Bias Free Gap Creation in Bilayer Graphene

A. R. Davenport, J. P. Hague

The Open University, Walton Hall, Milton Keynes, MK6 7AA, UK
anthony.davenport@open.ac.uk

Abstract

The experimental discovery of graphene by Novoselov and Geim *et al.* [1] has led to a major drive to develop graphene based microelectronics to replace silicon in computing devices.[2] Exceptional electrical, transport and thermodynamic properties make graphene a promising material for this task, although the carbon structure is naturally a zero-gap semiconductor. The goal is to change the electronic structure to make a useful semiconductor without destroying the properties that make graphene unique.[3]

We model bilayer graphene using a tight-binding approach with a small energy difference δ induced by the proximity of stacked sites in the AB stacking regime [4], plus an additional electron-phonon term describing supstrate and superstrate interactions related to the dimensionless electron-phonon coupling constant λ.

The electron-phonon interaction has been widely studied in condensed matter systems, most notably in theories of superconductivity.[5] There has been much work studying its role in graphene and graphitic structures both theoretically [6,7,8] and experimentally [9,10,11]. This work going beyond that of previous studies in an attempt to create a usable and tuneable gap in bilayer graphene purely by choosing the materials that will surround it.

A Green's function approached is used to explore the parameter space of interlayer hopping, temperature, phonon frequency and electron-phonon coupling constants. It can be seen from the imbedded picture of figure 1 that the four sites in its unit cell can be split into two unique sites, which we call X and Y (for sites without interlayer hopping and containing interlayer hopping respectively). By taking a simple momentum independent Ansatz and placing our greens function into the lowest order self-energy equation we obtain corrections to the on-site potential of each site.

Figure 1 shows that the small potential difference between sites X and Y is accentuated in our calculations with increasing electron-phonon coupling constants. We find that with medium sized coupling constants, seen in figure 2, an electron band gap could be created in bilayer graphene without the need for an external potential. There is a large range of band gaps up to $E_g = 1.3$ eV within the small coupling range $\lambda = 1.1\text{-}1.3$. These gaps surpass that achievable in biased bilayer systems, the small electron-phonon coupling range may be a significant factor within the electronics industry.

References

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Figures

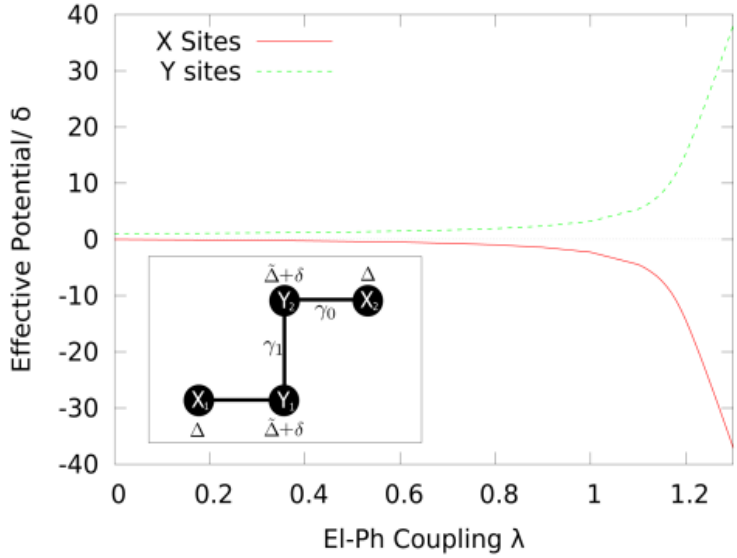

Figure 1: Bilayer graphene effective potential normalized to δ for X sites with intra-layer hopping and Y sites with both intra and interlayer hopping. As the electron-phonon coupling is increased, a near equal and opposite potential forms on X and Y sites, with values of the effective potential reaching 15δ at $\lambda = 1.2$.

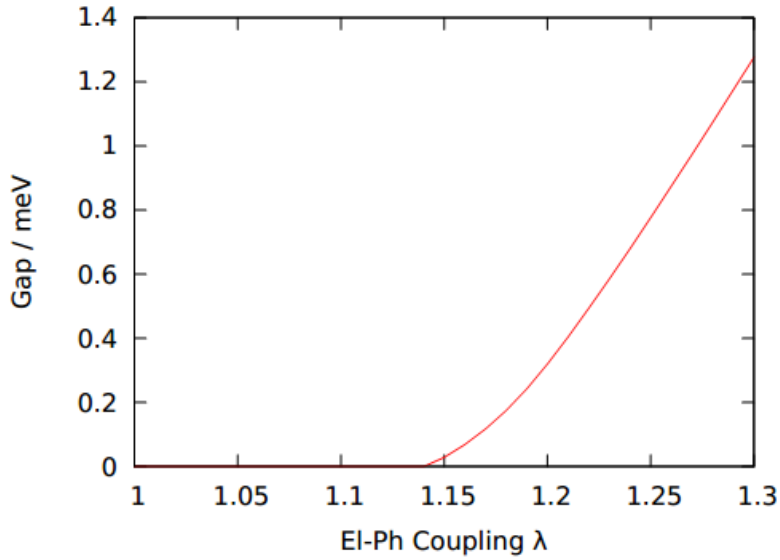

Figure 2: Formation of a bias-free gap in bilayer graphene. The gap opens at $\lambda \simeq 1.14$, increasing rapidly with electron-phonon coupling. A gap of $E_g \simeq 1$eV is found for dimensionless electron-phonon coupling constants of around $\lambda = 1.25$.