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Hypernetted-chain theory of charged impurity with mixture formalism

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The variational binary-mixture theory is applied to the case of a positron or proton embedded in electron gas. The Euler-Lagrange equation for the electron density fluctuation is solved. The numerical results are very similar to the ones obtained with our previous external-field formulation. The positron annihilation rate comes out slightly smaller than the experimental one from the mixture formalism. The singularity due to the bound state is shown to be outside of the metallic range. If we consider a massive impurity, the local-field correction to the dielectric function of the electron gas can be written in closed form in terms of the liquid structure function alone, which can be considered as a new self-consistency condition. We have also devised a new iteration method for the ground-state radial distribution function which does not apply the linearization technique.

I. VARIATIONAL EQUATION FOR IMPURITY

The variational inhomogeneous hypernetted-chain method (GHNC) has been previously shown to be working reasonably well in the case of a charged impurity embedded in the homogeneous electron gas.[1] The impurity problem can also be formulated as a zero-concentration limit of a binary mixture. The variational theory of binary mixtures has recently been utilized to obtain ground-state properties of two-component Bose fluids[2] and to study ^{3}He atoms in ^{4}He liquids.[3]

In order to treat the impurity in electron gas we consider the mixture of a Bose and a Fermi liquid. We use the trial function

$$\psi=\prod_{i,j}^{N_1N_2} f_{12}(\vec{r}_{1i}-\vec{r}_{2j})\prod_{i,j}^{N_1} f_{11}(\vec{r}_{1i}-\vec{r}_{2j})\prod_{i,j}^{N_2} f_{22}(\vec{r}_{2i}-\vec{r}_{2j})\phi_{11}\prod_{i=1}^{N_2} F(\xi_i)\ , \tag{1}$$

where N_1 is the number of electrons and N_2 the number of impurity particles, $f_{\alpha\beta}$ is a pair-correlation function between particles α and β, and ϕ_{11} is the Slater determinant of electrons. To allow for the possibility of having internal structure for the impurities we have also included the internal wave function F, depending only on the intrinsic coordinates ξ. By using the Lado approximation[4,5] for the squared Slater determinant and the kinetic energy in Jackson-Feenberg form one can readily utilize the formulas for boson mixtures presented in Ref. 2. Taking the zero-concentration limit $N_2=1$ there, we obtain for the total energy E the expression

$$E=N_1\epsilon_0(\rho_1)+\epsilon_c\ , \tag{2}$$

where $\epsilon_0(\rho_1)$ is the energy per particle of the homogeneous electron gas calculated at the density $\rho_1=N_1/V$. The correlation energy ϵ_c between the host system and the impurity is now given by

$$\epsilon_c=\epsilon_I+\frac{\hbar^2}{2\mu}\int[\nabla\sqrt{\rho(r)}]^2d\vec{r}+\int\rho(r)V(r)d\vec{r}+\frac{1}{2}\frac{1}{(2\pi)^3\rho_1}\int\delta^2(k)\chi(k)d\vec{k}\ . \tag{3}$$

Here ϵ_I is the internal energy of the impurity, $\rho(r)$ is defined to be ρ_1 times the distribution function g_{12} between the electron and the impurity, μ is their reduced mass, and $V(r)$ their interaction potential. Hence, the Fourier transform of the density fluctuation $\delta(r)$ of Ref. 1 is now given by

$$\delta(k)=\rho_1\int e^{i\vec{k}\cdot\vec{r}}(g_{12}-1)d\vec{r}\ .$$

The function $\chi(k)$ of Ref. 1 is now written in terms of the liquid structure factor $S(k)$ of the host electron gas in the form

$$\chi(k)=-\frac{\hbar^2}{4m}k^2\frac{S-1}{S^2}\left[\frac{m}{\mu}S+1\right]\ . \tag{4}$$

This expression is much simpler than the one in

Ref. 1. The function $\psi(r)$ of Ref. 1 would contain the effect three-body correlations which we neglect here. Otherwise the theory is formally the same. Hence we obtain the Euler-Lagrange equation

$$-\frac{\hbar^2}{2\mu}\nabla^2\sqrt{\rho}+[V(r)+W(r)]\sqrt{\rho}=0\ ,$$
$$W(r)=\frac{1}{(2\pi)^3\rho_1}\int\delta(k)\chi(k)e^{i\vec{k}\cdot\vec{r}}d\vec{k}\ , \tag{5}$$

for $\sqrt{\rho}$ either by directly varying the expression (2) with respect to $\sqrt{\rho}$ or by passing to the zero-concentration limit in the corresponding binary-mixture equation. In this connection it is interesting to note that if we take the impurity to be identical with the host particles we will recover from Eq. (5) the Euler-Lagrange (EL) equation describing the background while expression (3) tends to the chemical potential of the background and not to ϵ_0. If $V(r)$ in Eq. (5) is taken to be the Coulomb potential we see that ρ satisfies the usual cusp condition

$$\left.\frac{\rho'}{\rho}\right|_{r=0}=-\frac{2Q}{m}\frac{me^2}{\hbar^2}\ . \tag{6}$$

Since S behaves at small k like $\hbar/4e\sqrt{\pi m\rho}k^2$, one can easily deduce also the screening condition

$$\delta(k=0)=Q\ . \tag{7}$$

Although the expression for χ looks totally different in the two approaches the numerical results turn out to be very similar. This is understandable, since the major contribution to χ in both cases comes from Coulomb force, and hence we expect the overall features of the induced charge density to remain the same in both calculations. From Eq. (4) we see that the function $\chi(k)$ for small values of k is very sensitive to the behavior of $S(k)$. In particular S must have exactly the correct k^2 dependence in order to cancel out the Coulomb tail in Eq. (5). What is important is not really χ but the part where the Coulomb term is subtracted, i.e.,

$$\tilde{\chi}(k)=\chi(k)-\frac{4\pi e^2\rho_1}{k^2}\ . \tag{8}$$

From the EL equation for the homogeneous electron gas we can deduce that the second term in the power series of S is of fourth order in k. Hence, the value of $\tilde{\chi}(k=0)$ is directly proportional to the coefficient of this term. It turned out that the function S which was accurate enough in our earlier work[1] is not sufficiently accurate here to give any reasonable estimate of $\tilde{\chi}(k\approx 0)$. Therefore the present approach requires extreme accuracy for small k of $S(k)$. For this reason we have resorted to another expression of $S(k)$ obtained from the electron-gas EL equation in $\vec{k}$ space,

$$S(k)=\frac{k^2}{\{k^4+(4m/\hbar^2)[4\pi e^2\rho_1+k^2R(k)]\}^{1/2}}\ . \tag{9}$$

Here R is a functional of electron radial distribution function g_{11} such that

$$R(r)=-\frac{\hbar^2}{2m}\left[\frac{1-g_{11}}{g_{11}}\nabla^2 g_{11}-\frac{1}{2}\left[\frac{\nabla g_{11}}{g_{11}}\right]^2+\frac{1}{2}\left[\frac{\nabla f_0}{f_0}\right]^2+\nabla^2\ln f_0\right]\ . \tag{10}$$

In particular,

$$\tilde{\chi}(k=0)=R(k=0)=-\frac{\hbar^2}{4m}\rho_1\int\left[\left[\frac{\nabla f_0}{f_0}\right]^2+\left[\frac{\nabla g_{11}}{g_{11}}\right]^2\right]d\vec{r}\ ,$$

where the first term in the integral comes from the Lado approximation, f_0 being the correlation factor for noninteracting electrons.

Following the previous work[1,6] we can also here calculate the local-field correction $G(k)$ for the dielectric function. This is obtained by taking the impurity to be massive or $\mu\approx m$. Here we get the following result:

$$G(k)=-\frac{k^2}{4\pi e^2\rho_1}\tilde{\chi}(k)=-\frac{k^2}{4\pi e^2\rho_1}R(k)\ , \tag{11}$$

which is a closed-form expression in terms the electron liquid-structure function alone. It remains to be seen whether this expression remains valid even after the Lado approximation is done away with. In our previous work we used the above relation and the known[7] small-k behavior of G to force the function $\tilde{\chi}$ to have a correct value at the origin. In the present case no adjustment is needed since from Eqs. (10) and (11) we get the correct power law $G\sim k^2$ and with a nearly correct coefficient.

Similarly by using the properties of the Fourier transform one can derive for $G(k)$ the other asymptotic formula,

$$\lim_{k\to\infty} G(k)=1-g_{11}(0)\ , \qquad (12)$$

in agreement with our earlier results[1,6] and with those of Ref. 7.

From Eqs. (11) and (9) we obtain a very suggestive new expression for $S(k)$ in terms of local-field correction,

$$S(k)=\frac{1}{(1+\alpha\{[1-G(k)]/k^4\})^{1/2}}\ ,\qquad \alpha=\frac{4m}{\hbar^2}4\pi e^2\rho_1\ . \qquad (13)$$

When $G(k)\equiv 0$ this gives the uniform-limit result. Therefore $G(k)$ makes the correction for the cusp condition which requires a definite k^{-4} behavior for large k of $S(k)$. It is also seen that in the region where $G(k)>1$ one has an overshoot in $S(k)$. We believe that Eq. (13) provides perhaps the simplest possible self-consistent relation between $S(k)$ and $G(k)$ derivable from quantum theory rather than leaning to classical theory. The existence of such a relation has been discussed in connection with the Singwi-Tosi-Land-Sjölander (STLS) method,[8] which in lowest order gives a result very close to the one proposed by Hubbard.[9] The large-k asymptotic end of $G(k)$ come out correct in the Vashista-Singwi (VS) theory[10] as well as in STLS with higher-order corrections but in all above cases the function $S(k)$ from Eq. (13) would show no overshoot. Because of the Lado approximation the self-consistency condition (13) is only approximate but it may be a quite accurate one for calculations where one uses the dielectric function of electron gas as an input.[11]

II. NUMERICAL RESULTS

In order to solve the EL equation (5) numerically we had to improve first the accuracy of $S(k)$ of the host electron gas by solving the EL equation in Lado approximation both in $\vec{r}$ and $\vec{k}$ spaces with the help of Eq. (9). The iteration in $\vec{r}$ space was performed by direct numerical integration of the EL equation starting at $r=0$ with the correct cusp condition. Since no linearization is required here one never needs to invert matrices yet the convergence was good. We believe that the method can be extended also to full Fermi hypernetted-chain method (FHNC).

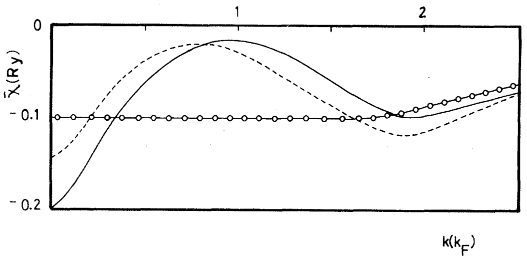

FIG. 1. Function $\tilde{\chi}$ for the proton ($\mu=m$) impurity at $r_s=3.39$. Full curve is from Eq. (4), dashed curve is the $c=0.6615$ calculation of Ref. 1. Curve with circles shows the function $\tilde{\chi}$ for the Coulomb-Bose system.

In Fig. 1 we compare the function $\tilde{\chi}$ obtained from Eq. (4) and the corresponding one of Ref. 1 where we had to adjust $\tilde{\chi}$ to have the correct value at $k=0$. Despite the apparent dissimilarities in the definitions, the numerical agreement is surprisingly good. A small part of the disagreement may result from the fact that in the present calculation, we have neglected the three-body terms in the electron-gas EL equation and the elementary diagrams in both cases. In particular from Fig. 1 we can see that $\tilde{\chi}(k=0)$ given by Eq. (4) is about 30% larger in absolute than the known exact value, which through Eq. (11) is related to the compressibility[7] of the homogeneous electron gas. On the other hand, as mentioned earlier, $\tilde{\chi}(k=0)$ is directly proportional to the coefficient of the k^4 term in the power series of $S(k)$. While it is well known[12,13] that, for example, in the ground state of the liquid ^{4}He the coefficient of the first power in the structure function determines the velocity of sound and hence the compressibility it seems that in the case of the long-range Coulomb force, the coefficient of the k^4 term, γ, is related to the compressibility κ of the interacting electron gas via the expression obtained from Eqs. (9)–(11),

$$\gamma=\frac{3}{4}\left[\left[\frac{\pi}{4}\frac{\hbar^2}{me^2}\right]^3\rho_1\right]^{1/2}\frac{\kappa-\kappa_0}{\kappa_0}\frac{1}{k_F^4}\ , \qquad (14)$$

where κ_0 is the compressibility of the noninteracting system.

To estimate the effect of the Fermi statistics, and in particular the effect of the Lado approximation, we have plotted in Fig. 1 the function $\tilde{\chi}(k)$ corresponding to the Coulomb-Bose system. The k^5 term missing in the boson $S(k)$ but present in the fermion system is responsible for the flatness of the boson $\tilde{\chi}(k)$ near $k=0$. The comparison of the $\tilde{\chi}$ functions corresponding to Bose and Fermi systems suggest that the behavior of $\tilde{\chi}$ at medium k is sensitive to the way one treats the statistics.[6]

In the treatment of proton and positron impurities we can proceed the way explained in Ref. 1. Here we have considered the $Q=1$ cases, proton or positron, and $Q=0$ cases, hydrogen or positronium, where Q is the charge of the impurity. The intrinsic wave function for $Q=1$ is 1 and for $Q=0$ that of positronium or hydrogen atom. In the latter cases the antisymmetry of the "dummy" electron with respect to others is neglected also here.

The induced density fluctuation at $r_s=2.07$ resulting from the proton impurity is plotted in Fig. 2. As expected it is essentially equivalent to our previous result, the only noticeable difference being near the region of the first minimum. From there on they both oscillate at the same phase and amplitude. In Fig. 3 the corresponding curves for positron impurity at $r_s=3.39$ are shown. Also here the agreement of the two different methods is remarkable. For comparison we have plotted in Fig. 2 also the density fluctuation of the Coulomb-Bose gas near the proton impurity. Here the deviation from the above fermion results is pronounced. In particular the oscillations in the tail of the density are completely out of phase and their wavelength is much longer thus indicating the importance of statistics in the oscillatory part of the density fluctuation. Using different approximation, e.g., FHNC (Refs. 14 and 15), one gets slightly different oscillations.[6]

III. DISCUSSION OF THE RESULTS

In Table I (Table II) we list the correlation energies ϵ_c from Eq. (3) and the height of the induced density fluctuation near the impurity for various values of r_s in the proton (positron) and hydrogen (positronium) cases and compare them with our best previous results. As before, we were not able to get any solution beyond certain values of r_s in the cases of proton and positron impurities while in the calculation of neutral impurities we had no difficulties. Similarly the other main characteristics of the present results follow closely the ones in Ref. 1. Compared with recent high-order field-theoretical calculations[16] we get more binding energy for the charged impurities while the neutral ones seem to come out very similar. In fact the correlation energies for the positronium impurity in the present calculation agree somewhat better with the ones of Ref. 16 than do our previous result. On the other hand, the height of the induced charge density near the impurity and consequently the annihilation rate in the case of positron impurity is now somewhat lower than the experimental results. However, if one adds $5-10\%$ correction for the core electrons the agreement becomes rather good.

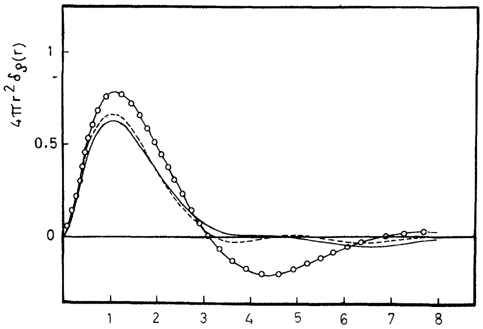

FIG. 2. Induced density fluctuation for proton impurity at $r_s=2.07$. Solid curve gives the result of the solution of Eq. (5). Dashed curve is the $Q=1$, $c=1$ calculation of Ref. 1. Curve with circles shows the density fluctuations in the Coulomb-Bose system.

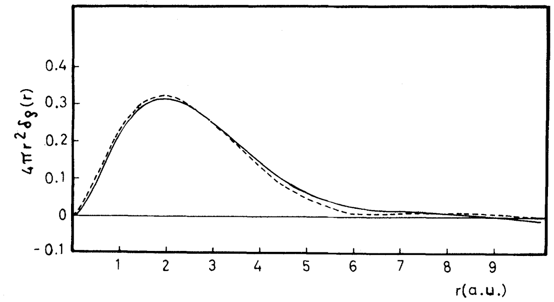

FIG. 3. Induced density fluctuation for positron impurity at $r_s=3.39$. Solid curve gives the result of the solution of Eq. (5). Dashed curve is the $Q=1$, $c=1$ calculation of Ref. 1.

Since a comprehensive discussion of earlier work concerning the impurity calculations is to be found in Refs. 1 and 16 we restrict ourselves to a comparison of present results with the ones of Sjölander and Stott.[17] In Fig. 4 we have plotted our annihilation rate together with the experimental results[18–20] and with the ones of Ref. 17. It is evident that our theoretical rate comes closer to the experimental result than does the one of Ref. 17, but perhaps a more interesting point is the appearance of the instability in both calculations. Looking at their Fig. 5 one observes that their density fluctuation $[ng(r)=\rho(r)]$ near $r=0$ does not satisfy the cusp condition which we do satisfy as well as the calculations in Ref. 16. It seems to us that if one would simply continue the exponentiallike behavior seen near $k_F \approx 0.5$ in their Fig. 5, down to zero, their annihilation rate would be improved and the cusp condition be better satisfied.

Concerning the instability, they suggested that it

TABLE I. Correlation energies and the height of the peak, $(\rho-\rho_1)/\rho_1=\delta(0)$ at $r=0$, for proton impurity. Columns 3 and 4: Correlation energies and the height of the peak for hydrogen impurity. Columns 5 and 6: Same ones corresponding to $Q=0$, $c=1$ calculations of Ref. 1.

	$Q=1$		$Q=0$		Ref. 1	
r_s	E_c (Ry)	$\delta(0)$	E_c	$\delta(0)$	E_c	$\delta(0)$
1.13	−1.986	3.9	−1.326	4.2	−1.550	4.9
2.07	−1.608	13.9	−1.082	13.3	−1.367	18.7
3.39	−1.705	65.9	−1.019	52.9	−1.282	62.8
5.65			−1.003	241.1	−1.243	253.2
7.91			−1.001	660.3	−1.227	682.4
11.3			−1.000	1924.2	−1.198	1988.2

may be due to the formation of a bound state at a certain value of r_s which then causes a divergence also in the annihilation rate. In their calculation this happened already within the metallic range, whereas in our $Q=1$ calculation this occurs around $r_s \gtrsim 8$, outside the range. However, in our proton case it already occurs at $r_s \gtrsim 3.5$. In both cases the instability was cured in our $Q=0$ calculation, where the bound state is explicitly introduced. Unfortunately our calculations are not as yet accurate enough to find out whether anything else interesting, such as having a jump in $\delta(r=0)$, etc., in connection with the singularity would happen or whether further corrections would simply push the singularity to higher r_s values.

Quite recently we have also applied the present mixture formalism to two systems of finite concentration, the liquid metallic hydrogen[21] and the electron-hole liquid[22] corresponding to proton and positron cases in the limit of zero concentration. In these systems similar instabilities are found at $r_s=1.6$ and 6.8, respectively. For the finite mixtures the bound-state formation finally causes a phase transition and hence for larger r_s values bound pairs have to be used as units. Clearly then the instability in the impurity systems could be considered as a precursor effect of a real phase transition in the two finite-mixture systems, where also the pressure seems to go through zero in the vicinity of the singular point. Since in Ref. 16 no singularity occurred, this point needs further clarification.

As a byproduct we have also calculated the dielectric function of electron gas. In Fig. 5 we have plotted the associated local-field correction $G(k)$ of Eq. (11). In comparison with our previous calculation[1,6] the maximum of $G(k)$ is at larger values of k and tends somewhat more slowly to the asymptotic value $1-g_{11}(0)$. In comparison with earlier calculations of $G(k)$ the residual uncertainties that we have seem to be much less than the factor of 3−4 at $k \approx 2k_F$ found even in quite recent literature.[23] Notably our result is in good agreement with the ones of Ref. 7.

In the present and in all other applica-

TABLE II. Correlation energies and the height of the peak. $(\rho-\rho_1)/\rho_1$ at $r=0$, for the positron impurity. Columns 3 and 4: Correlation energies and the height of the peak for positron impurity. Columns 5 and 6: Same ones corresponding to $Q=0$, $c=1$ calculations of Ref. 1.

	$Q=1$		$Q=0$		Ref. 1		Ref. 16	
r_s	E_c (Ry)	$\delta(0)$	E_c	$\delta(0)$	E_c	$\delta(0)$	E_c	$\delta(0)$
1.13	−1.425	1.4	−0.999	1.8	−0.714	1.5		
2.07	−1.009	3.3	−0.659	2.7	−0.676	4.1	−0.630	3.6
3.39	−0.819	8.6	−0.548	7.4	−0.594	11.5	−0.525	9.5
5.65	−0.786	35.4	−0.511	30.7	−0.543	40.3	−0.475	35.0
7.91	−0.985	136.2	−0.504	83.0	−0.524	99.3	−0.475	
11.3			−0.501	240.8	−0.511	269.1		

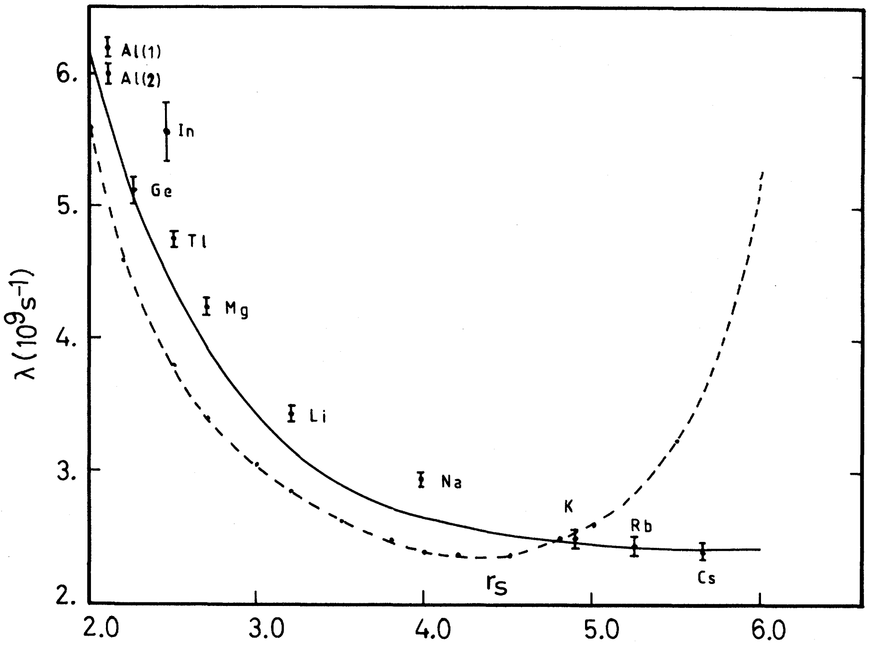

FIG. 4. Positron annihilation rate λ in metals. Solid curve gives the present $Q=1$ result, dashed curve is from Ref. 17, and bars are the experimental results of Refs. 18–20.

tions[1,21,22,24] we have made use of the Lado approximation in one of the kinetic-energy terms. From these quite a few applications we have become convinced that the Lado HNC with Jackson-Feenberg kinetic energy produces very accurate radial distribution functions. The other kinetic-energy expressions, which lead to intractable EL equations can be used afterwards to recalculate the energy. According to Ref. 25 this method gives for the total energy of electron-gas numbers which agree to within three places with the exact Monte Carlo results. Working out the full FHNC (Refs. 14 and 15) for mixtures and inhomogeneous systems is immensely more complicated and yet, we believe, results in little progress. Finally we should point out that elementary faults like having the radial distribution function become negative never occurs within the present theory.

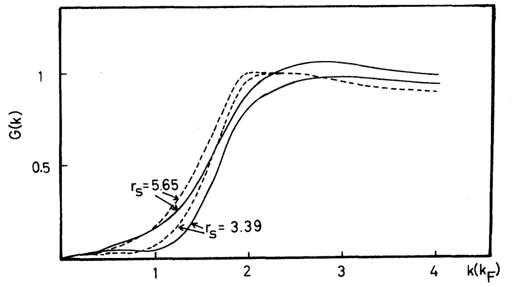

FIG. 5. Local-field correction function at $r_s=3.39$ and 5.65 from Eq. (11) (solid curve). Dashed curves are from Ref. 1.

In summary, we have shown that the variational binary-mixture theory works quite well for impurities embedded in an electron gas. Moreover this method and the one of Ref. 1 are shown to give practically equivalent results. The same is also true for the local-field correction of the dielectric function which agrees well with the best field-theoretical calculations.

Finally in order to be able to carry out the present calculations we had to devise a new method for solving the uniform-electron-gas problem more accurately, since normal linearization procedure was found inadequate in accuracy. In connection with this new method, which is based on calculating the correction function $R(k)$ to the uniform-limit approximation of the electron gas, we have shown that this correction is intimately connected with the local-field correction function $G(k)$. It remains to be shown that also in the full FHNC calculation this connection holds true and the coefficient of k^4 power is related to the compressibility of electron gas.[26] Owing to the Lado approximation the results are valid in the metallic range $r_s>2$ which, from the point of view of applications, is the interesting region. For $r_s \lesssim 2$ function $G(k)$ develops two zeros at finite k. This deficiency can be repaired by adopting the generalized mixture formalism,[27] which treats the statistics correctly but at the same time makes the theory much less transparent. On the other hand this region is already well understood in terms of STLS and VS methods.

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