Screening in a system with localized electrons

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Computer modeling is used to study the screening of an external electric field by a disordered system with localized electron states. The disordered system is an impurity band in a lightly doped compensated semiconductor. It is shown that at low temperatures the field averaged over the donor and acceptor coordinates or over a sufficiently large surface decreases with depth in the system over distances of the order of the average separation between the impurities, whereas the average of the absolute value of the field decreases with depth over a much greater distance governed by the field or temperature.

§ 1. QUALITATIVE CONSIDERATIONS

We shall consider a system in which electron states are localized in the vicinity of the Fermi level. We shall discuss specifically an impurity band in a lightly doped and compensated n-type semiconductor at temperatures much lower than the donor ionization energy, when each acceptor captures an electron and is charged negatively, whereas the remaining electrons fill only some of the donors. The vacant donors are positively charged and the filled donors are neutral. In spite of the absence of free electrons, a system of this kind screens the external field or charges introduced from outside because of a redistribution of electrons between donors. No particular difficulties are encountered in the description of such screening if the temperature is higher than the energy scatter of the levels (impurity band width). In this case the screening is of the Debye type and the screening radius is

$$r_s = \left( \frac{\varepsilon N_s}{4\pi(1-K)N_nd^2} \right)^{1/2},$$

where $\varepsilon$ is the electron charge; $\varepsilon_0$ is the permittivity of the lattice; $T$ is the temperature in energy units; $N_d$ is the donor concentration; $K = N_A/N_D$ is the degree of compensation; $N_A$ is the acceptor concentration.

At low temperatures the problem becomes complicated by the fact that the correlations associated with the electron-electron interactions are very important. At absolute zero the problem of the screening can be formulated as follows. We have to find the ground state of the system in an electric field and in the absence of the field, and then compare the energies and charge distributions.

In the present section we shall determine the charge distribution in an external field in the form that we shall postulate without—at this stage—justification and in the next sections we shall describe computer experiments carried out to study the problem.

A. Screening of absolute zero

We shall consider the half-space $x < 0$ which is filled with the system under consideration. We shall assume that outside this half-space there is a static electric field $E$ directed along the $x$ axis. The question is: does the field decay in the half-space $x > 0$? We can answer this question by postulating the following qualitative picture. Excess electrons migrate to the surface so as to screen the field. The density of the excess surface charge $\sigma$ is determined uniquely by the selected field: $4\pi r_0 \sigma = E$. If we bear in mind that the electron charge is discrete, we find that excess electrons form an irregular lattice with a period of the order of $\left( \frac{4\pi r_0}{E} \right)^{1/2}$. When the field is reduced, the period of this lattice tends to infinity. We can easily describe now the field pattern in the half-space. Near the "sites" of this lattice the field is compensated, whereas between the "sites" it penetrates into the half-space to a depth of the order of

$$r_0 = \left( \frac{4\pi r_0}{E} \right)^{1/2},$$

which becomes infinite in the limit $E \rightarrow 0$. Therefore, in a certain sense the screening is nonlinear. This circumstance is pointed out in Refs. 2 and 3, where it is attributed to the Coulomb gap, i.e., to the vanishing of the density of states at the Fermi level. Essentially, the preceding discussions are based on two assumptions, which are the only ones needed in the derivation of the Coulomb gap: the electron states are localized and the interaction is in accordance with the Coulomb law.

A full description of the screening can be provided if we can say at what distance from the surface is the screening lattice of excess electrons located. We shall assume that this distance is of the order of the average separation between impurities: $r_s \approx N_d^{-1/2}$. However, if the external field is considerably less than the fields exerted by one electron on another, then $r_s \propto r_0$. Moreover, by definition, the distance $r_s$ is independent of $E$. The low-temperature Debye radius of Eq. (1) reduces to this distance at the low-temperature limit of the validity of this equation, i.e., at $T \ll N_d^{1/2}/r_0$ (the case of strong compensation $1 - K \ll 1$ requires a separate discussion).

We shall now consider the field averaged in a plane parallel to the surface of the half-space. In view of the linearity of the electrostatic equations, this field is governed by the average charge which, in accordance with the above discussion, decreases steeply on increase in $x$ in the range $x > r_0$. Hence, it follows that the average field in this plane decreases at a distance of the order of $r_0$.

It is pointed out in Ref. 5 that in a planar surface layer the density of states responsible for the change in the carrier density because of a change in the Fermi level position does not
not have a Coulomb gap. This density is constant and gov-
erned by the total impurity concentration. In the geometry
under discussion the average thickness of the space charge
layer can be estimated from \( r_n = (R_g / \bar{u})^{-1/2} \), where \( g_0 \) is
the density of states for a moderate compensation of the or-
der of \( N_g^0 / \bar{u_0}^2 \). This estimate shows that the length \( r_n \) is of
the order of the average separation between impurities.

It therefore follows that the proposed description is
characterized by two different lengths representing the
screening effect. The square of the field averaged over a
plane parallel to the surface decreases at a distance of \( r_n \),
whereas the average field in such a plane decreases at a dis-
tance \( r_0 \). This is true of any geometry.

We shall consider a body of arbitrary shape and charac-
teristic size \( R \), subjected to a homogeneous electric field \( E \). If
this body is so large that \( R \gg r_n \), we can introduce a field
averaged over distances large compared with \( r_n \) but small
compared with \( R \). Such a field decreases with depth in
the body over a distance of the order of \( r_n \), whereas outside the
body it is identical with the field calculated on the assump-
tion that the body is metallic. However, the average square of
the field decreases only at a depth \( r_n \) and at distances short compared with \( r_n \) the field differs very little from the
average value. On the other hand, if the body is small, so that
\( R \ll r_n \), but still macroscopic, i.e., if \( R \gg r_0 \), then the dipole
moment induced in such a body does not have the same di-
rection as the external field and its magnitude is a random
quantity, i.e., it changes significantly on transition from one
configuration of donors and acceptors to another. This is
explained by the fact that if \( R \approx r_n \), then the screening
charge consists of about one electron.

In considering a body in an external field, we may face
the question what is the field at the point \( r \) when it is aver-
ergaged over all possible donor and acceptor configurations.
Within the framework of the proposed description of the
screening, the answer is as follows. When the screening
charge is averaged over the various configurations, its dis-
crete nature is lost completely. The average screening charge
is smeared out in a surface layer of thickness \( r_n \). If \( R \gg r_n \),
then the average field outside the body is the same as in the case
of metallic solid, whereas the average field inside the body falls
at a distance of the order of \( r_n \). This is true for \( r \gg r_n \) or \( r \ll r_0 \), but if \( R \approx r_n \), the induced dipole moment exhibits a
very strong dispersion on transition from one configuration
to another, although its average value is still the same as that
for a metal.

Unfortunately, we cannot provide a rigorous justifica-
tion of the proposed screening pattern, although in the next
sections we shall give supporting results of a computer mod-
eling. Moreover, we cannot say that this pattern is a definite
consequence of the localization states and of the discrete
nature of the electron charge. Let us examine, for example,
the screening of an external field in a classical Wigner crystal
which is formed by a classical electron class with a homogen-
eously charged three-dimensional background. In this case
we have both localization of one-electron states and the
core screening of the point charge, but it is clear that there is no large length
which depends on the field. The excess charge appears sim-
ply because of an increase or reduction in the lattice constant
of a Wigner crystal in the surface layer. Therefore, a weak
field is completely screened over a distance of the order of the
lattice constant and nonlinear screening does not appear.

It follows that in the case of a Wigner crystal the screening of
an external field does not occur in accordance with the pic-
ture proposed above. In our picture it is assumed that the
screening is due to a small number of excess electrons which
have little influence on the structure of the ground state in a
weak field. In the case of a Wigner crystal a weak field shifts
all the surface electrons. It seems to us that this mechanism
cannot operate in the case of a disordered system in which
the short-range order is governed by the donor and acceptor
configurations, and changes in this order require large en-
gies.

B. Estimate of the dispersion of the polarizability at zero
temperature

We shall consider a sphere of radius \( R \) in an external
field \( E \). It follows from the above discussion that the average
(over the system) density of the screening charge is \( -E \) and
the total screening charge in the sphere is \( -ER^2 \), \( R^2 \) is
the order of the average separation between impurities.

The average electric field \( E \) on a point \( r \), far enough from the
sphere, does not change significantly on transition from one
configuration to another. Therefore, it follows that the
average screening charge is \( -E \) on a sphere surface and \( 0 \) in
the interior.

In the opposite limiting case, \( ER \gg 1 \), for the majority of
the configurations of the donor and acceptor coordinates, i.e.,
for the majority of such spheres, a dipole consisting of two
charges separated by a distance \( R \) does not appear at all un-
der the action of the electric field. The probability of its ap-
pearance is of the order of \( f(R) \approx ER^2 / e < 1 \). The average
dipole moment \( \bar{P} \) of the order of \( f(R) \approx ER^2 / e \), i.e., it is of
the same order as for a conducting sphere of radius \( R \).

However, the dispersion of the dipole moment is

\[ \bar{P} - P = e \bar{E} \bar{P} = \alpha (\epsilon/\epsilon_0) \bar{E} \bar{P}, \]

where the second term is small compared with the first. The
relative fluctuation of the dipole moment

\[ P^2 - \bar{P}^2 = \alpha (\epsilon/\epsilon_0) \bar{E} \bar{P}, \]

is large. A fluctuation of the polarizability \( \alpha \), defined by the
relationship \( P = \alpha E \), is of the same order of magnitude. We
therefore find that the rms value of the relative deviation of
the polarizability of a sphere of radius \( R \) is of the order of

\[ \alpha \sqrt{\alpha} \approx \alpha \bar{E} \bar{P}. \]
We shall consider a sphere of radius $R$ with an excess charge at its center. The majority of the changes inside the sphere experience an electric field $E = e/\varepsilon_0 R^3$. It is found that for any sphere the length $\tau_E$ introduced above is of the order of the sphere radius. This is to be expected because for any radius $R$ the screening charge consists of one electron. In subsection 4 we have mentioned that the field averaged over a distance greater than $\tau_E$ fluctuates weakly in space and is not greatly affected when one distribution of coordinates is changed to another. When a point charge is screened, the field averaged over any sphere with a charge at the center fluctuates strongly. Therefore, the potential of a point charge is a strongly fluctuating random quantity at any distance.

Efron in fact assumed that the screening is of the insulator type, i.e., that the rms potential or the average of the absolute potential decreases in accordance with the Coulomb law

$$\langle \Phi \rangle = e/\varepsilon_0 R^3. \tag{5}$$

Here, $\Phi$ is the permittivity which appears because of the polarization of pairs of donors with an internal distance of the order of $\tau_E$, where $\tau_E \propto e$. (The value of $\Phi$ is of the order of infinity—see Ref. 6.) Essentially, Eq. (5) means that the main contribution to the permittivity appears for short distances because the permittivity does not exhibit spatial dispersion over distances $\gg \tau_E$. In this approximation the charge carriers are "electron polarons" which are electrons creating pair polarization during their motion. In fact, they can be regarded as electrons in a medium with the permittivity $\varepsilon_0$. Then, the density of the polaron states near the Fermi level is

$$\rho(0) = \frac{e^2}{\varepsilon_0 h^3} x_0^2. \tag{6}$$

However, we cannot exclude the possibility that $\rho(0)$ decreases in accordance with the power law: $\rho(0) \propto x_0^{q-1}$, where $q > 1$ is an unknown index. In this case the formula (6) becomes invalid. Unfortunately, the modeling for which the results are given in the next section cannot provide a sufficiently reliable value of the index $q$.

D. Screening and finite temperatures

We have mentioned earlier that at temperatures which are high compared with the impurity band width the screening is of the Debye nature. Naturally, in this case the surface density of the screening charge $\sigma$ is related to the field $E$ by the same expression $E = 4\pi\sigma$, but the charges undergo thermal motion, so that averaging with respect to time destroys completely the effects of the discreteness of the electric charge.

The question arises whether this suppression occurs at any temperature, no matter how low or only in the Debye range. It seems to us (although this cannot be regarded as proved) that low-temperature excitations in the system under consideration are electron transitions in donor pairs with large internal distances. These transitions do not alter basically the structure of the ground state, which is determined by the immobile charged acceptors. Therefore, if the temperature is sufficiently low, the charge positions vary little with time so that the discreteness of the electron range remains important even after averaging with respect to time. As at zero temperature, this discreteness may be manifested by the dispersion of the polarizability which appears as we go over from one impurity configuration to another. We shall still consider a sphere of radius $R$. It follows from the hypothesis of a Coulomb gap that the number of possible electron transitions from one donor to another located at a distance $R$ is very low if we consider only the transitions that require an energy which does not exceed $T$. If $T < 4\varepsilon_0 e^2/\varepsilon_0 R$, this number is independent of $\Lambda$ and proportional to $T$. These two statements are sufficient to show that the number in question is of the order of $\varepsilon_0 e^2/\varepsilon_0 R$. Hence, it follows that when temperature is lowered the dispersion becomes strong for $T > 4\varepsilon_0 e^2/\varepsilon_0 R$ and that

$$T < 4\varepsilon_0 e^2/\varepsilon_0 R. \tag{7}$$

 Naturally, the inequality $T < \varepsilon_0 e^2/\varepsilon_0 R$ should then be satisfied. Equation (7) reduces to Eq. (4) when $T = \varepsilon_0 e^2/\varepsilon_0 R$.

§ 2. COMPUTER MODELING

A. Absolute zero

The program of modeling at zero temperature was as follows. A method described in Ref. 7 was used to find the ground state of a system comprising $N$ donors and $N/2$ acceptors in a homogeneous electric field and in the absence of such a field. Half the donors should be neutral and the other half charged. The ground state is determined by finding the set of occupation numbers characterizing the charge state of each donor and ensuring a minimum of the total electrostatic energy of the system. The projection of the dipole moment on an axis parallel to the field is calculated for each of these states. The polarizability per one donor is found from

$$\alpha = (P_{\parallel} - P_{\perp})/eN, \tag{8}$$

where $P_{\parallel}$ and $P_{\perp}$ are, respectively, the projections of the dipole moment along the field direction in the presence and absence of the field. The vector $P$ is given by the expression

$$P = \sum_{i=1}^{N} \left( 1 - n_i \right) \mathbf{r}_i - \sum_{i=1}^{N} n_i \mathbf{r}_{\mathrm{ac}},$$

where $\mathbf{r}_i$ is the radius vector of a donor and $\mathbf{r}_{\mathrm{ac}}$ is the radius vector of an acceptor. If a donor $i$ is occupied, we have $n_i = 1$, but if it is vacant, we find that $n_i = 0$. The quantity $\alpha$ was averaged over many configurations of donors and acceptors and its dispersion was found. The modeling was carried out for sets with $N = 200$ and $N = 50$ in the form of a sphere and an ellipsoid of revolution (the latter only for $N = 200$).

The unit of length is the average distance between the donors $\xi_{\mathrm{HD}}$ and the energy and temperature are measured in units of $e^2/\varepsilon_0 \xi_{\mathrm{HD}}$. In terms of such units the radius of the sphere is $R = (\sqrt{3}/4\varepsilon_0)^{1/3}$. An electric field (in units of $eN^2/\varepsilon_0 \xi_{\mathrm{HD}}$) is 0.03, 0.05, 0.07, 0.1, 0.15, and 0.2. Within the limits of the calculation error, there is no systematic dependence of the average polarizability on the field. It is found that for a system in the form of a sphere the average value is $0.19 \pm 0.02$ for $N = 200$ and $0.16 \pm 0.03$ for $N = 50$. The polarizability is averaged over 40 configurations of the don-
nor and acceptor coordinates for $N = 200$ and over 85 configurations for $N = 50$.

In our units the polarizability of a metallic sphere is

$$\alpha_m = 3/4a = 0.239.$$  

The deviation of the observed average values from this $\alpha_m$ is due to the finite nature of the screening radius $r_o$. In the Appendix we shall derive an expression for the polarizability of a sphere $\alpha$ on the assumption that the screening is linear, i.e., that the density of the screening charge is $\varrho(r)/4\pi r_o^3$, where $\varrho(r)$ is the potential at the point $r$ and $r_o$ is the screening radius. In the Debye theory this expression should be identical with Eq. (1). In general, it can be calculated by substituting in Eq. (A.5) the values of $\alpha$ found by modeling. If $r_o/R < 1$, then Eq. (A.5) becomes

$$\alpha_n = \alpha_m r_o/R.$$  

It follows from Eq. (9) and from the above data that $r_o = 0.25$ both for $N = 200$ and $N = 50$. We shall now consider not a sphere but an elongated ellipsoid of revolution for the same set with $N = 200$ and with the axial ratio $r_3/r_1$. The average of 60 realizations of the polarizability was found to be $\alpha = 0.52 \pm 0.04$. The polarizability of the corresponding metallic ellipsoid would be $\alpha = 0.68$.

If we apply to the ellipsoid a formula similar to Eq. (9),

$$\alpha_n = \alpha_m r_o/r,$$  

where $S$ and $V$ are the surface area and the volume of the ellipsoid, we again obtain $r_o = 0.25$.

It follows that the polarizability averaged over the various configurations is the same as for a conducting solid of the same shape with a very small screening radius.

However, the directions and absolute values of the dipole moments of the individual configurations differ greatly from one another and from the situation encountered in an ideal conductor. This is manifested by the anomalously strong dispersion of the polarizability. Figure 1 shows this dispersion as a function of the electric field. The results should be compared with Eq. (4). We can see that when dispersion for $N = 200$ is multiplied by $(200/50)^{1/3} = 1.59$, the data for $N = 200$ and $N = 50$ become identical, in agreement with Eq. (4). We can also see that for large values of the dispersion [and Eq. (4) is only valid for such values!] the dependence is close to the square-root type.

The screening of a point charge at the center of a sphere can be studied by assuming that this is a unit charge and by finding the ground state of a system with $N = 200$ without and with a charge. Then, at six points in a sphere of radius $R$, at which the Cartesian coordinates intersect a sphere of radius $r$, we can define the value of $\varrho(r)$ as the difference between the electrostatic potentials at the center in the presence and absence of a charge ($i = 1, 2, \ldots, 6$). Then, calculating the average value for the sphere we obtain

$$\varrho(r) = \frac{1}{6} \sum_{i=1}^{6} \varrho_i(r).$$

The values of $r$ were selected to be as follows: $1/5, 2/5, 3/5, 4/5, 1, 2, 5$ in units of the radius $R$ of the sphere. This procedure was carried out for 60 configurations of the donor and acceptor coordinates and averaging was carried out over the realizations of the quantities $\varrho(r)$ and $|\varrho(r)|$. This gave $\varrho(r)$ and $|\varrho(r)|$, respectively. The results are presented in Fig. 2. If $r > R$, the potential fluctuates weakly and it amounts to $1/r$ in terms of the adopted units. However, if $r < R$, the fluctuations are so strong that very different results are obtained by different averaging methods. In particular, it is clear that $\varrho(r)$ decreases much more steeply than does $|\varrho(r)|$. For comparison, we plotted two figures in Fig. 2. The continuous curve represents the function

$$\varrho(r) = \exp\left[-\frac{r}{r_o}\right] - \frac{r_o}{r},$$

which applies to linear screening with the radius $r_o < R$, whereas the dashed curve is the function

$$\varrho(r) = \frac{1}{1/r_1 + 1/R + 1/R},$$

corresponding to the potential of a charged insulator sphere with a permittivity $\varepsilon$. It seems to us that $\varrho(r)$ fits well the curve of Eq. (11) with $r_o = 0.45$ in units of the average distance between the donors, whereas $|\varrho(r)|$ is close to the function (12) with $\varepsilon = 2.5$. This corresponds qualitatively to the ideas put forward in §1.

B. Modeling at finite temperatures

At finite temperatures the main results can be obtained by means of the fluctuation-dissipation theorem. The polarizability is calculated from

$$\alpha = \left<\Delta P^2\right>/2TN,$$  

where $\left<\ldots\right>$ denotes averaging over a cycle of Monte Carlo steps, i.e., it denotes averaging with respect to time, where the bar still represents averaging over the realizations. The results obtained below were obtained for sets with $N = 200$ and $N = 50$. The modeling program was described in Ref. 8. The number of the Monte Carlo steps increases as a result of cooling. The cycle ceases as soon as the number of electron transitions reaches 12 000. By increasing this number we can

**FIG. 1.** Dependence of the relative value of the rms deviation of the polarizability on the electric field. $\bigcirc$ for $N = 50$, averaging over 85 coordinate configurations; $\square$ for $N = 200$, values multiplied by $10^3$, averaging over 40 coordinate configurations. The curve represents Eq. (4).
demonstrate that 12,000 transitions are sufficient for the convergence of the process at all the investigated temperatures. The results of the calculation were averaged over the various configurations of donor and acceptor coordinates. The modeling was carried out at temperatures $T > 0.05$. Figure 3 shows the temperature dependence of the polarizability. This curve demonstrates the results of the Debye theory according to which the screening radius $r_\sigma$ is equal to $r_\sigma$, and it is described by Eq. (1) (see the Appendix). Since the donor concentration is taken to be unity, spheres with $N = 200$ and $N = 50$ have different radii and their polarizabilities per donor differ at high temperatures, when $r_\sigma$ becomes comparable with the sphere radius $R$. Figure 4 shows the dependence $r_\sigma(T)$ obtained using the function $\alpha(r_\sigma)$ calculated in the Appendix and the values of $\alpha$ are found from the modeling results. This figure shows also the dependence $r_\sigma(T)$ corresponding to the Debye theory. We can see that if $T \geq 0.2$, then we can in practice use the Debye theory which formally should be valid only for $T > 1$. This is clearly due to the fact that the Coulomb gap structure is destroyed at a very low temperature, as pointed out by Davies et al. This circumstance interfered with our attempt to check the hypothesis of two screening lengths at finite temperatures. The longer length should be manifested by an anomalous dispersion of the polarizability. Our results indicated an increase in the dispersion in the range $T < 0.2$ (Fig. 5). However, at the temperatures that could be considered in our analysis the dispersion did not reach 100% and we were unable to check Eq. (7). One would have to increase the size of the set used in the computations and to lower the temperature.

In addition to a modeling utilizing the fluctuation-dissipation theorem, we also carried out a modeling in which a system was "frozen" in a finite electric field and then thermal motion was "activated" and the polarizability was determined. However, this procedure did not give any basically new results.

The main conclusions were as follows: at absolute zero the screening is characterized by two lengths $r_\sigma$ and $r_{\sigma\sigma}$, and this is manifested by an anomalous dispersion of the polarizability...
FIG. 5. Temperature dependence of the relative value of the rms deviation of the polarizability: \( N = 50 \), averaging over 25 coordinate configurations; \( N = 200 \), averaging over 10 coordinate configurations (the value of \( N = 200 \) is multiplied by 2 in order to fit the high-temperature limits for the two sets).

ability in weak fields; when a point charge is screened, the potential at large distances from the charge is random and decreases slowly, whereas the average potential over all the configurations decreases rapidly; at finite temperatures the range of validity of the Debye theory with a radius \( r_1 \) defined by Eq. (1) extends deep into low temperatures. This circumstance does not allow us to "match" the data on the dispersion at zero temperature with those obtained for finite temperatures.

APPENDIX
Calculation of the polarizability of a sphere of radius \( R \) with a given screening radius \( r_1 \)

We shall select the origin of the coordinate system at the center of the investigated sphere. The potential outside the sphere is

\[
q^{(o)} = -E r \cos \theta + a E \cos \theta / r,
\]

(A.1)

where \( \theta \) is the angle between the vector \( r \) and the field \( E \). The potential inside the sphere is given by

\[
\Delta q^{(i)} = r_1 q^{(o)}.
\]

(A.2)

A solution of this equation is

\[
q^{(i)} = r^{(-\kappa)} \cos \theta [C_1 J_\kappa (r_1 r) + C_2 K_\kappa (r_1 r)],
\]

(A.3)

where \( C_1 \) and \( C_2 \) are constants and \( J_\kappa (x) \) and \( K_\kappa (x) \) are modified Bessel and Hankel functions, respectively. Dropping the terms which diverge at zero, we find that the potential inside the sphere is

\[
q^{(i)} = r^{(-\kappa)} \cos \theta [C_1 J_\kappa (r_1 r) + C_2 K_\kappa (r_1 r)],
\]

where \( C \) is a constant which must be determined.

Matching the functions \( q^{(o)} \) and \( q^{(i)} \) and their normal derivatives on the surface of the sphere \( (r = R) \), we obtain an equation which relates the polarizability \( \alpha \) to the screening radius \( r_1 \):

\[
2\alpha/R^3 + 1 = \frac{e^{-z}}{z} \left[ \frac{1}{2} \left( e^{2z} - 2e^z + 1 \right) + e^z \left( 2e^{-z} - 2e^{-2z} - 2z \right) \right],
\]

(A.5)

where \( z = R / r_1 \). If \( R > r_1 \), we find from Eq. (A.5) that

\[
a/R^3 = 1 - 3r_1/R.
\]

(A.6)

If \( R < r_1 \), then

\[
a/R^3 = 15\pi r_1^3.
\]

If we describe \( ro(T) \) using Eq. (1), we obtain from Eq. (A.6) the expression

\[
a/R^3 = \alpha R^3 / 15T.
\]

Translated by A. Tybudowicz