11-24-2009

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Recommended Citation

Sheehy, D., & Schmalian, J. (2009). Optical transparency of graphene as determined by the fine-structure constant. *Physical Review B - Condensed Matter and Materials Physics, 80* (19) https://doi.org/10.1103/PhysRevB.80.193411

Optical transparency of graphene as determined by the fine-structure constant

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(Dated: June 28, 2009)

The observed 97.7% optical transparency of graphene has been linked to the value 1/137 of the fine structure constant, by using results for noninteracting Dirac fermions. The agreement in three significant figures requires an explanation for the apparent unimportance of the Coulomb interaction. Using arguments based on Ward identities, the leading corrections to the optical conductivity due to the Coulomb interactions are correctly computed (resolving a theoretical dispute) and shown to amount to only 1-2%, corresponding to 0.03-0.04% in the transparency.

The optical transparency of graphene is determined by its optical conductivity $\sigma(\omega)$ and c, the speed of light[1]:

$$t(\omega) = (1 + 2\pi\sigma(\omega)/c)^{-2}. \quad (1)$$

Recent experiments[2] on suspended graphene found $t(\omega) \simeq 0.977$, independent of ω, in the visual regime (450nm $< \lambda <$ 750nm). This observation (see also Refs. 3,4,5) can be elegantly rationalized in terms of non-interacting Dirac particles with optical conductivity[6] $\sigma^{(0)}(k_B T \ll \omega \ll D) = \frac{\pi}{2} e^2/h$. Here D is the upper cut off energy for the linear dispersion, of order of several electron volts and T is the temperature. Assuming $\sigma = \sigma^{(0)}$ yields $t(\omega) \simeq 0.9774629(2)$, in excellent agreement with experiment. Thus, the optical transparency of *non-interacting* graphene $t(\omega) = (1 + \pi\alpha_{\rm QED}/2)^{-2}$ is solely determined by the value of the fine structure constant of quantum electrodynamics: $\alpha_{\rm QED} = e^2/(\hbar c) \simeq 1/137.035999(6)$. Despite the beauty of this reasoning, a natural question emerges: *Why can one ignore the electron-electron Coulomb interaction?* After all the Coulomb interaction in graphene is poorly screened and its strength is governed by its own, effective fine structure constant $\alpha = e^2/(\hbar v) \simeq 2.2$ that is significantly larger than $\alpha_{\rm QED}$ because of the smaller velocity[7] $v \simeq 10^6$m/s. The quantitative agreement between experiment and a non-interacting theory clearly requires a quantitative analysis of the size of interaction corrections to the optical conductivity and transparency of graphene.

In this Brief Report we determine the leading interaction corrections to the optical transparency and demonstrate that they amount to only 0.037% in the visual regime. This surprisingly small correction is the consequence of i) a perfect cancellation of the divergent (i.e. proportional to $\ln D/|\omega|$) parts of Feynman diagrams that contribute to the conductivity and ii) a near cancellation of the non-divergent contributions. While the first result has been stated earlier by us[8] as well as in Ref. 9, the latter effect has been a subject of a dispute[9,10,11]. Below we resolve this dispute and demonstrate that the leading perturbative correction to the conductivity was correctly analyzed by Mishchenko in Ref. 10. We show that perturbative corrections to the conductivity must be obtained by guaranteeing that momentum cutoffs, used to regularize divergences, are introduced in a fashion that respects Ward identities and thus guarantees charge conservation.

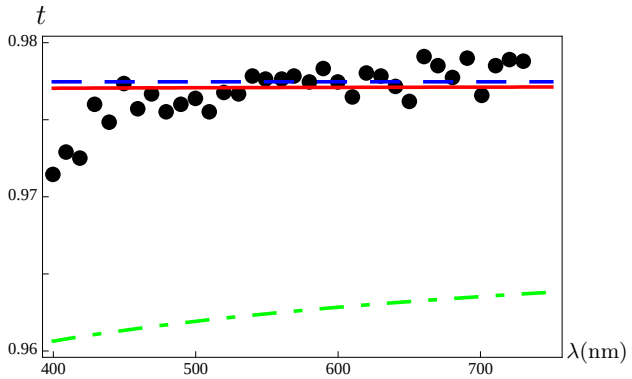

Figure 1: (Color Online) Optical transparency, Eq. (1), of graphene, from Ref. 2 (points) along with theoretical curves for the case of interacting graphene within the present theory, Eq. (9) with $\mathcal{C}_1 \simeq 0.01$ (solid red line), according to the theory of Ref. 9 ($\mathcal{C}_1 \simeq 0.51$; dot-dashed green line), and for noninteracting Dirac fermions (dashed blue line).

The low energy Hamiltonian for electrons in graphene[12] is obtained by expanding to leading order in gradients near the nodes of the tight-binding dispersion, yielding the following nodal-fermion Hamiltonian:

$$H = v\sum_{\mathbf{k},i} \psi_i^\dagger(\mathbf{k})\mathbf{k}\cdot\boldsymbol{\sigma}\psi_i(\mathbf{k}) + \frac{e^2}{2}\int d^2r d^2r' \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}. \quad (2)$$

Here $i = 1\cdots N$, with $N = 4$ counting the two spin indices and two independent nodes in the Brillouin zone, σ_μ are the Pauli matrices, and we have set $\hbar = 1$. It is simple to show that the charge density $\rho(\mathbf{r}) = \sum_{i=1}^N \psi_i^\dagger(\mathbf{r})\psi_i(\mathbf{r})$ and current density $\mathbf{j}(\mathbf{r}) = v\sum_{i=1}^N \psi_i^\dagger(\mathbf{r})\boldsymbol{\sigma}\psi_i(\mathbf{r})$ are related by the continuity equation:

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{j} = 0. \quad (3)$$

The optical conductivity is related by the Kubo formula to the retarded current-current correlation function:

$$\sigma(\omega) = \frac{e^2}{2\omega}\mathrm{Im}\big[f_{xx}^R(\mathbf{q}=\mathbf{0},\omega) + f_{yy}^R(\mathbf{q}=\mathbf{0},\omega)\big]. \quad (4)$$

Here, $f^R_{\mu\nu}(\mathbf{q},\omega)$ is the retarded correlation function determined from the Matsubara function $f_{\mu\nu}(Q) = \langle j_\mu(Q)\, j_\nu(-Q)\rangle$ by analytically continuing $i\Omega \to \omega + i0^+$. We use the convention $Q = (-i\Omega, \mathbf{q})$ and correspondingly write $j_0(Q) = \rho(Q)$ for the charge density.

The theory for the optical conductivity in graphene with electron-electron Coulomb interaction was developed in Refs. 8,9. Using renormalization group (RG) arguments it holds that the effective fine-structure constant of graphene, α, becomes a running coupling constant $\alpha(l)$ where l is the flow variable of the RG approach. In the case of graphene $\alpha(l)$ decreases logarithmically as one lowers the typical energy scale[8,9,13,14,15,16,17]. The optical conductivity $\sigma(\omega, T, \alpha)$ at frequency ω, temperature T and for the physical coupling constant α is related to its value at a rescaled frequency $\omega_R(l) = Z(l)^{-1}\omega$, rescaled temperature $T_R(l) = Z(l)^{-1}T$ as well as the running coupling constant via

$$\sigma(\omega, T, \alpha) = \sigma(\omega_R(l), T_R(l), \alpha(l)). \tag{5}$$

The scaling factor up to one loop is given by $Z(l) = e^{-l}\left(1 + \frac{\alpha}{4}l\right)$. Equation (5) implies that the conductivity is scale invariant under the RG flow. This result is true to arbitrary order in perturbation theory as can be shown following arguments by Gross[18]. It is physically due to the fact that the electron charge is conserved[19]. The scaling functions $\omega_R(l)$ and $T_R(l)$ grow under renormalization while $\alpha(l)$ decreases[8,19]. Thus, in the relevant collisionless regime $\omega \gg T$ is it sufficient to analyze the high frequency ($\omega_R(l) \simeq D$), weak coupling limit where

$$\sigma(D, 0, \alpha) = \sigma^{(0)}\left[1 + \mathcal{C}_1\alpha + \mathcal{C}_2\alpha^2 + \cdots\right]. \tag{6}$$

Here, the numerical coefficients $\mathcal{C}_i$ are determined by performing an explicit perturbation theory. The scaling law Eq. (5) yields the conductivity as a function of frequency where we replace α by the running coupling constant

$$\alpha \to \alpha(\omega) = \alpha/\left(1 + \frac{\alpha}{4}\log(D/\omega)\right), \tag{7}$$

here obtained to leading logarithmic accuracy[8,9,13,14,15,16,17]. The result is that interactions only give rise to additive corrections to $\sigma^{(0)}$ that are of the form

$$\sigma(\omega) = \sigma^{(0)}\left[1 + \mathcal{C}_1\alpha(\omega) + \mathcal{C}_2\alpha^2(\omega) + \cdots\right]. \tag{8}$$

Note, this behavior is correct in the collisionless regime $\omega \gg k_B T$. Qualitatively different behavior occurs in the opposite, hydrodynamic regime[17] $\omega \ll k_B T$.

Since $\alpha(\omega \to 0) = 0$, it follows from Eq. (8) that $\sigma(\omega \to 0) \to \sigma^{(0)}$. However, $\alpha(\omega)$ only vanishes as $4/\log(D/\omega)$ and corrections could easily be significant in the visible part of the spectrum where ω and D are comparable. The dominant correction is due to the $\mathcal{C}_1\alpha$ term and will be analyzed in this Brief Report. Combining Eqs. (7) and (8), and neglecting the higher-order terms, we have

$$\sigma(\omega) = \sigma^{(0)}\left[1 + \frac{\mathcal{C}_1\alpha}{1 + \frac{1}{4}\alpha\log(D/\omega)}\right]. \tag{9}$$

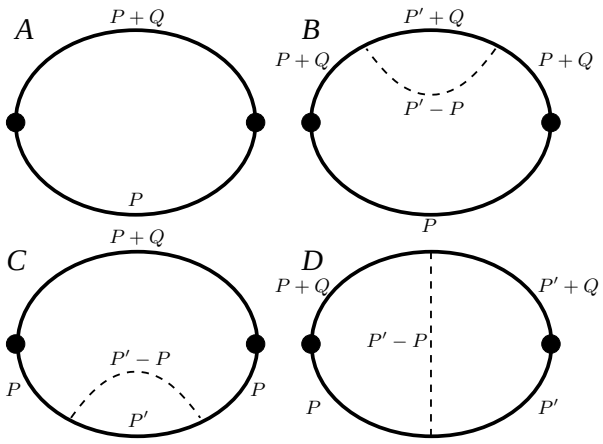

Figure 2: Feynman diagrams for the leading order contributions to $f_{\mu\nu}(Q)$ and $\sigma(\omega)$. Diagram A is the $\mathcal{O}(\alpha^0)$ contribution, while diagrams B, C, D are $\mathcal{O}(\alpha)$. Full lines represent fermions and dashed lines represent the Coulomb interaction.

Calculations of $\mathcal{C}_1$ were presented in Refs. 9 and 10, however with different results. While the authors of Ref. 9 obtained $\mathcal{C}_1 = (25 - 6\pi)/12 \simeq 0.513$, Mishchenko[10] obtained a significantly smaller value $\mathcal{C}_1 = (19 - 6\pi)/12 \simeq 0.0125$, which was however disputed in Ref. 11. Determining the correct value of $\mathcal{C}_1$ is important for two reasons. First, there is no obvious mistake in either Ref. 9 or Ref.10. It is clearly important from a purely theoretical point of view to settle this issue and set the criteria for correct calculations of interaction effects in graphene. Second, as we discuss in more detail below and illustrate in Fig. 1, the coefficient determined in Ref. 9 is not consistent with experiment, impling that qualitatively new phenomena or even higher order corrections would have to be invoked to understand the observations of Ref. 2.

We now obtain $\sigma(\omega)$ by calculating the correlation function $f_{\mu\nu}(Q)$ which, as follows from Eq. (3), satisfies

$$Q_\mu f_{\mu\nu}(Q) = 0, \tag{10}$$

with the repeated index summed over $\mu = 0, x, y$. When calculating $f_{\mu\nu}(Q)$, the leading contributions to which are shown in Fig. 2, we must ensure that Eq. (10) is satisfied at each order in α.

The zeroth-order contribution, Fig. 2A, corresponds to the current-current correlation function $f^{(0)}_{\mu\nu}(Q)$ of non-interacting Dirac particles and yields[16]

$$f^{(0)}_{\mu\nu}(Q) = \frac{N}{16|Q|}\left(Q^2\delta_{\mu\nu} - Q_\mu Q_\nu\right), \tag{11}$$

which obeys Eq. (10). Performing the analytic continuation and inserting the result into the Kubo formula yields, after restoring proper units, $\sigma^{(0)} = \frac{\pi e^2}{2h}$ for $N = 4$. This leads to the 97.7% optical transmission discussed above.

Next we analyze the three leading corrections to $\sigma^{(0)}$ as shown in Fig. 2B-D. The diagrams in Fig. 2B and C yield the same contribution with interactions entering via

self energy insertions with the leading self energy

$$\Sigma(\mathbf{p}) = -e^2 \int_{P'} V(\mathbf{p}-\mathbf{p}')G(P'), \tag{12}$$

where $\int_{P'} ... = T\sum_{\omega'} \int_{p'} \frac{d^2p'}{(2\pi)^2} ...$ and $V(\mathbf{p}) = \frac{2\pi}{|\mathbf{p}|}$ is the Fourier-transformed Coulomb interaction. The fermion propagator is given by

$$G(P) = \frac{-i\omega\sigma_0 - v\mathbf{p}\cdot\sigma}{\omega^2 + v^2p^2}. \tag{13}$$

The self energy, Eq. (12), diverges logarithmically and must be regularized, for example by introducing an upper momentum cut off $\Lambda \simeq D/v$. We will show that the discrepancy between previous calculations of $\sigma(\omega)$ can be traced to the fact that, in Eq. (12), there are two obvious ways to introduce the ultraviolet (UV) cut-off Λ.

Thus, upon evaluating the frequency summation and momentum integrals, we obtain

$$\Sigma(\mathbf{p}) = \frac{1}{4}\alpha v \mathbf{p}\cdot\boldsymbol{\sigma} \ln\left[\frac{4\Lambda c}{p}\right], \tag{14}$$

where the number c depends on the cutoff procedure, with $c = \mathrm{e}^{-1/2}$ if we evaluate the momentum integral using the cutoff $|\mathbf{p}'| < \Lambda$, i.e. by confining fermion states to a circle near the node. (Note we always discard contributions that vanish for $\Lambda/p \to \infty$). On the other hand, if we evaluate the momentum integral by restricting $|\mathbf{p}-\mathbf{p}'| < \Lambda$, i.e. by having a finite Coulomb interaction at short distances (see also Ref. 11), we find that $c = \mathrm{e}^{1/2}$. This corresponds to replacing the Coulomb potential via $V(\mathbf{p}) \to V_\Lambda(\mathbf{p}) = 2\pi\theta(\Lambda - |\mathbf{p}|)/|\mathbf{p}|$. We emphasize that the log-divergent contribution to $\Sigma(\mathbf{p})$ is independent of the regularization procedure, with the difference being in the subleading contributions.

As we will show, the two different values that have been determined for $\mathcal{C}_1$ in Refs. 9 and 10, respectively, are directly related to the two different values for c in the self energy as it enters in the diagrams of Fig. 2B and C. The diagram Fig. 2D is unaffected by the regularization procedure. Which result for c, i.e. which regularization procedure, is correct? The answer comes from the Ward identity, which, as we show next, is only satisfied if we implement the momentum cutoff by restricting the momenta in the Coulomb potential to $|\mathbf{p}-\mathbf{p}'| < \Lambda$, implying that Mishchenko's result[10] is correct.

To demonstrate that the proper cut off procedure is to restrict $|\mathbf{p}-\mathbf{p}'| < \Lambda$ in the Coulomb potential, we analyze the leading interaction corrections (Fig. 2B,C, and D), which we call $f^{(1)}_{\mu\nu}(Q)$. These satisfy:

$$\begin{aligned} Q_\mu f^{(1)}_{\mu\nu}(Q) &= N\alpha \int_P \int_{P'} V_\Lambda(\mathbf{p}-\mathbf{p}') \\ &\times \mathrm{Tr}\left\{G(P'+Q)G(P+Q)G(P'+Q)\sigma_\nu \right. \\ &\left. -G(P')\sigma_\nu G(P')G(P)\right\}. \end{aligned} \tag{15}$$

This result was obtained from the three diagrams Fig. 2B-D by simply using the identity

$$G(P)(i\Omega\sigma_0 - \mathbf{q}\cdot\sigma)\,G(P+Q) = G(P) - G(P+Q), \tag{16}$$

and the cyclic property of the trace. At this point, the UV cutoff only enters via $V_\Lambda(\mathbf{p})$, so that we can shift $P \to P-Q$ and $P' \to P'-Q$ in the first term, again use the cyclic property of the trace, and obtain

$$Q_\mu f^{(1)}_{\mu\nu}(Q) = 0, \tag{17}$$

the required result. Note that other regulation schemes for the UV behavior will *not* necessarily work in this way. In particular, regulating the momenta by restricting the Green-function momentum arguments amounts to replacing $G(P) \to G(P)\Theta(\Lambda - |\mathbf{p}|)$; with such a replacement, Eq. (16) and thus Eq. (15) will not be valid. We conclude, then, that in graphene momenta must be regularized using $V_\Lambda(\mathbf{p})$.

The same conclusion can be arrived at by considering the leading corrections to the current vertex

$$\Lambda_\mu(P,Q) = -\alpha \int_K G(K)\sigma_\mu G(K+Q)V_\Lambda(\mathbf{k}-\mathbf{p}). \tag{18}$$

Again using Eq. (16), we obtain

$$\begin{aligned} Q_\mu\Lambda_\mu &= -\alpha \int_K \left(G(K+Q) - G(K)\right) V_\Lambda(\mathbf{k}-\mathbf{p}), \\ &= \Sigma(P+Q) - \Sigma(P), \end{aligned} \tag{19}$$

which is the correct Ward identity. Once again, alternate schemes for cutting off the momentum integrals are not guaranteed to yield a proper Ward identity of this form. Our finding that a regularization in terms of a hard fermion cut-off violates charge conservation is analogous to the observation in QED that incorrect regularization schemes yield unphysical results such as a photon mass[20].

Our final tasks are to evaluate the contributions to the current-current correlation function and to determine the conductivity using the Kubo formula Eq. (4). We first consider the diagrams B and C, which are identical. Recognizing the self-energy insertion, we have (with an overall 2 for the two diagrams):

$$f^{(1)}_{\mu\nu}|_{BC} = -2N \int_P \mathrm{Tr}[G(P)\sigma_\mu G(P+Q)\sigma_\nu G(P)\Sigma(\mathbf{p})]. \tag{20}$$

Evaluating the trace, and performing the frequency integral and analytical continuation yields

$$\mathrm{Im} f^{(1)R}_{\mu\mu}(\mathbf{q}=\mathbf{0},\omega)|_{BC} = -\frac{N\alpha\omega}{16} \ln\frac{8v\Lambda c e^{-1/2}}{\omega}, \tag{21}$$

where the repeated μ index refers to the sum over the xx and yy components as in Eq. (4). Analyzing the diagram D of Fig. 2, which can be written as

$$f^{(1)}_{\mu\nu}|_D = -N \int_P \mathrm{Tr}[G(P)\Lambda_\mu(P,Q)G(P+Q)\sigma_\nu], \tag{22}$$

it turns out that the result does not depend on the details of the regularization procedure and yields

$$\mathrm{Im} f^{(1)R}_{\mu\mu}(\mathbf{q}=\mathbf{0},\omega)|_D = \frac{N\alpha\omega}{16}\left(\ln\frac{8v\Lambda}{\omega} + \frac{19-6\pi}{6}\right). \tag{23}$$

By examining Eqs. (21) and (23), it is clear that the dependence on the high energy scale Λ vanishes, in agreement with general scaling arguments[8,9]. Plugging these results into Eq. (4) yields Eq. (9) with coefficient

$$\mathcal{C}_1 = \frac{19-6\pi}{12} - \frac{1}{2}\ln c e^{-1/2}. \qquad (24)$$

We indeed see that the correct cut-off procedure, with $c = e^{1/2}$, yields $\mathcal{C}_1 = \frac{19-6\pi}{12}$, whereas the other cutoff procedure, corresponding to $c = e^{-1/2}$, yields[9] $\mathcal{C}_1 = \frac{25-6\pi}{12}$.

We have verified[19] that the same result holds within alternate regularization procedures that do not use sharp cutoffs, as long as the Ward identity is satisfied. For example, replacing the Coulomb interaction $V(\mathbf{r}) \to V_\eta(\mathbf{r}) = \frac{e^2 r_0^{-\eta}}{r^{1-\eta}}$ with r_0 a length scale and $\eta > 0$ (putting the physical system, at $d = 2$, slightly below its own upper critical dimension) regulates all integrals in a way consistent with Eq. (17). We obtain (for $\eta \to 0$)

$$\begin{aligned} \mathrm{Im} f^{(1)R}_{\mu\mu}|_{BC} &= -\frac{N\alpha\omega}{16}\left(\frac{1}{\eta} + \ln\frac{4v}{\omega r_0} - \gamma_E\right), \qquad (25) \\ \mathrm{Im} f^{(1)R}_{\mu\mu}|_{D} &= \frac{N\alpha\omega}{16}\left(\frac{1}{\eta} + \ln\frac{4v}{\omega r_0} - \gamma_E + \frac{19-6\pi}{6}\right), \end{aligned}$$

with γ_E the Euler constant. Once again, while the separate contributions diverge with $\eta \to 0$, their sum is convergent and yields the coefficient $\mathcal{C}_1 = \frac{19-6\pi}{12}$.

As we have discussed, Eq. (9) implies that the correction to $\sigma^{(0)}$ is small at low photon energies $\omega \ll D$ regardless of the value of $\mathcal{C}_1$. However, at larger (i.e., optical[2,5]) frequencies, the second term may become significant, depending on the value of the number $\mathcal{C}_1$. Nair *et al.*[2] find the conductivity to be $\sigma/\sigma^{(0)} = (1.01 \pm 0.04)$. If we take the value $\mathcal{C}_1 \simeq 0.513$ from Ref. 9, however, Eq. (8) predicts a large frequency-dependent correction to the conductivity that is not consistent with these error bars, giving, for example at photon wavelength $\lambda = 600nm$ (or $\hbar\omega = 2.07$eV), $\sigma/\sigma^{(0)} \simeq 1.667$, assuming the bandwidth $D = 7.24$eV. In contrast, using $\mathcal{C}_1 = 0.0125$ of Ref. 10, yields for the same parameters, $\sigma/\sigma^{(0)} \simeq 1.016$, consistent with the error bars of Nair *et al.*[2]. In Fig. 1 we show the optical transparency that result from both values for $\mathcal{C}_1$ (using bandwidth $D = 7.24$eV), along with the free-Dirac fermion result as function of wavelength λ in comparison with experiment.

Given the smallness of interaction corrections, with $\sigma/\sigma^{(0)} \simeq 1.016$ for the correct value of $\mathcal{C}_1$ (a correction comparable to corrections due to the true tight-binding band structure), it is unlikely that optical measurements will reveal interaction effects. Electron-electron interactions are much more visible in the enhanced diamagnetic response[8] or the hydrodynamic transport[17].

In summary, we determined the leading corrections to the optical conductivity and transparency of graphene and find that they are very small and determined by the fine structure constant α_{QED} up to corrections of order 1-2% in the conductivity and $0.03 - 0.04\%$ in the transparency. Correctly regularizing the UV-divergent contributions required using Ward identity arguments to resolve previous discrepancies in recent literature (a controversy that persists[21]). Our work demonstrates that there are no discrepancies in $\sigma(\omega)$ obtained by different theoretical methods[10], such as the Kubo formula, the density polarization approach or kinetic approaches, if charge conservation is guaranteed at all stages of the calculation. Our methods confirm and, more importantly, justify the result first obtained by Mishchenko[10] and provide a general prescription for calculating interaction corrections in graphene.

Acknowledgments — We gratefully acknowledge useful discussions with I. Vekhter, as well as the Aspen Center for Physics where part of this work was carried out. This research was supported by the Ames Laboratory, operated for the U.S. Department of Energy by Iowa State University under Contract No. DE-AC02-07CH11358, and by the Louisiana Board of Regents, under grant No. LEQSF (2008-11)-RD-A-10.

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