Retardation Effects in Ion-Ion Collisons*

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The modification of the two center screened electronic Coulomb potential due to relativistic kinematical effects is investigated in the Coulomb gauge. Both nuclear and electronic charges were approximated by Gaussian distributions. For ion velocities $v/c = 0.1$ the effect may roughly be approximated by a 0.1 % increase in the effective strength for the monopole term of the two center potential. Thus for ion kinetic energies not exceeding a few MeV/nucleon this relativistic contribution induces small effects on the binding energy of the 1 σ-electrons except for super critical charges.

Besides relativistic effects arising from the fast motion of the electrons [1] (as considered in a fixed nuclear frame) relativistic contributions due to the ion relative motion could also play a non-negligible role for velocities $v/c \geq 0.1$. The size of this effect may be inferred from a simple consideration: Two point charges are moving with constant velocity on a streight line in opposite directions. If we assume both equal charges and masses they move with $\bar{v} = 1/2\, v$ with respect to the center-of-mass (C.M.) frame. If we further consider electrons in molecular orbitals (their reference frame is the C.M. frame) then in the Coulomb gauge the two center Coulomb potential at small separation distances gets increased by $(\bar{v}/c)^2$ $= 0.25\%$ for $v/c = 0.1$ in the direction perpendicular to the direction of motion [2]. The contribution on the monopole term is obtained after angular averaging and amounts to $\frac{1}{3}(\bar{v}/c)^2 = 0.08\%$. Surprisingly enough as we will show below this value is even a rather close estimate for the realistic case where two screened Coulomb potentials move on Coulomb trajectories.

Let us separately consider each of the four potentials connected with the nuclear and electronic charge densities respectively and assume all to be Gaussian shaped density distributions. Then any of the re-

tarded Coulomb potentials in the Coulomb gauge is given by

$$V_i(\mathbf{r}, t)_{\mathrm{ret}} = e^2 \int d^3r'\, d\tau\, \frac{\rho_i(\mathbf{r}', \tau)}{|\mathbf{r} - \mathbf{r}'|}\, \delta\left(\tau - t + \frac{|\mathbf{r} - \mathbf{r}'|}{c}\right) \quad (1)$$

with charge density distributions

$$\rho_i(\mathbf{r}', \tau) = Z_i \left(\frac{\lambda_i}{\pi}\right)^{3/2} \exp\{-\lambda_i[\mathbf{r}' - \mathbf{R}_i(\tau)]^2\} \quad (2)$$

with

$$\int d^3r'\, \rho_i(\mathbf{r}', \tau) = Z_i$$

$\mathbf{R}_i(\tau)$ describes the trajectory of the moving charge eZ_i with mass m_i in the C.M. frame. As usual eZ_i is counted positive for the nucleus, negative for the electronic cloud. $1/\sqrt{\lambda_i}$ are suitable size parameters being of the order of 5 fm for the nuclear and 1 au for the electronic charges. Since the deviations from Coulomb trajectories due to screening effects are sufficiently small for ion kinetic energies as large as a few MeV/nucleon we will use Coulomb trajectories $X(\tau)$ (X = relative distance between the two nuclei)

$$\tau = \pm \frac{a}{v}[\varepsilon \sqrt{y^2 - 1} + \ln(y + \sqrt{y^2 - 1})] \quad (3)$$

with

$$y = \frac{x-a}{\varepsilon \cdot a}, \qquad a = \frac{e^2 Z_1 Z_2}{M v^2},$$

$$\varepsilon^2 = 1 + \left(\frac{b}{a}\right)^2, \qquad X_{\min} = a(1+\varepsilon), \tag{4}$$

$$R_i = \frac{M}{m_i} X \dots i = 1, 2$$

M is the reduced mass, v the asymptotic relative velocity which is given by the incoming velocity of the projectile and b is the impact parameter. $X_{\min}$ describes the distance of closest approach corresponding to $\tau = 0$. For simplicity we will drop the index "i" throughout the following.

With these definitions we may solve (1) by performing the angular integration. This can easily be done by introducing the new variable $\mathbf{r}' - \mathbf{r} = \mathbf{u}$, since

$$\int d\varphi \sin \vartheta \, d\vartheta \exp[-2\lambda \mathbf{u} \cdot \mathbf{q}] = \frac{2\pi}{2\lambda u q} [e^{2\lambda u q} - e^{-2\lambda u q}] \tag{5}$$

where

$$\mathbf{q} = \mathbf{r} - \mathbf{R}(\tau), \qquad q = |\mathbf{q}|, \qquad \tau = t - \frac{u}{c}.$$

Finally, after time integration, we get for each of the moving charges

$$V(\mathbf{r}, t)_{\text{ret}} = Z e^2 \sqrt{\frac{\lambda}{\pi}} \int_0^\infty \frac{du}{q} [e^{-\lambda(u-q)^2} - e^{-\lambda(u+q)^2}], \tag{6}$$

$$\mathbf{q} = \mathbf{r} - \mathbf{R}(\tau), \qquad \tau = t - \frac{u}{c}.$$

The expression (6) is especially convenient since the non-retarded Coulomb potential is readily obtained by considering $c \to \infty$ leading to $\tau \to t$, thus making q independent of u which reduced (6) to

$$V(\mathbf{r}, t)_{\text{non-ret}} = \frac{Z e^2}{q} \operatorname{erf}(q \sqrt{\lambda}). \tag{7}$$

As the monopol term proved to be most important [3] we will project it out from (6) and (7) respectively

$$V(\mathbf{r}, t)_{\text{ret}} = \sum_{lm} Y_{lm}(\Omega) \cdot \varphi_l(r, t)_{\text{ret}}$$

$$\varphi_0(r, t)_{\text{ret}} = \frac{Z e^2 \sqrt{\pi}}{2r} \int_0^\infty du \, \frac{1}{R} \{\operatorname{erf}[\sqrt{\lambda}(u - |r - R|)]$$

$$+ \operatorname{erf}[\sqrt{\lambda}(u + |r - R|)] - \operatorname{erf}[\sqrt{\lambda}(u - |r + R|)]$$

$$- \operatorname{erf}[\sqrt{\lambda}(u + |r + R|)]\}$$

$$R = \left| \mathbf{R}\left(t - \frac{u}{c}\right) \right|. \tag{8}$$

This expression is not particularly simpler in the non-retarded case. Numerical difficulties arise if $1/\sqrt{\lambda}$ gets very small (point charge). Then it is useful to solve (1)

directly for a point charge [4] or to take the limit $\lambda \to \infty$ in the angular integrated form of (6), in essence leaving the error functions in (8) in its integral representations and taking the limit $\lambda \to \infty$. The result is simple

$$\varphi_0(r, t)_{\text{ret}} = \frac{Z e^2 \sqrt{\pi}}{r} \int_{u_{\min}}^{u_{\max}} \frac{du}{R}, \qquad R = R\left(t - \frac{u}{c}\right) \tag{9}$$

where $u_{\min}$ and $u_{\max}$ are to be determined from the implicit equations

$$\left| r - R\left(t - \frac{u_{\min}}{c}\right) \right| = u_{\min}$$

$$\left| r + R\left(t - \frac{u_{\max}}{c}\right) \right| = u_{\max}. \tag{10}$$

In the non-retarded case (10) is readily solved and we obtain

$$\varphi_0(r, t)_{\text{non-ret}} = Z e^2 \sqrt{\pi} \begin{cases} \dfrac{2}{R} & \dots \ r < R \\[2mm] \dfrac{2}{r} & \dots \ r > R. \end{cases} \tag{11}$$

The total potential acting on an electron referred to the C.M. frame as its reference frame is given through the superposition principle by a sum over all four Coulomb potentials connected with the nuclear and electronic charge densities.

The Equations (5–8) are an essential consequence of the assumed Gaussian shaped density distributions. This, however, is not a severe restriction, because it has already been shown [5] that by rather short sums over suitably chosen Gaussian distributions realistic densities may be approximated very well. If a precise calculation needs to be done, such a superposition may be used; we restricted ourselves here to one Gaussian each for the electronic and nuclear charge distribution of each atom. Furthermore we considered $Z_1 = Z_2$ only, which cuts down the computational effort by a factor two.

Our attention was focussed on the impact parameter dependence and the r-dependence of the deviation from the non-retarded Coulomb potential along the trajectory $\mathbf{R}(t)$. So in Figure 1 three impact parameters b and three points along $\mathbf{R}(t)$ have been chosen. Presently in heavy-ion atomic physics predominantly close collisions are investigated, therefore small values for b and R have been selected. Not much difference was observed in the retardation effect between corresponding positions $\mathbf{R}(t)$ on the in- and outcoming way even though the problem is no more symmetric in time as obvious from (10) together with (3) (u must be positive, but t changes sign). The main interest in retardation effects for $v/c \approx 0.1$ is probably in reactions with $Z_1 + Z_2$ near to the super critical charge $Z \approx 170$ where the K-shell electron
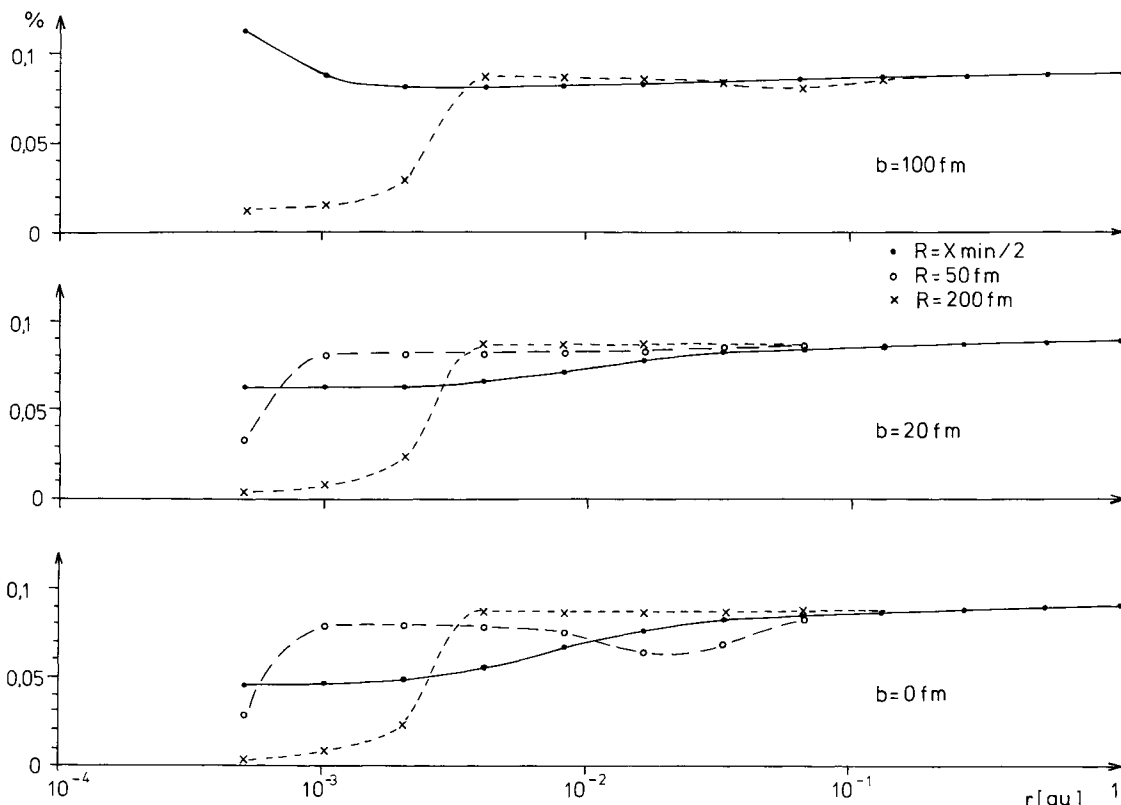
Fig. 1. Percentage deviation of the retarded two center Coulomb potential (monopole term) from the non-retarded one as a function of r [au]. Bombarding energy is 5 MeV/nucleon for two colliding ^{208}Pb neutral atoms. R is half the relative distance of the two nuclei. Three values of the impact parameter b are shown

binding energy changes like some high power in Z. Using perturbation theory a 0.1 percent change in the effective potential strength may become some percent effects on the binding energy. However, other dynamical effects acting on the electrons are at least one order of magnitude larger [6].

Our calculations neglected some relativistic kinematical effects like the Lorentz contraction of the moving charge in the direction of motion, relativistic corrections to the non-relativistic Coulomb trajectories or changes to molecular orbitals coming from a relativistic C.M. transformation. We kept the charges spherical and neglected these effects, because they are higher order corrections to the retarded Coulomb potential in the velocity range chosen. For very fast ions this approximation will no longer be valid. Already for the assumed ion velocities $v/c \approx 0.1$ the neglected Lorentz contraction of the electronic charge causes the retarded screened Coulomb potential for a neutral atom to become slightly negative for distances $r \geq 2R_0$ (this region has been excluded from the figures). R_0 is the radius of the electron cloud. However, the absolute value of the screened Coulomb potential is already several orders of magnitude smaller than the Van der Waals potential at those distances and therefore retardation effects of the kind described here are negligible far out.

References

1. Breit, G.: Phys. Rev. **34**, 553 (1929)
   Breit, G.: Phys. Rev. **39**, 616 (1932)
2. Becker, R., Sauter, F., Ed.: Theorie der Elektrizität, Vol. I, p. 186ff. Stuttgart: Verlag B.G. Teubner 1969
3. Jakubaßa, D.H.: Phys. Lett. **58** A, 163 (1976)
4. Jackson, A.D.: Classical Electrodynamics, p. 464ff. New York: John Wiley & Sons Inc. 1962
5. Kolb, D., Cusson, R.Y., Harvey, M.: Nucl. Phys. A **215**, 1 (1973)
   Kolb, D., Cusson, R.Y.: Z. Physik **253**, 282 (1972)
6. Smith, K., Müller, B., Greiner, W.: J. Phys. B: Atom. Molec. Phys. **8**, 75 (1975)
   Jakubaßa, D.H., Kleber, M.: Z. Physik A **277**, 41 (1976)

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