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Discrepancies in quantum electro-dynamics

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Abstract

Experimental tests of quantum electro-dynamics (QED) have developed dramatically for simple atomic systems such as hydrogen. However, a range of anomalies has been discovered recently. There has also been significant progress for medium-Z hydrogenic and helium-like atoms. In this area tests are often based on X-ray spectroscopic measurements. Future prospects for critical insight into the nature and convergence of QED in multi-electron systems will be discussed.

Keywords: Quantum electrodynamics; Helium-like atoms; Hydrogenic atoms

1. Introduction: background

There has been extensive and widespread interest in testing atomic physics in simple systems recently. Of course, this interest lay behind the discovery of the Lyman and Balmer series in hydrogen a hundred years ago, and was the origin of the early understanding of atomic structure and the Bohr model. Further, it was the anomaly in the Bohr predictions of the discrete energy levels in hydrogen which led to (relativistic) quantum mechanics and the Dirac equation for the electron in a bound atomic orbit; and it was the anomaly of the Lamb shift in the non-degeneracy of the 2s and 2p sub-shell energy levels, also in hydrogen, in the Lamb and Rutherford experiment, which led to the confirmation of quantum electro-dynamics (QED) as an applied quantum field theory of the interaction between light and charge.

QED is the first quantifiable result of second quantization. In first quantization, the Bohr model was able to interpret hydrogen Lyman and Balmer series spectra as transitions between quantized electron orbitals and the corresponding quantized energy levels of those atomic systems. With quantum mechanics in 1925–26, this was seen as conserved angular momenta and conserved energies for a particular stable eigenfunction, which corresponded to particular quantum numbers of the electronic wavefunctions. Within 2 years Dirac had redeveloped this to provide relativistic quantum mechanics for a spin-1/2 particle—the electron orbiting the nucleus of a hydrogenic system. However, the Lamb and Rutherford experiments of 1950–52 demonstrated that this understanding was not sufficient to explain the spectroscopic structure observed, even for hydrogen.

2. Zero-point energies

As Feynman observed, it is necessary also to consider the radiation field (and not just the electronic and nuclear orbits) as a quantized system, so that in any particular system there may be, e.g. one nucleus, one electron and, one or two photons (of a certain energy). This second quantization implied that even in the presence of zero real photons (i.e. even in a vacuum state) there would be a zero-point energy just like the energy $1/2(\hbar\omega)$ of a simple harmonic oscillator in the ground state. This vacuum state energy corresponded to a root-mean-square electric field, carried by (virtual) photons interacting for a time limited by the uncertainty principle. These fields cause oscillations in the isolated

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system given by the Dirac equation, and hence smear the charge distribution of the electron as it moves around the nucleus. This smearing can be imagined as a convolution of the original orbit with a symmetric Gaussian shift of the radius of any part of the electron wavefunction. For p states, which have zero amplitude at the nucleus, this broadening on a smooth potential of locally constant slope might be seen to give no average effect (the potential increases to higher radius, but decreases to lower radius, so for a symmetric broadening the shift of energy levels is zero to first order). However, for s states the finite amplitude of the electron wavefunction at the nucleus is caused to oscillate only to higher radius (in any direction), so that the energies of s states are raised by the electron self-energy arising from quantum electrodynamics. Hence the two states 2s and 2p, which were degenerate in Dirac theory, are non-degenerate in QED. Additional terms including vacuum polarization diagrams were seen to also contribute to the overall energies, transition rates, and gyromagnetic ratios of the bound electrons, and QED developed rapidly.

3. Difficulties of QED calculations

There are particular theoretical difficulties with any quantum field theory. Unlike the Dirac equation, QED has no finite closed form, even for the simplest bound state of a single hydrogen atom. Each system involves the calculation of energy shifts due to any number of virtual (quantized) photons of any energy—an infinite series of Feynman diagrams. This series in α/π is asymptotically divergent, and the calculation of sufficient orders to consider the limitation of this exceeds current computational power. For multi-electron atoms there is an additional series expansion in $1/Z$. Each Feynman diagram represents an infinite series of terms with higher orders of charge density $\rho \propto (Z\alpha)^3 \cdot$ It is not analytic for low Z. Even individual terms in this approach yield infinite results, and renormalisation and regularisation are required to yield a finite result in order to compare theory with experiment.

4. Experimental agreements in classic tests on hydrogen and helium

Despite these confronting mathematical difficulties, even within a couple of years of the development of QED (1953), the experimental and theoretical Lamb shifts for the hydrogen 2s–2p transition of a mere $0.0359\,\mathrm{cm}^{-1}$ were in agreement to four significant figures.

Work has continued to concentrate on hydrogen itself, where in recent work at the Max Planck Institute for Quantum Optics, Theodor Hänsch and colleagues have measured the ultraviolet transition frequency between the 1s and 2s states of atomic hydrogen to be $2.466\,061\,413\,187\,103\,(46) \times 10^{15}\,\mathrm{Hz}$—an accuracy of 15 significant figures (Niering et al., 2000)! This measurement proves QED as the best tested theory in nature (with general relativity), accurate to one part in 10^{14}. As the authors have stated, 'It's so accurate that simply repeating the measurement a year from now would provide a better and more direct verification (or falsification) of the constancy of the fine-structure constant over cosmological time than any astrophysical data we have.' Consequently, major goals have related to the possible temporal dependence of the fine structure constant and the speed of light, and the size of the proton radius.

The very success of this is a demonstration of the predictive power of physics. However, current issues in the investigation of hydrogen now lie in determinations of the proton form factor and polarisability, rather than the QED terms. In other words, further research in this area is now principally in fundamental or nuclear physics. Additionally, some may feel slight scepticism at the good agreement with hydrogen, in that QED was of course presented as a theory for hydrogen. It is fair to ask if QED provides valid predictions for the rest of the periodic table!

Recent work has also concentrated on helium, particularly as a test of electron correlation and QED. For neutral helium, tests have confirmed QED to a high degree (Drake, 2001), although the treatment of terms in a perturbative series expansion for both QED contributions and for the electron–electron correlation in this low-Z system is a difficult problem, and many references have discussed the difficulty of ordering terms to avoid double-counting of particular physical processes. The double-counting will always be wrong, but it has been an extremely difficult problem to isolate independent diagrammatic contributions.

For 1s–2s and 1s–2p transitions in helium, which primarily measure the 1s Lamb shift, the first major theoretical calculation by Drake (1988) was discordant by several significant figures from earlier experiment, but had a theoretical uncertainty implied at the 0.5% level, or some 40 times less than corresponding experiments. At the time, a view was widespread that experimental research was not competitive in this area; that the experimental errors were quite dominant; and that the theoretical understanding of these systems was complete. However, within 5 years (Drake et al., 1993; Forrey et al., 1995), further theoretical work had been completed which led to a large shift of theory with an increase in the theoretical error bar of a factor of 10. Further theoretical and experimental work has now converged to agreement within 1σ but with even larger quoted uncertainties (Drake and Martin, 1998; Bergeson et al., 1998; Drake and Goldman, 2000). However, the current comparison of the helium fine structure represents an as yet unexplained 15σ discrepancy (Drake, 2002). Hence the interplay between experiment and theory is a necessary driver and is able to allow the development of significant insight in both theoretical and experimental high-precision work.

For He^+, the situation is a little different, in that major discrepancies have now been observed (van Wijngaarden et al., 1991). A difficult and complex experiment in Canada showed discrepancies from theory of many standard deviations. The analogous experiment, applied to hydrogen (van Wijngaarden et al., 1998) showed no such discrepancy, and the conclusion was made that this might be due to residual magnetic fields near the experiment. A test reapplication of the results to He^+ appears to have confirmed this experimental limitation, and new results appear to confirm theory (van Wijngaarden et al., 2001). However, an independent confirmation of this result is called for.

The other classic test of QED lies in g-2 experiments. Dirac theory would predict the gyromagnetic ratio of the electron (from its spin = 1/2) to be exactly 2. Careful measurements (e.g. by Van Dyck et al. (1995) and Dehmelt (1990)) yielded $g_e = 2 \times (1 + 1.159652188(4) \times 10^{-3})$ instead. This was predicted by early QED theory to be due to the creation and annihilation of virtual photons in the photon field, even in a vacuum where the number of photons is zero and this process is dominated by the zero point energy corresponding to fluctuations in the electromagnetic field. The recent corresponding theoretical value for this is $g_e = 2 \times (1 + 1.159652133(29) \times 10^{-3})$ (Hughes and Kinoshita, 1999) or 11 significant figures of accuracy. This has been one of the most stringent tests of a regime of QED for low electric-field strengths. Additional and separate g-2 tests of bound QED have been developed recently with atomic traps, and further progress is expected in the next few years (Verdu et al., 2002).

High Z systems (particularly uranium) have been investigated to test QED, nuclear physics, and the region of high coupling coefficients $Z\alpha$ (Beyer et al., 1995; Stohlker et al., 2000) to 5%. Lithium-like systems have also probed QED terms, although the complexity of the excited three-electron system creates additional theoretical difficulty. Neutral atoms (Cs and Rb) have been used to test electro-weak theory and parity violation, while other neutral atoms have been investigated at synchrotrons and elsewhere for relativistic atomic theory and wavefunctions, but not for tests of QED. Exotic atomic systems including antihydrogen, positronium, muonium and muonic atoms have been of particular interest in testing QED in extreme regimes, in coupling near divergence (i.e. in regimes where $Z\alpha$ approaches 0 or 1), and in renormalisation. There has been strong continued interest in hydrogenic and helium-like atoms, with only one or two electrons, as tests of QED and electron correlation.

5. Current discrepancies

These successes underlie our current confidence in the predictive power of QED. However, several key discrepancies remain and question the limits of that confidence.

The highly accurate measurements of hydrogen and helium, mentioned above, are also in strong disagreement with current QED theory. The latest CODATA revision of the determination of physical constants (Mohr and Taylor, 1999, 2000) found an unresolved discrepancy in the determination of the Rydberg. When all (hydrogen, helium and proton/deuteron radius) data are refined simultaneously, normalised residuals are 1.5σ. Also, the normalised residuals show a systematic deviation between theory and experiment, corresponding to $126/n^3$ kHz for $nS_{1/2}$ states. Therefore, a second (recommended) refinement omitted the proton/deuteron radius data and allowed this to vary freely to give a fitted result. The result was a radius some 8σ discrepant from scattering measurements. The authors commented that the most likely sources for this difference are a deviation of the proton charge radius and/or the deuteron charge radius predicted by the spectroscopic data from the values deduced from scattering experiments, an uncalculated contribution to the energy levels from the two-photon QED correction that exceeds the estimated uncertainty for this term, or a combination of these.

In summary, this could be resolved by further investigations into the size and shape of the low-Z nuclei or by further theoretical investigation along current directions into higher order terms of QED. However, this may also suggest that the current perturbative expansion is showing some limitations, or that the renormalisation approach needs reinvestigation. Of course, it is also possible that the approach of QED has some particular flaws or limitations which experiment might be beginning to illuminate. It is worthwhile reflecting that whereas general relativity (also tested to a very high level) has an infinite manifold of well-constructed alternate theories to explain gravity, testable to greater or lesser degree, QED has virtually no rivals to explain the interaction of light with matter. The standard response of particle (and field theory) to an anomaly in the experimental data has been to consider an as-yet-unknown additional particle, which will modify the interaction and lead to an observable shift by perturbative expansions and computations. Of course, electro-weak theory is such a successful explanation. But grand unification appears to require something much more profound, with different symmetries and a different underlying principle. String or twistor theories, or the invocation of multiple collapsed dimensions, show some promises in these areas, but without any experimental verification to date.

However, there are a couple of testable alternative hypotheses. A proposal of 'positional indeterminacy', which is like invoking a quantisation of space, has shown some promise with regard to key experimental anomalies as discussed above (Ruzzene, 2000). At the current time, this proposal predicts the sign and magnitude of some discrepancies, but is contraindicated by the latest He^+ result. However, the theory also predicts discrepancies for medium-Z systems, which are within a factor of two of current experimental uncertainty. Hence new experimental results may confirm or disprove this model as currently constituted.

Another key discrepancy lies in the quoted theoretical accuracies. This exists both for hydrogenic computations and for helium-like computations. It is extremely difficult to gauge the accuracy of a theoretical work. Estimates of convergence and consistency necessarily omit key terms that might be dominant, or more dominant than previously considered. This is particularly the case in QED studies. For example, Drake et al. (1993) quotes uncertainties of 0.5% for QED, but there were up to 5% errors in the total QED component of energies (Plante et al., 1994). Later, a different computation (Persson et al., 1996) claimed a 5–10% uncertainty due to correlation effects for $Z<32$ for the same systems, and later a 2.5% discrepancy was found from the Persson result for $Z=32$ (Yerokhin et al., 1997).

Also, for hydrogenic systems, the pioneering work of Mohr (1985) and Johnson and Soff (1985) quoted 0.3 ppm uncertainties for medium-Z 1s–2p transitions. However, lowest order two-loop terms are of the order of percent in these systems, so this earlier uncertainty was unable to anticipate the higher magnitude of these additional theoretical corrections.

It should be stressed that all of this development is necessary and healthy, and has been a product of strenuous research by outstanding theorists. Some have claimed a more serious concern compared to this incremental improvement of theoretical understanding and the understanding of theoretical limitations to uncertainties. It has been seriously considered that a divergence in both the $Z\alpha$ and α/π expansions are possible in QED (Sapirstein, 1998; Karshenboim, 2000). It has been noted similarly that in many systems, higher order terms may yield corrections as large or larger than lower order terms (Jentschura, 2000).

Lowest-order QED terms scale as $(Z\alpha)^4 n^{-3}$, with higher order terms scaling to the sixth and higher powers. Such higher terms may only be a few percent of the lowest order terms; and yet these are the critical areas of current theoretical development, and also are the region where the convergence of all higher terms remains ill defined and may be probed by medium-Z experiments. Medium-Z measurements also probe higher-order (photon exchange) QED theory, in particular $\alpha^2(Z\alpha)^6$ and higher terms causing recent dilemmas. These expansions are not analytic at low or high Z (Karshenboim, 2000).

In consequence of all this, it is worthwhile noting that significant discrepancies currently exist in medium-Z tests of QED. Results from different experimental groups in the medium-Z region are inconsistent, and the problem of correlation in three-body systems is complex and unresolved. Further, theoretical predictions differ from one another by an amount approximately equal to the current experimental uncertainty.

Recently it has been observed that EBITs have led to a new opportunity in the possibility of testing 2-electron QED effects (Chantler et al., 2000). A significant realisation of recent years is that complementary endeavours are investigating different fundamental issues and making major contributions to different fields. Modest increases in experimental precision over current work—by a factor of three in an appropriate system—may demonstrate the limitations of current theoretical approaches and may suggest a more sound theoretical approach to QED.

There has been excellent work developing laser resonance experiments at accelerators, and recently at EBITs (Lea et al., 1994; von Brentano et al., 1993; Myers et al., 1995; Klein et al., 2001). Part of this area has been reviewed recently (Myers, 2001). Significant unexplained anomalies between theory and experiment remain in this field, and it is an area of active interest. The origin of these discrepancies is not yet clear. Other tests in this regime have pursued lifetime or quench studies which may be based on laser–optical or X-ray transitions (Serpa et al., 1998), or on radiative recombination and radiative electron capture (Stolker et al., 1997, 1999), and related processes involving X-ray or visible emission from continuum states. The remainder of this review will concentrate on X-ray spectroscopic transitions between discrete levels, where narrow natural widths permit high-resolution measurements.

6. Medium-Z, helium-like anomaly

In the medium-Z regime for helium-like ions a series of experiments has yielded an apparent anomaly with respect to theory, as shown in Fig. 1. The particular experiments of Beiersdorfer et al. (1989a, b) led to a claim that theory was in error by 3σ, based on a series of 2 standard deviations of experiment from theory. The conclusion is neither clearly supported nor clearly refuted by other work. If theory is in error, then the

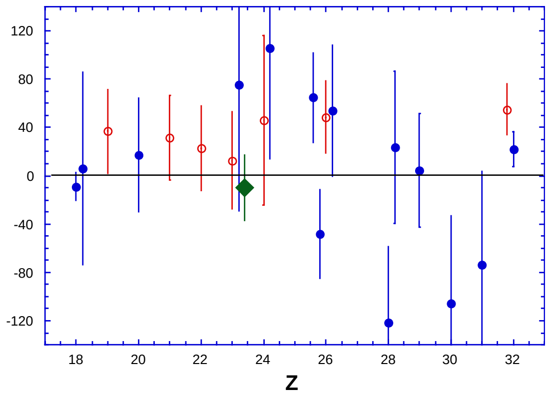

Fig. 1. Helium-like QED theory for the dominant w line (1s–2p $^1P_1$–$1s^2$) (Drake, 1988), atomic number $Z = 15-40$ (straight line) versus PLT tokamak measurements and EBIT measurements by Beiersdorfer et al. (1989, open circles) compared to other experimental results (filled circles). Solid diamond is Chantler et al. (2000) where other references are also provided.

Z-dependence of this error is of major concern to theoreticians around the world. If certain experimental systematics are responsible, a series of critical experiments should identify key systematics.

7. EBIT experiments

The major QED measurements to date use accelerator-based beam-foil spectroscopy or plasma-based spectroscopy. Excellent measurements are usually limited by Doppler shift uncertainties from fast beams. Electron beam ion traps (EBITs) avoid this limitation, by trapping the ions in a weak radial and longitudinal trap. Negligible thermal motions occur. Limiting experimental precision comes from other, controllable, contributions, namely statistics and the calibration of the dispersion function of the spectrometer and detector systems used. EBIT physics also addresses processes of interest in astrophysical theory, plasma diagnostics, and laser research.

There are two techniques which have been applied to high-precision research in QED using EBIT sources (Hölzer et al., 1998; Paterson et al., 1997; Chantler et al., 1999). The use of curved crystals (Johann geometry) dramatically increases the statistics, and also makes the experiment insensitive to positional misalignment of 5–500 μm (major limitations of other techniques). We have recently designed and constructed a prototype two-dimensional backgammon detector (based on NIST and Japanese precursors) promising high performance compared with earlier work.

8. Excited-state QED

The results for helium-like vanadium are sensitive to the QED contributions of the 2s state as well as the ground (1s) level. This sensitivity, at the 40% level, is of course exceeded by experiments which directly measure the excited level (e.g. 2s–2p) transitions. However, it is interesting that direct measurements of the ground state Lamb shift are now also sensitive to the contributions of QED to these higher levels. This level of accuracy implies that higher-state QED should not be assumed in such investigations or such analysis, but should also be directly investigated.

9. Two-electron QED

Two-electron QED is the QED contribution due to two-electron Feynman diagrams, but also due to the difference between one-electron diagrams in the different (one versus two electrons) potential. Different theoretical approaches yield quite different estimates of this QED contribution. Hence these experiments will isolate one of the most difficult questions regarding QED theoretical implementation to atomic systems. Currently only three medium-Z measurements have a claim to be sensitive to two-electron QED for the 1s Lamb shift in medium-Z atoms. Our work on vanadium is one of these three, and the other two, for quite different Z, are sensitive at the 50% level but have neglected certain systematic contributions at this level in their analyses (curved crystal dynamical diffraction shifts, crystal defects, absolute calibration, theoretical uncertainty) (Deslattes et al., 1984; Maclaren et al., 1992). This investigation is beginning, and should bear fruit in the next few years.

10. Second-order QED

A key interest is in the sensitivity of these new measurements to second-order QED. Within a helium-like system, the definition of the relevant sum is not so well defined due to correlation terms of a similar order; but a good guideline is given by the corresponding result for hydrogenic systems. On this basis, several medium-Z measurements are indeed sensitive to second-order QED now.

11. Discrepancies between different theoretical predictions

A clear statement of the critical level for testing theory lies in the discrepancy between current theoretical predictions across the central range of atomic number.

Different theories predict differing levels of agreement with experimental data for helium-like transitions in the medium-Z regime (Vainshtein and Safranova, 1985; Indelicato, 1988; Drake, 1988; Plante et al., 1994; Cheng et al., 1994; Yerokhin et al., 1997). For $Z = 26$, theory differs by 30 ppm from one another, and this level is consistent across the range of medium-Z. The problem of isolating contributions from different correlation diagrams in these few-electron systems has been part of this discrepancy. The variation between theories is about 1–2 standard deviations of experimental results. For example, the experiment on vanadium has yielded results for vanadium with an accuracy of 27 ppm or 5.7% of the Lamb shift. Hence, significantly reducing the current experimental error budget, by relatively small factors of two or three, will lead to further critical investigations of theoretical approaches. We can look forward to this prospect in the near future.

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