\,(35)$ has been derived with a relative uncertainty of $2.5 \cdot 10^{-10}$.

A competing alternative approach for the determination of the fine structure constant is given by the combination of the Rydberg constant R_∞ , the ratio of the Planck constant over the mass of a rubidium atom M_{Rb} and the mass ratio M_{Rb}/m_e :

$$\alpha_{\text{recoil}}^2 = \frac{2R_\infty h}{cm_e} = \frac{2R_\infty}{c} \frac{M_{\text{Rb}}}{m_e} \frac{h}{M_{\text{Rb}}}. \quad (2.3)$$

At the moment the dominant uncertainty is caused by the determination of the ratio h/M_{Rb} , which has been quantified in the group of Francois Biraben in 2011 [5].

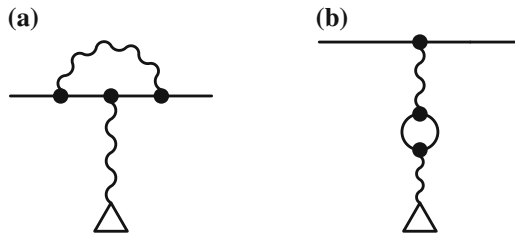


Fig. 2.1 Feynman diagrams of the first-order QED corrections (one-loop corrections) of the free electron g -factor. The electron is symbolized as a *straight line*, the photons as *curved lines* and the magnetic field as a *triangle*. Like in all the following Feynman diagrams, the time arrow points to the *right*. In **a** the Schwinger term (self-energy) is shown. In **b** the vacuum-polarization term is illustrated

Here, the recoil velocity of a single rubidium atom $v_{\text{recoil}} = \frac{\hbar k}{M_{\text{Rb}}}$ is measured, when it absorbs a photon of momentum $\hbar k$. This approach determines the fine structure constant $\alpha_{\text{recoil}}^{-1} = 137.035\,999\,037\,(91)$ with a relative uncertainty of $6.6 \cdot 10^{-10}$. The comparison of this value with the one obtained independently from the g -factor of the free electron represents the most stringent test of QED.

2.3 The g -Factor of the Bound Electron

In contrast to the g -factor of the free electron, where the electron is exposed to only small electromagnetic trapping fields, at our experiment we are interested to test QED under extreme conditions, by measuring g -factors in presence of strong electric fields. The strongest electric field which are accessible on the laboratory scale is the binding field of a heavy, highly charged nucleus.³ In Fig. 2.2 the relativistic prediction of the mean electric fields of $1s_{1/2}$ and $2s_{1/2}$ electrons are plotted versus the nuclear charge.⁴ Already in the low Z region ($Z \gtrsim 8$) the bound-electron perceives a larger electric field strength than by the brightest laser sources, which reach intensities of about $2 \cdot 10^{22} \text{ W/cm}^2$ [16]. The field strengths in heavy hydrogenlike ions approach the Schwinger limit, where the vacuum gets unstable, since the external electric field accelerates apart the virtual electron-positron pairs. In a homogeneous electric field spontaneous electron-positron pair creation has been predicted for: $E_S = \frac{m_e^2 c^3}{e \hbar} = 1.3 \cdot 10^{16} \text{ V/cm}$ [17–19]. At the surface ($r_{\text{surf}} = \sqrt{5/3} r_{\text{rms}}$) of a uranium nucleus ($Z = 92$) the electric field is $E(r_{\text{surf}} = 7.6 \text{ fm}) = 2.3 \cdot 10^{19} \text{ V/cm}$ [20].

Perturbative BS-QED - Series Expansions in (α/π) , $(Z\alpha)$ and $(1/Z)$

The fundamental approach of QED calculations in atomic systems, referred to as bound-state quantum electrodynamics (BS-QED), has been developed in the 1950s. Treating e.g. a hydrogenlike ion which contains a nucleus and an electron as a complete two-body problem, at least two QED series-expansions have to be considered:

- Firstly, the radiative corrections, regarding the interaction between the electron and the external magnetic field, require a series-expansion in orders of (α/π) , similar to the expansion for the free electron, see Eq. (2.2).

³Even stronger fields can be reached by muonic ions or even more exotic atomic systems. However, the measurement time is strongly limited by their short lifetimes.

⁴Here, the relativistic expectation value of $1/r^2$ has been used from [15]. For nuclear charges larger than 30, such a relativistic calculation is essential, e.g. for uranium ($Z = 92$) the mean electric field derived by the non-relativistic Schrödinger equation is a factor of 2.8 smaller than the relativistic calculation. The mean electric field of a $1s_{1/2}$ electron is:

$$E_{\text{mean}}(1s_{1/2}) = \frac{Ze}{4\pi\epsilon_0} \left\langle \frac{1}{r^2} \right\rangle = \frac{Ze}{4\pi\epsilon_0} \frac{2(Z\alpha)^2 (m_e c / \hbar)^2 (2\sqrt{1 - (Z\alpha)^2} + 1)}{\sqrt{1 - (Z\alpha)^2} (3 - 4(Z\alpha)^2)}. \quad (2.4)$$

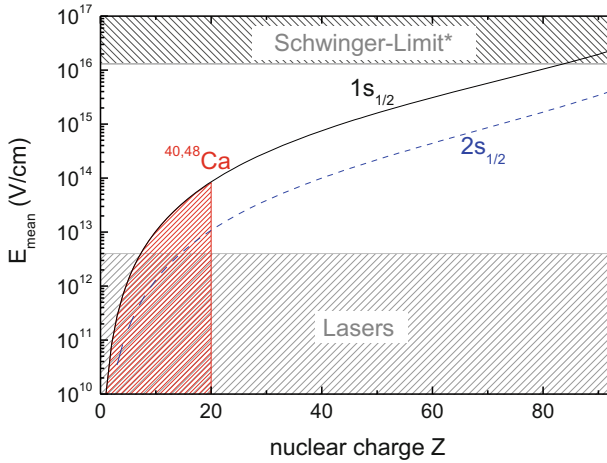


Fig. 2.2 Illustration of the mean electric field in highly charged ions as a function of the nuclear charge Z . The *red-hatched* area marks the field strength we have experimental access to. The lower *gray-hatched* area illustrates the electric field-strength accessible by the brightest laser sources and the upper *gray-hatched* area designates the Schwinger limit (for a homogeneous electric field), where the vacuum gets unstable. The *black* (*blue*) line represents the mean electric field strength, which acts on a single $1s_{1/2}$ ($2s_{1/2}$) - electron (Color figure online)

- Secondly, radiative corrections also occur in the interaction between the electron and the nucleus, which require an additional expansion in orders of $(Z\alpha)$. Studying heavy highly charged ions, the convergence of this series-expansion deteriorates. For example for hydrogenlike helium ($Z = 2$) the series-expansion converges quickly in powers of $(2 \cdot \alpha) \approx 0.01$, whereas for hydrogenlike lead ($Z = 82$) the series-expansion converges much slower in powers of $(82 \cdot \alpha) \approx 0.60$.
- Beyond that, in many-electron systems the interactions between the bound-electrons require a third series-expansion in orders of $(1/Z)$, where the n th order corresponds to Feynman diagrams with n photons, which are exchanged between the bound-electrons.⁵

To circumvent a series-expansion in $(Z\alpha)$, which is especially problematic for heavy highly charged nuclei, already in 1951 Wendell H. Furry reduced the two-body problem, where the electron (one body) interacts with the nucleus (other body), to an effective one-body problem of the electron, treating the nucleus classically as an time-independent static external potential $V(\vec{r})$ [21], e.g. as a Coulomb potential: $V_{\text{nucl}}(r) = (Ze)/(4\pi\epsilon_0 r)$. He added this potential to the Dirac equation of the single electron wave function $\psi(\vec{r}, t)$:

⁵The following explanation roughly outlines the $1/Z$ parameter of the perturbative expansion of the interelectronic interaction: In general, the parameter of the perturbative expansion is given by the matrix-element of the perturbation operator over the typical energy difference. The matrix-element of the Coulomb repulsion scales with $\alpha / \langle r_{12} \rangle$, where $\langle r_{12} \rangle$ (distance between two electrons) scales inversely with $(\alpha Z)^{-1}$. The energy difference typically scales with $(\alpha Z)^2$.

$$\left(i \hbar \partial_t + i \hbar c \vec{\alpha} \cdot \vec{\nabla} - \beta m c^2 - e V_{\text{nuc}}(\vec{r}) \right) \psi(\vec{r}, t) = 0, \quad (2.5)$$

where $\beta \equiv \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}$, $I_2 \equiv \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\vec{\alpha} \equiv \begin{pmatrix} 0 & \sigma_{1,2,3} \\ \sigma_{1,2,3} & 0 \end{pmatrix}$ and $\sigma_{1,2,3}$ are the Pauli matrices. As a consequence of this approach, also referred to as the *Furry picture*, the interaction with the nuclear potential is already included in the propagator of the electron. In Feynman diagrams this approach is symbolized by a double line for the electron propagator. Limitations of this picture, which e.g. presumes an infinitely heavy nucleus, will be discussed in Sect. 2.3.3.

In this thesis, we will focus on bound-electron g -factors in two different electron-configurations: (1) in the already mentioned hydrogenlike configuration and (2) in the lithiumlike configuration, which has two core electrons on the 1s-level and one valence electron on the 2s-level. Various physical effects contribute to the g -factors of the respective valence electron:

$$g(\text{H-like}) = g_{\text{Dirac}}^{\text{H-like}} + \Delta g_{\text{QED}}^{\text{H-like}} + \Delta g_{\text{nuc}}^{\text{H-like}}, \quad (2.6)$$

$$g(\text{Li-like}) = g_{\text{Dirac}}^{\text{Li-like}} + \Delta g_{\text{QED}}^{\text{Li-like}} + \Delta g_{\text{nuc}}^{\text{Li-like}} + \Delta g_{\text{int}} + \Delta g_{\text{sQED}}, \quad (2.7)$$

where $g_{\text{Dirac}}^{\text{H-like, Li-like}}$ is the Dirac value for the particular valence electron, $\Delta g_{\text{QED}}^{\text{H-like, Li-like}}$ are the corresponding radiative corrections of the valence electron and $\Delta g_{\text{nuc}}^{\text{H-like, Li-like}}$ contain nuclear corrections. In lithiumlike systems the interactions between the three electrons are included in the interelectronic interaction corrections Δg_{int} and the corresponding radiative corrections, the so-called screened QED corrections, Δg_{sQED} . In Fig. 2.3 the relative g -factor contributions for (a) hydrogenlike ions and (b) lithiumlike ions are listed in dependence on low and medium atomic numbers Z , which are accessible at our experimental apparatus. In the following these corrections are briefly introduced and the present status of the BS-QED calculations is summarized.

2.3.1 g_{Dirac} - Dirac Values of the Bound-Electron g -Factor

As seen in Fig. 2.3a, for atomic numbers larger than eight the dominant contribution of the bound-electron g -factor in a hydrogenlike ion is a relativistic correction. This contribution has been calculated already in 1928 by Gregory Breit [24]. Focusing on the zeroth-order approximation of BS-QED for a hydrogenlike ion, by solving its Dirac equation (2.5) in the presence of a magnetic field, he derived the following analytical expression:

$$g_{\text{Dirac}}^{\text{H-like}} = 2 + \Delta_{\text{Breit}}^{\text{H-like}} = \frac{2}{3} \left[1 + 2\sqrt{1 - (Z\alpha)^2} \right] = 2 - \frac{2}{3}(Z\alpha)^2 - \frac{1}{6}(Z\alpha)^4 + \dots \quad (2.8)$$

A detailed derivation of this expression from the Dirac equation by means of the minimal coupling is given for example in chapter four of the textbook “Fundamental

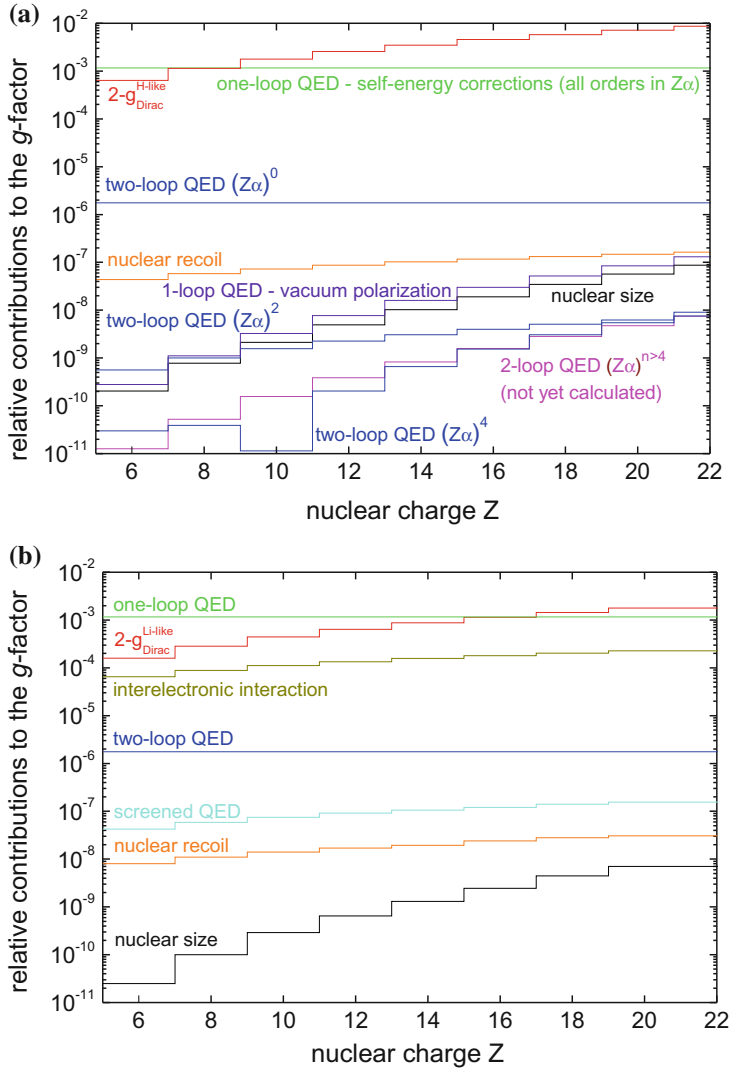


Fig. 2.3 Relative contributions to the bound-electron g -factor **a** for hydrogenlike ions [22] and **b** for lithiumlike ions [23]: Relativistic Breit correction (red), 1-loop QED without vacuum-polarization (bright green), 1-loop QED only vacuum-polarization (violet), 2-loop QED up to the fourth order in $(Z\alpha)$ (blue), 2-loop QED not yet calculated (magenta), nuclear recoil (orange), nuclear size (black), interelectronic interaction (green) and screened QED (turquoises). Only ions with an even atomic number are plotted, since we focus on spinless nuclei

Physics in Particle Traps” [25]. Due to the leading-order scaling of $(Z\alpha)^2$ the Breit correction reduces the g -factor of hydrogenlike helium ($Z = 2$) by only 71 ppm (parts per million) and by 13% for hydrogenlike lead ($Z = 82$).

In lithiumlike systems this effect amounts to:

$$g_{\text{Dirac}}^{\text{Li-like}} = 2 + \Delta_{\text{Breit}}^{\text{Li-like}} = \frac{2}{3} \left[1 + \sqrt{2 + 2\sqrt{1 - (Z\alpha)^2}} \right] = 2 - \frac{1}{6}(Z\alpha)^2 - \frac{5}{96}(Z\alpha)^4 + \dots, \quad (2.9)$$

see also Fig. 2.3b.

2.3.2 Δg_{QED} - Radiative Corrections

The recapitulation of the radiative corrections in hydrogenlike systems, which occur in the dynamics between the bound electron and the external magnetic field, is structured in terms of their (α/π) series-expansion. In lithiumlike systems very similar contributions occur in the zeroth order in $(1/Z)$, where photon exchange between the electrons does not occur.

One-loop BS-QED Corrections of the Order $(\alpha/\pi)^1$

In Fig. 2.4 all six Feynman diagrams of the first-order in (α/π) are presented for hydrogenlike systems. In 1997 the three self-energy diagrams (a-c) have been solved for the first time within the Furry picture in all orders in $(Z\alpha)$ [26]. In 2004 these calculations have been improved and extended also to lithiumlike systems in all orders of $(Z\alpha)$ [27]. Besides self-energy corrections, also the vacuum-polarization

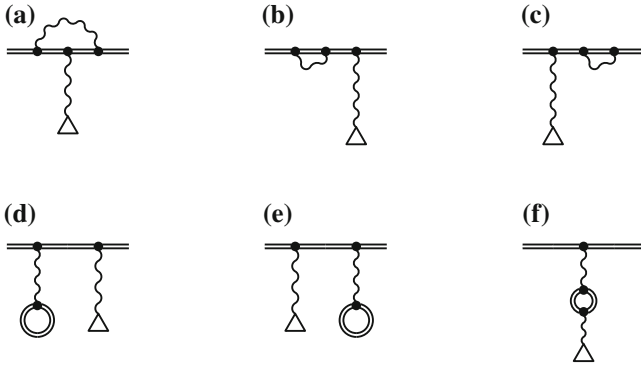


Fig. 2.4 One-loop BS-QED radiative corrections for hydrogenlike ions. **a–c** represent the self-energy diagrams; **d–f** the vacuum-polarization diagrams, which contain the electric-loops in **d** and **e** and the magnetic-loop in **f**. The *double line* symbolizes the electron propagator, calculated in the Furry picture

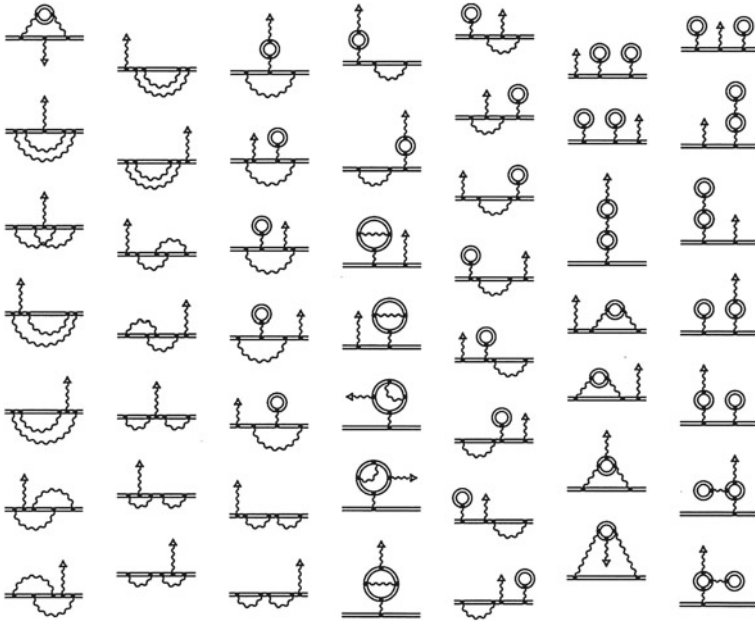


Fig. 2.5 Two-loop BS-QED corrections for hydrogenlike ions [20, T. Beier]

corrections have been evaluated [28], which are at least four orders of magnitudes smaller in the nowadays accessible low and medium Z region.

Two-Loop BS-QED Corrections of the Order $(\alpha/\pi)^2$

Already the two-loop BS-QED corrections contain 50 Feynman diagrams, see Fig. 2.5. At present solutions for these second and higher-order corrections in (α/π) are not available in all orders in $(Z\alpha)$. Expanding the two-loop corrections in orders of $(Z\alpha)$, contributions of the order $(\alpha/\pi)^2(Z\alpha)^4$ have been derived in 2005 for all ns states (hydrogenlike, lithiumlike, sodiumlike ...) [29]. Nowadays uncalculated terms of $(Z\alpha)^5$ or higher-order in the two-loop QED expansion dominate the theoretical uncertainty of bound-electron g -factors in hydrogenlike systems.

2.3.3 Δg_{nucl} - Nuclear Corrections

Until now, the nucleus has been treated as a point charge, fixed in space, which is added as an external Coulomb potential to the Dirac equation, see Eq. (2.5). The following nuclear properties require corrections of the bound-electron g -factor.

Nuclear Magnetic Moment

A nuclear magnetic moment leads to an additional splitting of the bound-electron energy levels. This so-called hyperfine structure also modifies the bound-electron g -factor [20]. Since the nuclear magnetic moment is caused by the spins of the constituents of the nucleons, i.e. the spins of the quarks and gluons, which combine to complicated structures via complex interactions, it cannot be rigorously calculated, but has to be measured. Furthermore it is not sufficient to describe the nuclear magnetic moment by a point-like dipole, but by a smeared-out nuclear magnetization, referred to as the *Bohr–Weisskopf* effect [30]. Avoiding these contributions, in this thesis we focus solely on spinless nuclei with even number of protons and neutrons.

Δg_{ns} - Nuclear Size and Δg_{nd} - Nuclear Deformation

The size of the nucleus is considered by modifications of the nuclear potential in the Dirac equation, see Eq.(2.5). The modeled nuclear potential in principal relies on the root-mean-square charge radius, $r_{\text{nucl}}^{\text{rms}} = \sqrt{\langle r^2 \rangle}$, which has to be measured in experiments. In 2002 the corresponding relativistic g -factor correction has been derived analytically for ns and $np_{1/2}$ electron states, which reside in our experimentally accessible nuclear charge range ($Z = 1 - 20$), [31]. In the non-relativistic limit this g -factor contribution scales with $\Delta g_{\text{ns}} = \frac{8}{3\pi^3} (Z\alpha)^4 m_e^2 \langle r^2 \rangle$. Due to the Z^4 -scaling the knowledge of the nuclear charge distribution sets the limit of g -factor calculations for heavy highly charged ions. The determination of $r_{\text{nucl}}^{\text{rms}}$ via the measurement of a bound-electron g -factor has been demonstrated by the measurement of the g -factor of hydrogenlike silicon [32].

In a recent study [33] the leading relativistic nuclear quadrupole and hexadecapole deformation corrections have been derived analytically. For heavy highly charged ions, e.g. hydrogenlike uranium, the relative nuclear deformation contribution to the g -factor is about 10^{-6} . In the low and medium Z systems, studied in this thesis, the nuclear shape correction is not relevant at the current level of precision ($\Delta g_{\text{nd}}(^{12}\text{C}) = -7.9(5.3) \cdot 10^{-16}$ and $\Delta g_{\text{nd}}(^{28}\text{Si}) = -2.85(52) \cdot 10^{-13}$).

Δg_{rec} - Nuclear Mass/Recoil

So far the nucleus has been treated as a static point-charge (or charge distribution), fixed in space. This time-independent approximation, which would be exact for infinitely heavy ions, enabled the tremendous simplification of BS-QED, by reducing the two-body problem to an effective one-body problem for the bound electron. The motion of the nucleus itself (recoil motion) due to the finite nuclear mass requires BS-QED calculations beyond the Furry picture. In 2001 this effect has been calculated as a correction of the bound-electron g -factor to first-order in m_e/M and to all orders in $Z\alpha$ [34]. To zeroth order in $(1/Z)$, this formula describes also the recoil correction for electrons in ns states. In the lowest relativistic order the nuclear recoil correction scales as follows: $\Delta g_{\text{rec}} = -\frac{m_e}{m_{\text{ion}}} \frac{(\alpha Z)^2}{n^2}$. This thesis includes a dedicated measurement of the recoil contribution by measuring the g -factor difference of $^{40}\text{Ca}^{17+}$ and $^{48}\text{Ca}^{17+}$, see Sect. 2.7 and Chap. 6 for more details.

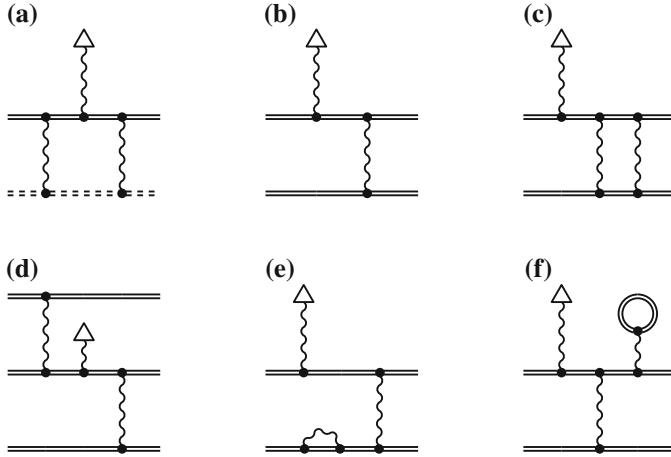


Fig. 2.6 BS-QED diagrams of some particular physical effects: **a** Nuclear polarization (The nucleus is presented as a *double dashed line*.), **b** interelectronic interaction (one photon exchange with one core electron), **c** interelectronic interaction (two photon exchange with one core electron), **d** interelectronic interaction (one photon exchanges with two core-electrons), **e** screened QED (self-energy), **f** screened QED (vacuum-polarization). These diagrams just highlight one diagram of the particular physical effect and not the complete set of diagrams of the corresponding order

Δg_{np} - Nuclear Polarization

Intrinsic nuclear dynamics enable virtual electromagnetic excitations, by the exchange of two photons between the nucleus and the bound electron. This so-called nuclear polarization correction is evaluated in a $(1/Z)$ series expansion. The lowest-order Feynman diagram is shown in Fig. 2.6a. Similar to the nuclear size corrections, the nuclear polarization correction is limited to the phenomenological description of the nucleon-nucleon interaction and in that way can set an ultimate accuracy limit of QED tests in heavy highly charged ions. The effect has been calculated for the bound-electron g -factor in 2002 [35] and has been improved in a recent paper [36], evaluating the zeroth and first-orders in $(1/Z)$ in heavy highly charged ions, e.g. $\Delta g_{np}(^{208}\text{Pb}^{81+}) = -1.977 \cdot 10^{-7}$. As the nuclear shape corrections, for the ions, studied in this thesis, the nuclear polarization correction is not relevant at the current level of precision.

2.3.4 Many-Electron Corrections

Focusing on the g -factor of a $2s$ electron in a lithiumlike electron configuration, which has got two core electrons ($1s$) and one valence electron ($2s$), one has to consider the interactions between these electrons. We distinguish between two different g -factor contributions.

Δg_{int} - Interelectronic Interaction Corrections for Lithiumlike Ions

The interelectronic interaction contribution contains all Feynman diagrams with photon exchanges between the electrons, like for example diagrams (b–d) in Fig. 2.6, excluding diagrams with additional self-energy or vacuum-polarization loops. In an unusual way this correction requires also the analysis of the negative-energy Dirac states, which contribute to the interelectronic interaction correction of the g -factor with the same order of magnitude as the positive-energy states. In 2002 the one-photon exchange diagrams (first-order in $1/Z$) have been evaluated to all orders in $(Z\alpha)$ within a rigorous QED approach [37]. A recent paper from 2014 presents an extension of these rigorous QED calculations to the two-photon exchange diagrams (second order in $1/Z$) [38]. At present the interelectronic interaction contribution to the bound-electron g -factor dominates the theoretical uncertainty of lithiumlike g -factors in the low- and medium- Z region ($Z < 30$).

Δg_{sQED} - Screened QED Corrections for Lithiumlike Ions

The screened QED corrections include all Feynman diagrams with photon exchanges between the electrons, which contain additionally self-energy or vacuum-polarization loops. As an illustration, diagrams (e) and (f) in Fig. 2.6 show some leading-order screened QED corrections. Since the convergence of the screened QED contributions differs for various atomic numbers, at present three different approaches are used: (1) For lower Z the convergence in a rigorous QED approach becomes worse, so that perturbation theory only in leading-order in $(Z\alpha)$ is applied. (2) In the medium- Z region an effective screening potential is introduced in the QED calculations to all orders in $(Z\alpha)$. (3) For heavy highly charged ions a rigorous QED approach is used [38].

2.4 Measurement Principle of the Bound-Electron g -Factor

In a homogeneous magnetic field $\vec{B} = B\vec{e}_z$ the Zeeman effect describes the shift of the bound-electron energy levels in dependence on the specific total angular momentum J and the corresponding projection m_J parallel to the magnetic field:

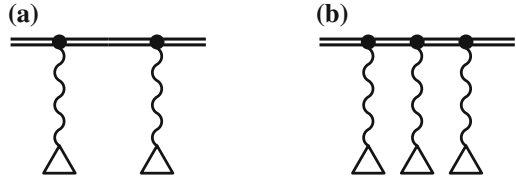
$$\Delta E_Z(J, m_J, B) = g_J m_J \mu_B B. \quad (2.10)$$

In this context the ns states energetically split into two states, the spin-up $|\uparrow\rangle$ and spin-down $|\downarrow\rangle$ states. The corresponding energy difference, the so-called Zeeman (level) splitting, amounts to:

$$\Delta E_{Z\text{-Splitting}} = \Delta E_Z(|\uparrow\rangle) - \Delta E_Z(|\downarrow\rangle) = h \frac{g}{4\pi} \frac{e}{m_e} B = h \cdot \nu_L, \quad (2.11)$$

where ν_L is the Larmor frequency, also called the spin precession frequency. For the determination of the magnetic field, the cyclotron frequency ν_c of the ion is

Fig. 2.7 Leading-order diagrams of the 2nd and 3rd order Zeeman shifts



measured:

$$v_c = \frac{1}{2\pi} \frac{q_{ion}}{m_{ion}} B. \quad (2.12)$$

The combination of Eqs. (2.11) and (2.12) provides an experimental access to the bound-electron g -factor:

$$g = 2 \frac{m_e}{m_{ion}} \frac{q_{ion}}{e} \frac{v_L}{v_c} = 2 \frac{m_e}{m_{ion}} \frac{q_{ion}}{e} \Gamma, \quad (2.13)$$

which depends on the electron/ion mass-ratio, electron mass over ion mass, the charge ratio, which is a simple ratio of integers, and the Larmor- to cyclotron frequency ratio $\Gamma \equiv \frac{\nu_L}{\nu_c}$.

Higher-Order Zeeman Shifts

Multiple interactions between the bound electron and the external magnetic field, as for example illustrated in Fig. 2.7, lead to higher-order Zeeman shifts, which are non-linear in the magnetic field. Studying this effect, the Zeeman shift can be evaluated in a series-expansion:

$$\Delta E(J, m_J, B) = \Delta E^{(1)}(J, m_J, B) + \Delta E^{(2)}(J, m_J, B) + \Delta E^{(3)}(J, m_J, B) + \dots \quad (2.14)$$

where: $\Delta E^{(i)}(J, m_J, B) = g_J^{(i)} \cdot m_J \cdot (\mu_B B)^i / (m_e c^2)^{i-1}$ and $i \in \mathbb{N}$, see also Fig. 2.8. In the case of $J = 1/2$, the first-order coefficient $g_J^{(1)}$ is related to the theoretically predicted bound-electron g -factor described above: $g = g_{1/2}^{(1)}$. The higher-order shifts can be calculated, see [39]. Considering the symmetry relation: $g_J^{(2)} \cdot (m_J) = g_J^{(2)} \cdot (-m_J)$, the quadratic correction does not alternate the Zeeman splitting for $J = 1/2$ levels, so that for example hydrogenlike and lithiumlike ions are not effected. Nevertheless the third order Zeeman shift, where $g_J^{(3)} \cdot (m_J) = -g_J^{(3)} \cdot (-m_J)$, is the leading-order correction of the Zeeman splitting in hydrogenlike and lithiumlike ions. For $^{40}\text{Ca}^{17+}$ and $^{12}\text{C}^{5+}$ these higher-order Zeeman splittings are much smaller than the relative experimental uncertainty of a few $1 \cdot 10^{-11}$, see Table 2.1.

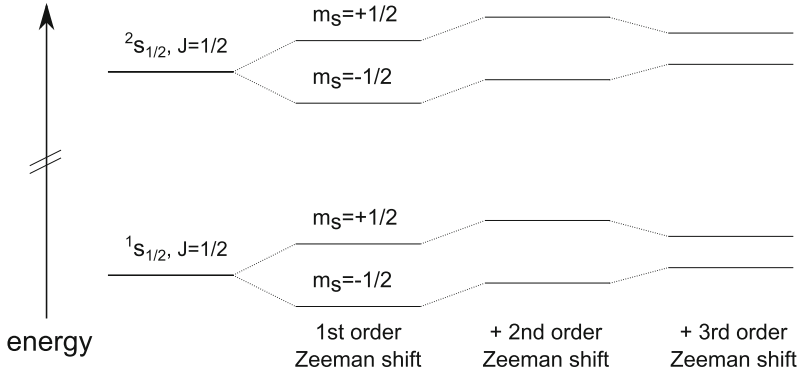


Fig. 2.8 Level scheme of the higher-order Zeeman shifts for the $1s_{1/2}$ and $2s_{1/2}$ states. In the case of $^{12}\text{C}^{5+}$ and $^{40}\text{Ca}^{17+}$ the 2nd order Zeeman effect shifts all the Zeeman sublevels in equal measure up, so that the Zeeman splitting is not influenced and the 3rd order Zeeman effect slightly diminishes the Zeeman splitting. The way of representing the shifts is exaggerated

Table 2.1 2nd and 3rd Zeeman shifts for hydrogenlike carbon $^{12}\text{C}^{5+}$ and lithiumlike calcium $^{40}\text{Ca}^{17+}$ in a magnetic field of 3.76 T [40]

Ion	$ \Delta E^{(2)} / \Delta E^{(1)} $	$ \Delta E^{(3)} / \Delta E^{(1)} $
$^{12}\text{C}^{5+}$	$2.2 \cdot 10^{-7}$	$2.6 \cdot 10^{-16}$
$^{40}\text{Ca}^{17+}$	$3.2 \cdot 10^{-7}$	$3.8 \cdot 10^{-16}$

2.5 Status of the Bound-Electron g -Factor Measurements

In parallel to the great improvements of the theoretical predictions of the bound-electron g -factor in the last 15 years, a tremendous progress has been made on the experimental determination of the bound-electron g -factor. One major breakthrough has been achieved in 2000, when, in the group of Günter Werth, Nikolaus Hermanspahn, Harmut Häffner and colleagues managed to trap a single hydrogenlike carbon ion in a Penning trap setup and measured the g -factor with the newly developed double-trap technique $(\delta g/g)_{\text{exp}} = 2.5 \cdot 10^{-9}$ [41]. The theoretical uncertainty of that time was of the same order of magnitude $(\delta g/g)_{\text{theo}} = 3.5 \cdot 10^{-9}$.⁶ In 2003 José Verdú and colleagues, also from the group of Günter Werth, published the g -factor of hydrogenlike oxygen $(\delta g/g)_{\text{exp}} = 2.3 \cdot 10^{-9}$ [42]. The corresponding theoretical prediction at that time had a relative uncertainty of $(\delta g/g)_{\text{theo}} = 3.0 \cdot 10^{-10}$. Seven years later Sven Sturm and colleagues had developed a number of experimental improvements, e.g. an improved trap design, a significantly enlarged spatial separation of the two Penning traps, to improve the magnetic homogeneity [43], completely newly developed cryogenic detection systems to reduce the ion's temperatures,

⁶In this paragraph I quote the theoretical g -factors, which have been published together with the measurements at that time. Most calculations improved in the last years.

feedback techniques, pressure and room temperature stabilizations and beside that a new phase-sensitive detection technique, PnA [44], which will be also explained in this thesis in Sect. 3.4.2. In 2011 Sven Sturm and colleagues published the g -factor of hydrogenlike silicon, $^{28}\text{Si}^{13+}$ ($(\delta g/g)_{\text{exp}} = 5.0 \cdot 10^{-10}$ and $(\delta g/g)_{\text{theo}} = 8.5 \cdot 10^{-10}$), which at present represents the most stringent test of BS-QED [32]. All QED contributions have been tested with a relative uncertainty of $8 \cdot 10^{-7}$; without the $(Z\alpha)^0$ contributions, the relative uncertainty is still $3 \cdot 10^{-4}$. Two years later Anke Kracke and colleagues measured the g -factor of lithiumlike silicon, $^{28}\text{Si}^{11+}$ ($(\delta g/g)_{\text{exp}} = 1.1 \cdot 10^{-9}$ and $(\delta g/g)_{\text{theo}} = 2.5 \cdot 10^{-8}$), which represents the most stringent test of many-electron BS-QED calculations [45]. To date, all the calculated bound-electron g -factors have been in good agreement with the corresponding measurements.

Next Steps - Bound-Electron g -Factor Measurements Presented in this Thesis

In this thesis I will present an improved g -factor value of hydrogenlike carbon. From the result a new value for the electron's atomic mass has been derived, which reduces the uncertainty of the current literature value of the atomic mass of the electron m_e by a factor of 13. Furthermore, I will present high-precision g -factor measurements of the lithiumlike calcium isotopes $^{40}\text{Ca}^{17+}$ and $^{48}\text{Ca}^{17+}$. Their g -factor difference represents a unique test of BS-QED beyond the Furry picture.

In the last two sections of this chapter I will highlight firstly the status of electron mass measurements (Sect. 2.6) and secondly the status of isotope shift measurements (Sect. 2.7).

2.6 The Electron and Its Atomic Mass

In 1897 Joseph J. Thomson and colleagues discovered the electron as a unique particle in cathode ray experiments [46]. In his Nobel lecture in 1906 he denominated the electron mass with a relative precision of the order of 6% ("...the mass of the corpuscle is only about 1/1700 of that of the hydrogen atom.") [47]. Nowadays, the electron is regarded as a massive, electrically charged, point-like, elementary spin-1/2 particle. A possible substructure would be smaller than $2 \cdot 10^{-20}$ m [48]. The Kobayashi–Maskawa phase in the quark sector of the SM can induce an electric dipole moment (EDM) of $d_e < 1 \cdot 10^{-38} e \cdot \text{cm}$ via higher-order quark loops [49]. Larger electron EDMs are predicted in several SM extensions. At the moment, the upper limitations of the sought-after electron EDM amounts to $8.7 \cdot 10^{-29} e \cdot \text{cm}$ at a 90% confidence level [50]. As the lightest electrically charged lepton of the SM, the electron is a stable particle. This outstanding property assigns the electron a prominent role in nature. Its intrinsic characteristics, especially its mass, which is one of the 19 fundamental input parameters of the SM, profoundly determines the atomic structure of our universe.

2.6.1 *Benefits of an Improved Electron Mass*

These days at least two fields of high-precision physics benefit from an improved electron mass:

- **The determination of the fine structure constant:**

Introduced already in Sect. 2.2, the most stringent test of QED, which is based on the theoretical prediction and the measurement of the anomalous magnetic moment of the free electron, requires an experimentally determined value for the fine structure constant α . At present, the most precise value relies on four fundamental constants, see Eq. (2.3): (1) the Rydberg constant ($\delta R_\infty/R_\infty = 5.0 \cdot 10^{-12}$) [51], (2) the rubidium mass ($\delta M_{\text{Rb}}/M_{\text{Rb}} = 1.2 \cdot 10^{-10}$) [52], (3) the ratio Planck constant over rubidium mass ($\delta(h/M_{\text{Rb}})/(h/M_{\text{Rb}}) = 1.2 \cdot 10^{-9}$) [5] and (4) last but not least the mass of the electron.

Further progress on this impressive QED test is motivated in particular by the $2.5 - 3.6\sigma$ discrepancy between the theoretically predicted and the measured anomalous magnetic moment of the muon $\delta a_\mu/a_\mu(\text{exp}) = 5.4 \cdot 10^{-7}$ [53, 54]. Since the radiative loop contributions from hypothetical heavier new particles with masses $m_{\text{new phys}}$ scale with $m_{(\mu,e)}^2/m_{\text{new phys}}^2$, the muon has a 40000 times enhanced sensitivity to “new physics” compared to the about 200 times lighter electron. A confirmation of such a discrepancy also in the anomalous magnetic moment of the free electron requires amongst others a value of the fine structure constant with a relative uncertainty of about $4 \cdot 10^{-11}$. With the new value of the electron mass, reported in this thesis, we approach such requests.

- **Tests of QED in strong electric fields:**

Mentioned in Sect. 2.5, nowadays the most stringent tests of BS-QED are based on high-precision measurements of the bound-electron g -factor of hydrogenlike ions. Here, the measurement principle strongly depends on the electron mass, see Eq. (2.13). Already the uncertainty of the g -factor of hydrogenlike silicon in 2011 has been dominated by the uncertainty of the electron mass [32]. For further planned bound-electron g -factor measurements an improved electron mass is of great importance.

2.6.2 *Electron Mass Measurements in History*

Some remarkable achievements in trapping physics of charged particles have been associated with measurements of the electron mass. In this section I will summarize the tremendous experimental progress, which improved the relative uncertainty of the electron mass by more than three orders of magnitudes in the last 40 years, see also Fig. 2.9. I will start with the first direct determination of the electron mass in a Penning trap 37 years ago. In such a direct approach, which is the most common measurement principle in high-precision mass spectrometry of charged particles

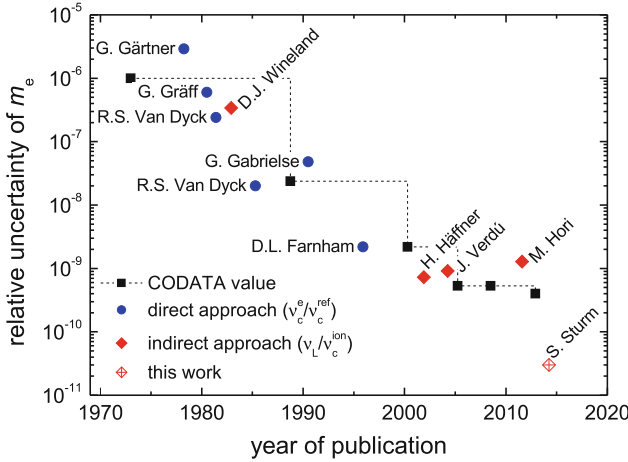


Fig. 2.9 A historical overview of the relative uncertainties of the electron mass measurements in the last four decades. *Blue markers*: Direct measurements of the cyclotron frequency ratio $\nu_c^{\text{ref}}/\nu_c^e$ [55–59]. *Red markers*: Indirect measurements of the Larmor-to-cyclotron frequency ratio ν_L/ν_c^{ion} [41, 42, 60–63]. *Black markers*: Literature values by the CODATA [51, 64–68] (Color figure online)

(elementary particles, ions, molecules), the cyclotron frequency ratio of the particle of interest, in this case of the electron $\nu_c^e = \frac{1}{2\pi} \frac{e}{m_e} B$, and a reference particle $\nu_c^{\text{ref}} = \frac{1}{2\pi} \frac{q_{\text{ref}}}{m_{\text{ref}}} B$ is measured in a homogeneous magnetic field:

$$m_e = \frac{e}{q_{\text{ref}}} \frac{\nu_c^{\text{ref}}}{\nu_c^e} m_{\text{ref}}, \quad (2.15)$$

where e and q_{ref} are the charge states of the electron and of the reference particle, respectively, and m_{ref} is the mass of the reference particle, which must have a smaller relative uncertainty than the electron mass. For the electron mass this direct approach has been applied for the first time by G. Gärtner and E. Klempt in 1978 [55]. They loaded alternately clouds of a few thousand protons and a few thousand electrons into a Penning trap and measured in a destructive manner the particle loss by resonant cyclotron excitations. In the following 17 years this direct measurement principle has been improved, reducing the size of the particle clouds and optimizing the frequency detection techniques. In this context four papers have to be mentioned: (1) In 1980 G. Gräff, H. Kalinowsky and J. Traut [56] introduced a time-of-flight (ToF) technique to measure the electron-proton mass ratio. (2) In 1981 R.S. Van Dyck Jr. and P.B. Schwinberg used for the first time non-destructive radio frequency (rf) resonance techniques [57]. They alternately confined clouds of about 10 electrons and 40 ions in the same magnetic field of a Penning trap and detected the induced image charges of the excited clouds. (3) In the following years R.S. Van Dyck Jr. and colleagues improved their experimental setup [58]. (4) In 1995 D.L. Farnham, R.S. Van Dyck Jr. and

P.B. Schwinberg published their last direct measurement of the electron mass, by measuring the cyclotron frequencies of a single carbon nucleus ($^{12}\text{C}^{6+}$) and a small electron cloud (5-13 electrons) via non-destructive rf-resonance detection techniques [59]. Their measurement principle has been limited by the large relativistic shift of the electron and the corresponding large uncertainty of the electron cyclotron frequency due to the smallness of the electron mass.

In parallel to this direct approach, D.J. Wineland, J.J. Bollinger and W.M. Itano developed an alternative approach for precision mass spectrometry in Penning traps already in 1982 [60]. They measured on the one hand the cyclotron frequency of a small cloud of lithiumlike $^9\text{Be}^+$ ions, using a laser-beam fluorescence technique, and on the other hand a hyperfine transition of these ions via an rf-optical double-resonance technique. For the determination of the electron mass they had to rely on theoretical predictions for the bound-electron g -factor.

Before I will come to the state-of-the-art measurement principle for the electron mass, which has been developed within the group of Günter Werth, I want to mention two further, more exotic measurements of the electron mass: (1) In the context of a CPT test, the masses of protons and antiprotons have been measured by Gerald Gabrielse and colleagues in 1990 [61]. They alternatively trapped small clouds of protons and antiprotons in a cylindrical Penning trap. Here, they measured also the mass ratios antiproton-to-electron and proton-to-electron, determining in that way also a value of the electron mass. (2) In 2011 Masaki Hori and colleagues performed two-photon laser spectroscopy of antiprotonic helium, a bound-state including a helium nucleus, an antiproton and an electron. Relying on matter-antimatter symmetry, $m_{\bar{p}} = m_p$, they derived a value for the electron mass [62].

2.6.3 *State-of-the-art Measurement Principle of the Electron Mass*

In the beginning of this millennium, Günter Werth, Heinz-Jürgen Kluge and Wolfgang Quint presented an improved and advanced variant of the indirect approach to circumvent the determination of the cyclotron frequency of the free electron and the corresponding large relativistic shifts. Instead of measuring the cyclotron frequency of the free electron ν_c^e , the electron was bound to a light nucleus and the ratio between the Larmor frequency of the bound electron and the cyclotron frequency of the hydrogenlike ion has been measured, exactly like for the determination of the bound-electron g -factor, see Sect. 2.4. Relying on calculations for the bound-electron g -factor, Eq. (2.13) can be resolved to the electron mass:

$$m_e = \frac{g_{\text{theo}}}{2} \frac{e}{q_{\text{ion}}} \frac{v_c}{v_L} m_{\text{ion}} = \frac{g_{\text{theo}}}{2} \frac{e}{q_{\text{ion}}} \frac{m_{\text{ion}}}{\Gamma}. \quad (2.16)$$

Due to the $(Z\alpha)^5$ scaling of the higher-order two-loop QED corrections, which dominate the uncertainty of bound-electron g -factor calculations for hydrogenlike ions,

Table 2.2 Binding energies of atomic carbon, ^{12}C from the *NIST Atomic Spectra Database* [70]

Ionization state	Binding energy (eV)
I [71]	11.260 30
II [72]	24.384 5 (9)
III [73]	47.887 78 (12)
IV [74]	64.493 58 (19)
V [75]	392.090 49 (3)

see Fig. 2.3, it is favorable to use light nuclei. For the first time this measurement principle has been used by Hartmut Häffner and colleagues in 2001, in the group of Günter Werth. Here, they determined the Larmor-to-cyclotron frequency ratio of hydrogenlike carbon [69]. Two years later José Verdú and colleagues measured also the Larmor-to-cyclotron frequency ratio of hydrogenlike oxygen [42]. Both measurements have already been mentioned in the context of historical bound-electron g -factor measurements in Sect. 2.5.

In this thesis the measurement on hydrogenlike carbon is repeated with a significantly improved experimental setup, which enables a 25-fold improvement in comparison to the former measurement on hydrogenlike carbon.

We have also chosen hydrogenlike carbon, since the atomic mass of carbon ^{12}C defines the atomic mass unit and thus has no uncertainty. In Table 2.2 the binding energies of carbon ^{12}C are listed. Since for the first ionization energy no uncertainty is listed in [71] and a further calculated value in [76] deviates by 0.7 meV, we assume a conservatively estimated error of 1 meV for the first ionization state. With a total binding energy of $E_{\text{bind}} = 540.116\,6\,(14)\,\text{eV}$ and the conversion factor of $1\,\text{u} = 931.494061(21) \cdot 10^6\,\text{eV}/c^2$ [51] the mass of $^{12}\text{C}^{5+}$ is calculated:

$$\begin{aligned}
 m(^{12}\text{C}^{5+}) &= 12\text{u} - 5 \cdot m_e + E_{\text{bind}} \\
 &= 11.997\,257\,680\,291\,7\,(18)\text{u} \quad (0.15\,\text{ppt}). \quad (2.17)
 \end{aligned}$$

2.6.4 State-of-the-art Calculations of the Bound-Electron g -Factor of Hydrogenlike Carbon

In the framework of bound-state QED the g -factor of $^{12}\text{C}^{5+}$ has been calculated with a relative uncertainty of $1.2 \cdot 10^{-11}$: $g = 2.001\,041\,590\,176\,(24)$ [63]. Beyond that, the theoretical uncertainty has been even further reduced by a factor of 5 by estimating the dominant unknown term - the leading higher-order contribution in two-loop QED calculations: $g_{2L}^{\text{ho}}(Z) \approx (\alpha/\pi)^2 (Z\alpha)^5 b_{50}$ - from the discrepancy between the experimentally and determined g -factor of hydrogenlike silicon, $^{28}\text{Si}^{13+}$, see Table 2.3 and supplement of [63]. The final state-of-the-art value for the theoretically predicted bound-electron g -factor value is [63]:

Table 2.3 Theoretical contributions to the bound-electron g -factor of hydrogenlike carbon $^{12}\text{C}^{5+}$. Abbreviations: “h.o.” higher-order, “SE:” self-energy contribution, “SE-FS:” mixed self-energy and nuclear finite size contribution, “VP-EL:” electric-loop vacuum-polarization contribution, “VP-ML:” magnetic-loop vacuum-polarization contribution, “rad-rec:” leading term of the mixed radiative-recoil contribution [63]

Theoretical contributions		$^{12}\text{C}^{5+}$
Dirac finite nuclear size one-loop QED		1.998 721 345 391 (1)
		0.000 000 000 407
	$(Z\alpha)^0$	0.002 322 819 466 (1)
	$(Z\alpha)^2$	0.000 000 742 160
	$(Z\alpha)^4$	0.000 000 093 422
	h.o. SE	0.000 000 008 283 (4)
	h.o. SE-FS	−0.000 000 000 002 (2)
	h.o. VP-EL	0.000 000 000 556
	h.o. VP-ML	0.000 000 000 038
$\leq$ two-loop QED	$(Z/\alpha)^0$	−0.000 003 515 108
	$(Z/\alpha)^2$	−0.000 000 001 123
	$(Z/\alpha)^4$	0.000 000 000 060
	h.o.	−0.000 000 000 003 (3)
Nuclear recoil	m_e/M	0.000 000 087 725
	rad-rec	−0.000 000 000 068
	h.o.	−0.000 000 000 028
Nuclear polarization		0.000 000 000 000
Nuclear deformation		0.000 000 000 000
Total theory		2.001 041 590 176 (6)

$$g_{\text{theo}}(^{12}\text{C}^{5+}) = 2.001\,041\,590\,179\,8\,(47) \quad (2.4\text{ ppt}). \quad (2.18)$$

2.7 Testing BS-QED Beyond the Furry Picture

As already specified in the context with bound-electron g -factors, see Sect. 2.3.3, high-precision measurements within the atomic level scheme are sensitive to various nuclear properties, such as the nuclear mass, the nuclear charge distribution, the nuclear spin, the nuclear magnetization distribution and nuclear level schemes. Here, measurements on different isotopes are of particular interest, since the differences of these measurements, the so-called *isotope shifts* (IS), are exclusively caused by the nuclear differences.

2.7.1 Isotope Shift Measurements

High-precision measurements of isotope shifts represent one of the vital investigations in atomic physics [77]. In this context many atomic transitions have been studied with various techniques, e.g. X-ray measurements also in muonic atoms, elastic electron scattering experiments, laser and X-ray spectroscopy and dielectronic recombination measurements. Isotope shifts arise mainly from the combined effects of (1) the finite nuclear mass and (2) the volume of the nuclear charge distribution.⁷ The recoil shift which is also called mass shift (MS) usually dominates the isotope shifts in light atoms and has a large relativistic nuclear recoil contributions in heavy highly charged ions. The nuclear size shift which is also called volume or field shift (FS) is caused by the spatial overlap of the nuclear charge distribution and the electronic wave functions. The FS scales as Z^5 or even Z^6 and thus dominates the isotope shifts in heavy atoms.

A successful test of the relativistic mass shift has been performed by Rosario Soria Orts and colleagues in 2006 [78]. They measured the isotope shift of the magnetic-dipole (M1) transitions of boron- and berilliumlike argon ions at the Heidelberg electron beam ion trap with relative uncertainties of 4.9 and 8.3%.

To my knowledge, the first measurement of an isotope effect in bound-electron g -factors has been performed by W.M. Hughes and H.G. Robinson in 1969 [79]. They measured the bound-electron g -factor ratio (not the difference) of hydrogen (H) and deuterium (D), using optical pumping of rubidium and a spin-exchange detection of H and D atomic Zeeman resonances.

2.7.2 The Isotope Shift of the Bound-Electron g -Factors of Two Different Lithiumlike Calcium Isotopes, $^{40}\text{Ca}^{17+}$ and $^{48}\text{Ca}^{17+}$

In the second part of my thesis, I will focus on the bound-electron g -factor difference of the lithiumlike isotopes $^{40}\text{Ca}^{17+}$ and $^{48}\text{Ca}^{17+}$. In the case of ^{40}Ca and ^{48}Ca the nuclear charge radii are surprisingly similar: $r_{\text{nuc}}(^{40}\text{Ca}) = 3.4776(19)$ fm and $r_{\text{nuc}}(^{48}\text{Ca}) = 3.4771(20)$ fm [80], so that the nuclear size contribution basically cancels in the g -factor difference. To 99.96% the g -factor difference is dominated by the recoil contribution.

⁷In principle, also nuclear polarizations contribute to isotope shifts. However, at the present level of precision this contribution can be neglected.

2.7.3 Theoretical Calculations of the Isotope Shift

$$\Delta g = g(^{40}\text{Ca}^{17+}) - g(^{48}\text{Ca}^{17+})$$

For ns states the recoil contribution is of pure relativistic origin. The corresponding full relativistic theory can be formulated only in the framework of QED. As already stated in Sect. 2.3.3, the recoil correction is the only contribution, which requires BS-QED calculations beyond the external field approximation, the so-called Furry picture. In a recent paper the recoil contribution has been evaluated to all orders in $(Z\alpha)$ for the $2s$ state of the calcium isotopes [81]. The corresponding radiative, second-order in (m_e/m_{ion}) and interelectronic interaction (first and higher-orders) recoil corrections have been calculated [82–86]. The theoretical uncertainty of the recoil contributions is dominated by the uncalculated higher-order relativistic and QED corrections. In Table 2.4 the different theoretical contributions to the g -factor difference of $^{40}\text{Ca}^{17+}$ and $^{48}\text{Ca}^{17+}$ are listed.

Since we measured the absolute g -factor values of $^{40}\text{Ca}^{17+}$ and $^{48}\text{Ca}^{17+}$, I also list the corresponding state-of-the-art g -factor contributions in Table 2.5. Although most recent progress has been made on the interelectronic interaction contributions, by the rigorous QED evaluation of the second-order contributions (two-photon exchange diagrams) [38], the interelectronic interaction contribution still dominates the theoretical uncertainty.

2.7.4 The Atomic Masses of $^{40}\text{Ca}^{17+}$ and $^{48}\text{Ca}^{17+}$

The experimental determination of the isotope difference between the bound-electron g -factors of $^{40}\text{Ca}^{17+}$ and $^{48}\text{Ca}^{17+}$ requires (1) two high-precision frequency ratio measurements of $\Gamma(^{40}\text{Ca}^{17+})$ and $\Gamma(^{48}\text{Ca}^{17+})$, see Eq. (2.13), which will be

Table 2.4 Theoretical contributions of the bound-electron g -factor difference of the lithiumlike calcium isotopes $^{40}\text{Ca}^{17+}$ and $^{48}\text{Ca}^{17+}$ [81]

Effects	Contributions to $\Delta g/10^{-9}$
Nuclear recoil: one-electron non-QED $\sim m_e/m_{\text{nucl}}$	12.246
Nuclear recoil: one-electron non-QED $\sim (m_e/m_{\text{nucl}})^2$	−0.006
Nuclear recoil: one-electron QED $\sim m_e/m_{\text{nucl}}$	0.123
Nuclear recoil: one-electron QED $\sim \alpha(m_e/m_{\text{nucl}})$	−0.009 (1)
Nuclear recoil: interelectronic-interaction	−2.051 (25)
Finite nuclear size	0.004 (10)
Total theory [$\Delta g = g(^{40}\text{Ca}^{17+}) - g(^{48}\text{Ca}^{17+})$]	10.305 (27)

Table 2.5 Theoretical contributions to the bound-electron g -factors of the lithiumlike calcium isotopes: $^{40}\text{Ca}^{17+}$ and $^{48}\text{Ca}^{17+}$ [38, 81]

Theoretical contributions	$^{40}\text{Ca}^{17+}$	$^{48}\text{Ca}^{17+}$
Dirac value (point nucleus)	1.996 426 010 90	
One-loop QED	0.002 325 555 (5)	
Two-loop QED	−0.000 003 520 (2)	
Interelectronic interaction	0.000 454 290 (9)	
Screened QED	−0.000 000 370 (7)	
Finite nuclear size	0.000 000 014 41 (2)	0.000 000 014 41 (2)
Nuclear recoil	0.000 000 061 85 (15)	0.000 000 051 54 (12)
Total theory	1.999 202 042 (13)	1.999 202 032 (13)

presented in Chap. 6. (2) Above that, high-precision values of the $^{40}\text{Ca}^{17+}$ and $^{48}\text{Ca}^{17+}$ masses are essential, see also Eq. (2.13), which will be summarized in the following.

The Mass of $^{48}\text{Ca}^{17+}$

In a recent measurement campaign the atomic mass of ^{48}Ca has been directly determined with the Penning trap mass spectrometer SHIPTRAP [87], measuring the cyclotron frequency ratio of singly charged $^{48}\text{Ca}^+$ ions and C_4^+ carbon clusters as a reference [81]:

$$R = \frac{\nu_c(^{48}\text{Ca}^+)}{\nu_c(\text{C}_4^+)} = \frac{m(\text{C}_4^+)}{m(^{48}\text{Ca}^+)} = 1.000\,990\,101\,75\,(39) \quad (0.39\text{ ppb}). \quad (2.19)$$

Both cyclotron frequencies are determined as the sum of the two trap radial-motion frequencies, see Eq. (3.12). For this purpose small clouds (≤ 5 ions) of $^{48}\text{Ca}^+$ and C_4^+ are alternately produced with a laser-ablation ion source [88]. They are separately transferred into a preparation Penning trap for cooling and centering via mass-selective buffer-gas cooling [89]. Afterwards, the particular cyclotron frequency is measured in the so-called measurement Penning trap, using the novel Phase-Imaging Ion-Cyclotron Resonance technique (PI-ICR) [90, 91].

The mass of a C_4^+ cluster is calculated, considering the dissociation energy $E_{\text{diss}} = 18.0(1.7)\text{ eV}$ [92], the ionization energy $E_{\text{ion}} = 11.0(7)\text{ eV}$ [93] and the missing electron: $m(\text{C}_4^+) = 4 \cdot 12\text{u} - 1 \cdot m_e - \Delta m(E_{\text{diss}}) + \Delta m(E_{\text{ion}}) = 47.999\,451\,412\,6\,(20)\text{ u}$. The mass differences between all three possible cluster structures - linear, rhombus and triangular pyramidal - are already covered by the uncertainties of the dissociation and ionization energies. For the determination of the mass of lithiumlike calcium $^{48}\text{Ca}^{17+}$ we have to correct the mass of singly charged calcium: $m(^{48}\text{Ca}^{1+}) = R/m(\text{C}_4^+)$ by the 16 missing electron masses and the corresponding binding energies:

$\Delta m(E_{\text{bind}}) = 7.2438(43) \cdot 10^{-6} \text{ u}$ [70].⁸ Here, the relative isotope dependence of the binding energy is smaller than $3 \cdot 10^{-12}$.⁹ Finally we extract the mass of $^{48}\text{Ca}^{17+}$ [81]:

$$m(^{48}\text{Ca}^{17+}) = m(^{48}\text{Ca}^{1+}) - 16 \cdot m_e + \Delta m(E_{\text{bind}}) = 47.943\,204\,044\,(19) \text{ u} \quad (0.4 \text{ ppb}). \quad (2.20)$$

The Mass of $^{40}\text{Ca}^{17+}$

The masses of $^{40}\text{Ca}^{17+}$ and $^{40}\text{Ca}^{19+}$ have been measured directly by Szilard Nagy and colleagues in 2006 at the SMILETRAP Penning trap mass spectrometer [95], using a time-of-flight technique and H_2^+ ions as a reference. The atomic mass of ^{40}Ca which has been published in the atomic mass evaluation (AME) 2012 [96] is based on these two measurements, corrected by the masses of the missing electrons and their binding energy. Here, calculated binding energies from [97] have been used: 6732.139 eV for the lithiumlike ion and 13017.129 eV for the hydrogenlike ion. Calculating backwards from the AME 2012 value, $m(^{40}\text{Ca}) = 39.962\,590\,864\,(22) \text{ u}$, we determine the mass of a lithiumlike ^{40}Ca ion:

$$m(^{40}\text{Ca}^{17+}) = 39.953\,272\,233\,(22) \text{ u} \quad (0.6 \text{ ppb}). \quad (2.21)$$

This value slightly deviates from the value published in [95], since the mass of hydrogen changed by $1.6 \cdot 10^{-9} \text{ u}$, comparing AME 2003 and AME 2012.

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⁸Binding energies from NIST table [70]: $E_{\text{bind}} = 18804(4) - 11756.4449(80) = 6747.5(4.0) \text{ eV}$ and $1 \text{ u} = 931494061(21) \text{ eV}/c^2$.

⁹In general the binding energies of different isotopes varies due to their different masses (mass shift) and their different charge distributions (field shift). For calcium the field shift dominates, which scales with Z^5 to Z^6 [77]. Since the binding energy of a 1s electron in uranium differs by 200 eV between a hypothetical point-charge distribution and the measured charge distribution [94], the field shift for 1s electrons in calcium isotopes should be smaller than $\Delta m/m = 200 \text{ eV}/92^5 \cdot 20^5/40 \text{ GeV} = 2.6 \cdot 10^{-12}$. For 2s electrons this effect is even smaller.

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