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FINITE SIZE OF NUCLEUS AND VACUUM POLARIZATION IN HEAVY ATOMS

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НОВОСИБИРСК

distinction at small distances of a potential from the Coulomb one should be taken into account. The influence of the finite size of the nucleus on the induced-charge density has been investigated analytically in [7] at distances $R \ll r \ll \lambda_c$ (R is the nuclear radius, $\lambda_c = 1/m$ is the Compton wavelength of electron, m is the electron mass). At arbitrary distances but only for some concrete nuclei this problem has been investigated numerically in the papers cited above. Recently the influence of nuclear finite size on the contribution of self-energy diagram has been studied in [15].

In the present paper we consider analytically the change of induced-charge density $\delta\rho_{fs}(r)$, arising from the nuclear finite size, at distances much larger than R. We restrict ourself by the case $Z\alpha < 1$. A simple expression for $\delta\rho_{fs}(r)$ is obtained. The consideration is based on the use of the integral representation for the electron Green function in a Coulomb field. The expression obtained is very convenient for numerical calculations.

2 Green function and the induced-charge density

Let us pass to the calculations. According to the rules of the diagram technique the expression for the density of induced charge is of the form

$$\delta\rho(r) = -ie\int\frac{d\epsilon}{2\pi}Tr\gamma^0 G(\vec{r},\vec{r}|\epsilon), \tag{1}$$

where $G(\vec{r},\vec{r}\,'|\epsilon)$ is the electron Green function which we present as follows:

$$G(\vec{r},\vec{r}\,'|\epsilon) = \left\langle \vec{r}\left|\frac{1}{\gamma^0(\epsilon+V(r))-\vec{\gamma}\vec{p}-m}\right|\vec{r}\,'\right\rangle. \tag{2}$$

Here γ_μ are the Dirac matrices and $V(r)$ is the potential energy of an electron in the field of a nucleus. For $Z\alpha < 1$ the contour of integration over the energy ϵ in (1) goes from $-\infty$ to $+\infty$ below the real axis in the left half-plane of the variable ϵ and above it in the right one. The Green function has cuts along the real axis of ϵ from $-\infty$ to $-m$ and from m to $+\infty$, corresponding to a continuous spectrum. It also has simple poles, corresponding to a discrete spectrum, in the interval $(0, m)$. Using the analytical properties of the Green function we deform the contour of integration over ϵ in (1) so that it coincides finally with the imaginary axis.

Let us represent the potential energy $V(r)$ in the form

$$V(r) = -\frac{Z\alpha}{r} + U(r). \tag{3}$$

The function $U(r)$ is the difference between the potential energy of an electron in the real field of a nucleus and in a Coulomb field. So it differs from zero at the same distances as the nuclear-charge density $\rho(r)$.

Let us introduce the notation $\hat{P} = \gamma^0(\epsilon + Z\alpha/r) - \vec{\gamma}\vec{p}$. It is easy to check using the expansion over $U(r)$ that the following relation is fulfilled:

$$\frac{1}{\hat{P}-\gamma^0 U(r)-m} = \frac{1}{\hat{P}-m} + \\ +\frac{1}{\hat{P}-m}\left[\gamma^0 U(r) + \gamma^0 U(r)\frac{1}{\hat{P}-\gamma^0 U(r)-m}\gamma^0 U(r)\right]\frac{1}{\hat{P}-m}. \tag{4}$$

We represent $\delta\rho(r)$ as follows:

$$\delta\rho(r) = \delta\rho_c(r) + \delta\rho_{fs}(r) \tag{5}$$

where $\delta\rho_c(r)$ is the induced-charge density in the Coulomb field. Substituting (4) in (2) and then in (1), we obtain the following expression for $\delta\rho_{fs}(r)$:

$$\delta\rho_{fs}(r) = e\int\frac{d\epsilon}{2\pi}\int\!\!\int d\vec{r}\,'d\vec{r}\,''Tr\gamma^0 G_c(\vec{r},\vec{r}\,'|i\epsilon)\Big[\gamma^0 U(r')\delta(\vec{r}\,'-\vec{r}\,'') + \\ +\gamma^0 U(r')G(\vec{r}\,',\vec{r}\,''|i\epsilon)\gamma^0 U(r'')\Big]G_c(\vec{r}\,'',\vec{r}|i\epsilon), \tag{6}$$

where $G_c(\vec{r},\vec{r}\,'|i\epsilon)$ is the electron Green function in the Coulomb field. It easy to see that at least one of the arguments of the Green functions in (6) is small because of the presence of functions $U(r)$. Therefore, at the calculation of the Green functions in (6) only the angular moment $j = 1/2$ is significant. In Ref. [16] the convenient integral representation is derived for G_c that is valid in the whole complex ϵ plane. With the help of formulae (19) and (20) of [16] we find the contribution of angular moment $j = 1/2$ to the Coulomb Green function at imaginary energy (for simplicity, in the following we also use the notation G_c for this contribution):

$$G_c(\vec{r},\vec{r}\,'|i\epsilon) = -\frac{i}{4\pi rr'k}\int_0^\infty ds\exp\left[2iZ\alpha\epsilon s/k - k(r+r')\coth s\right]\times \\ \times\Big\{[1-(\vec{\gamma}\vec{n})(\vec{\gamma}\vec{n}\,')][(\gamma^0\epsilon - im)\frac{y}{2}I'_{2\nu}(y) - iZ\alpha I_{2\nu}(y)\gamma^0 k\coth s] + \\ +I_{2\nu}(y)\Big[[1+(\vec{\gamma}\vec{n})(\vec{\gamma}\vec{n}\,')](\gamma^0\epsilon - im) + \tag{7}$$

$$+mZ\alpha\gamma^0(\vec{\gamma},\vec{n}+\vec{n}\,') - \frac{k^2(r-r')}{2\sinh^2 s}(\vec{\gamma},\vec{n}+\vec{n}\,') - (\vec{\gamma},\vec{n}-\vec{n}\,')k\coth s\Big]\Big\}.$$

Here $I_{2\nu}(y)$ is modified Bessel function of the first kind, $\vec{n}=\vec{r}/r$, $\vec{n}\,'=\vec{r}\,'/r'$, $y=2k\sqrt{rr'}/\sinh s$, $\nu=\sqrt{1-(Z\alpha)^2}$, $k=\sqrt{m^2+\epsilon^2}$. If $\lambda_c\sim r\gg r'$, then the region $\epsilon\sim 1/r$ gives the main contribution to the integral over ϵ in the expression for $\delta\rho_{fs}(r)$. In this case in (7) $s\sim 1$, the argument of Bessel function $y\sim(r'/r)^{1/2}\ll 1$ and we can use the asymptotics

$$I_{2\nu}(y)\approx\frac{1}{\Gamma(2\nu+1)}\left(\frac{x}{2}\right)^{2\nu}, \tag{8}$$

If $r\gg\lambda_c\gg r'$, then $\epsilon\sim(\lambda_c/r)^{1/2}$, $k\approx m$, $e^{2s}\sim(r/\lambda_c)$ and $y\sim(r'/\lambda_c)^{1/2}\ll 1$. So, we can use the asymptotics of Bessel function again. Besides, it is convenient to perform in (7) the integration by parts over s in term proportional to $(r-r')$.

Let us use a trick substantially simplifying the calculations. In the present paper we consider spherically symmetric nuclear-charge distribution. It is obvious that the induced-charge density is also spherically symmetric function of r. So, we can multiply both sides of (6) by $d\vec{n}/(4\pi)$ and take the integral over the angles of unit vector $\vec{n}$. Making these transformations we obtain for $\delta\rho_{fs}(r)$:

$$\delta\rho_{fs}(r)=\frac{2e}{\pi^2\Gamma(2\nu+1)r^{2(1-\nu)}}\int_{-\infty}^{\infty}d\epsilon k^{4\nu}\iint_0^{\infty}\frac{ds_1ds_2}{(\sinh s_1\sinh s_2)^{2\nu}}\times$$
$$\exp\Big[2iZ\alpha\epsilon(s_1+s_2)/k-kr(\coth s_1+\coth s_2)\Big]\times$$
$$\left[\coth s_1\coth s_2+2m^2/k^2-1\right]F, \tag{9}$$

where

$$F=\int_0^{\infty}dr'(r')^{2\nu}U(r')+$$
$$+\frac{1}{32\pi}Tr\iint d\vec{r}\,'d\vec{r}\,''(r'r'')^{\nu-1}U(r')U(r'')\times \tag{10}$$
$$\Big[1-(\vec{\gamma}\vec{n}\,'')(\vec{\gamma}\vec{n}\,')+\nu[1+(\vec{\gamma}\vec{n}\,'')(\vec{\gamma}\vec{n}\,')]+iZ\alpha\gamma^0(\vec{\gamma},\vec{n}\,'-\vec{n}\,'')\Big]\gamma^0G(\vec{r}\,',\vec{r}\,''|0),$$

It is taken into account in (10) that in (9) $\epsilon\ll 1/R$ (R is the nuclear radius) gives the main contribution to the integral over energy. The arguments of

the Green function G in (10) satisfies the inequalities $r',r''<R\ll\lambda_c$. So one can set in (10) the energy ϵ to be equal to zero. In addition, at distances $r\sim R$ the function G does not depend on the electron mass. Thus, we can see that the factor F in (9) doesn't depend on r and on the parameter of integration ϵ. On the other hand, all dependence on the nuclear-charge distribution is contained in the factor F. Therefore, the contributions to $\delta\rho_{fs}(r)$ of large distances and small distances are factorized. The integrals in (9) are convergent and our expression doesn't require the renormalisation.

3 Calculation of the factor F

Let us pass to the calculation of F. Quite similarly to (4) we obtain the relation

$$\frac{1}{\hat{P}-\gamma^0U(r)-m}=\frac{1}{\hat{P}-m}+\frac{1}{\hat{P}-m}\gamma^0U(r)\frac{1}{\hat{P}-\gamma^0U(r)-m}, \tag{11}$$

or

$$G(\vec{r},\vec{r}\,'|i\epsilon)=G_c(\vec{r},\vec{r}\,'|i\epsilon)+\int d\vec{r}\,''G_c(\vec{r},\vec{r}\,''|i\epsilon)\gamma^0U(r'')G(\vec{r}\,'',\vec{r}\,'|i\epsilon) \tag{12}$$

We must find the asymptotics of Green function at $kr\sim kr'\ll 1$ ($k=\sqrt{m^2+\epsilon^2}$). At these distances $s\sim kr\ll 1$ gives the main contribution to the integral in (7). Replacing $1/\sinh s$ and $\coth s$ by $1/s$ in (7) and using ([17], p.303)

$$\int_0^{\infty}\frac{dx}{x}I_a(x)e^{-px}=\frac{1}{a(p+\sqrt{p^2-1})^a},$$
$$\int_0^{\infty}dxI_a(x)e^{-px}=\frac{1}{\sqrt{p^2-1}(p+\sqrt{p^2-1})^a}, \tag{13}$$

we obtain the asymptotics of the Coulomb Green function at small distances:

$$G_c(\vec{r},\vec{r}\,'|i\epsilon)\approx\frac{i}{8\pi\nu rr'}\left[\Theta(r-r')\left(\frac{r'}{r}\right)^{\nu}+\Theta(r'-r)\left(\frac{r}{r'}\right)^{\nu}\right]\times$$
$$\times\left[iZ\alpha\gamma^0[1-(\vec{\gamma}\vec{n})(\vec{\gamma}\vec{n}\,')]+(\vec{\gamma},\vec{n}-\vec{n}\,')+\nu\,\mathrm{sign}(r-r')(\vec{\gamma},\vec{n}+\vec{n}\,')\right] \tag{14}$$

This asymptotics doesn't depend on ϵ and m. It is seen from (12) that the asymptotics of the function G is also independent of these quantities. Let us represent the solution of the equation (12) in the form

$$G(\vec{r},\vec{r}'|i\epsilon) \approx \gamma^0[1-(\vec{\gamma}\vec{n})(\vec{\gamma}\vec{n}')]A_1(r,r') + \gamma^0[1+(\vec{\gamma}\vec{n})(\vec{\gamma}\vec{n}')]A_2(r,r') + \\ +(\vec{\gamma},\vec{n}-\vec{n}')\,iZ\alpha A_3(r,r') + (\vec{\gamma},\vec{n}+\vec{n}')\,iZ\alpha A_4(r,r'), \qquad (15)$$

where A_{1-4} are some functions. Substituting (15) in (12) we obtain a simple system of equations for A_{1-4}. Using (15) and (10) we get the following expression for F:

$$F = \int_0^\infty dr\, r^{2\nu} U(r) + 4\pi \iint_0^\infty dr\, dr'\, (rr')^{\nu+1} U(r) U(r') \times \\ \times \left[A_1(r,r') + \nu A_2(r,r') - (Z\alpha)^2 A_3(r,r')\right]. \qquad (16)$$

It follows from (16) that it is sufficient for us to find the functions

$$a_i(r) = 4\pi r^{\nu+1} \int_0^\infty dr' (r')^{\nu+1} U(r') A_i(r,r'), \quad (i = 1-4). \qquad (17)$$

Let us multiply both sides of the equations for $A_i(r,r')$ by $4\pi(rr')^{\nu+1}U(r')$ and then take the integral over dr'. As a result we obtain the system of equations for a_i. It is convenient to represent this system in the form

$$a_1(r) \mp \nu a_2(r) + (Z\alpha)^2 a_3(r) = \\ = Z\alpha \int_0^\infty dx U(x)\theta_\pm \left[a_2(x) \pm \nu a_3(x) - a_4(x)\right], \qquad (18)$$

$$a_1(r) + a_3(r) \pm \nu a_4(r) = \\ = \frac{1}{Z\alpha} \int_0^\infty dx U(x)\theta_\pm \left[\pm \nu a_1(x) + a_2(x) - (Z\alpha)^2 a_4(x) \pm \nu x^{2\nu}\right],$$

where $\theta_+ = \Theta(r-x)$, $\theta_- = -(r/x)^{2\nu}\Theta(x-r)$. From (18) and (16) we obtain the following relations:

$$F = 2\nu Z\alpha a_3(\infty),$$
$$a_1(\infty) + \nu a_2(\infty) = -(Z\alpha)^2 a_3(\infty), \quad a_1(\infty) + a_3(\infty) = \nu a_4(\infty). \qquad (19)$$

Actually, due to the rapid convergence of integrals we can use an arbitrary distance larger than nuclear radius as upper limits of integration in (18) and (19). Let us consider the functions

$$L(r) = \nu a_1(r) + a_2(r) + (Z\alpha)^2 a_4(r), \\ M(r) = Z\alpha[a_2(r) + \nu a_3(r) + a_4(r)]. \qquad (20)$$

From (18) by simple differentiation we obtain for this functions:

$$\nu \frac{d}{dr} M(r) = U(r)\left[L(r) + \nu r^{2\nu} - Z\alpha M(r)\right] \qquad (21)$$
$$\nu \frac{d}{dr} r^{-2\nu} L(r) = U(r) r^{-2\nu}\left[Z\alpha(L(r) + \nu r^{2\nu}) - M(r)\right].$$

Using (19), we get $M(\infty) = F$, $L(\infty) = 0$. Therefore, to calculate F it is sufficient to find $f(r)$:

$$f(r) = \frac{\nu r^{2\nu} M(r)}{L(r) + \nu r^{2\nu}}, \qquad (22)$$

since $F = f(\infty)$. From (21) we obtain for $f(r)$ the following closed equation:

$$\frac{d}{dr} f(r) = U(r)\left[r^{2\nu} - \frac{2Z\alpha f(r)}{\nu} + \frac{f^2(r)}{\nu^2 r^{2\nu}}\right]. \qquad (23)$$

It is convenient to make the substitution: $f(r) = \nu r^{2\nu} H(r)$. It is necessary to get the boundary condition for $H(r)$ at $r = 0$. In order to do that let us return to (21) and find the asymptotics of functions $M(r)$ and $L(r)$ at $r \to 0$. At small r we can leave in $U(r)$ only its singular part $Z\alpha/r$. It allows us to search the solution of (21) in the form $M(r) = br^\gamma$, $L(r) = cr^\gamma - \nu r^{2\nu}$, where b and c are some constants. From (21) we find $\gamma = \nu \pm 1$. However, the solution with $\gamma = \nu - 1$ doesn't satisfy the system for $M(r)$ and $L(r)$ written in the integral form because of the divergence of the integral over r at lower limit. So, finally we obtain: $\gamma = \nu + 1$ and $H(0) = b/c = Z\alpha/(1+\nu)$.

Solving the equation (23) at $Z\alpha \ll 1$ by the iteration over $U(r)$, we obtain in the first approximation

$$f^1(r) = \int_0^r U(x) x^{2\nu}\, dx. \qquad (24)$$

At small r the function $f^1(r)$ is equal to $Z\alpha r^{2\nu}/2\nu$ and is in agreement with the asymptotics $f(r) \approx Z\alpha\nu r^{2\nu}/(1+\nu)$, following from the boundary condition for $H(0)$, at $Z\alpha \to 0$ only.

Fig. 1 shows the dependence of $F/ < r^2 >^\nu$ on $Z\alpha$, where $< r^2 > = (Z|e|)^{-1} \int \rho(r) r^2 d\vec{r}$ is the mean squared radius of the nuclear charge-density, for the case of homogeneously charged sphere. For the othere nuclear charge distributions $\rho(r)$ (the charged spherical shell and the distribution used in [7] and consistent with the experimentally obtained) the corresponding curves coincides practically with that shown in Fig. 1. For all these distributions both total charge $Z|e|$ and mean squared radius $< r^2 >$ are equal. With the accuracy of a few percent all the curves are described by the formula

$$\mathcal{F} = \frac{Z\alpha\nu}{1+\nu}[< r^2 > /3]^\nu . \qquad (25)$$

For comparison the dependence of quantity $F^1/ < r^2 >^\nu$ on $Z\alpha$ ($F^1 = f^1(\infty)$, see (24)) is also shown in Fig. 1. It is seen that at $Z\alpha \sim 1$ the value of F essentially differ from that of F^1 obtained to the first order in $U(r)$.

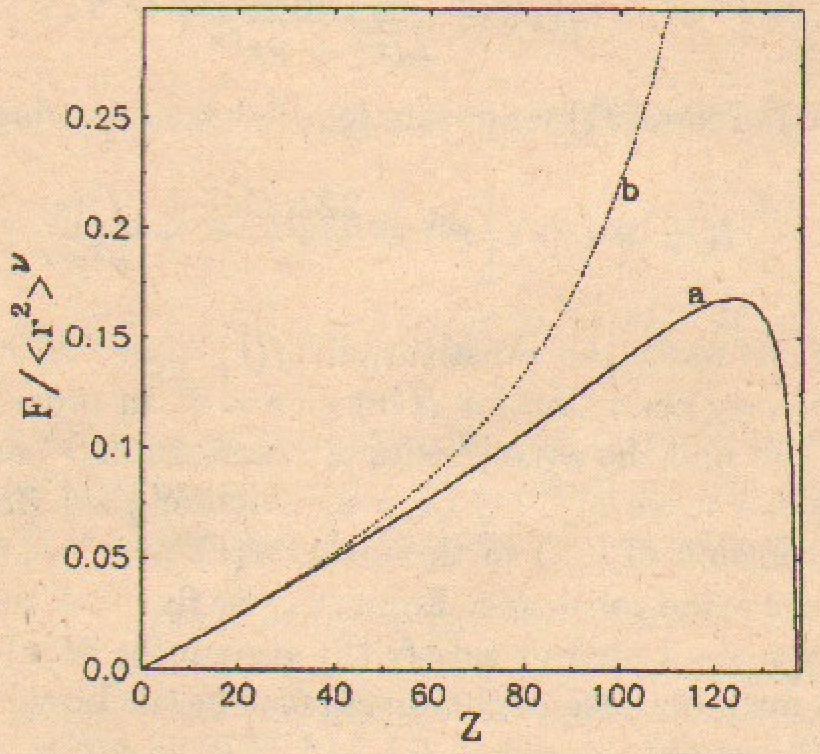

Fig. 1. a)—Factor F as a function of the nuclear charge Z; b)—Factor F^1, obtained to the first order in $U(r)$, as a function of Z.

In Ref. [7] the analytical expression has been obtained for $\delta\rho_{fs}(r)$ being valid at $R \ll r \ll \lambda_c$. The method of calculations in [7] essentially distinguished from that of ours. At small distances we can get the asymptotics of formula (9) and compare it with the result of [7]. Taking into account the factorization of large and small distance contributions, the function F should coincide with the corresponding factor of Ref. [7]. It is indeed so if we take into account the missed factor $r^{2\nu}$ in the right hand side of equation (30) from [7] (eq.(31) for the asymptotics contains this factor).

4 Asymptotics

Let us consider the behaviour of $\delta\rho_{fs}(r)$ at large and small distances in comparison with the Compton wavelength of an electron. At $r \gg \lambda_c$ $Z\alpha \sim 1$ the main contribution to the integral in (9) is made by the region $s_{1,2} \sim \ln(mr) \gg 1$, $|\epsilon|/m \sim (mr)^{-1/2} \ll 1$. Making the corresponding expansion and taking the elementary integrals at $mr \gg 1$, we obtain:

$$\delta\rho_{fs}(r) = \frac{e\, m^{3+2\nu} F}{\sqrt{\pi}\, 4^\nu\, \Gamma^2(\nu+1/2)} \frac{e^{-2mr}}{(mr)^{5/2}} \int_0^\infty dx x \exp[-\nu x - x^2/4mr] . \qquad (26)$$

If $\nu^2 \gg 1/mr$ then the integral in (26) is equal to $1/\nu^2$. If $\nu^2 \ll 1/mr$, then it is equal to $2mr$.

At small distances $R \ll r \ll \lambda_c$ the main contribution to the integral over ϵ is made by the range of integration $|\epsilon| \sim 1/r \gg m$. Replacing k in (9) by $|\epsilon|$, taking the integral with respect to ϵ and introducing the variables $T = s_1 + s_2$ $\tau = s_1 - s_2$, we get

$$\delta\rho_{fs}(r) = \left(\frac{eF}{r^{2\nu+3}}\right) \frac{\Gamma(4\nu+1)}{\pi^2\, 2^{2\nu}\, \Gamma^2(2\nu+1)} \times \qquad (27)$$

$$\times \int_0^\infty dT \int_0^T d\tau \frac{\cos(2Z\alpha T)\cosh\tau\,(\cosh T - \cosh\tau)^{2\nu}}{(\sinh T)^{4\nu+1}}$$

It is convenient to take the integral in (27) by the following way. First we pass from the variable τ to the variable x by the substitution $\sinh\tau = \sinh x \sinh T/(\cosh x + \cosh T)$ and take the integral over T. This integral is expressed via the Legendre function of the first kind $P^{-2\nu-1/2}_{2iZ\alpha-1/2}(\cosh x)$ and its derivative (see. [18], eq. (8.713(3))). Then we take the integral over x with the help of eq. (7.132(2)) from [18]. Finally we obtain the following result for the asymptotics at small distances:

$$\delta\rho_{fs}(r) = \left(\frac{eF}{r^{2\nu+3}}\right) \frac{2\nu\,\Gamma(4\nu+1)}{\pi^2\,(2\nu+1)} \left|\frac{\Gamma(\nu+iZ\alpha)}{\Gamma(2\nu+1)}\right|^4 \qquad (28)$$

This result is in agreement with that of [7].

Let us consider now the limit case $Z\alpha \to 0$. Setting $Z\alpha = 0$ in the integral in (9) and taking the integral first over s_1, s_2 and than over ϵ, we obtain after the simple calculations:

$$\delta\rho^{(0)}_{fs}(r) = \frac{2eF^{(0)}m^2}{\pi^2\, r^3} [K_0(2mr) + (mr + 1/mr)K_1(2mr)] , \qquad (29)$$

where $K_{0,1}(x)$ — are the modified Bessel function of the third kind, $F^{(0)} = \int_0^\infty r^2 U(r) dr$. The result (29) coincides with that obtained in the first order of perturbation theory from the usual relation in the momentum representation between the induced-charge density $\delta\rho(\vec{k})$ and the renormalized polarization operator $P(-\vec{k}^2)$ (see [19], section 114):

$$\delta\rho(\vec{k}) = -V(\vec{k})P(-\vec{k}^2)\,, \qquad (30)$$

where $V(\vec{k})$ is the nuclear potential in the momentum representation. Let us replace $\delta\rho(\vec{k})$ and $V(\vec{k})$ in (30) by $\delta\rho_{fs}(\vec{k})$ and $U(\vec{k})$ respectively and perform the inverse Fourier transform. Since $U(r)$ is not equal to zero only at small distances of the order of the nuclear radius, we can substitute $U(\vec{k})$ in the integral over $\vec{k}$ by $U(\vec{k}=0)$. As a result we obtain (29).

5 Conclusion

Simple analytical expression (9) for the indused-charge density, obtained exactly in $Z\alpha$, is valid for the distances much larger than the nuclear size R. This expression is very convenient for numerical calculations. The comparison of our results with the numerical results from [9] shows that formula (9) is applicable starting from $r \sim 10R$. Fig. 2 shows the dependence of $\delta\rho_{fs}(r)$

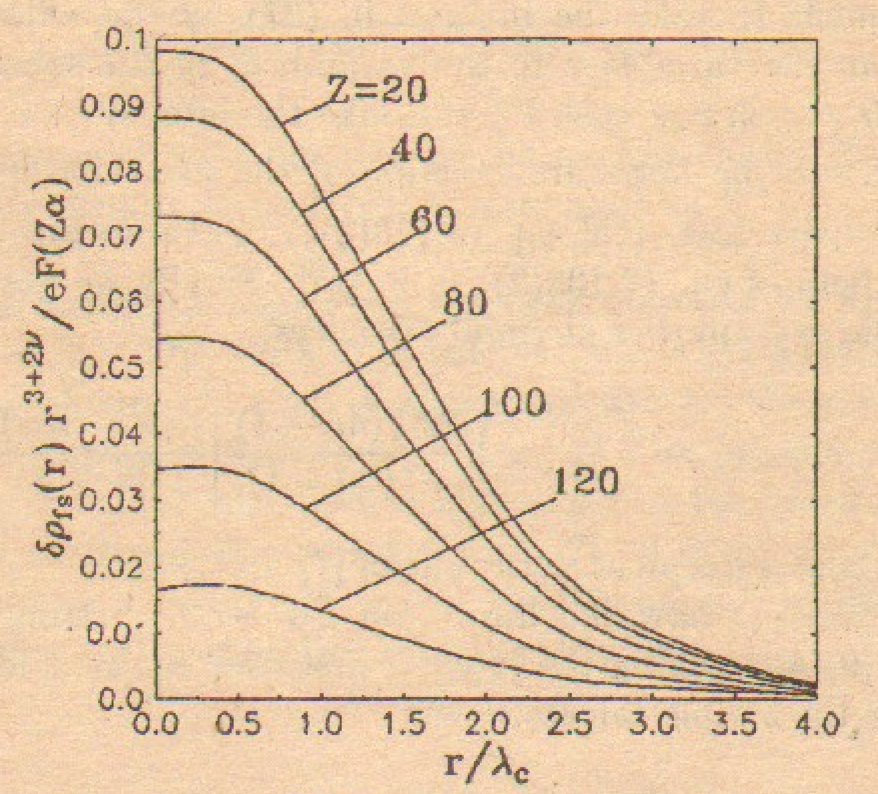

Fig. 2. The dependence of $\frac{r^{3+2\nu}}{eF}\delta\rho_{fs}$ on r for various Z.

on r for various $Z\alpha$. It is seen that the dependence on $Z\alpha$ is very essential.

Since the total induced charge is equal to zero, we can write the expression for the induced potential $\delta\phi_{fs}(r)$ as follows:

$$\delta\phi_{fs}(r) = 4\pi \int_r^\infty r'(1 - r'/r)\delta\rho_{fs}(r')\,dr'\,. \qquad (31)$$

Fig. 3 shows the dependence of the potential $\delta\phi_{fs}(r)$ on $Z\alpha$. Emphasize again that all dependence on the nuclear charge density $\rho(r)$ is contained in the factor F (10). Moreover, for the realistic distributions $\rho(r)$ this factor is determined by the value of mean squared radius $< r^2 >$ (see (25)).

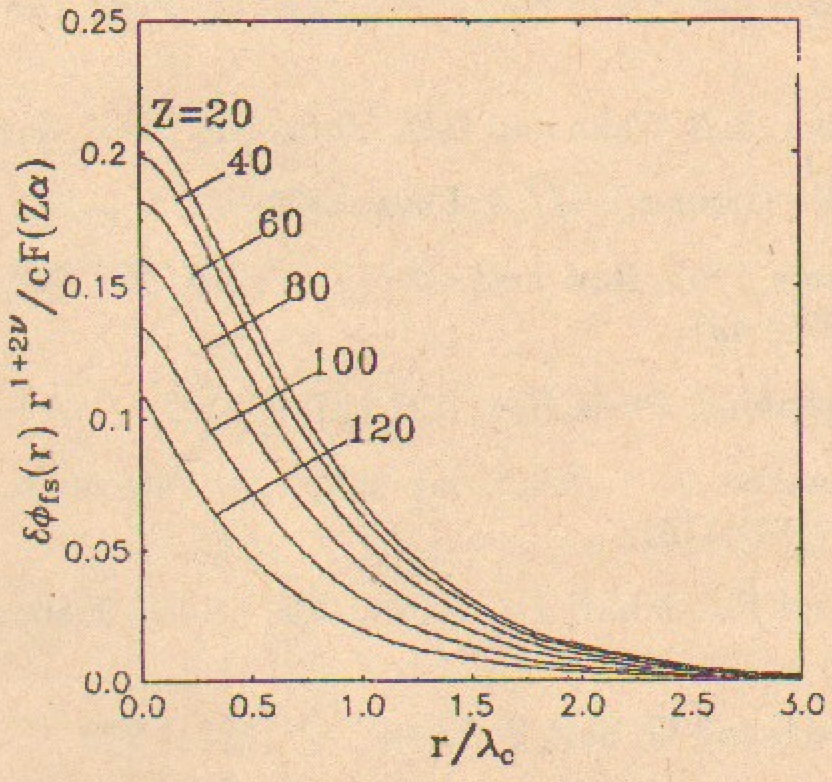

Fig. 3. The dependence of $\frac{r^{1+2\nu}}{eF}\delta\phi_{fs}$ on r for various Z.

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