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Numerical study of impurity effects in Graphene[1] ZHOU LI, FRANK MARSIGLIO, Dept. of Physics, University of Alberta, STEPAN GRINEK, JIE CHEN, Dept. of ECE, University of Alberta — It is known that long-range Coulomb impurities could induce a novel supercritical regime in gapped graphene [1]. For short range impurities, the electron wave function is less localized near the band edge and thus numerical results may depend on the size and boundary conditions of the simulated graphene. For six attractive impurities forming a quantum well with radius=a(a is the distance between two nearest neighbor atoms in graphene), we found that the bound states will not merge into the continuum. The results from a finite size exact diagonalization with open boundary conditions agree well with that from an infinite size study based on Green's functions. Also an efficient numerical approach based on kernel polynomial methods [2] will be adopted to evaluate the Green's function accurately in the regime with strong interference effects and compared to T-matrix results.

[1] V.M. Pereira et.al, Phys. Rev. B, 78, 8, 2008, pp. 085101.
[2] L.Covaci et.al, Phys. Rev. Lett. 105, 167006 (2010)

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