Monte-Carlo simulation of the tight-binding model of graphene with partially screened Coulomb interactions

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Abstract

We present results of Hybrid-Monte-Carlo simulations based on the work of Ref. [1] of the tight-binding theory of graphene, coupled to an electric two-body potential which is generated by a Hubbard-Stratonovich field [2, 3]. We have investigated the spontaneous breaking of sub-lattice symmetry, which occurs when the effective fine-structure constant $\alpha_{\rm eff}$ is large and which corresponds to a transition from a conducting to an insulating phase (Fig. 1). We chose a form of the potential which correctly accounts for screening of the two-body Coulomb interactions of valence-electrons by electrons in lower orbitals (Fig. 2): At short range we used the exact results of the calculation within the constrained random phase approximation (cRPA) presented in Ref. [4]. At long range we used a pheonomenological model to generate screening, which is motivated by the same formalism. We compare our results to previous simulations presented in Ref. [5], which correctly accounted for short-range screening, but over-estimated screening at long distances. These authors located the phase transition at $\alpha_c \approx 3.14$. We find that sub-lattice symmetry-breaking is largely insensitive to the exact form of the long-range part of the potential. Our results confirm the expectation that suspended graphene ($\alpha_{\rm eff} \approx 2.2$) is a conductor, when screening is correctly accounted for.

References

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[4] T. O. Wehling et al., "Strength of effective Coulomb interactions in graphene and graphite," Phys. Rev. Lett. 106, 236805 (2011) arXiv:1101.4007.

[5] M. V. Ulybyshev et al., "Monte-Carlo study of the semimetal-insulator phase transition in monolayer graphene with realistic inter-electron interaction potential," Phys. Rev. Lett. 111, 056801 (2013) arXiv:1304.3660.

Figures

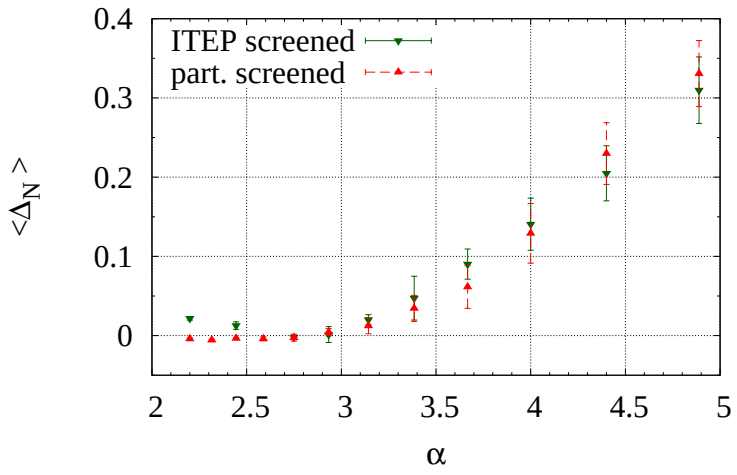

Figure 1: Difference of particle number-density of sub-lattices (i.e. order-parameter for phase-transition to gapped phase) as function of effective fine-structure constant for two versions of long-range screening.

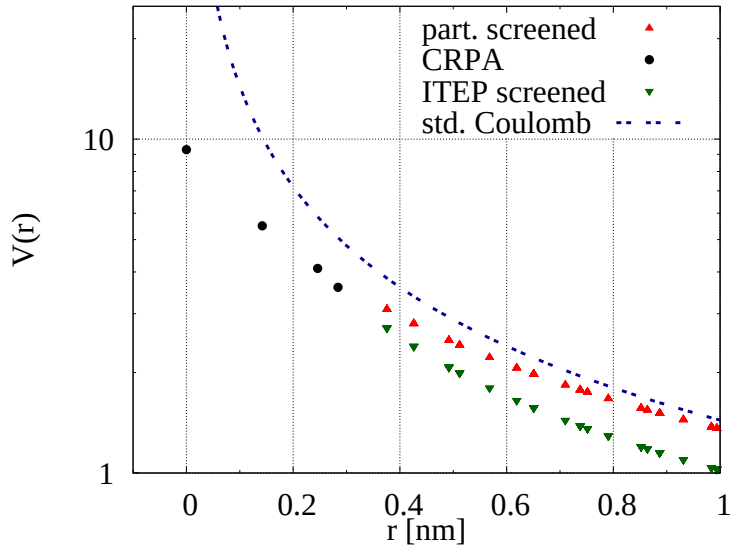

Figure 2: Unscreened Coulomb potential, screened potential as in Ref. [5] ("ITEP screened") and partially screened Coulomb potential. Exact results of cRPA formalism at short distances (Ref. [4]).