Self-energy screening approximations in multi-electron atoms

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HIGHLIGHTS

► We develop a self-energy screening approximation suitable for multi-electron atoms.
► This approximation is tested in a number of few- and many-electron systems.
► We obtain superior agreement with experiment compared with existing approximations.
► An implementation of this approximation is provided for use with GRASP2K.

ARTICLE INFO

ABSTRACT

Atomic structure calculations have reached levels of accuracy which require evaluation of many-electron QED contributions. Since exact analytic solutions do not exist, a number of heuristics have been used to approximate the screening of additional electrons. Herein we present an implementation for the widely used GRASP atomic-structure code based on Welton's concept of the electron self-energy. We show that this implementation provides far superior agreement compared with a range of other theoretical predictions, and that the discrepancy between the present implementation and that previously used is of comparable magnitude to other sources of error in high-accuracy atomic calculations. This improvement is essential for ongoing studies of complex atomic systems.

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1. Quantum electrodynamics and self-energy

Both classically and in quantum field theory, the electromagnetic field of the electron can interact with the electron itself. In both cases, this interaction results in an infinite energy associated with the electron (Sakurai, 1967). In quantum field theory, this interaction corresponds to an electron emitting a virtual photon, which is then reabsorbed by the electron – the Feynman diagram for this interaction is presented in Fig. 1. The energy associated with the interaction between the electron and its own electromagnetic field is the self-energy of the electron.

This self-energy results in observable effects. Most famously it is responsible for the Lamb shift (Lamb and Retherford, 1947; Bethe, 1947). In order to obtain a finite numerical result, the infinite portion of the integral is required to be removed by the process of renormalisation, which can also include a finite energy cut-off. Since the classical electromagnetic self-energy is thereby removed or renormalised, this energy shift is a purely quantum-mechanical phenomenon. It arises due to the interaction of the

electron with the quantised electromagnetic field. In quantum field theory, these quantum fluctuations of the electromagnetic field strength are also responsible for spontaneous emission.

Early self-energy corrections were carried out to first-order in $Z\alpha$ (Bethe, 1947). In the early 1970s, Mohr provided an atomic self-energy formulation within the bound-state Furry formalism in a suitable form for direct numerical evaluation, used to evaluate the self-energy for ground-state hydrogenic atoms (Mohr, 1974). Later work extended this to include $n=2$ hydrogenic systems (Mohr, 1983) and more recent studies have evaluated hydrogenic self-energies for $n=3$, 4, 5 (Mohr and Kim, 1992; Indelicato et al., 1998; Le Bigot et al., 2001). There have been no generalisations of the self-energy calculations to arbitrary N-electron atomic systems.

Without exact solutions, atomic structure packages use an approximation to the self-energy. This can be obtained by taking the exact hydrogenic results of Mohr and successors and reducing them by some screening factor to allow for multiple electron interactions. These factors aim to represent some scaling from the hydrogenic system to the system of interest, yet their form is of a wide variety. From Mohr (1974) we have that $E_{SE}^H = (\alpha/\pi)(Z\alpha)^4 F(Z\alpha)m_e c^2$. Approaches used to derive a multielectron self-energy include using the mean radius to determine an effective Z for that

Fig. 1. Feynman diagram for the first-order QED contribution to the electron self-energy.

Fig. 2. Feynman diagrams for the self-energy screening correction in two-electron systems.

wavefunction (Dyall et al., 1989; Parpia et al., 1996), scaling Mohr's hydrogenic results by the ratio of the wavefunction amplitude at the origin to that of a hydrogenic wavefunction at the origin (Kim et al., 1991), by the projection of the wavefunction onto a hydrogenic wavefunction (in source code Jonsson et al., 2007), by the *weighted* projection of the wavefunction onto a hydrogenic wavefunction (Jonsson et al., 2007), or some other similarly calculated ratio.

The GRASP packages (Grant et al., 1980; Dyall et al., 1989; Parpia et al., 1996; Jonsson et al., 2007) are amongst the most widely used atomic structure programs with several thousand citations for the various versions. However, even the most recent versions of GRASP make use of outdated self-energy values and screening factors (Indelicato et al., 2007; Blundell, 1993b). Recent theoretical evaluation of photoionisation in complex systems is reaching sub-eV accuracy with the GRASP2K package (Lowe et al., 2010, 2011; Chantler et al., 2010, 2012), and therefore improvement of these QED approximations is necessary.

The next most significant quantum-field-theoretical effect on atomic energy levels is vacuum polarisation. The vacuum polarisation can be computed to second-order from the expectation value of the Uehling potential (Uehling, 1935; Wichmann and Kroll, 1956), and to fourth-order from the expectation value of the Källén-Sabry (Källén and Sabry, 1955) potential. In GRASP2K both of these contributions are evaluated using the methods outlined in Fullerton and Rinker (1976). The use of computed wavefunctions to evaluate these expectation values means that the dominant contributions of electron screening are automatically included.

In the Welton concept for the electron self-energy, the interaction of the electron with the electromagnetic field does not cause any real energy changes. Rather, the interaction perturbs the motion of the electron, causing it to explore a larger region of space than it would otherwise (Welton, 1948). In the case of an atomically bound electron, this reduces the overlap between the electron and the nucleus, and it is this change of potential and screening which causes the energy shift of the electron (Fig. 2).

Due to fluctuations in the electromagnetic field, Welton (1948) showed that a free electron will experience oscillations in position, with a mean-square radius of

$$\langle (\Delta \mathbf{x})^2 \rangle = \frac{2}{\pi} \frac{e^2}{\hbar c} \left(\frac{\hbar}{mc} \right)^2 \int_{k_0}^{k} \frac{dk}{k}. \tag{1}$$

This integral diverges at both the upper and lower limit. The upper limit is truncated at $k = mc/\hbar$ and the divergence at the lower limit disappears for an electron in any sort of potential. Following the concept of Welton (1948), we consider an electron moving in a potential $V(\mathbf{x})$. Denoting the part of the electron motion due to fluctuations in the electric field as $\Delta \mathbf{x}$, the instantaneous potential energy can be written as

$$V(\mathbf{x} + \Delta \mathbf{x}) = (1 + (\Delta \mathbf{x} \cdot \nabla) + \tfrac{1}{2}(\Delta \mathbf{x} \cdot \nabla)^2 + \cdots) V(\mathbf{x}). \tag{2}$$

The average potential energy is then

$$\langle V(\mathbf{x} + \Delta \mathbf{x}) \rangle = (1 + \tfrac{1}{6} \langle (\Delta \mathbf{x})^2 \rangle \nabla^2 + \cdots) V(\mathbf{x}), \tag{3}$$

and the contribution to the potential energy due to the electron's perturbed motion is proportional to $\nabla^2 V(\mathbf{x})$. This suggests

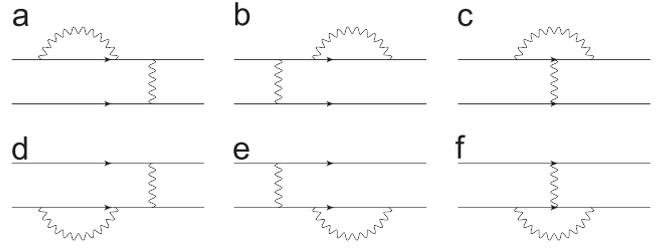implementing a screening factor

$$E_{SE} = \frac{\langle \phi | \nabla^2 V(\mathbf{x}) | \phi \rangle}{\langle \phi^H | \nabla^2 V(\mathbf{x}) | \phi^H \rangle} E_{SE}^H. \tag{4}$$

Approximations based on this approach have been implemented in some codes (Indelicato et al., 2007; Indelicato and Desclaux, 1990; Kim et al., 1991; Indelicato et al., 1987; Blundell, 1993a). Indelicato and Desclaux (1990) and Kim et al. (1991) replace Eq. (4) with a screening based on the two-electron correction to the self-energy for states with $|\kappa| \geq 2$,

$$E_{SE} = \frac{\langle \phi | \beta \boldsymbol{\alpha} \cdot \boldsymbol{E} | \phi \rangle}{\langle \phi^H | \beta \boldsymbol{\alpha} \cdot \boldsymbol{E} | \phi^H \rangle} E_{SE}^H, \tag{5}$$

where $\boldsymbol{\alpha}$ are the Dirac matrices.

Eq. (4) is zero when we are considering a wavefunction with $|\kappa| \geq 2$ around an infinitely dense nucleus, resulting in no screening. We propose the use of finite nuclei in our calculations, so have kept the first order term (Eq. (4)) consistently throughout our implementation instead of using Eq. (5) as previous authors have.

We have found excellent agreement using Eq. (4) with the perturbation theory calculations of Indelicato and Mohr (2001) and the all-orders calculations of Artemyev et al. (2005), and have therefore retained it for all wavefunctions. Blundell (1993a) uses a screening implementation including only the leading term, however Blundell only investigated a small number of test cases to compare phenomenological methods with more rigorous ones.

In the present work, we provide our proposed implementation of Eq. (4) for the GRASP2K software package. We demonstrate that this implementation provides better agreement with available theoretical two- and three-electron screening calculations than any of the other approximations used in the literature, and we demonstrate that it is competent to address many-electron systems with physically plausible behaviour.

2. The Thomas-Fermi nuclear potential

The Fermi model for the nuclear charge distribution is useful for finite-difference methods because all derivatives are finite and continuous. The model is defined as

$$\rho(r) = \frac{\rho_0}{1 + e^{(r-c)/a}} \tag{6}$$

where a and c are constants relating to the nuclear size and skin thickness. By Poisson's equation

$$\nabla^2 V(r) = \frac{\rho_0}{\epsilon_0 (1 + e^{(r-c)/a})} \tag{7}$$

which allows convenient numeric determination of $\nabla^2 V(r)$ for use in computation which we have implemented in GRASP2K.

We also considered contributions to $V(r)$ from the mean electron distribution, since $\nabla^2 V(r)$ is proportional to the charge

density. We found that this did not alter the self-energy screening when smoothed over a range of atomic numbers, but did introduce a great deal of non-physical noise associated with the finite grid on which it was calculated. For this reason we have implemented the more robust analytic approach.

3. Implementation

The reference hydrogenic values used in GRASP2K's self-energy calculations are those from Mohr (1983). This work calculated self energy values for electrons in hydrogenic systems with $n=1$, or 2 and $10 \leq Z \leq 40$. Since then, Mohr and others have performed new high accuracy calculations that have extended this range significantly.

Mohr and Kim (1992) use improved numerical techniques to extend hydrogenic calculations to states with principal quantum number $n=3$, 4, and 5 and $1/2 \leq j \leq 3/2$ and for nuclear charge $10 \leq Z \leq 110$. Le Bigot et al. (2001) use high-accuracy computational methods to calculate the low-energy part of the self energy. This allowed extension of self energy calculations of Mohr (1983) to include electrons with $n=3$, 4, or 5 and angular momentum $5/2 \leq j \leq 9/2$ for hydrogenic computations.

Mohr and Soff (1993) also performed complete self-energy calculations for a number of hydrogenic states using finite nuclear charge distributions. These were in the range $26 \leq Z \leq 100$ and for the states $1S_{1/2}, 2S_{1/2}$, and $2P_{1/2}$. Beier et al. (1998) extended this work and determined finite nuclear size corrections for all hydrogenic atomic systems in the range $26 \leq Z \leq 110$. These results form the basis of the finite nuclear size corrections included in our modified GRASP2K. However, we also desired that the nuclear size corrections reflect the nuclear conditions chosen by the user which are not necessarily the same RMS charge radii used by Beier et al. (1998). Mohr and Soff (1993) derived an empirical relation between the self-energy correction and nuclear radius, however the coefficients for this functional form were only given for three elements. We have extrapolated these coefficients logarithmically across the range $1 \leq Z \leq 110$ for inclusion in GRASP2K. Logarithmic extrapolation provided the best consistency with the values determined by Mohr. Results are presented in Fig. 3.

Finally, results of Le Bigot et al. (2001) were extrapolated linearly from the lowest value originally calculated ($Z=60$) to $Z=1$. The accuracy of this extrapolation is likely to suffer, but at low Z the contribution from these high-energy angular

momentum is tiny so even a poor approximation is better than the previously used method to treat the electron as if it had lower angular momentum. Hence this is now implemented.

Yerokhin and Shabaev (1999) and Sapirstein and Cheng (2006) have also computed one-loop self-energy contributions to hydrogen-like atoms. Their results are consistent with those of Mohr and collaborators to within 1%. In most cases the discrepancy is much smaller than 1%. The use of these values instead of Mohr's would not significantly alter our results or conclusions. We use the references listed as they represent the most complete collection of values available, as presented in Fig. 3.

4. Results

Direct experimental QED measurements in multi-electron systems are difficult to make. Furthermore, there are no entirely analytic determinations of the QED energy in arbitrary multi-electron systems. Instead we compare our numerical results with the available theoretical results, which have been determined using a number of high accuracy techniques.

Dominant screening naturally occurs where the self-energy terms themselves are largest, namely for ground state terms including $1s^2$ configurations, as presented in Fig. 4. In the helium-like system, advanced theoretical computations have generated detailed predictions, and alternate heuristics or Welton approaches can be directly compared to these.

Yerokhin and Shabaev (1995) and Yerokhin et al. (1997) have used partial-wave techniques to derive results for a number of helium-like and lithium-like systems. Artemyev et al. (2005) extended their work to include all orders of contribution in $Z\alpha$, and claim a high degree of accuracy in the high-Z region. Indelicato and Mohr (2001) use a different approach, applying perturbation theory to determine self-energy screening contributions for a wide range of nuclear charge and electron quantum number. For the systems considered here, Indelicato and Mohr (2001) results generally indicate slightly less screening than Artemyev et al. (2005), but both follow similar trends.

Four different approximation methods have been used, and comparison is made to whichever theoretical results are available for the system in question. The GRASP2K package, as it exists on the Computer Physics Communications library, approximates the screening coefficient by taking the overlap integral of the wavefunction and a hydrogenic wavefunction in the region $r \leq 0.0219 a_0$. We
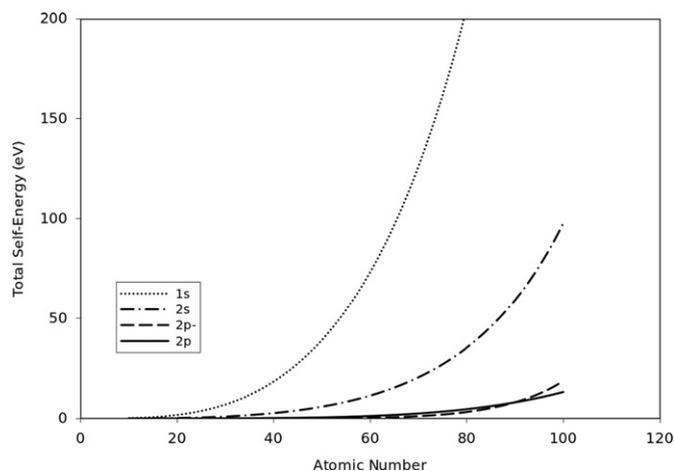
Fig. 3. Total self-energy for electrons in hydrogenic orbitals, using Mohr (1983), Mohr and Kim (1992), Mohr and Soff (1993), Beier et al. (1998), and Le Bigot et al. (2001) with extrapolation methods described in text.
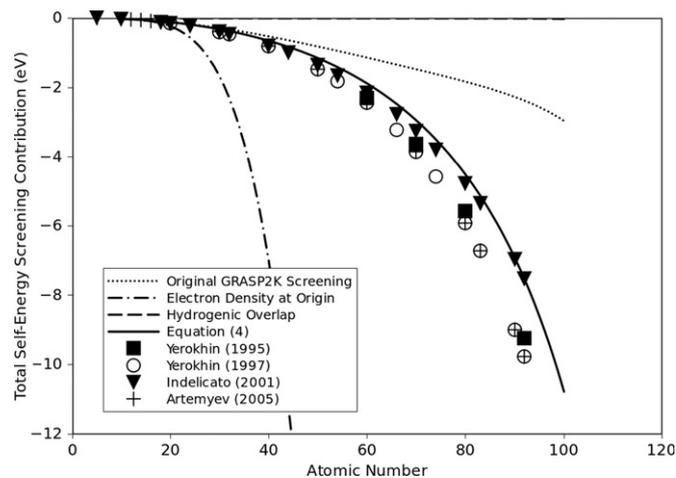
Fig. 4. Screening contributions to helium-like ground state self-energy $1s^2$ $^1S_0$. Comparison of past screening heuristics with the new approach (lines) and with high-accuracy theoretical calculations (symbols) gives a strong indication of the improvement obtained.

have included this approximation in our results, labelled 'Original GRASP2K Screening'. An alternative method used previously is the total overlap integral of the actual wavefunction with a hydrogenic wavefunction. We have re-considered this approximation method and it is labelled 'Hydrogenic Overlap' in our results (however, this gives a largely null or hydrogenic screening independent of Z).

For the sake of completeness we have included a method based on the ratio of the electronic wavefunctions at $r=0$. The rationale behind this method is the identification of the electron-self energy as arising from the nuclear Laplacian, which is non-zero only at $r=0$ for a point nucleus. This method provides poor results for finite-nuclear charge distributions. Finally, we include the new approximations based on the Welton interpretation. This method is derived in detail in Section 2. These alternatives are then compared to the results of Yerokhin and Shabaev (1995), Yerokhin et al. (1997), Artemyev et al. (2005), Indelicato and Mohr (2001), and Persson et al. (1993).

In this most significant case, the new implementation is far superior to other implementations following Welton's concept, and indeed is in very close agreement with that of Indelicato and Mohr (2001). Arguably the advanced methods of Artemyev et al. (2005) are currently the most accurate available, and there is a significant but relatively small discrepancy of our implementation from these.

For configurations of $1s2p$, the dominant screening arises from the $1s$ electron which is however relatively weakly screened by the $2p$ electron Figs. 5 and 6. In both cases, the new implementation agrees well with advanced methods.

The screening contribution to the $2p_{3/2}-2p_{1/2}$ fine structure energy separation is a useful test of this implementation, and is presented in Fig. 7. Here the new implementation clearly reflects the structure and functional relationship of the self-energy screening and is accurate to better than 1 eV for all Z.

It is clear from Figs. 4–8 that Eq. (4) reproduces the accurate theoretical results much better than any of the other three approximations. In the case of the hydrogenic systems, the original GRASP2K provides reasonable results, and produces results that track the changes in screening quite well, however Eq. (4) produces numerically superior results in all cases.

To probe the many-electron system, we provide a few illustrative comparisons. In the case of the lithium Lamb shift, Eq. (4) is the only method that produces valid results. All three other methods fail to match the functional form of the isoelectronic
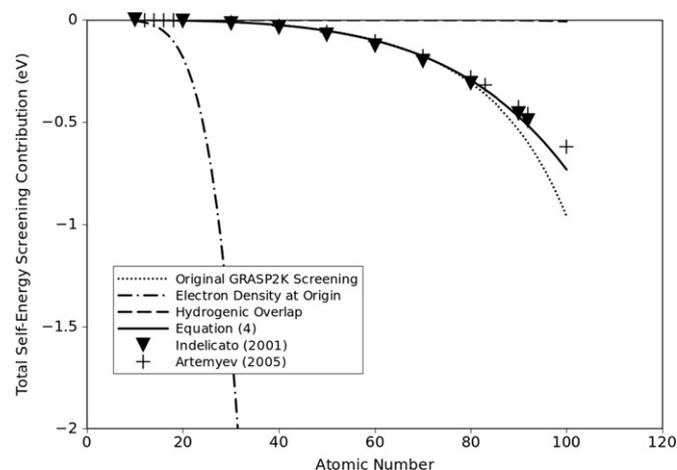

Fig. 6. Self-energy screening contributions to the $1s2p_{1/2}^1 J = 1$ isoelectronic sequence. Comparison of the existing screening method available in GRASP2K with new approximations (lines) and high-accuracy theoretical results (symbols). Similarly to Fig. 5, Eq. (4) and the original GRASP2K approximation diverge at high-Z. Interestingly, they diverge in opposite directions. Eq. (4) provides better comparison to theory in both cases.

Fig. 7. Self-energy screening contributions to the $1s^1 2p_{1/2}^1 J = 1 \rightarrow 1 s^1 2p_{3/2}^1 J = 1$ fine structure energy separation. Both the original approximation and Eq. (4) capture the functional form of the screening contribution. However, only Eq. (4) provides reasonable agreement with advanced theoretical predictions.

Fig. 5. Self-energy screening contributions to the helium-like $1s2p_{3/2} J = 1$ isoelectronic sequence. Comparison of the existing screening method available in GRASP2K with new approximations (lines) and high-accuracy theoretical results (symbols). Eq. (4) produces similar results to the original screening method at low Z, but at high Z diverges and shows better agreement with advanced theory.
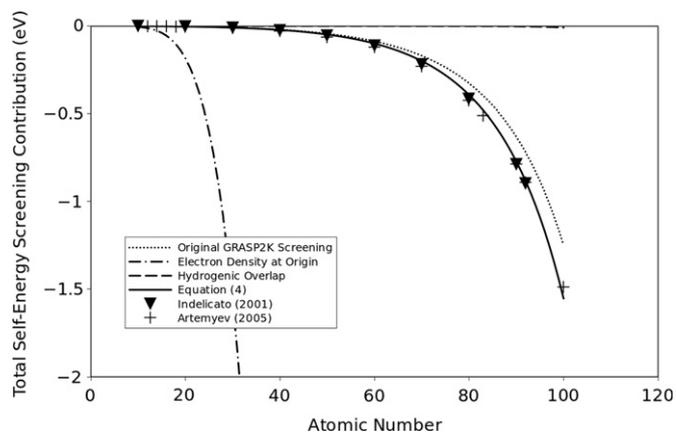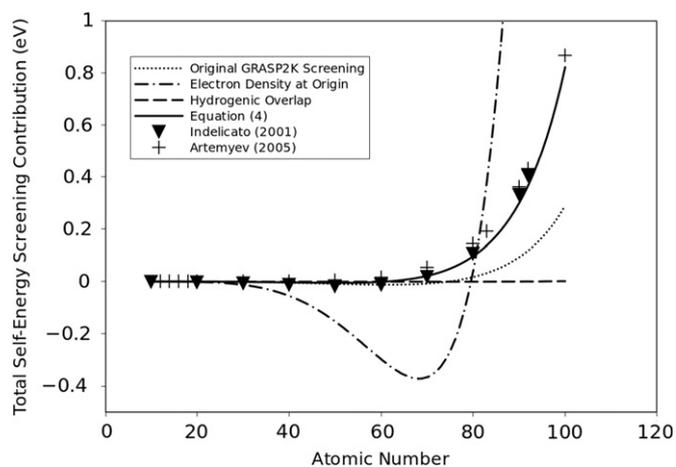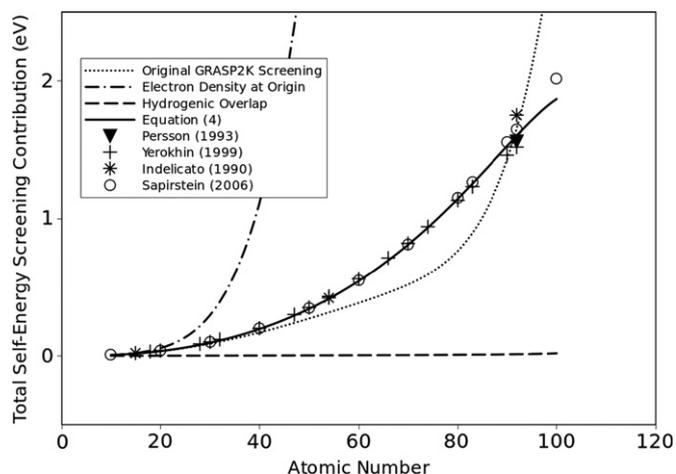

Fig. 8. Self-energy screening contributions to the Lamb-shift in the lithium-like isoelectronic sequence. In this more complex atom, the other available approximations do not even capture the form of the sequence. Our approximations agree well with the high-accuracy theoretical work of both Persson and Yerokhin.

sequence. We have also plotted the three-electron screening calculated by Indelicato and Desclaux (1990). Our results are very similar for Z=15 and Z=54 but are 0.15 eV lower for high-Z Li-like uranium, which places them in better agreement with Persson et al. (1993) and Yerokhin and Shabaev (1995).

This method can be applied to arbitrary N-electron systems, and in Fig. 9 we present screening contributions to the ground state of the neon-like isoelectronic sequence. Here we have no obvious detailed prediction with which to compare, yet it is reasonable to have some confidence in the prediction compared to earlier methods.

A comparison of our results to the results of Sapirstein and Cheng (2006) in copper-like atoms is presented in Fig. 10. Here we are comparing a relatively small value, and therefore present the relevant functional $F(Z\alpha)$ for this valence electron. Sapirstein and Cheng (2006) calculate the self-energy of the 4s electron in copper using a screened Kohn-Sham potential. This comparison is useful as it tests the screening approximation in a many-electron atom where screening effects are comparable in magnitude to the unscreened self energy. Both the original GRASP2K screening method and that based on Eq. (4) show excellent agreement with Sapirstein and Cheng (2006), with a maximum discrepency of < 0.05eV for either method.
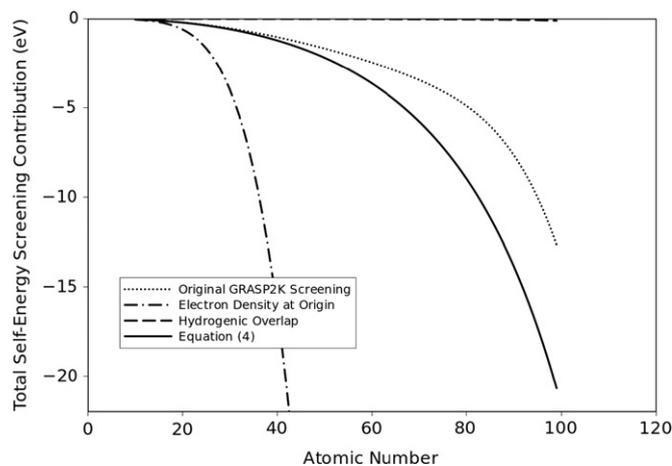

Fig. 9. Self-energy screening contribution to the Ne-like ground state isoelectronic sequence. The absolute discrepency between the screening approximations increases with both the number of electrons in the system and nuclear charge.
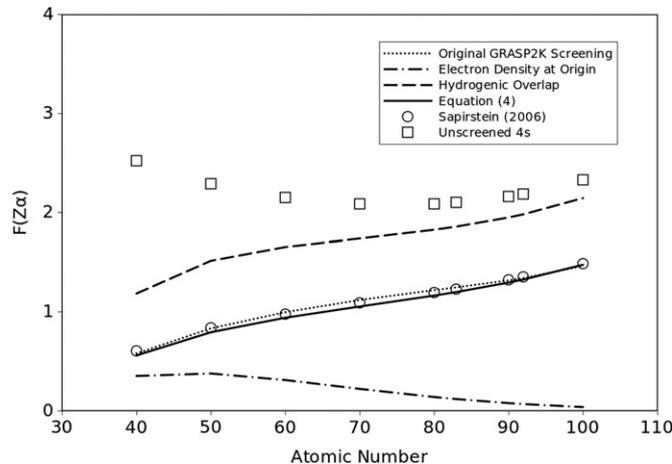

Fig. 10. $F(Z\alpha)$ for the 4s electron in copper-like ions. The results of the screening methods described in text are compared to the work of Sapirstein and Cheng (2006), and to the unscreened values.

For medium-Z, neutral or near-neutral systems the self-energy screening is essential to high-accuracy calculations. The contribution to the $K\alpha$ spectrum in the 3d transition metals is of order 0.1–1 eV, and the differences between the screening methods are smaller than, but of comparable magnitude to, the primary uncertainty in these calculations which arises due to convergence issues.

5. Conclusion

High accuracy atomic structure calculations are necessary in a wide range of fields. Previously, inaccuracies in atomic structure calculations were primarily due to errors introduced through the central field approximation and poor wavefunction convergence. These calculations are now at the stage where computational inaccuracies are of a similar magnitude to inaccuracies in quantum-electrodynamic approximations. In order to calculate accurate atomic data these approximations must be improved.

We have presented here a modification to the widely used GRASP2K atomic structure package which improves the determination of the leading-order QED contribution to multi-electron systems. As well as updating the program to use the latest available hydrogenic values and modifying it to account for finite-nuclear-size effects, we have also implemented a self-energy screening approximation based on the Welton interpretation of the self-energy. These have been compared to available theoretical values for selected 2-, 3- and many-electron systems and we have found that the new approximations are in much better agreement with advanced dedicated approaches. The new version of the software is available for download at supplementary material with this manuscript, on-line; or is available on the author's homepage at http://www.ph.unimelb.edu.au/~chantler/.

Appendix A. GRASP2K implementation

The modified version of the GRASP2K, "rci2" package now uses Eq. (4) to calculate the electron self-energy screening by default, and also presents the user with additional non-default options. The user is able to select a screening approximation from the following options:

$$E_{SE}^1 = E_{SE}^H \tag{A.1}$$

$$E_{SE}^2 = \frac{\langle \phi | \nabla^2 V(\mathbf{x}) | \phi \rangle}{\langle \phi^H | \nabla^2 V(\mathbf{x}) | \phi^H \rangle} E_{SE}^H. \tag{A.2}$$

$$E_{SE}^3 = \frac{\langle \psi_{r<0.0219} | \psi_{r<0.0219} \rangle}{\langle \psi_{r<0.0219}^H | \psi_{r<0.0219}^H \rangle} E_{SE}^H \tag{A.3}$$

$$E_{SE}^4 = \frac{\psi(r=0)}{\psi^H(r=0)} E_{SE}^H \tag{A.4}$$

$$E_{SE}^5 = \langle \psi^H | \psi \rangle E_{SE}^H \tag{A.5}$$

E_{SE}^2 is the method described in this paper. E_{SE}^3 uses the ratio of the actual wavefunction density in a small region around the nucleus to the equivalent density for a hydrogenic orbital as a screening parameter, E_{SE}^4 uses the ratio of the actual wavefunction density at $r=0$ to the ratio of a hydrogenic wavefunction at $r=0$, and E_{SE}^5 uses a monopole projection of the actual wavefunction onto a hydrogenic wavefunction.

The "rci2" package now presents an additional prompt is asking the user to select a radial wavefunction file containing hydrogenic wavefiles. This file must be in a GRASP2K unformatted file (GRASP2K contains tools for converting file formats if

necessary). If the user does not wish to provide this then one of the non-default options can be chosen.

As the modifications have been written to the Fortran77 standard there should be no additional compilation complexities. There is also an option for a full debugging output. This will write subshell-specific screening coefficients, effective $F(Z\alpha)$ values, and finite nuclear-size contributions to a 'screening.sum' file. The changes are provided as a .patch file. In order to install, the GRASP2K package can be downloaded from the CPC software library. The .patch file should then be copied into the GRASP2K root directory and the command 'patch $-p1 <$ slfenrgy.patch' will install it. GRASP2K can then be compiled as usual.

Appendix B. Supplementary data

Supplementary data associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.radphyschem.2013.01.004.

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