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The Self-Energy of Electrons in Critical Fields

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Corrections of order $a$ but all orders of $Za^2$.

We find a shift of $\pm 11.0$ keV. This shift is almost canceled by the vacuum-polarization, leaving a negligible effect for all quantum-electrodynamic

parameters. The $\sqrt{s}$ is chosen to be $1.0$ GeV. The self-energy correction this process is treated to all orders in $Za^2$.

We have calculated the energy shift of $\pi^{-}$-electrons in heavy atoms due to

Abstract:

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The self-energy of electrons in critical fields...
The K-electron binding energy $E_{1s}$ increases strongly as a function of the nuclear charge $Z$. For $Z = 150$, $E_{1s}$ amounts to about the electron rest mass and hence one enters the truly relativistic domain. For $Z \geq 170$ the binding energy exceeds twice the electron rest mass and the K-shell electron gets imbedded as resonance in the negative energy continuum, which opens the possibility of spontaneous positron production. For a current discussion of the behaviour of electrons in these critical fields we refer to ref. 1 and references therein.

The major motivation of our investigations was the question whether field theoretical corrections, such as vacuum-polarization and self-energy may prevent such an extraordinary strong binding. These processes are visualized by the Feynman-diagrams in fig. 1. The double lines indicate the exact propagators and wave functions in the Coulomb field of the nucleus. The dominant vacuum-polarization contribution is provided by the attractive Uehling potential. Its influence on electronic binding energies for superheavy systems has been calculated by various authors.\textsuperscript{2-4} For the critical nuclear charge $Z_{cr}$ the Uehling potential leads to an energy shift $\Delta E_{VP}^{(n=1)} \approx -11.8 \text{ KeV}$\textsuperscript{4}, which decreases $Z_{cr}$ by 1/3 of a unit. The remaining vacuum-polarization effects in lowest structure of $Z_\alpha^n$ with $n=1$ were evaluated by M. Gyulassy\textsuperscript{5,6} and by Rinker and Wilets\textsuperscript{7}. These authors made use of the angular momentum decomposition of the electron propagator in spherically symmetric potentials that was developed by Wichmann and Kro1\textsuperscript{8}. The obtained energy shift of $\Delta E_{VP}^{(n=1)} \approx 1.15 \text{ KeV}$\textsuperscript{5} is very small compared with the total K-shell binding energy of 1 MeV.

Electronic self-energy corrections for high-Z systems have been first studied in the pioneering work of Brown, Langer and Schaefer\textsuperscript{9-11}. In these theoretical investigations the traditional expansion\textsuperscript{12} of the Feynman diagrams in powers of the coupling constant ($2\alpha$) of the external field was avoided. This method was further refined and successfully applied in computations of electron energy shifts in high - Z elements by Desiderio and Johnson\textsuperscript{13}, who allowed for a realistic nuclear charge distribution as well as the electron-electron interaction in the Hartree-Fock approximation. The precise analysis of self-energy corrections by P. Nohr\textsuperscript{14} is based on the Coulomb potential for point-like nuclei. Due to the singular nature of the potential these calculations are restricted to nuclear charges below $Z = \alpha^{-1} \approx 137$. Cheng and Johnson\textsuperscript{15} continued the calculations of ref. 13 up to $Z = 160$, where a repulsive energy shift for K-shell electrons of $\Delta E_{SE} = 7.3 \text{ KeV}$ was found.

Recently Liesen et al.\textsuperscript{16} measured the ionization probability $P(b)$ of the strongest bound electron states versus the classical impact parameter $b$ in collisions of Pb and Ca with a combined charge $Z_1 + Z_2 = 178$. For almost central collision deviations from an empirical scaling law for $P(b)$ were found. The authors speculated that a strong self-energy shift of the quasimolecular ion-state could be responsible for the observed modification of the ionization probability.

In our calculations we employed the methods developed by Desiderio and Johnson\textsuperscript{13}, which may be slightly simplified by restriction to K-shell electrons. The energy shift of a $1_{1/2}$-electron due to the quantum-electrodynamical self-energy correction finally can be expressed in a form amenable to direct numerical evaluation ($\hbar = c = m = 1$)

$$\Delta E = \Delta E^{'0}(Z'=Z) - \Delta E^{'0}(Z'=0) + i \Delta R^0 + \Delta E^{'2} + \Delta E^{'C}.$$ \hspace{1cm} (1)
The contraction of the main term of the Coulombic wave function for a given nuclear charge \( Z \) is
\[
\frac{Z(1 + \frac{1}{Z^2})}{2} \int \frac{d^3r}{\rho} \phi^2(r) \rho(r) < (x) | (y) = \sum \frac{Z}{\rho(r)} \phi^2(r) \rho(r) < (x) | (y)
\]
The contraction term is determined by
\[
\int \frac{d^3r}{\rho} \phi^2(r) \rho(r) < (x) | (y)
\]
and
\[
x \rho x \ (xd) \phi(x) \phi(y) \int \frac{d^3r}{\rho} \phi^2(r) \rho(r) < (x) | (y)
\]
Denote the momentum of a given complex energy \( E \) and angular momentum \( J \) by
\[
\gamma
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\[
\begin{align*}
\langle x | (y) \rangle & \gamma \\
\langle x \rangle & \gamma \\
\langle x \rangle & \gamma \\
\langle x \rangle & \gamma \\
\langle x \rangle & \gamma \\
\langle x \rangle & \gamma \\
\langle x \rangle & \gamma \\
\langle x \rangle & \gamma \\
\end{align*}
\]
In formula (3) \( j_k \) and \( h_\lambda^{(1)} \) are the spherical Bessel-function and Hankel-function of first kind for purely imaginary arguments.

The coupled differential equations (4) were solved numerically using the predictor-corrector methods of ref. 17. For hydrogen-like systems the external potential energy \( V(x) \) is determined by the nuclear charge distribution, for which a homogeneously charged sphere with a radius \( R = 1.2A^{1/3} \text{fm} \) has been assumed. All integrations were performed numerically with Gaussian quadratures.

To check our computer code, we computed the self-energy contribution to the K-shell binding energy in mercury (\( Z=80 \)). Assuming a fictitious nuclear mass number \( A=1 (\text{He}^{1.2} \text{fm}) \) we obtained \( \Delta E_{SE} = 206.1 \text{eV} \) which is about 0.7 eV smaller than the result of Cheng and Johnson\(^{15} \)) for a point-like nucleus.

For the superheavy system \( Z = 130 \) we found \( \Delta E_{SE} = 2.537 \text{ keV} \) for a nucleus with \( A=1, \) as compared with the point-nucleus value\(^{15} \) of \( \Delta E_{SE} = 2.586 \text{ keV} \pm 0.156 \text{keV} \). These numbers are drastically reduced if one takes into account a realistic nuclear size determined by \( A = z \cdot \lambda. \) This lowers the energy shift to \( \Delta E_{SE} = 1.896 \text{ keV}. \) The complementary result of Cheng and Johnson is \( \Delta E_{HF}^{SE} = 1.844 \text{keV} \pm 0.029 \text{keV}, \) where, in addition, electron screening effects within a mean field Hartree-Fock (HF) potential were taken into account. For \( Z=150 \) the present calculation leads to \( \Delta E_{SE} = 4.963 \text{ keV} \) and for \( Z = 160 \) to \( \Delta E_{SE} = 7.759 \text{ keV}, \) respectively. The latter number differs by 393 eV from the corresponding HF-values of ref. 15), where the numerical error was estimated to \( \pm 354 \text{ eV}. \)

Presumably this slight disagreement is caused by the considerable difference of a HF-potential from a Coulomb potential for finite size nuclei. Our calculation for \( Z=169 \) yielded \( \Delta E_{SE} = 10.819 \text{ keV}. \) For the critical nuclear charge \( Z=170 \) we adjusted the nuclear mass number and hence the nuclear radius such that the K-electron energy eigenvalue differed only by \( 10^{-3} \text{ eV} \approx 10^{-3} \text{ eV} \) from the border line of the negative energy continuum. As the most important result we found an energy shift of \( \Delta E_{SE} = 10.989 \text{ keV}, \) which still represents only a 1% correction to the total K-electron binding energy. Therefore it may safely be neglected in investigations of ionization probabilities\(^{16} \) in superheavy quasimolecular systems. If one adds to this the vacuum-polarization contributions of ref. 4) and 5) for critical external potentials, the total energy shift due to radiative corrections of order \( \alpha \) amounts only to 300 eV. This tiny effect is at present far outside of any measurable consequences. The various calculations for the self-energy correction of K-electrons in high-Z atoms are summarized in fig. 2. On a logarithmic scale the energy shift is displayed versus the nuclear charge \( Z. \) For \( Z > 70 \) it is well described by an exponential increase.

We conclude that radiative corrections as vacuum-polarization or self-energy may not prevent the K-shell binding energy from exceeding \( 2m_e^2 \) in superheavy systems with \( Z > Z_{cr} = 170. \)
The results of the present calculations for extended nuclei are indicated by crosses. The squares represent the values obtained by Chang and Johnson (19) for a Hartree-Fock potential and extended nuclei. The error bars for the present calculations in the Coulomb field of point-like nucleons are much smaller than the errors due to the uncertain results of P, E, and self-energy (20). The double lines indicate the exact point of the nuclear charge. The large circles are the result of the self-energy shift of K-shell electrons as a function of the external field in the Coulomb field of a nucleus.

Figure 2: Feynman diagrams for the lowest order vacuum polarization (a).