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Numerical simulations of graphene conductivity with realistic inter-electron potential

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There was a long time disagreement in literature between theoretical calculations and experimental data about conductor-insulator phase transition in graphene. This contradiction was resolved in the papers [Phys. Rev. Lett. 111, 56801 (2013)] and [Phys. Rev. B 89, 195429 (2014)] where chiral condensate was studied taking into account screening of Coulomb potential by σ -electrons of carbon atoms. Unfortunately there was no explicit evidence that conductivity drops down simultaneously with appearance of chiral condensate. Therefore it is required to perform direct calculations of graphene conductivity in tight-binding model.

We performed Monte-Carlo simulations of graphene tight-biding model with realistic electron-electron interaction and calculated the dependence of conductivity on dielectric permittivity of substrate.

According to our calculations suspended graphene has conductivity $\sigma = 0.325 \pm 0.003 e^2/\hbar$ which is very close to experimental value $\sigma = (1.01 \pm 0.04)e^2/4\hbar$. The phase transition in conductivity is also shifted to unphysical region epsilon<1 due to influence of σ -electrons.

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