The effects of electron-phonon interactions on bandgaps.

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Abstract. I compute the spectral functions of a 1D Holstein polaron moving in a modulated potential, to examine the effects of electron-phonon interactions on band gaps. The imaginary time Green function is computed using diagrammatic quantum Monte Carlo, which exactly sums the diagrammatic series. From the imaginary time Green function, spectral functions are computed. The electron-phonon interaction flattens the electronic dispersion and leads to an increase in the gap at momentum $k = \pi/2$. At strong coupling, polaron sidebands form in the gap. These results demonstrate the strong effect that electron-phonon interactions can have on band gaps.

1. Introduction
The size of bandgaps is a crucial feature in developing semiconductor devices, and is especially important in LED design, semiconductor lasers and influences the usefulness of semiconductors to make transistors. An open question persists about how interactions influence band gaps, with the effects of electronic correlations on band insulators remaining an important topic in condensed matter theory [1].

The Hamiltonian considered here represents a Holstein model [2] which is augmented with a modulated potential of magnitude $\Delta$,

$$H = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + \sum_i \Delta (-1)^i n_i + g \omega_0 \sum_i n_i (b_i^\dagger + b_i) + \omega_0 \sum_i (b_i^\dagger b_i + 1/2)$$

Here, electrons hop between sites because of an overlap integral of magnitude $t$. The modulated potential represents the energy shift in a superstrate due to a commensurate substrate with two types of atoms, and the Holstein electron-phonon coupling term represents an interaction of strength $g$ with a polarisable substrate. Phonons are created on site $i$ with the operator $b_i^\dagger$, $c_i^\dagger$ creates electrons, $n_i$ is the number operator for electrons and $\omega_0$ is the frequency of the Einstein phonons described by the last term in the Hamiltonian. Even indexed sites with energy offset $+\Delta$ will be denoted as A sites and odd index sites with energy offset $-\Delta$ will be denoted as B sites. This model is similar to the ionic Hubbard model [1] with the Coulomb repulsion replaced by an electron-phonon interaction. It is common to introduce a dimensionless electron-phonon coupling, which is defined here as $\lambda = g^2 \omega_0 / 2t$.

In the absence of electron-phonon interaction, the Hamiltonian leads to energy bands of the form $E_{A,B}(k) = \pm \sqrt{\gamma^2(k) + \Delta^2}$ where $\gamma(k) = -2t \cos(k)$ i.e. there is an energy gap with...
magnitude $2\Delta$ at momentum $k = \pi/2$ as illustrated in Figure 1. It is the aim of this paper to demonstrate the influence of electron-phonon interactions on this band gap.

![Figure 1](image1.png)  
**Figure 1.** Bare dispersion at $\lambda = 0$ showing various modulated potential sizes, $\Delta$.

Figure 2. Example of a diagram in the expansion. Curved lines represent phonons and the straight line the electron. Filled circles represent interaction vertices. Also shown are the signs of the constituent propagators. It can be seen that any possible minus sign problems associated with the anomalous propagators cancel because there are always an even number of such propagators.

2. Method

I use a form of diagrammatic quantum Monte Carlo to compute the exact imaginary time Green functions for the polaron [3, 4]. A small modification is required to deal with a binary basis. In the presence of a modulated potential, it is appropriate to represent non-interacting Green functions as a matrix. For imaginary time, $\tau > 0$ and at absolute zero, the Green functions are defined as follows:

$$G = \begin{pmatrix} G_{AA} & G_{AB} \\ G_{BA} & G_{BB} \end{pmatrix} = \begin{pmatrix} -\langle c_A(\tau)c_A^\dagger(0) \rangle & -\langle c_A(\tau)c_B^\dagger(0) \rangle \\ -\langle c_B(\tau)c_A^\dagger(0) \rangle & -\langle c_B(\tau)c_B^\dagger(0) \rangle \end{pmatrix},$$ \hspace{2cm} (2)

where,

$$G_{AA} = \frac{1}{2} \left[ \exp(-E_A\tau) + \exp(-E_B\tau) \right] + \frac{\Delta}{2 \sqrt{\gamma^2 + \Delta^2}} \left[ \exp(-E_A\tau) - \exp(-E_B\tau) \right]$$ \hspace{2cm} (3)

$$G_{BB} = \frac{1}{2} \left[ \exp(-E_B\tau) + \exp(-E_A\tau) \right] + \frac{\Delta}{2 \sqrt{\gamma^2 + \Delta^2}} \left[ \exp(-E_B\tau) - \exp(-E_A\tau) \right]$$ \hspace{2cm} (4)

$$G_{AB} = G_{BA} = \frac{1}{2} \frac{\gamma}{\sqrt{\gamma^2 + \Delta^2}} \left[ \exp(-E_B\tau) - \exp(-E_A\tau) \right].$$ \hspace{2cm} (5)

For $\tau < 0$ and absolute zero, all Green functions are zero valued because the polaron only contains a single electron. In its most basic form, the algorithm proceeds by inserting and removing interaction lines into or from the electron propagator. Since $G(\tau < 0) = 0$, vertices are time ordered between times 0 and $\tau$, where $\tau$ is the length of the diagram. This time ordering averts any major sign problems. The propagators of the Holstein interaction represent local phonons with a local interaction term, so the interaction lines have the form $\exp(-\omega_0\tau)\delta_{XX}$ where $X \in \{A, B\}$ represents sub-lattice type and $\delta_{XX}$ is the Kronecker delta function (i.e. phonons on A sites can only interact with electrons on site A). By fixing the lattice type of the vertices at the ends of the diagram and inserting multiple lines with both A and B end vertices, the full interacting Green function can be calculated.

It is worth noting that there is an unusual symmetry between the two non-interacting bands in the anomalous Green functions, $G_{AB}$ and $G_{BA}$, such that reassigning A and B sites introduces
a minus sign. This is not a problem, as there are always an even number of anomalous non-interacting Green functions in the full diagonal Green functions $G_{AA}$ and $G_{BB}$. Therefore any negative signs arising from reassigning the bands cancel to give a net positive sign, as demonstrated by the example in Figure 2. The factor $\gamma(k)$ can be negative or positive depending on the momentum, however the average sign has been found to be $\langle s \rangle > 0.9999$ for all cases discussed here. The $\tau$ dependent Green function is measured here using the estimator given in Ref. [4] which is free of systematic errors.

3. Results

![Figure 3](image1.png)  
**Figure 3.** Momentum dependent electronic spectrum when $\lambda = 0.5$ for (a) band A electrons (b) B band electrons.

![Figure 4](image2.png)  
**Figure 4.** Momentum dependent electronic spectrum when $\lambda = 1.0$ for (a) band A electrons (b) B band electrons.

I briefly discuss some of the results obtained for this model. For illustration purposes, a large non-interacting half band gap $\Delta = 1$ is chosen so that the bands are clearly resolved. The Green functions $G_{AA}$ and $G_{BB}$ are computed for a range of momenta and $\lambda$ values by making $10^9$ measurements to obtain an accuracy of greater than 0.5% at 500 imaginary time points ranging
from $\tau = 0$ to $\tau = 5$. To obtain spectral functions, a numerical procedure is used to invert the integral transform relating the $\tau$-dependent Green function and the spectral function,

$$G(\tau) = \int_0^\infty \exp(-E\tau)A(E),$$

where $A(E)$ is the spectral function. In this way, the analytic continuation of the Green function is carried out. A continuous-frequency Monte Carlo approach is used to determine spectral functions, with sets of several thousand delta functions free to change frequency and magnitude. These are sampled according to the weight, $\exp(-\chi^2/\alpha)$. $\alpha$ is decreased until the spectrum meets the historic maximum entropy condition of $\chi^2 = N_d$ where $N_d$ is the number of data points. It is anticipated that the more sophisticated stochastic analytic inference will be used for a future improvement in spectral function resolution [5].

I start by showing spectral functions for A and B type electrons at $\lambda = 0.5$ (Fig. 3) and $\lambda = 1.0$ (Fig. 4). For all figures, $\omega_0 = t = 1$. Two bands can be seen, with spectral weight at high energies for A type electrons, and at lower energies for B type electrons. There is a gap at $k = \pi/2$. Both spectra have the same basic form as shown in figure 1. As the electron-phonon interaction is increased from $\lambda = 0.5$ to $\lambda = 1.0$, there is a slight increase in the band gap, and some band flattening occurs. This band flattening has also been seen for polarons in the absence of a modulated potential [6]. There is an increase in the width of the excitation peaks indicating a decrease in quasi-particle lifetime, and a polaron side band can be seen forming above the electron band in figure 4(b) around $k = \pi/2$ which is the signature of an excitation consisting of an electron and a single phonon.

![Figure 5.](image-url)  
(a) Evolution of the spectral weight of A site electrons as the electron-phonon interaction $\lambda$ is increased. (b) As panel (a) for B site electrons.

To examine the $\lambda$ dependence of the gap more clearly, I show the evolution of the spectral functions at $k = \pi/2$ in figure 5. As the electron-phonon interaction increases, the energy of the B type band decreases more rapidly than the energy of the A type band, which leads to a band gap increase. The polaron side band can also be seen. Since a phonon needs to be created for decays from the top band into the polaron side band, it is anticipated that such transitions are rarer than those into the ground state. To show the gap more clearly, both A and B type spectra are shown on a waterfall plot in figure 6.

4. Summary and conclusions

In this paper, I computed spectral functions of a polaron in a 1D modulated potential, demonstrating that in one dimensional systems, electron-phonon interactions could be used
Figure 6. Spectral functions of A and B type electrons at $k = \pi/2a$. Note the increase in the band gap as the electron-phonon coupling is increased, and the polaron side band.

...to modify substrate induced bandgaps. By analysing the spectral function, it was found that the electron-phonon interaction initially leads to an increase in the gap, although with stronger interactions polaron side bands form in the gap.

Photoemission results suggest that a bandgap of the order of 0.25 eV is formed in graphene placed on a substrate of SiC [7] and a bandgap has been predicted for graphene on hexagonal boron nitride [8]. This raises the possibility that a similar electron-phonon mediated enhancement might be accessible for graphene. Work to explore this possibility is currently in progress.

Acknowledgments
I am pleased to acknowledge EPSRC grant no. EP/H015655/1 and useful discussions with Pavel Kornilovitch, Sasha Alexandrov, Mervyn Roy, Peter Maksym, Ed McCann, Nigel Mason and Nick Braithwaite.

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