16 MARS 1982

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GSi - 82 - 6a
PREPRINT

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FEBRUARY 1982

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GSi 82-6a

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The self-energy of electrons in critical fields⁺

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Abstract:

We have calculated the energy shift of K-electrons in heavy atoms due to the self-energy correction. This process is treated to all orders in $Z\alpha$, where Z denotes the nuclear charge. For the superheavy system $Z = 170$, where the K-shell binding energy reaches the pair-production threshold ($E_{1s}^B \sim 2mc^2$), we find a shift of +11.0 keV. This shift is almost cancelled by the vacuum-polarization, leaving a negligible effect for all quantum-electrodynamical corrections of order α but all orders of $Z\alpha$.

⁺Work supported by the Bundesministerium für Forschung und Technologie and in part (G.S.) by the Deutsche Forschungsgemeinschaft (Heisenberg-Programm)

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.²⁻⁴ For the critical nuclear charge Z_{cr} the Uehling potential leads to an energy shift $\Delta E_{vp}^{(n=1)} = -11.8 \text{ KeV}^4$, which decreases Z_{cr} by $1/3$ of a unit. The remaining vacuum-polarization effects in lowest order of the fine-structure constant α but in all orders of $(Z\alpha)^n$ with $n \geq 1$ were evaluated by M. Gyulassy^{5,6} and by Rinker and Wilets⁷. These authors made use of the angular momentum decomposition of the electron propagator in spherically symmetric potentials that was developed by Wichmann and Kroll⁸. The obtained energy shift of $\Delta E_{vp}^{(n \geq 1)} = \pm 1.15 \text{ KeV}^5$ 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 Schaefer⁹⁻¹¹. In these theoretical

investigations the traditional expansion¹²⁾ of the Feynman diagrams in powers of the coupling constant $(Z\alpha)$ 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 Johnson¹³, 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. Mohr¹⁴⁾ 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 $Z = \alpha^{-1} \sim 137$. Cheng and Johnson¹⁵⁾ 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.¹⁶⁾ measured the ionization probability $P(b)$ of the strongest bound electron states versus the classical impact parameter b in collisions of Pb and Cm 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 $1s\sigma$ -state could be responsible for the observed modification of the ionization probability.

In our calculations we employed the methods developed by Desiderio and Johnson¹³⁾, which may be slightly simplified by restriction to K-shell electrons. The energy shift of a $1s_{1/2}$ -electron due to the quantum-electrodynamical self-energy correction finally can be expressed in a form amenable to direct numerical evaluation ($\hbar = c = m = 1$)

$$\Delta E = \Delta E'_{\text{O}} (Z'=Z) - \Delta E'_{\text{O}} (Z'=0) + i\pi R_{\text{O}} + \Delta E^{(2)} + \Delta E_{\text{C}}. \quad (1)$$

Here the residuum term is given by

$$i\pi R_0 = -\alpha \int_0^\infty dr \int_0^r dx \left\{ \frac{2}{3} \frac{x}{r^2} q(r)q(x) - \frac{1}{r} p(r) p(x) \right\}$$

with

$$q(x) = 2 g_{1s}(x) F_{1s}(x),$$

$$p(x) = g_{1s}^2(x) + F_{1s}^2(x).$$

$\Delta E(2)$ is

$$\Delta E(2) = -\frac{5\alpha}{4\pi} \langle V(x) \rangle_{1s} - \frac{2\alpha}{\pi^2} \int_0^\infty q^-(p) \frac{\xi \ln \xi}{\xi-1} p^2 dp$$

$$+ \frac{\alpha}{\pi^2} \int_0^\infty g_{1s}(p) F_{1s}(p) Z(\xi) p^3 dp + \frac{\alpha E_{1s}}{2\pi^2} \int_0^\infty q^+(p) Z(\xi) p^2 dp$$

with $\xi = p^2 - E_{1s}^2 + 1$ and

$$Z(\xi) = \frac{\xi}{\xi-1} \left(1 + \frac{\xi-2}{\xi-1} \ln \xi \right).$$

$g_{1s}(p)$ and $F_{1s}(p)$ denote Bessel-transforms of the radial component of the

Dirac wavefunction,

$$g_{1s}(p) = \int_0^\infty g_{1s}(x) j_0(px) x dx,$$

$$F_{1s}(p) = \int_0^\infty F_{1s}(x) j_1(px) x dx$$

and

$$q^\pm(p) = g_{1s}^2(p) \pm F_{1s}^2(p).$$

$\langle V(x) \rangle_{1s}$ is the expectation value of the potential energy and E_{1s} the energy eigenvalue of the K-shell electron.

The counter term ΔE_C is determined by

$$\Delta E_C = -\frac{\alpha}{2\pi} \langle V(x) \rangle_{1s} \int_0^\infty \frac{du}{(u^2+1)^{1/2}}$$

The contribution of the main term $\Delta E_0^i(Z')$ for a given nuclear charge Z' can be written as

$$\Delta E_0^i = -\frac{2\alpha}{\pi} \int_0^\infty \omega d\omega \int_0^\infty dr \int_0^r dx \sum_{\kappa=\pm 1}^{\pm \infty} \text{Re} \left[\frac{|K|}{\Delta_\kappa(E_{1s} - i\omega)} \right]$$

$$+ \frac{i(\kappa-1)^2}{2(\bar{\kappa}+1)} B_{\bar{\kappa}} q^{\infty+}(r) q^{0+}(x)$$

$$+ \frac{\bar{\kappa}}{2\bar{\kappa}+1} B_{\bar{\kappa}-1} [q^{\infty-}(r) + \frac{\kappa+1}{\bar{\kappa}} q^{\infty+}(r)] [q^{0-}(x) + \frac{\kappa+1}{\bar{\kappa}} q^{0+}(x)]$$

$$+ \frac{\bar{\kappa}+1}{2\bar{\kappa}+1} B_{\bar{\kappa}+1} [q^{\infty-}(r) - \frac{\kappa+1}{\bar{\kappa}+1} q^{\infty+}(r)] [q^{0-}(x) - \frac{\kappa+1}{\bar{\kappa}+1} q^{0+}(x)]$$

$$- B_{\bar{\kappa}} p^{\infty}(r) p^0(x) \Big] \quad (2)$$

with $\bar{\kappa}$ being the orbital angular momentum related to κ and $\bar{\kappa}$ related to $-\kappa$, respectively. Here we have used the abbreviations

$$q^{\infty,0\pm}(x) = g_{1s}(x, E_{1s}) F_{\kappa}^{\infty,0}(x, E_{1s} - i\omega) \pm F_{1s}(x, E_{1s}) G_{\kappa}^{\infty,0}(x, E_{1s} - i\omega),$$

$$p^{\infty,0}(x) = g_{1s}(x, E_{1s}) G_{\kappa}^{\infty,0}(x, E_{1s} - i\omega) + F_{1s}(x, E_{1s}) F_{\kappa}^{\infty,0}(x, E_{1s} - i\omega),$$

$$B_{\bar{\kappa}} = h_{\bar{\kappa}}^{(1)}(i\omega r) j_{\bar{\kappa}}(i\omega x). \quad (3)$$

$\Delta_\kappa(E)$ denotes the Wronskian for a given complex energy E and angular momentum quantum number κ :

$$\Delta_\kappa(E) = F_{\kappa}^{\infty}(x, E) G_{\kappa}^{00}(x, E) - F_{\kappa}^0(x, E) G_{\kappa}^{\infty}(x, E).$$

$F_{\kappa}^{0,\infty}$ and $G_{\kappa}^{0,\infty}$ are solutions of the radial Dirac equation for complex energies which are either regular at the origin ($x=0$) or at infinity ($x=\infty$)

$$\frac{dG_{\kappa}}{dx} = -\frac{\kappa}{x} G_{\kappa} + (E + 1 - V(Z')) F_{\kappa},$$

$$\frac{dF_{\kappa}}{dx} = - (E - 1 - V(Z')) G_{\kappa} + \frac{\kappa}{x} F_{\kappa}. \quad (4)$$

In formula (3) j_λ 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 $R = 1.2A^{1/3}$ 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 $A=1$ ($R=1.2$ fm) we obtained $\Delta E_{SE} = 206.1$ eV which is about 0.7 eV smaller than the result of Cheng and Johnson¹⁵⁾ for a point-like nucleus. For the superheavy system $Z = 130$ we found $\Delta E_{SE} = 2.537$ keV for a nucleus with $A=1$, as compared with the point-nucleus value¹⁵⁾ of $\Delta E_{SE} = 2.586$ keV $\pm .156$ keV.

These numbers are drastically reduced if one takes into account a realistic nuclear size determined by $A = 2.5 \cdot Z$. This lowers the energy shift to $\Delta E_{SE}^{HF} = 1.896$ keV. The complementary result of Cheng and Johnson is $\Delta E_{SE}^{HF} = 1.844$ keV $\pm .029$ 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 $\Delta E_{SE} = 4.963$ keV and for $Z = 160$ to $\Delta E_{SE} = 7.759$ keV, respectively. The latter number differs by 393 eV from the corresponding HF-values of ref. 15), where the numerical error was estimated to ± 354 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 $\Delta E_{SE} = 10.839$ 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} eV $\sim 10^{-9} E_{1s}^{cp}$ from the border line of the negative energy continuum. As the most important result we found an energy shift of $\Delta E_{SE} = 10.989$ 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 probabilities¹⁶⁾ in superheavy quasimolecular systems. If one adds to this the vacuum-polarization calculations of ref. 4) and 5) for critical external potentials, the total energy shift due to radiative corrections of order α 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 $Z \geq 70$ 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 $2mc^2$ in superheavy systems with $Z \gtrsim Z_{cr} \sim 170$.

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Figure Captions:

Fig. 1: Feynman diagrams for the lowest order vacuum-polarization (a) and self-energy (b). The double lines indicate the exact propagators and wave functions in the Coulomb field of a nucleus.

Fig. 2: The self-energy shift ΔE of K-shell electrons as a function of the nuclear charge Z . The calculations are performed to first order in α but to all orders in the coupling constant ($Z\alpha$) of the external field. The dots denote the numerical results of P. Mohr¹⁴⁾ for 1s-electrons in the Coulomb field of point-like nuclei. The squares represent the values obtained by Cheng and Johnson¹⁵⁾ for a Hartree-Fock potential and extended nuclei. The results of the present calculations for extended nuclei are indicated by crosses.

Fig.2

Fig.1