Substrates, electron-phonon interactions and the modification of graphene band gaps

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While the zero bandgap in graphene leads to exceptional electronic properties, it hampers attempts to make transistors for digital applications. This presentation describes how the presence of substrates might be used to solve this problem. Recent experimental work has shown that there may be bandgaps in graphene on certain substrates: There has been significant debate regarding whether a gap is present in monolayer graphene on silicon carbide [1,2] and ARPES measurements have found a gap in graphene on a monolayer of intercalculated gold on ruthenium [3]. While there is significant controversy about the origin of the gap seen in Ref. [1] and the nature of the reconstruction of the surface of the SiC system (see e.g. [4]), the authors of Ref. [3] have found evidence for the opening of the gap in the ruthenium system due to a breaking of the symmetry of the two carbon sub-lattices in graphene. Given this surprise gap opening, there are likely to be many other systems in which gaps can be generated by a substrate.

The existence of substrates that can modify the electronic structure of graphene raises the interesting possibility of using the substrate to induce interactions between the electrons in the monolayer. In a two dimensional material, effective electron-electron interactions can be induced via a strong interaction between the electrons in the layer and phonons in a strongly polarizable substrate because of limited out of plane screening [5]. I calculate the effects of electron phonon interaction on electrons in both a linear chain (1D analogue) and a honeycomb lattice (graphene) where a gap has been opened with a modulated potential. I present results for both systems, computed using the numerically exact diagrammatic quantum Monte Carlo technique. The results show an increase in the gap on increased electron-phonon coupling, until the gap becomes filled when polaron side bands form. This demonstrates the potential to use substrate (or superstrate) induced electronic correlations to engineer the electronic properties of graphene.

References

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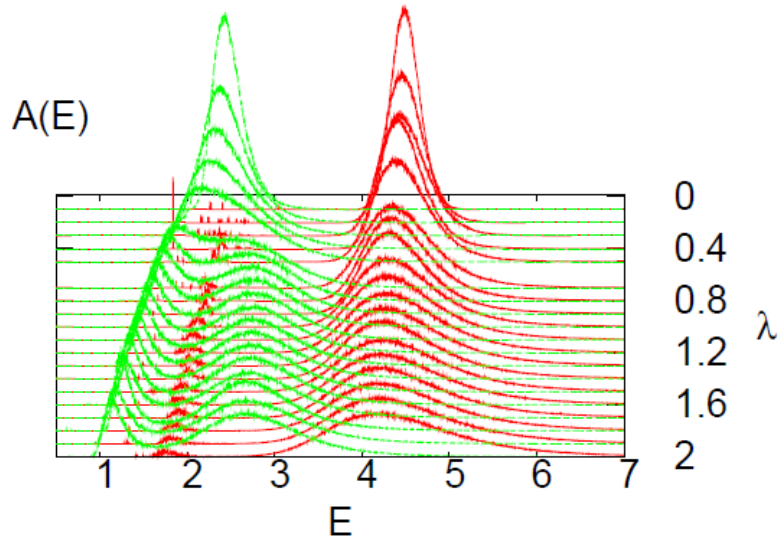
Figures



Spectral functions A(E) of A and B type electrons at the edge of the Brillouin zone on a chain with modulated potential used as a 1D analogue of the graphene substrate system. Note the increase in the band gap as the electron-phonon coupling (λ) is increased, and the polaron side band which forms in the gap at large coupling.