## Self-Energy of Electrons in Critical Fields

Gerhard Soff

Gesellschaft für Schwerionenforschung, D-6100 Darmstadt, Germany

and

## Paul Schlüter, Berndt Müller, and Walter Greiner

Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, D-6000 Frankfurt am Main, Germany (Received 23 February 1982)

The energy shift of K electrons in heavy atoms due to the self-energy correction has been calculated. 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  $(E_{1s}^{\ b} \sim 2mc^2)$ , a shift of + 11.0 keV is found. This shift is almost cancelled by the vacuum polarization, leaving a negligible effect for all quantumelectrodynamical corrections of order  $\alpha$  but all orders of  $Z\alpha$ .

PACS numbers: 31.10.+z, 31.20.-d, 31.30.Jv

The K-electron binding energy  $E_{1s}^{b}$  increases strongly as a function of the nuclear charge Z. For Z = 150,  $E_{1s}^{b}$  amounts to about the electron rest mass and hence one enters the truly relativistic domain. For  $Z \gtrsim 170$  the binding energy exceeds twice the electron rest mass and the Kshell electron gets imbedded as a resonance in the negative energy continuum, which opens the possibility of spontaneous positron production. For a current discussion of the behavior of electrons in these critical fields we refer to Reinhardt, Müller, and Greiner,<sup>1</sup> and references therein.

The major motivation of our investigation 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.<sup>2-4</sup> For the critical nuclear charge  $Z_{cr}$  the Uehling potential leads to an energy shift  $\Delta E_{VP}^{(n=1)} = -11.8$ keV,<sup>4</sup> which decreases  $Z_{cr}$  by one third of a unit. The remaining vacuum-polarization effects in lowest order of the fine-structure constant  $\alpha$  but in all orders of  $(Z\alpha)^n$  with n > 1 were evaluated by Gyulassy<sup>5,6</sup> and by Rinker and Wilets.<sup>7</sup> These authors made use of the angular momentum decomposition of the electron propagator in spherically symmetric potentials that was developed by Wichmann and Kroll.<sup>8</sup> The obtained energy shift of  $\Delta E_{VP}^{(n>1)} = +1.15 \text{ keV}^5$  is very small compared with the total K-shell binding energy of 1 MeV.

Electronic self-energy corrections for high-Zsystems were first studied in the pioneering work of Brown and co-workers.<sup>9-11</sup> In these theroretical investigations the traditional expansion<sup>12</sup> 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 Johnson,<sup>13</sup> 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 Mohr<sup>14</sup> is based on the Coulomb potential for pointlike nuclei. Because of the singular nature of the potential these calculations are restricted to nuclear charges below  $Z = \alpha^{-1} \sim 137$ . Cheng and Johnson<sup>15</sup> continued the calculations of Ref. 13 up to Z = 160. where a repulsive energy shift for K-shell electrons of  $\Delta E_{SE} = +7.3$  keV was found.

Recently Liesen et al.<sup>16</sup> measured the ionization probability P(b) of the strongest bound electron states versus the classical impact parameter

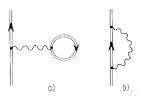


FIG. 1. Feynman diagrams for the lowest-order (a) vacuum polarization and (b) self-energy. The double lines indicate the exact propagators and wave functions in the Coulomb field of a nucleus.

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 1so state could be responsible for the observed modification of the ionization probability. In our calculations we employed the methods developed by Desiderio and Johnson,<sup>13</sup> 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 ( $\hbar = c = m = 1$ ),

(1)

 $\Delta E = \Delta E_0'(Z'=Z) - \Delta E_0'(Z'=0) + i\pi R_0 + \Delta E^{(2)} + \Delta E_c.$ 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

$$Q(x) = 2G_{1s}(x)F_{1s}(x), P(x) = G_{1s}^{2}(x) + F_{1s}^{2}(x).$$

 $\Delta E^{(2)}$  is

$$\Delta E^{(2)} = -\frac{5\alpha}{4\pi} \left\langle V(x) \right\rangle_{1s} - \frac{2\alpha}{\pi^2} \int_0^\infty Q^-(p) \frac{\xi \ln\xi}{\xi - 1} p^2 dp + \frac{\alpha}{\pi^2} \int_0^\infty G_{1s}(p) F_{1s}(p) Z(\xi) p^3 dp + \frac{\alpha E_{1s}}{2\pi^2} \int_0^\infty Q^+(p) Z(\xi) p^2 dp$$

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 wave function,

$$G_{1s}(p) = \int_0^\infty G_{1s}(x) j_0(px) x \, dx \,, \quad F_{1s}(p) = \int_0^\infty F_{1s}(x) j_1(px) x \, dx \,,$$

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  $\Delta E_c$  is determined by

$$\Delta E_c = -\frac{\alpha}{2\pi} \langle V(x) \rangle_{1s} \int_0^\infty \frac{d\omega}{(\omega^2 + 1)^{1/2}}.$$

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

$$\Delta E_{0'} = -\frac{2\alpha}{\pi} \int_{0}^{\infty} \omega \, d\omega \int_{0}^{\infty} dr \int_{0}^{r} dx \sum_{\kappa=\pm 1}^{\pm\infty} \operatorname{Re} \left\{ \frac{-|\kappa|}{\Delta_{\kappa} (E_{1s} - i\omega)} \left[ \frac{(\kappa - 1)^{2}}{l (l + 1)} B_{\overline{l}} Q^{\infty +}(r) Q^{0^{+}}(x) + \frac{l}{l 2l + 1} B_{l-1} \left( Q^{\infty -}(r) + \frac{\kappa + 1}{l} Q^{\infty +}(r) \right) \left( Q^{0^{-}}(x) + \frac{\kappa + 1}{l} Q^{0^{+}}(x) \right) + \frac{l + 1}{2l + 1} B_{l+1} \left( Q^{\infty -}(r) - \frac{\kappa + 1}{l + 1} Q^{\infty +}(r) \right) \left( Q^{0^{-}}(x) - \frac{\kappa + 1}{l + 1} Q^{0^{+}}(x) \right) - B_{l} P^{\infty}(r) P^{0}(x) \right] \right\},$$
(2)

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

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

$$P^{\infty,0}(x) = G_{1s}(x, E_{1s})G_{\kappa}^{\infty,0}(x, E_{1s} - i\omega) + F_{1s}(x, E_{1s})F_{\kappa}^{\infty,0}(x, E_{1s} - i\omega), \quad B_{1} = h_{1}^{(1)}(i\omega r)j_{1}(i\omega r).$$
(3)

1466

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

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

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

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

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

In formula (3)  $j_1$  and  $h_1^{(1)}$  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 Shampine and Gordon.<sup>17</sup> For hydrogenlike systems the external potential energy V(x) is determined by the nuclear charge distribution, for which a homogeneously charged sphere with a radius  $R = 1.2 \text{ A}^{1/3}$  fm has been assumed. All integrations were performed numerically with Gaussian quadratures. A more complete report of our calculations will be published elsewhere.<sup>18</sup>

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 Johnson<sup>15</sup> for a pointlike 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 value<sup>15</sup> of  $\Delta E_{SF} = 2.586 \pm 0.156$  keV. These numbers are drastically reduced if one takes into account a realistic nuclear size determined by A = 2.5Z. This lowers the energy shift to  $\Delta E_{SF}$ = 1.896 keV. The complementary result of Cheng and Johnson is  $\Delta E_{SE}^{HF} = 1.844 \pm 0.029$  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 evaluated as  $\pm 354$  eV. The estimated error in our computation is less than 300 eV for Z = 160and Z = 170. Thus the slight disagreement for Z = 160 is smaller than the numerical uncertainty of both calculations. Presumably it is also partly caused by the considerable difference of a HF

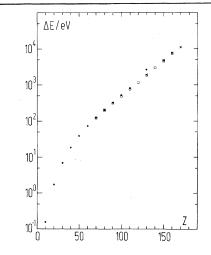


FIG. 2. The self-energy shift  $\Delta E$  of K-shell electrons as a function of the nuclear charge Z. The calculations are performed to first order in  $\alpha$  but to all orders in the coupling constant  $(Z\alpha)$  of the external field. The dots denote the numerical results of Mohr (Ref. 14) for 1s electrons in the Coulomb field of pointlike nuclei. The squares represent the values obtained by Cheng and Johnson (Ref. 15) for a Hartree-Fock potential and extended nuclei. The results of the present calculations for extended nuclei are indicated by crosses.

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 ~  $10^{-9}$  $\times E_{1s}^{b}$  from the borderline 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 probabilities<sup>16</sup> in superheavy quasimolecular systems. If one adds to this the vacuum-polarization calculations of Refs. 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 Kelectrons in high-Z atoms are summarized in Fig. 2. On a logarithmic scale the energy shift is displayed versus the nuclear charge Z. For  $Z \ge 70$  it is well described by an exponential increase.

We conclude that radiative corrections such as vacuum polarization or self-energy may not prevent the *K*-shell binding energy from exceeding  $2mc^2$  in superheavy systems with  $Z > Z_{cr} \sim 170$ .

This work was supported by the Bundesministerium für Forschung und Technologie and in part by the Deutsche Forschungsgemeinschaft (Heisenberg-Programm).

<sup>1</sup>J. Reinhardt, B. Müller, and W. Greiner, Phys. Rev. A 24, 103 (1981).

<sup>2</sup>F. G. Werner and J. A. Wheeler, Phys. Rev. 109, 126 (1958).

<sup>3</sup>W. Pieper and W. Greiner, Z. Phys. 218, 327 (1969). <sup>4</sup>G. Soff. B. Müller, and J. Rafelski, Z. Naturforsch. Teil A 29, 1267 (1974).

<sup>5</sup>M. Gyulassy, Phys. Rev. Lett. <u>33</u>, 921 (1974).

<sup>6</sup>M. Gyulassy, Nucl. Phys. <u>A244</u>, 497 (1975).

<sup>7</sup>G. A. Rinker and L. Wilets, Phys. Rev. A 12, 748 (1975).

<sup>8</sup>E. H. Wichmann and N. M. Kroll, Phys. Rev. 101, 843 (1956).

<sup>9</sup>G. E. Brown and G. W. Schaefer, Proc. Roy. Soc. London, Ser. A 233, 527 (1956).

<sup>10</sup>G. E. Brown, J. S. Langer, and G. W. Schaefer,

Proc. Roy. Soc. London, Ser. A 251, 92 (1959).

<sup>11</sup>G. E. Brown and D. F. Mayers, Proc. Roy. Soc. London, Ser. A 251, 105 (1959).

<sup>12</sup>G. W. Erickson and D. R. Jennie, Ann. Phys. (N.Y.) <u>35,</u> 271, 447 (1965). <sup>13</sup>A. M. Desiderio and W. R. Johnson, Phys. Rev. A <u>3</u>,

1267 (1971).

<sup>14</sup>P. J. Mohr, Ann. Phys. (N.Y.) 88, 26, 52 (1974).

<sup>15</sup>K. T. Cheng and W. R. Johnson, Phys. Rev. A <u>14</u>, 1943 (1976).

<sup>16</sup>D. Liesen, P. Armbruster, F. Bosch, S. Hagmann, P. H. Mokler, H. J. Wollersheim, H. Schmidt-Böcking, R. Schuch, and J. B. Wilhelmy, Phys. Rev. Lett. 44,

983 (1980).

<sup>17</sup>L. F. Shampine and M. K. Gordon, Computer Solution of Ordinary Differential Equations: The Initial Value Problem (Freeman, San Francisco, 1975).

<sup>18</sup>P. Schlüter *et al.*, to be published.

## Large-Scale Collision-Free Instability of Two-Dimensional Plasma Sheets

H. Goldstein<sup>(a)</sup> and K. Schindler

Theoretische Physik IV, Ruhr-Universität Bochum, D-4630 Bochum 1, West Germany (Received 10 November 1981)

The stability of a two-dimensional plasma sheet with a small field component parallel to the normal direction of the sheet is studied by means of the energy principle of collision-free kinetic theory. Numerical computations-show that, depending on the parameter regime, unstable perturbations exist. The mode resembles a tearing mode. The typical wavelength along the main magnetic field direction is comparable with the scale length of the equilibrium.

PACS numbers: 52.35.+g, 52.30.+r

Sudden changes in the topology of magnetic fields (reconnection) has been suggested to provide, under suitable conditions, a powerful mechanism to release free energy from magnetized plasma in the laboratory,<sup>1</sup> in space,<sup>2</sup><sup>-6</sup> and near stars.<sup>7</sup> Although a substantial amount of knowledge has been accumulated on this topic, a number of basic questions have remained open.

The present paper deals with generalized (two dimensional) collision-free plasma sheets. Since the strictly one-dimensional case, in which electron Landau resonance dominates, is reasonably understood,<sup>2,8</sup> we concentrate on the two-dimensional case where a magnetic field component  $B_z$  normal to the current sheet (Fig. 1) is sufficiently large to suppress electron Landau resonances. In addition, we are motivated to study this case by the fact that the near-Earth geomag-

netic tail, where space craft provide in situ observations, falls into that regime. Here, one of the important problems is to identify the elementary plasma processes that govern the observed dynamic characteristics occurring in connection with geomagnetic activity.

In the literature two main branches of approach can be distinguished: (a) The undisturbed equilibrium is quiet in the sense that noise from microinstabilities does not play a significant role: The plasma is collision free even on large space and time scales,<sup>3,9,10</sup> (b) Microinstabilities, e.g., the lower-hybrid drift instability, lead to sufficiently pronounced transport phenomena, such that the plasma behaves as a dissipative fluid on large scales.<sup>3,11</sup>

Since the respective domains of applicability of these two types of processes are not yet clear,