Notes on the impacts of electric field on nanostructures

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Contents

1 One dimensional non-interacting systems

1.1 One-band model

We first consider a one dimensional chain consisting of N sites with the following Hamiltonian

$$H = \sum_{n=1}^{N} [\epsilon_{\rm G} + n\Delta] c_n^\dagger c_n + t \sum_{n=1}^{N-1} \left(c_n^\dagger c_{n+1} + \text{H.c.} \right), \tag{1}$$

where $\epsilon_{\rm G}$ is the on-site energy, $\Delta = eEa$, with e being the charge of an electron, E is the electric field, and a is the lattice constant. The annihilation (creation) operators corresponding to Wannier states $w_n(x)$ localized at $n-th$ site is denoted with $c_n^{(\dagger)}$.

In the absence of electric field $\Delta = 0$, the Hamiltonian is diagonalized in the basis of Bloch states $\Psi_k(x) = \sum_n e^{ikna} w_n(x)$, with spectrum $\epsilon_k = \epsilon_0 + 2t\cos(ka)$, with momentum quantum number $k \in [-\pi/a, \pi/a]$. However with the application of electric field, the transnational invariance is destroyed and hence the momentum is not a good quantum number anymore. Following the procedure of Ref. [1], we can look for a linear combination of Wannier states $f_l^\dagger = \sum_m U_{l,m} c_m^\dagger$ than can diagonalize Hamiltonian Eq. 1. Hence we require

$$[H, f_l^\dagger] \stackrel{!}{=} E_l f_l^\dagger \Rightarrow \sum_m c_m^\dagger \left[(m\Delta - E_l) U_{l,m} + t\{U_{l,m-1} + U_{l,m+1}\} \right] \stackrel{!}{=} 0, \tag{2}$$

which because of the linear independence of Wannier functions implies the following recursive relation

$$\{U_{l,m-1} + U_{l,m+1}\} + \frac{m - (E_l/\Delta)}{2t/\Delta} U_{l,m} = 0 \tag{3}$$

which is characteristic of Bessel's functions of order $m - (E_l/\Delta)$.

Figure 1 shows the numerical evaluation of the spectrum as well as the eigenstates of Eq. 1 as a function of quantum number i. While in the absence of electric field, the eigenstates are the Bloch states, for finite field the eigenstates exhibits Oscillatory behaviour followed by exponential decay. This is similar behaviour as the Airy functions which are the wavefunctions of a particle in a tilted box (particle in a box with additional external electric field). Figure 2 shows the first few eigenenergies as a function of electric field. We see the formation

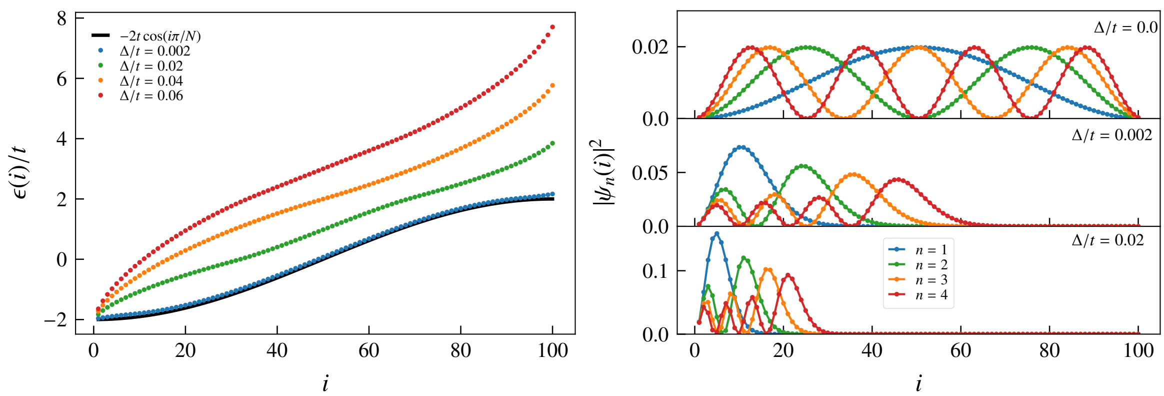

Figure 1: Left: The energy spectrum for various electric field strengths for $N = 100$, $\epsilon_{\rm G} = 0$. Right: The magnitude of first few eigenstates for various fields.

of Stark ladders for larger m.

1.2 Two-band Model

We now turn our focus to a two-band model with the folowing tight binding Hamiltonian

$$H = \sum_{o=1,2} \sum_{n=1}^{N} [\epsilon_o + n\Delta] c_{o,n}^\dagger c_{o,n} + \sum_{o,o'=1,2} t_{o,o'} \sum_{n=1}^{N-1} \left(c_{o,n}^\dagger c_{o',n+1} + \text{H.c.} \right) + \eta\Delta \sum_{n=1}^{N} \left(c_{1,n}^\dagger c_{2,n} + \text{H.c.} \right), \tag{4}$$

where the first term describes the modification of the onsite-energy for different orbitals $o = 1, 2$, the second terms is the tunnel coupling and the last term has been included to account for the possibility of orbital excitations with the aid of electric field.

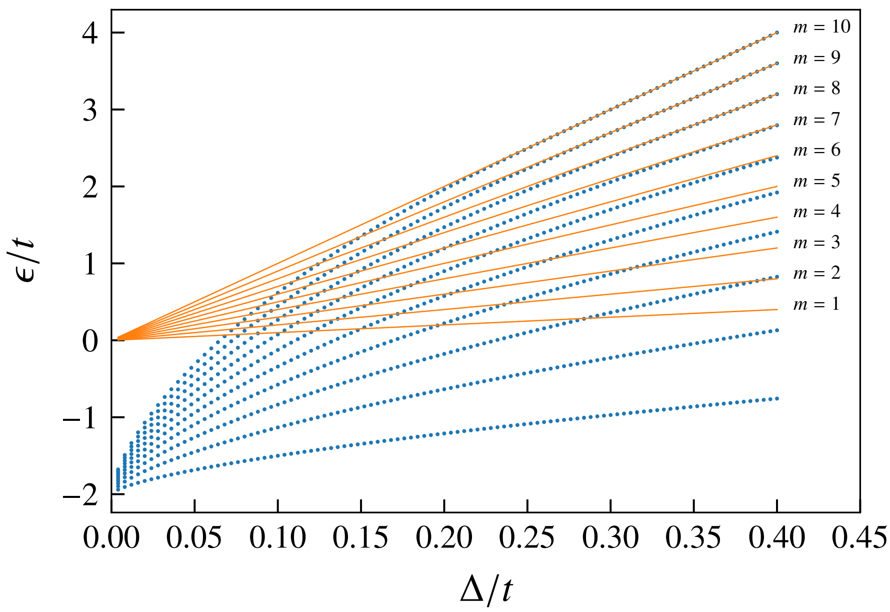

Figure 2: The spectrum as a function of applied field Δ/t (filled circles). The solid lines show the stark ladders $E_m = m\Delta$.

1.2.1 In the absence of interband coupling ($t_{1,2} = t_{2,1} = 0, \eta = 0$)

In the absence of inter-band coupling, we investigate whether the Stark ladders will be formed. In the absence of gate voltage $\epsilon_1 = \epsilon_2 = 0$, we indeed get the Stark ladders with a double degeneracy. For finite gate voltage as shown in figure 3, we have two branches of Stark ladders. However due to overlap of ladders for electrons and holes the spectrum is more complex. In figures 4 and 5 we look at the spectrum and density of state for various

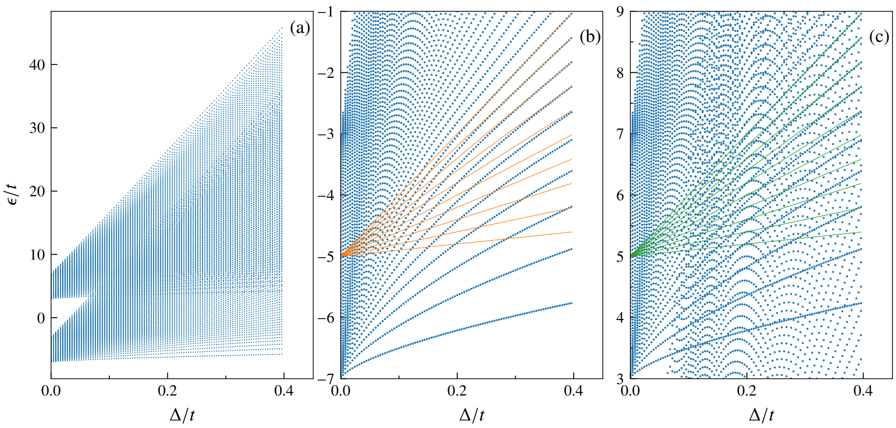

Figure 3: (a) The spectrum as a function of applied field Δ/t. (b)-(c) Compasison a selected region of the spectrum with the stark ladders for electron and holes $E_m = \epsilon_{e/h} + m\Delta$ (solid lines).

gate voltages at a fixed electric field. We can identify three distinct regions: (1) for vanishing gate voltages we have one set of doubly degenerate Stark ladder similar to the one band model (with additional degeneracy). (2) for intermediate gate voltages the ladder stars to split and we see interference pattern and finally (3) for large gate voltages, there is a finite gap and we see two separate Stark ladders. I noticed similar analysis is done in Ref. [2].

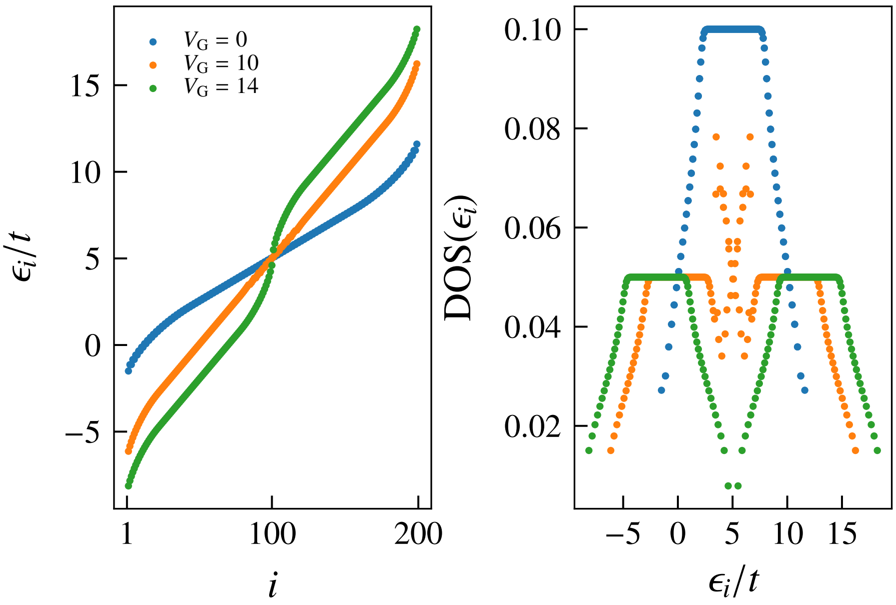

Figure 4: Left: The energy spectrum for applied field $\Delta/t = 0.1$, $N = 100$ and various gate voltages. Right: The corresponding density of state as a function of energy.

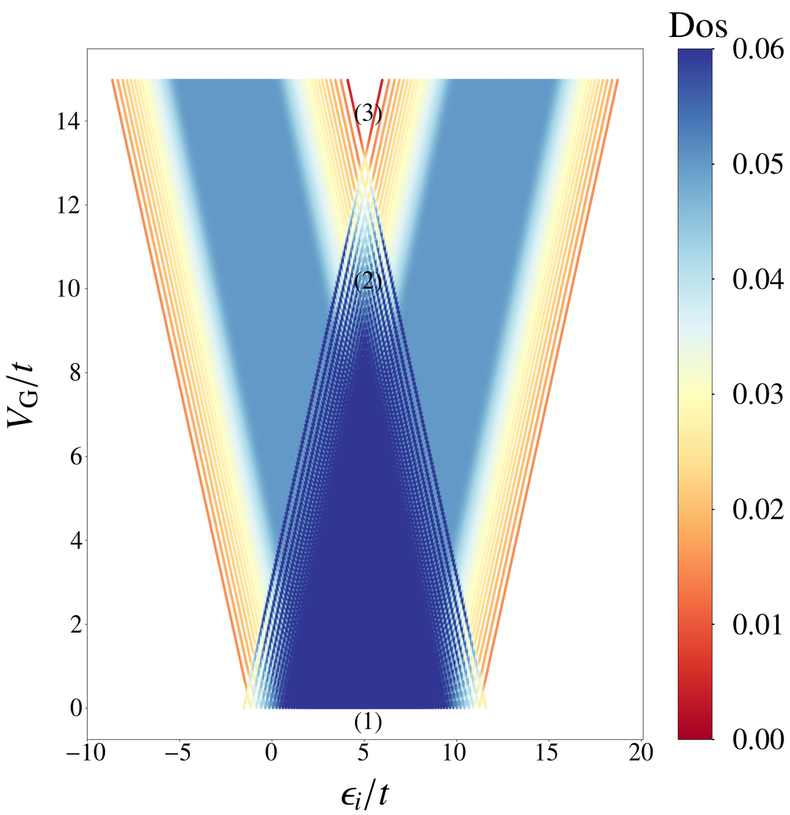

Figure 5: Density of state as a function of eigenenergies and gate voltage.

2 kwant simulation

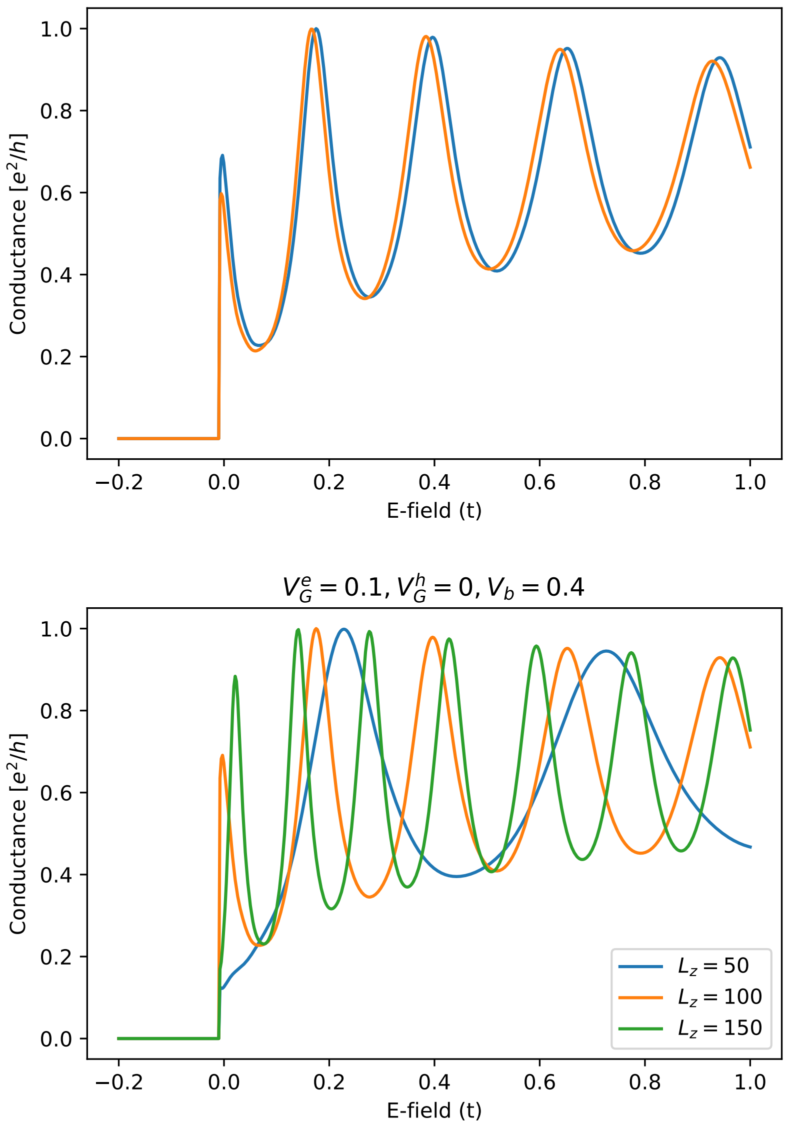

Figure 6: Conductance as a function of electric field.

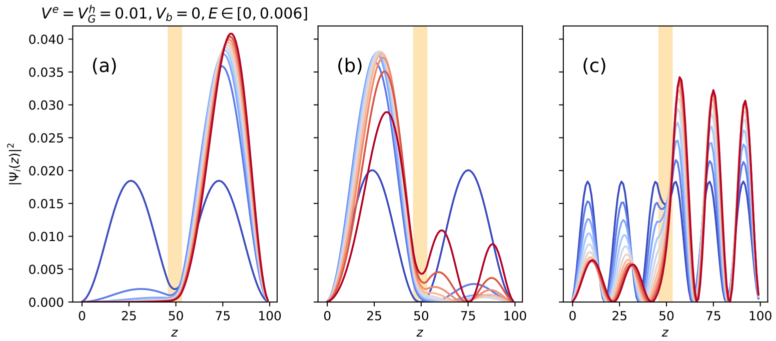

Figure 7: Position dependance of wavefunctions for varying electric field.

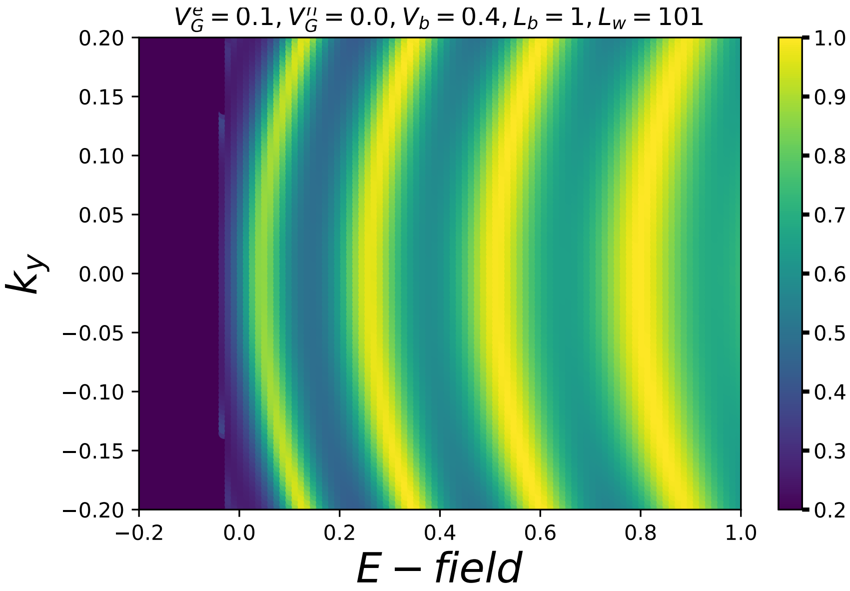

Figure 8: Transmission as a function electric field and k_y.

3 Realistic parameters

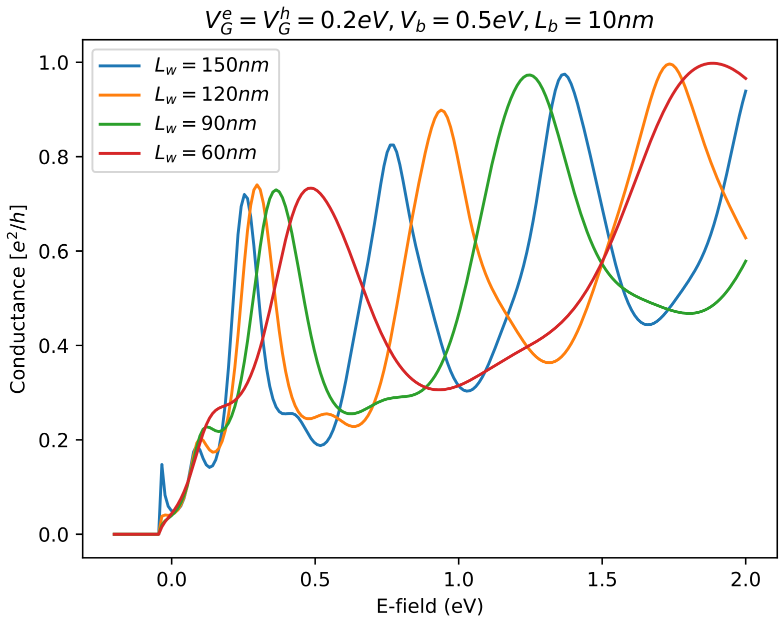

Figure 9: Conductance as a function electric field for various well-lengths.

References

[1] K. Hacker and G. Obermair. Stark ladders in a one-band-model. *Zeitschrift für Physik A Hadrons and nuclei*, 234(1):1–5, Feb 1970.

[2] T. Kawaguchi and M. Saitoh. Stark ladders in a two-band tight-binding model. *Journal of Physics: Condensed Matter*, 3(47):9371–9380, nov 1991.

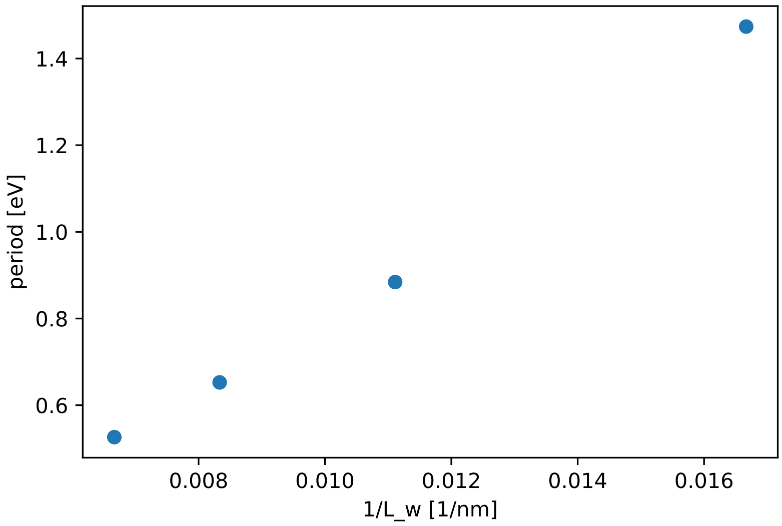

Figure 10: Transmission as a function electric field and k_y.

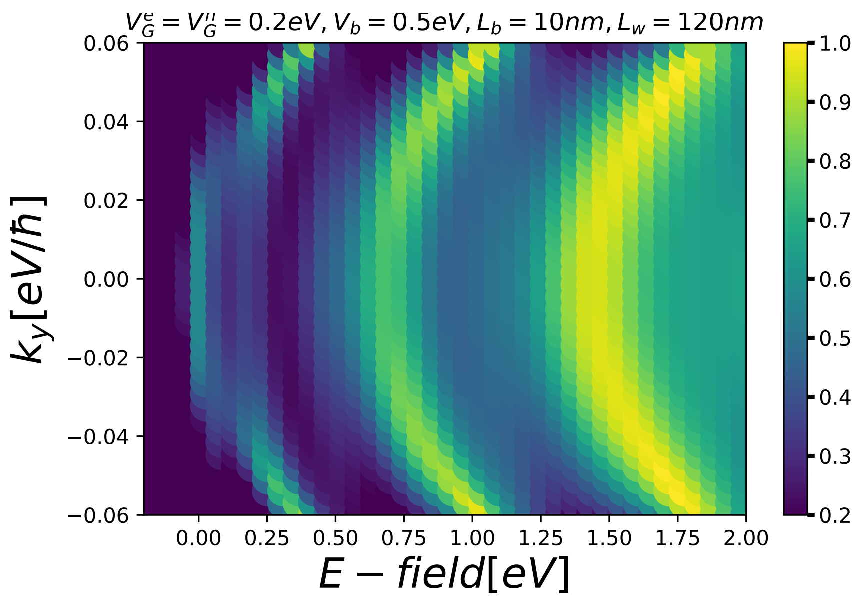

Figure 11: Length dependance of period of oscillations.

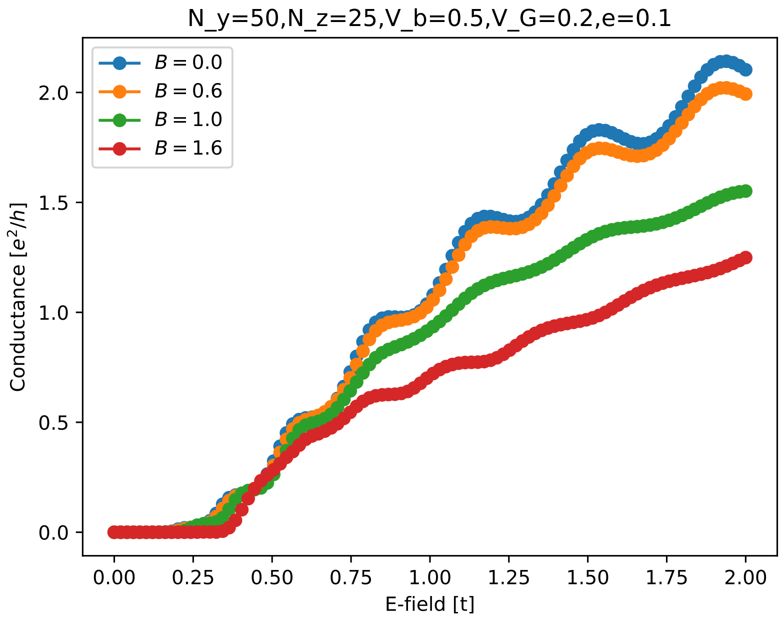

Figure 12: Length dependance of period of oscillations.

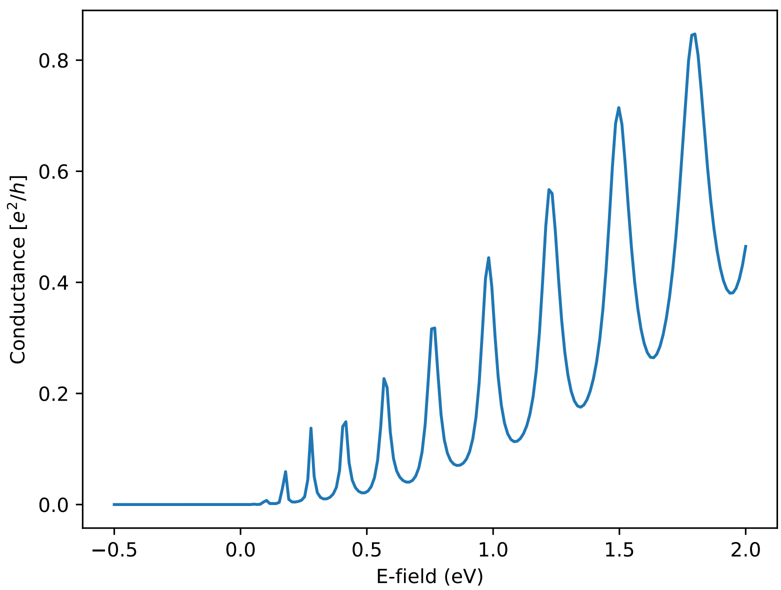

Figure 13: Conductance as a fucntion bias Voltage.

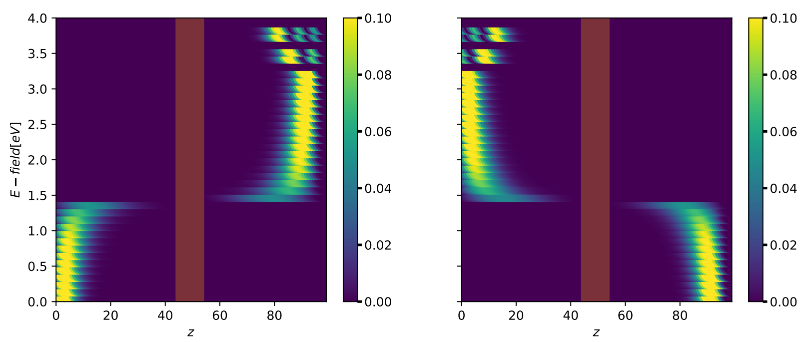

Figure 14: Local density of state for electrons and holes.

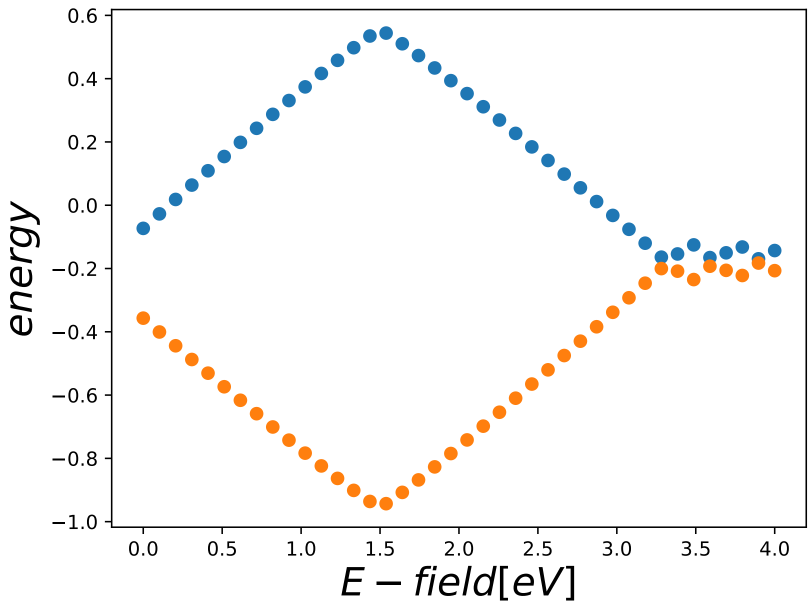

Figure 15: buttom/top of e/h band as a function of E-field.