Comparison Between Experiment and Theory in Heavy Electronic Systems

B. Fricke

Fachbereich Physik, Gesamthochschule Kassel, D-3500 Kassel,
W. Germany

Introduction

Most talks in this symposium dealt with electronic and muonic
systems with small or medium Z and one or two electrons or one
muon, respectively. The quantum-electrodynamical effects in
these systems are relatively small, but due to the very accurate
measurements one is able to study them up to very high orders.
On the other hand, the talk of Dr. Rafelski dealt with extreme
electronic systems with Z around 170, where the QED effects are
expected to be relatively big, but also relatively inaccurate
from a computational point of view. Although these are systems
with very many electrons, they have been treated there as one-
electron systems, first, because most electrons are outer
electrons, and thus do not play any important role and second,
because the influence of the few other inner electrons does not
change the predictions qualitatively, which are mainly connected
with the question of the diving of the 1s level into the negative
continuum. I would like to discuss here the area between these
two extremes. These are systems

    a) with large and very large Z, where
    b) the many-body effects become important, and
    c) the observable effects are neither small nor big.

This area is the region of the binding energies of the innermost
electrons of very heavy atoms (Z > 80).

The experimental data in this region result either from photo-
electron spectroscopy[1] with an accuracy of the order of eV at
binding energies of about 100 keV or from the observation of
normal X-rays with an accuracy which is already below 1 eV [2].

The main assumption in every theoretical discussion of a many-electron system is an extremely good knowledge of the self-consistent field solution of the many-body Dirac equation. These calculations, which have to be accurate relativistic Dirac-Fock calculations with no Slater approximation, have been performed by a number of groups[3]. This Dirac-Fock value results to about 99 % of the binding energy of the innermost electrons in heavy systems. The remaining 1 % of the observable effect arises from the QED corrections vacuum polarization and vacuum fluctuation as well as the part of the electron-electron interaction, which is not taken into account in the Dirac-Fock calculation, which is the magnetic interaction between the electrons and retardation. In addition to these four effects one has to take into account the influence of the extended nucleus with a realistic nuclear charge distribution directly in the Dirac-Fock calculations.

Magnetic interaction and retardation

According to the proposal of Gaunt[4] the unretarded interaction between two Dirac currents given by the Dirac matrices $\vec{\alpha}$ can be written like

$$H_G = - \frac{e^2}{r_{12}} \, \vec{\alpha}_1 \cdot \vec{\alpha}_2 \quad . \tag{1}$$

Breit[5] proposed the quantum mechanical analogon to Darwin's retarded Hamilton function, which now usually is called the Breit operator

$$H_{Br} = -\frac{e^2}{2r_{12}} \, (\vec{\alpha}_1 \cdot \vec{\alpha}_2 + (\vec{\alpha}_1 \cdot \vec{n}) \, (\vec{\alpha}_2 \cdot \vec{n})) \text{ with } \vec{n} = \frac{\vec{r}_{12}}{|\vec{r}_{12}|} \quad . \tag{2}$$

An even more accurate expression has been derived by Bethe and Salpeter[6], which is due to the exchange of a transverse photon $(R = r_{12})$

$$H'_{Br} = - \frac{1}{2} e^2 \, \vec{\alpha}_{1i} \cdot \vec{\alpha}_{2j} \left[\delta_{ij} \frac{\cos \, \omega \, R}{R} + \frac{\partial^2}{\partial R_i \partial R_j} \frac{\cos \, \omega \, R - 1}{\omega^2 R} \right], \tag{3}$$

where ω is the energy transferred by the virtual photon.

In direct two-electron matrix elements of H'_{Br} the photon energy $\omega = o$; in this case H'_{Br} reduces exactly to H_{Br}. The same result is obtained when all contributions of the order ω^2 or higher $(O((\frac{v}{c})^4)$ are neglected. Therefore the normal Breit operator H_{Br} is a good approximation for small Z, because of $v \ll c$ in this region. An alternative expression for the Breit operator is

$$H''_{Br} = - \frac{e^2}{2r_{12}} (\vec{\alpha}_1 \cdot \vec{\alpha}_2 \cos \omega \ r_{12} + (1 - \cos \omega \ r_{12})) \quad . \quad (4)$$

Both expressions H'_{Br} and H''_{Br} are good for the region of large Z.

	$\langle H'_{Br} \rangle$	$\langle H_{Br} \rangle$
Ne(Z = 10)	0.033	0.033
Xe(Z = 54)	11.420	11.549
Pb(Z = 82)	48.393	49.521
No(Z = 102)	107.203	110.516

Tab. 1

Contribution of the magnetic and retardation contribution to the total energy of an atom in a.u. for the operators H_{Br} and H'_{Br}.

Table 1, which is taken from the paper of Mann[7] contains the expectation values of the two operators H'_{Br} and H_{Br} for different Z in a.u. Only for very large Z appreciable discrepancies occur. One has to have in mind that one s electron contributes to these values already by more than 40 %. In addition, one gets somewhat different numbers, when different wave functions are taken into the calculation.

Vacuum polarization

Within the last few years calculations of the vacuum polarization effect by Gyulassy[8] and Rinker[9] have been performed, which explicitly took into account Coulomb wavefunctions to describe the intermediate states of the virtual electron and positron cloud.

This method of calculation leads to values which are correct
even for the region of high Z elements. If one compares these
calculations with the usual $Z\alpha$ and α expansion, usually applied
for low Z calculations, one has to state that the lowest order
Uehling term plus higher orders in $(Z\alpha)^n$ with $n = 2,3,\ldots$ plus
all higher order terms in α^n are included.

Vacuum fluctuation (self-energy)

If Coulomb wavefunctions are taken explicitely as intermediate
states in the calculation of the lowest order vertex correction,
the results for the vacuum fluctuation correction are expected
to be quite accurate, even in the region of $Z\alpha \approx 1$.
Mohr[10] used this method to calculate the self-energy with analytical
Coulomb wavefunctions for very high Z systems. Desiderio and
Johnson[11] as well as Cheng and Johnson[12] even went beyond that
approximation. They took into account numerical Dirac-Fock-Slater
wavefunctions with an extended nucleus as intermediate states. This
is the only way to continue the calculations into the region
$Z > 137$. Usually the result is expressed as

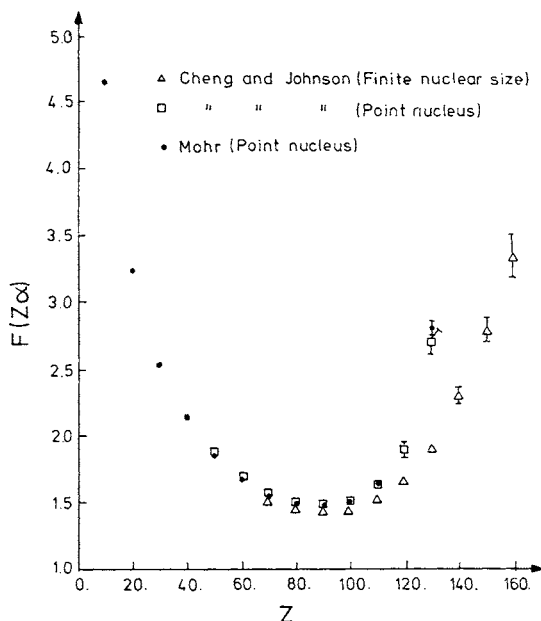$$\frac{\alpha}{\pi} \, \frac{(Z\alpha)^4}{n^3} \, mc^2 \, F(Z\alpha) \quad .$$

Fig. 1

Values for the
function $F(Z\alpha)$
in the expression
of the self-energy
for large and
very large Z (see
ref. 12 and 10).

A comparison of the function $F(Z\alpha)$ for the various calculations for the 1s electronic state can be seen in figure 1, where for low Z elements the results of Cheng et al.[12] and Mohr[10] agree well, whereas for high Z Mohr's values of $F(Z\alpha)$ increase much stronger than Cheng's results. The reason for this difference is the effect of the extended nucleus which is taken into account in the numerical wavefunctions of Cheng et al.[12]. Due to numerical uncertainties, the calculations of Cheng et al.[12] were not continued with the present version of the program above Z = 160. Therefore the very important question, if the self-energy of the innermost level may become so big for Z $\approx$ 173 that a diving of this level into the negative continuum can be prevented, cannot be answered up to now. There are experimental indications in the heavy ion collision of Cm on Pb which could be interpreted in this way. But actual calculations have not been performed so far.

Order of magnitude of the effects

In table 2 we list the contributions to the binding energies of the four effects discussed above for the innermost electrons of the elements Z = 90 and Z = 100.

		Z = 90	Z = 100
Magnetic contribution:	1s	+492 eV	+715 eV
	$2p_{1/2}$	+100 eV	+153 eV
Retardation:	1s	- 36 eV	- 41 eV
	$2p_{1/2}$	- 10 eV	- 13 eV
according to ref. 7,13,14			
Vacuum polarization:			
1. order Uehling term	1s	- 80 eV	-148 eV
with extended nucleus	$2p_{1/2}$	- 2 eV	- 4 eV
higher orders (ref.8 and ref. 9)	1s	+ 4 eV	+ 8 eV
Vacuum fluctuation:	1s	+306 eV	+457 eV
according to ref. 10 to ref. 12	$2p_{1/2}$	+ 7 eV	+ 15 eV

Table 2: Contributions of the four corrections to the 1s and $2p_{1/2}$ level of Z = 90 and 100.

These values have to be compared with the binding energy of about
141 keV for the 1s state of Z = 100, which is the result of the
solution of the SCF Dirac-Fock equation[13]. The agreement between
the experimental results and theory is good within a few eV.

Where do we stand now?

Recently, Deslattes et al.[15] compared all available results of
experimental inner shell X-ray energies with theoretical
calculations. They showed (see fig. 2) that there seems to be a
linear trend proportional to Z for the difference between experi-
mental and theoretical values for the K_{α_1} line.
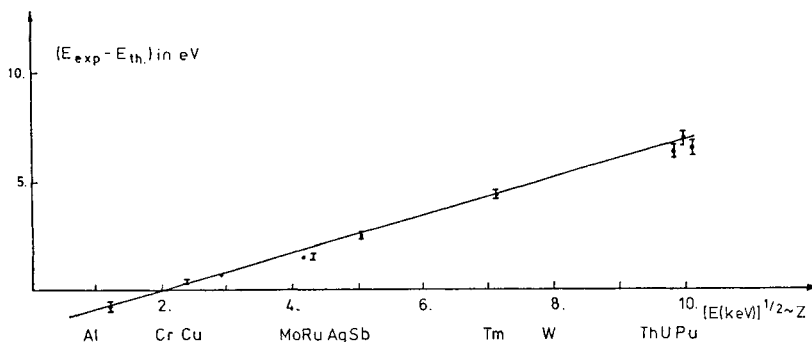

Fig. 2: Difference between experimental and theoretical
values for the K_{α_1} line.

Up to now there is no answer for this discrepancy.

To avoid any calibration problem between different experiments
which may be the reason for this systematic discrepancy, Borchert
et al.[16] measured X-ray energies for low Z and high Z elements
simultaneously in different orders of the Bragg reflection. Their
results show an agreement for the measured X-ray energy difference
and theory which is always better than 2 eV.

According to latest comparisons, the discrepancy shown in fig. 2
decreases again for the high Z elements. If this is true it is
easy to be understood[17] why Borchert et al.[16] did not measure any
big difference. They always compared one element on the increasing
low Z part of the curve with a high Z element on the decreasing
upper part of the curve, so that the relative difference between
both discrepancies remained smaller than 2 eV.

Finally one should mention the large discrepancy which shows up
between experimental $K_\alpha^h{}_1$ hypersatellite lines and theoretical
values[18,19]. For Hg it is still of the order of 30 eV.

To close the gap between experiment and theory in the future, to
my mind one main effort must be undertaken from the theoretical
side. Because we are dealing with complicated systems of many
electrons, which are connected in a self-consistent way, one has
to look into the self-consistency effects on the whole atom and its
total energy which will arise from all three effects, the magnetic
interaction, the vacuum polarization, and vacuum fluctuation. The
second is easier, because the main part of it can be inserted as
an additional local potential in the SCF calculations. Also the
first can be (and already has been) included in the SCF
calculation[20]. The most complicated will be the third. Up to now
there is no direct way to include the vacuum fluctuation in the
calculation itself. Although these indirect QED effects are small,
one has to study them in the light of these discrepancies with
great care.

How large are the contributions for $Z \approx 170$?

The magnetic contribution and retardation never has been
calculated for the region of superheavy elements, but from an
extrapolation of ref. 7 one may expect that the contribution to
the 1s binding energy for $Z = 170$ is in the order of +20 to +40 keV.
The vacuum polarization contribution as calculated by ref. 8 and 9
is expected to be $\approx$ -10 keV. The vacuum fluctuation, as calculated
by Cheng and Johnson[12], can only be extrapolated for these very

high Z systems (see the discussion about this question in the part on vacuum fluctuation). If we assume $F(Z\alpha) \approx 4.5$ for $Z = 170$, we get a contribution of $\approx +18$ keV.

Thus, the total QED contribution to the 1s level of $Z = 170$ is expected to be in the order of $\approx +40$ keV. This number has to be compared with the influence of the extended nucleus. For $Z = 170$ an uncertainty in the nuclear radius of $\Delta R = 0.1$ fm [21] leads to a change in the 1s binding energy of 3 keV. Thus, an uncertainty of about 1 fm in the nuclear radius already amounts to the same order of magnitude as the sum of the QED contributions.

Consequences

We have seen that QED effects in many-electron atoms in the region between $Z = 80$ to 100 are in the order of 10^{-3} to 10^{-2} of the binding energy for the innermost electrons. Of course, it would be most interesting to measure one-electron systems, even at these high Z. Because this will be very complicated to achieve experimentally, one might spend further effort to get better results from one-hole systems instead. Of course, theoretically this is much more complicated.

Although for superheavy systems theoretical values are still very inaccurate and experiments are not available, it is still of great principal interest. Great effort should be undertaken to get also some results from this region. Maybe, experiments at the heavy ion accelerators one day will give some answers to this important question.

References

1. One example is F.T. Porter and M.S. Freedman, Phys. Rev. Lett.
   $\underline{27}$, 293 (1971)

2. G.L. Borchert, P.G. Hansen, B. Jonson, H.L. Ravn and J.P.
   Desclaux in Atomic Masses and Fundamental Constants 6 (Eds.
   J.A. Nolen and W.B. Benenson) N.Y. and London Plenum Press,
   p. 189

3. J.P. Desclaux, Comp. Phys. Comm. $\underline{9}$, 31 (1975), program
   developed by J.B. Mann, described in J.B. Mann and J.T. Waber,
   J. Chem. Phys. $\underline{53}$, 2397 (1970);
   in addition there exists a number of analogous programmes e.g.
   by Meyers

4. J.A. Gaunt, Proc. Roy, Soc. (London) $\underline{A122}$, 513 (1929)

5. G. Breit, Phys. Rev. $\underline{34}$, 553 (1929); $\underline{36}$, 383 (1930); $\underline{39}$, 616 (1932)

6. H.A. Bethe and E.E. Salpeter in Quantum Mechanics of one and two
   electron atoms, Academic Press N.Y. 1957, p. 181

7. J.B. Mann and W.R. Johnson, Phys. Rev. $\underline{A4}$, 41 (1971)

8. M. Gyulassy, Phys. Rev. Lett. $\underline{33}$, 921 (1974)

9. G.A. Rinker and L. Wilets, Phys. Rev. $\underline{A12}$, 748 (1975)

10. P.J. Mohr, Ann. Phys. (N.Y.) $\underline{88}$, 26, and 52 (1974)

11. A.M. Desiderio and W.R. Johnson, Phys. Rev. $\underline{A3}$, 1267 (1971)

12. K.T. Cheng and W.R. Johnson, Phys. Rev. $\underline{A14}$, 1943 (1976)

13. B. Fricke, J.P. Desclaux and J.T. Waber, Phys. Rev. Lett. $\underline{28}$,
    714 (1972)

14. K.N. Huang, M. Aoyagi, M.H. Chen, B. Crasemann and H. Mark,
    At. Data Nucl. Data Tables $\underline{18}$, 243 (1976) and references therein

15. R.D. Deslattes, E.G. Kessler, L. Jacobs and W. Schnitz, Phys.
    Lett. $\underline{71A}$, 411 (1979)

16. G.L. Borchert, P.G. Hansen, B. Jonson, H.L. Ravn and J.P.
    Desclaux, 6 Int. Conf. on Atomic Masses, 1979

17. R.D. Deslattes, private communication, Dec. 1980

18. K. Schreckenbach, H.G. Börner and J.P. Desclaux, Phys. Lett. 63A, 330 (1977)

19. N. Beatham, I.P. Grant, B.J. Mc Kenzie and S.J. Rose, Physica Scripta 21, 423 (1980)

20. W. Johnson, private communication
    J.P. Desclaux, "   "   "

21. B. Fricke, W. Greiner and J.T. Waber, Theor. Chim. Acta 21, 235 (1971)