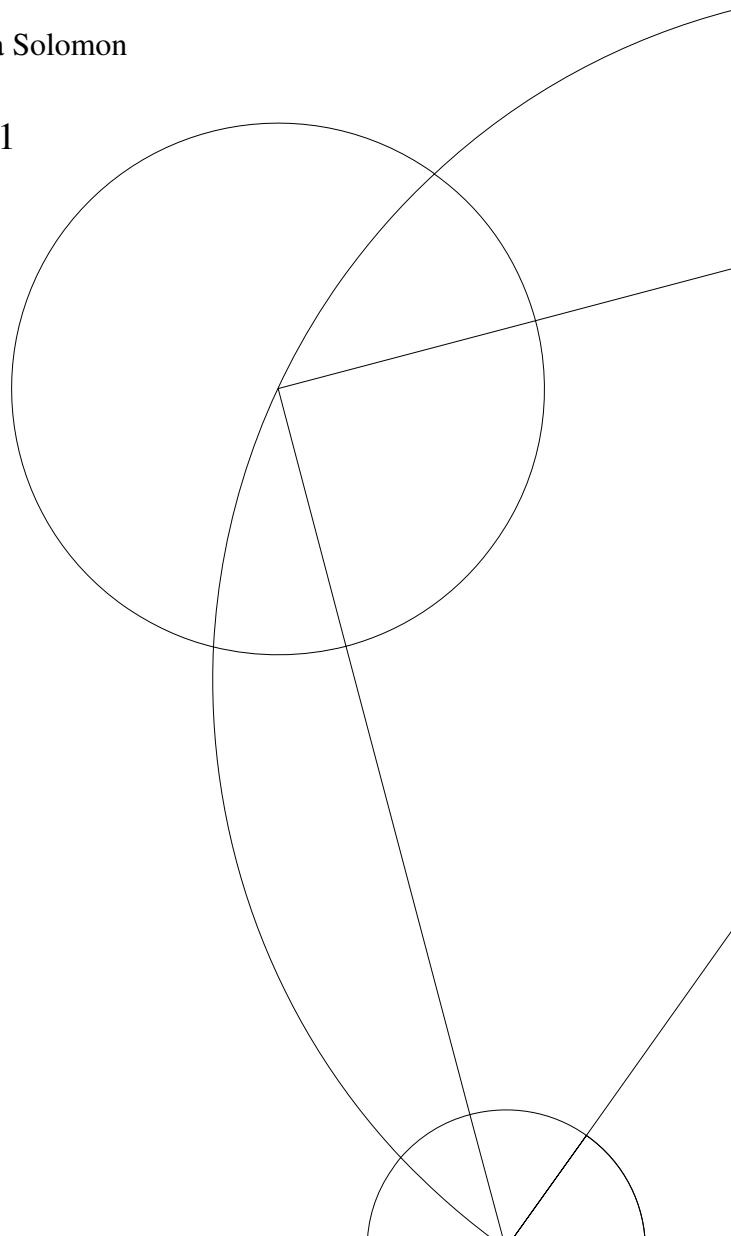


# **TOWARDS MOLECULAR QUANTUM GATES: INVESTIGATION OF THE INTERFERENCE EFFECTS IN TRANSMITTED PHASE THROUGH MOLECULES**

Amalie Terese Jiao Paulsen

Supervisor: Gemma Solomon

June 2021



---

## CONTENTS

---

1	INTRODUCTION	1
2	THEORY	2
2.1	Molecular junctions . . . . .	2
2.2	Atoms and their electronic structure . . . . .	3
2.3	Electronic transport theory . . . . .	4
3	SIMULATIONS, DATA AND DISCUSSION	8
3.1	Python script for theoretical computation . . . . .	8
3.2	The phase of linear conjugated systems at the Fermi energy . . . . .	9
3.3	Reproducing $\pi/4$ phase gate from Childs' paper . . . . .	10
3.4	Changing the phase of linear conjugated systems . . . . .	11
3.4.1	Impact of $\alpha$ . . . . .	11
3.4.2	Impact of $\beta$ and $\beta_l$ . . . . .	13
3.5	The phase of cyclic molecules connected to linear chains . . . . .	19
3.5.1	Cyclic molecules connected to 1 atom . . . . .	20
3.5.2	Cyclic molecules connected to 3 and 5 atoms . . . . .	20
3.6	Towards a candidate for a $\pi/4$ phase gate . . . . .	23
4	CONCLUSION	26
	Appendices . . . . .	28
A	Investigation of narrowing . . . . .	28
B	Investigation $\pi$ in even molecules - maple . . . . .	30
C	Investigating $\pi$ even molecules . . . . .	37
D	Investigating alpha for cyclic molecules . . . . .	39
E	Phase as a function of beta for 5 -linear . . . . .	45
F	Phase as a function of beta for 6 - linear . . . . .	48
G	Shift in transmission for 5 - linear . . . . .	52
H	Shift in transmission for 6 - linear . . . . .	61
I	phase of cyclic systems . . . . .	71
	Bibliography	73

# 1

---

## INTRODUCTION

---

The beauty of classical electronic devices is the simple building blocks of transistors.[1] These are collected into different gates that combined with a thousand others result in an immense calculation power. However, there are crucial limits to perform certain tasks such as factorization and simulations of cell response to pharmaceutical drugs.[2], [3] This is all due to the whole calculation process of classical computers. Therefore, there is a comprehensive search for another way to build a computer which can be dated back to Richard Feynman(1982).[4] The field has been under great development in the last 10 years, but the perfect building blocks for the quantum computer has not yet been found. However, the approach of using molecular junctions in quantum gates is a very promising field. This is because the number of molecules available are almost infinite. As molecules are natural in the nm-size, observing quantum mechanical effects like quantum interference are possible at room temperature .[5] This is a great advantage opposed to other technologies which rely on cooling to extreme temperatures.[6] Unfortunately, there are some huge gaps in the knowledge of single molecular junctions. One of the greatest being the phase of the transmitted electron wave function. Gaining more knowledge about the phase will streamline the development of phase gates for quantum computers.

*This project aims to investigate the phase of the transmitted wave function through single molecular junctions using a variety of linear conjugated systems.*

This is done in order to find some tendencies of the phase when using different molecular systems. In the end we encapsulate some requirements for using molecular junctions as candidate systems for  $\pi/4$  quantum phase gates.

The theory used in this project is presented in section 2 along with the method used for the computations. In section 3, we present the results from analyzing the behavior of conjugated linear systems and conjugated linear systems with cyclic side chains. Encapsulating the results from the analysis will give a deeper understanding of the phase tendencies as well as getting us closer to a  $\pi/4$  quantum phase gate.

# 2

---

## THEORY

---

### 2.1 MOLECULAR JUNCTIONS

A molecular junction can be achieved by connecting a molecule to two electrodes as seen in fig. 1 A). The yellow dots are representing the electrodes, and the green dots are representing an arbitrary molecule. The grey dots only represent the coupling between the molecule and the electrode. The electrodes are often made of inert metal plates like gold or silver.[7], [8] Applying a voltage difference between the electrodes make the electrons move from one electrode to the other through the molecule.[9] Due to the small size of the junction we only look at the electron properties in terms of its wave function obeying the rules of quantum mechanics.[9] This project examines the theoretical phase of the transmitted wave function through a single molecular junction using Landauer formalism. A central observation when studying the phase is that phase coherence is maintained across the molecule which is a premise used through the paper without proof.

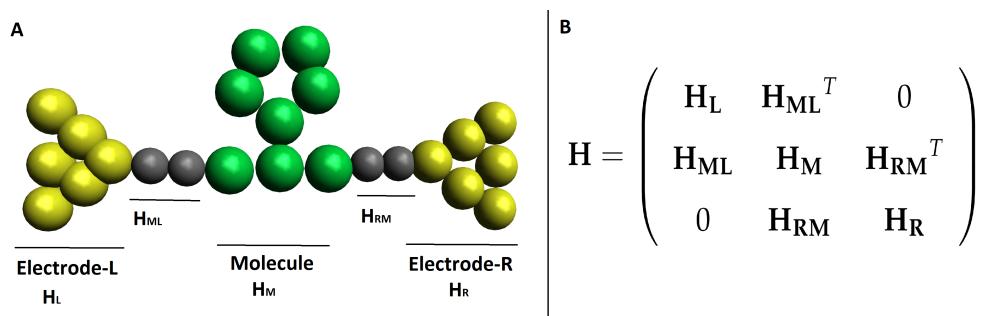


Figure 1: A) A model of a molecular junction. The gold atoms are the electrodes and the green ones are the molecule. The grey dots are not real atoms but represent the coupling between the electrodes and the molecule. B) is a general representation of the extended Hückel for the molecular junction.

## 2.2 ATOMS AND THEIR ELECTRONIC STRUCTURE

The model of the molecular junction in fig. 1 A) makes it possible to examine the transmitted electron wave function through multiple types of molecules. The investigated molecules are represented by their electronic structure. This is done by writing up their molecular orbitals (MO) using linear combination of atomic orbitals (LCAO). Thereby, each molecule is represented by a weighted sum of an atomic orbital basis. A type of LCAO-method is the Extended Hückel theory which is used in this project.

### *The extended Hückel theory*

The Hückel theory describes planer conjugated systems. The great success of Hückel theory is predicting that bonds of conjugated system act like they are sharing all the bonds rather than having alternating double single bonds.[10] In this project we have 1 Orbital pr. site and 1 electron in each orbital. The Hückel theory only take the p electrons in the outer orbitals into account which are the electrons in the  $\pi$ -bond framework [11]. The basis set is then constituted solely of the  $\pi$ -electrons neglecting  $\sigma$  -  $\pi$  interactions. The approximations of the Hückel theory are:[9], [10], [12] All orbitals are orthogonal to each other (This simplification means that either the electron feels the full potential from a nucleus, or it does not feel the potential at all). Nearest neighbour interactions - electrons are only able to feel the Coulomb interaction of their own nucleus and the nucleus next to it. All other resonances are set to 0. All atoms make an equal contribution to the MO basis, and their Coulomb integrals are set to  $\alpha$ . The size of the resonance between neighbor atoms are denoted  $\beta$ . Overlap integrals and remaining resonances are set to 0. This means the Hückel Hamiltonian can be expressed as:

$$\mathbf{H}_{\mathbf{M}i,j} = \langle i | H | j \rangle = \begin{cases} \alpha & \text{for } i = j \\ \beta & \text{for } i = j \pm 1 \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

$\mathbf{H}_{\mathbf{M}i,j}$  is the i,j'th component in the Hückel Hamiltonian of the molecule. The Hückel Hamiltonian can be extended to contain the Hückel of the molecule  $\mathbf{H}_M$ , the electrodes  $\mathbf{H}_L$  and  $\mathbf{H}_R$  as well as the coupling elements between them  $\mathbf{H}_{RM}$  and  $\mathbf{H}_{LM}$ . Often the extended Hückel Hamiltonian is

represented as a block matrix seen in fig. 1 B)[9], [13], [14].

For a 2 atom linear conjugated molecular system the extended Hückel Hamiltonian becomes:

$$\mathbf{H} = \begin{pmatrix} \alpha' & \beta' & 0 & 0 \\ \beta' & \alpha & \beta & 0 \\ 0 & \beta & \alpha & \beta' \\ 0 & 0 & \beta' & \alpha' \end{pmatrix}, \mathbf{H}_M = \begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix}, \mathbf{H}_{ML} = \begin{pmatrix} \beta' \\ 0 \end{pmatrix}, \mathbf{H}_{RM} = \begin{pmatrix} 0 \\ \beta' \end{pmatrix} \quad (2)$$

Where  $\alpha$  and  $\alpha'$  are the on site energies of the atoms and of the electrodes, respectively.  $\beta$  is the strength of the coupling between neighbour atoms and  $\beta'$  is the coupling element between the molecule and the electrodes.

## 2.3 ELECTRONIC TRANSPORT THEORY

### *Landauer formalism*

The conductance in macroscopic systems obeys Ohm's law which states a linear dependence of the conductance with the width. However, in mesoscopic systems this approximation does not hold, and instead we use the Landauer formalism written as: [9], [15]

$$I = \frac{2e}{h} \int_{-\infty}^{\infty} d\epsilon [f_L(\epsilon) - f_R(\epsilon)] T(\epsilon) \quad (3)$$

$f(\epsilon)$  is the Fermi function and is introduced to account for the Pauli principle.  $T(\epsilon)$  is the transmission probability of the electron through the molecule. Since many electrons contribute to the current, the integral is taken over all the quantum-states occupied at a given energy. The factor 2 accounts for the spin degeneracy. The theory predicts an energy dependence of the electron transport through a molecule. [16]

The Fermi function describes the probability of an orbital being occupied at a given temperature: [9], [15], [17]

$$f_{L(R)}(\epsilon) = \frac{1}{e^{\frac{\epsilon - \mu_{L(R)}}{kT}} + 1}, 0 \leq f_{L(R)}(\epsilon) \leq 1. \quad (4)$$

$\epsilon$  is the energy state of the electron and  $\mu_{L(R)}$  is the chemical potential of the left(right) electrode.  $\mu_{L(R)}$  is a measure of how many electronic states which are occupied on each side.

A voltage can change the chemical potential of an electrode. The biaswindow:  $f_L(\epsilon) - f_R(\epsilon)$  in eq. 3 is a function of the difference in chemical potentials between the two electrodes and thereby the applied bias voltage. A difference in the chemical potentials will create a current. When there is no bias voltage applied, the two electrodes are in equilibrium with each other, and hence no electrons can run through.

### *Transmission function*

The transmission function describes the transmission probability of an electron travelling through a system. The probability is dependent of the number of conduction channels in the system. The simulated molecular junctions used in this project will only have one conductance channel. Therefore, the transmission probability behaves like a regular probability ranging from 0 to 1. The transmission function is dependent of the electron energy: [9], [18], [19]

$$T(\varepsilon) = \text{Tr} \left\{ \boldsymbol{\Gamma}^L \mathbf{G}^{\text{ret}}(\varepsilon) \boldsymbol{\Gamma}^R \mathbf{G}^{\text{adv}}(\varepsilon) \right\}, \quad 0 \leq T(\varepsilon) \leq 1 \quad (5)$$

Where  $\mathbf{G}^{\text{ret}}$  and  $\mathbf{G}^{\text{adv}}$  are the retarded and advanced Green's function, respectively.  $\boldsymbol{\Gamma}^{\text{L(R)}}$  is the spectral density matrix describing the coupling between the left (right) electrode and the molecule. The strength of the coupling between the left(right) electrode and the i'th and j'th element in the molecule are given by[18], [19]:

$$\boldsymbol{\Gamma}_{ij}^{\text{L(R)}}(\varepsilon) = \sum_{\alpha} V_{i\alpha}^{L(R)} d_{\alpha(\beta)}^{L(R)}(\varepsilon) d_{\alpha(\beta)}^{L(R)}(\varepsilon) V_{\alpha(\beta)j}^{L(R)} \quad , \quad d_{\alpha(\beta)}^{L(R)}(\varepsilon) = \sqrt{2\pi\delta(\varepsilon - \varepsilon_{\alpha(\beta)}^{L(R)})} \quad (6)$$

$V^{L(R)}$  is the coupling matrix between the molecule and the left(right) electrode,  $\alpha(\beta)$  denote the left(right) lead, and  $d_{\alpha(\beta)}^{L(R)}(\varepsilon)$  is the density of states(DOS) of the left(right) electrode. DOS is an expression of the number of states available at energy  $\varepsilon$ . As the electrodes are made of inert metal plates, the energy dependence of the density of states are neglected. Thereby, the wide band approximation can be used which states a constant DOS.[7] Here we set DOS to 1. The spectral density matrix then only constitute of the outer product of the potentials making the  $\boldsymbol{\Gamma}^{\text{L(R)}}$  be expressed as:

$$\boldsymbol{\Gamma}^{\text{L}} = \mathbf{V}^{\text{L(R)}} \otimes \left( \mathbf{V}^{\text{L(R)}} \right)^T \quad (7)$$

### *Non Equilibrium Green's function method*

The Green's function method is highly used when solving the Schrodinger equation for a molecular system as these are almost impossible to solve otherwise.[9] When using Green's function to calculate the current in a molecular junction, the energy is assumed to be complex. The following retarded and advanced Green's function for a single particle problem are obtained: [9], [15]

$$\mathbf{G}^{\text{ret}}(\varepsilon) = \frac{1}{\varepsilon - \mathbf{H}_M + i\eta} \quad , \quad \mathbf{G}^{\text{adv}}(\varepsilon) = \frac{1}{\varepsilon - \mathbf{H}_M - i\eta} \quad (8)$$

When placing the two Green's functions next to each other, it becomes clear that they are Hermitian

conjugate of each other. The two versions of Green's function represent two different boundary conditions corresponding to the incoming- and outgoing- version of the same wave.  $\varepsilon$  is the energy of the incoming electron,  $i\eta$  represent an infinitesimal imaginary part of the energy.  $\mathbf{H}_M$  is the Hückel of isolated molecule. However, in the molecular junction the molecule is not alone but bound to two electrodes which is effecting the molecule. The influence of the electrodes is described below using perturbation theory.

### Perturbation theory

Perturbation is a way of describing a complex quantum system in terms of a more simple and mathematically known one. When perturbing the known Hamiltonian for the isolated molecule, we get the following expression for the electronic structure of the molecule: [12]

$$\mathbf{H}'_M = \mathbf{H}_M - \sum = \begin{vmatrix} \alpha - i * a & \beta \\ \beta & \alpha - i * a \end{vmatrix} \quad (9)$$

Where  $\mathbf{H}'_M$  is the perturbed version of  $\mathbf{H}_M$ .  $\mathbf{H}'_M$  describes the molecule connected to the electrodes.  $a$  is the strength of the electrode coupling,  $\alpha$  is the energy of the atom orbital, and  $\beta$  is the hopping element that describes the amount of energy an electron gain by moving to an adjacent orbital.[9], [12]  $\sum$  is the self energy described below.

### Self energy

The self energy of the Green's function can be expressed in terms of a real and an imaginary part of the molecule-electrode coupling elements:

$$\Sigma_{aa}(\varepsilon) = \Lambda_{aa}(\varepsilon) \mp \frac{i}{2}\Gamma_{aa}(\varepsilon), \quad \Gamma = \Gamma^L + \Gamma^R \quad (10)$$

Where  $\Gamma$  is the full spectral density matrix of the molecular junction, and  $\mathbf{aa}$  is the diagonal elements. As discussed above, we are using the wide band approximation and setting DOS to a constant. This neglects the energy dependence of the self energy. As a result, the real part vanishes, and the imaginary part in the self energy becomes a constant.

$$\Sigma_{aa}(\varepsilon) \simeq \mp \frac{i}{2}\Gamma_{aa} \Rightarrow \Sigma \simeq \frac{i(\Gamma^L + \Gamma^R)}{2} \quad (11)$$

$\Gamma^{L(R)}$  is the spectral density of the left(right) electrode. We get the following expression for the two Green's functions when using the perturbed Hamiltonian:

$$\mathbf{G}^{\text{ret}}(\varepsilon) = \frac{1}{\varepsilon + i\eta - \mathbf{H}_M + \Sigma}, \quad \mathbf{G}^{\text{adv}}(\varepsilon) = \mathbf{G}^{\text{ret}\dagger} \quad (12)$$

The expressions of the Green's functions are dependent of the Hückel Hamiltonian and therefore electronic structure of the molecule.

### *Change of basis*

We change basis from AO to molecular conductance orbital(McO) in order to calculate the phase of the transmitted wave function.[18] This is done by diagonalizing Green's function:

$$\begin{aligned}\mathbf{G}^{\text{ret}'}(\varepsilon) &= \mathbf{C}_{\text{ret}}^{-1} \mathbf{S}^{-1} \mathbf{G}^{\text{ret}}(\varepsilon) \mathbf{C}_{\text{ret}} = \mathbf{C}_{\text{ret}}^{-1} \mathbf{G}^{\text{ret}}(\varepsilon) \mathbf{C}_{\text{ret}} \\ \mathbf{G}^{\text{adv}'}(\varepsilon) &= \mathbf{C}_{\text{adv}}^{-1} \mathbf{S}^{-1} \mathbf{G}^{\text{adv}}(\varepsilon) \mathbf{C}_{\text{adv}} = \mathbf{C}_{\text{ret}}^{\dagger} \mathbf{G}^{\text{adv}}(\varepsilon) \mathbf{C}_{\text{ret}}^{-1\dagger}\end{aligned}\quad (13)$$

$\mathbf{S}^{-1}$  is the overlap matrix which is set to the identity matrix as a part of the Hückel approximation stating that only adjoint orbitals can be felt.  $\mathbf{C}_{\text{ret}(\text{adv})}$  is the eigenvectors of  $\mathbf{G}^{\text{ret}(\text{adv})}$ . The coupling element in the AO basis is defined as: [18].

$$t_{\alpha\beta}^{\text{AO}}(\varepsilon) = \sum_{i,j} \mathbf{V}_{\alpha,i}^L \mathbf{G}^{\text{ret}}{}_{i,j}(\varepsilon) \mathbf{V}_{j,\beta}^R \quad (14)$$

Where  $i,j$  denote a matrix element, and  $\alpha$  and  $\beta$  are representing the electrode leads. As for the Green's function, we similarly change basis from AO to McO basis:

$$t_{\alpha\beta}^{McO}(\varepsilon) = \sum_{i,j} \mathbf{C}_r^{\dagger} \mathbf{V}_{\alpha,i}^L \mathbf{G}^{\text{ret}'}{}_{i,i}(\varepsilon) \mathbf{C}_r^{\dagger} \mathbf{V}_{j,\beta}^R = \sum_i \mathbf{V}_{\alpha,i}^{L\dagger}(\varepsilon) \mathbf{G}^{\text{ret}'}{}_{i,i}(\varepsilon) \mathbf{V}_{i,\beta}^{R\dagger}(\varepsilon) \quad (15)$$

The total coupling are a sum of the individual MO contributions (for both AO and McO):

$$t_{\alpha\beta}(\varepsilon) = \sum_i t_{\alpha\beta i} \quad (16)$$

Each MO has a different phase. This result in quantum interference effects when the electron tunnel through all the MO in the junction.[16]. The transmission function both show constructive and destructive interference effect. The interference effects indicate that phase coherence is maintained across the molecule.[20] In this project we use the coupling to calculate both the transmission and the phase. The transmission function can then be expressed as:

$$T(\varepsilon) = t_{\alpha\beta}(\varepsilon) t_{\alpha\beta}^{\dagger}(\varepsilon) \quad (17)$$

### *Phase*

The phase of the transmitted wave function can be calculated from the real and imaginary coupling elements[18]:

$$\theta_{\alpha\beta}(\varepsilon) = \arctan [\text{Im}(t_{\alpha\beta}(\varepsilon)) / \text{Re}(t_{\alpha\beta}(\varepsilon))] \quad (18)$$

When the electrons are interacting with the McO, it is changing the phase. The change in phase is a function of the coupling which are a function of Green's function and the potentials between the electrodes. On the basis of this, the phase must depend on the structure of the molecular junction. This dependence will be examined in the following section.

# 3

---

## SIMULATIONS, DATA AND DISCUSSION

---

### 3.1 PYTHON SCRIPT FOR THEORETICAL COMPUTATION

A theoretical molecular junction is programmed in python 3 using Jupyter Notebook 6.1.4. A part of script is written by William Bro-Jørgensen. The goal of this project is to examine how we can control the phase of the transmitted wave function in order to suggest a candidate for a  $\pi/4$  phase gate. We want to see if we can come up with a rule set for how to change the phase in terms of the geometry of the molecule as well as the different parameters of the Hückel Hamiltonian. Essentially, we want to be able to predict the phase of the transmitted wave function at a transmission of 1 and at the Fermi energy.

Going through the experimental section, we will start by looking at some general trends for the phase of linear conjugated systems. Subsequently, we will replicate a  $\pi/4$  phase gate developed by Childs' et. al. [21]. This is done in order to see what factors are at play when changing the phase of the transmitted wave function. The approach used in the article are further used in the following sections. Then the phase of linear conjugated systems with cyclic side chains are studied. Finally, we will use the gained knowledge in order to suggest a candidate for a  $\pi/4$  phase gate.

Unless anything else is stated, all the energies are in units of electron volt( $eV$ ). Most commonly, the type of atoms and molecules used in between the electrodes are carbon atoms or hydrocarbon molecules. Nonetheless, when the parameters of the carbon atoms are modified, the chemical structure changes. At some point it is not obvious which type of molecule to map the parameters on. This is why we will mention the investigated molecules in terms of their geometry and number of constituents atoms and not by the exact type of atoms.

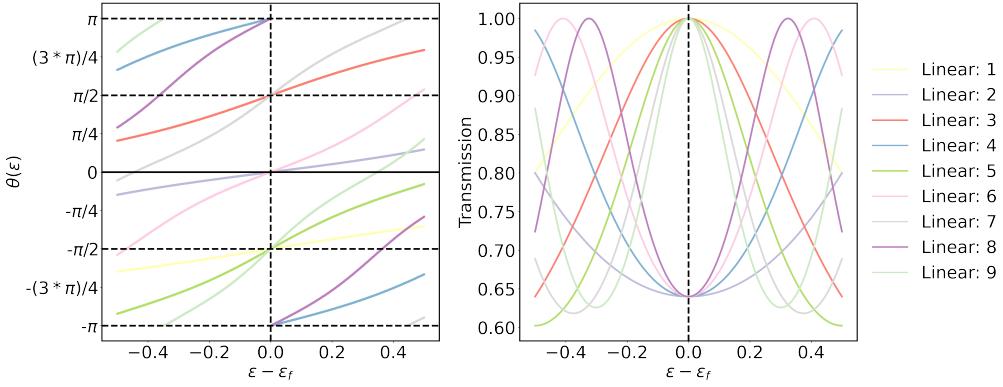


Figure 2: Phase (left) and Transmission(right) as a function of energy for 9 linear molecules. The parameters are set to  $\alpha_l = 0.$ ,  $\alpha = 0.$ ,  $\beta = -1.$  and  $\beta_l = -1..$

### 3.2 THE PHASE OF LINEAR CONJUGATED SYSTEMS AT THE FERMI ENERGY

Linear conjugated chains is the most simple form of conjugated systems. Therefore, an excellent starting point for finding phase trends is investigating linear conjugated systems.

The initial parameters of the examined linear conjugated systems are:  $\alpha_l = 0$ ,  $\alpha = 0$ ,  $\beta = -1$  and  $\beta_l = -1$ . Looking at fig. 2 - 9 different linear conjugated systems are plotted. Both the phase(left) and transmission(right) are as a function of energy (energy minus the Fermi energy). At the Fermi energy, a tendency is emerging of the phase only taking on values which is an integer of  $\pi/2$  meaning  $-\pi, -\pi/2, 0, \pi/2$  and  $\pi$ . This trend can be written as:

- linear: 2 and 6 have a phase of 0.
- linear: 3 and 7 have a phase of  $\pi/2$ .
- linear: 4 and 8 have a phase of  $\pi$  or  $-\pi$ .
- linear: 1, 5 and 9 have a phase of  $-\pi/2$ .

Herewith, there is a cyclic pattern where the phase of the 2-atom linear junction starts at  $\pi/2$  and each time you add an atom, the phase increases with  $\pi/2$ , until it reaches  $\pi$ . Then the cyclic patters start again from  $-\pi$ . However, it's not all the phases which have a transmission of 1 at the Fermi energy. In fact, it is only every other (the odd number of linear systems). If the linear molecules are used in a phase gate, it's crucial that they have a transmission of 1 at the Fermi energy.

Our goal is to come up with a suggestion of a phase gate containing 2 molecules which gives a  $\pi/4$  phase difference of the transmitted wave functions. Nonetheless, if one want to obtain a phase difference of  $\pi/4$  between two molecules, there is a requirement to find a way to get another phase than  $\pi/2$  of the individual molecules. Further, this should be obtained at a transmission of 1 and at

the Fermi energy. The approach for finding a molecule with the right phase is inspired by the article by Childs' et al [21]. In 2009 they suggested a molecular junction containing a molecule with perfect transmission at momentum  $-\pi/4$  and  $-3 * \pi/4$  (see figure 3). The molecule from the article are reproduced in order to understand what parameters are at play.

### 3.3 REPRODUCING PI/4 PHASE GATE FROM CHILDS' PAPER

Childs' et. al. used a 7-atom molecular junction. 3 of the atoms constituted a linear chain where each end was connected to an electrode. The rest of the 4 atoms formed a cyclic molecule connected to the second atom in the linear chain as shown in fig. 3 B). However, they didn't give the exact values of the parameters which has led to multiple trial and errors. In order to find the closest match we locked  $\alpha_l$  and  $\alpha$  at 0 and looped over the following parameters:

1. The gamma component ( $\beta_l$ )
2. The strength of the coupling between neighbor atoms- the strength of the bonds ( $\beta$ )

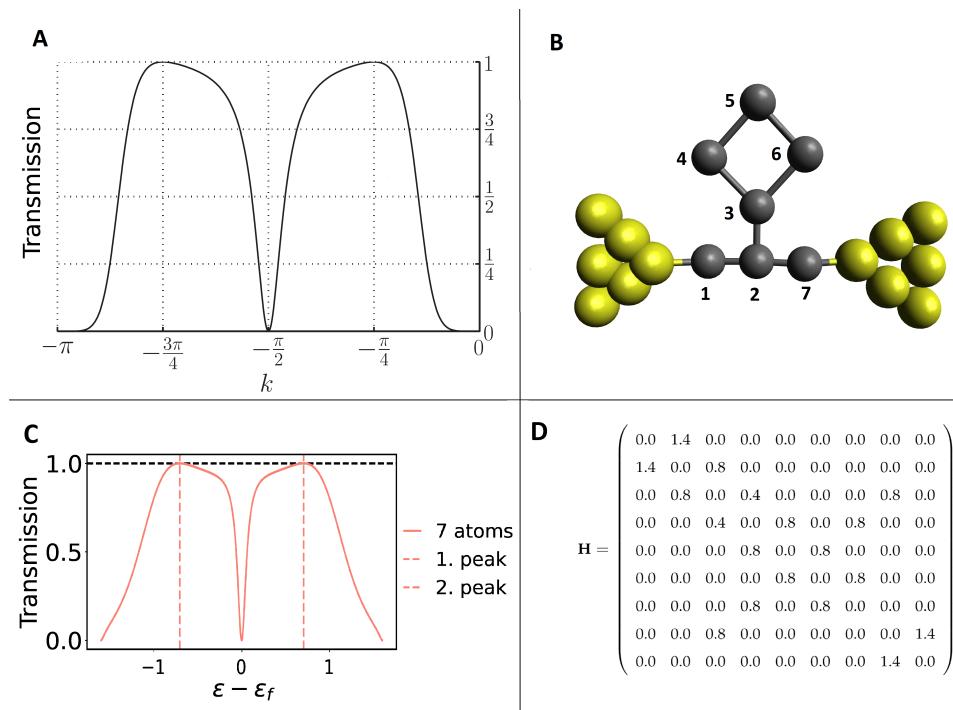


Figure 3: A) Plot of the transmission as a function of momentum from Childs' article-2009 [21]. On the x-axis is the momentum and on the y-axis is the transmission. You see 2 transmission peaks. 1 peak at  $-\pi/4$  and 1 at  $-3\pi/4$ . B) A model of the molecule Childs' et. al. are using in their phase gate. The numbers are given in order to convert to the Hückel Hamiltonian. C) A reproduction of the pi/4 phase gate made by Childs' et. al. D) The extended Hückel Hamiltonian used to reproduce the transmission graph from Childs' et. al. paper from 2009.

After approximately a thousand runs the following values was obtained:  $\alpha = 0.$ ,  $\alpha_l = 0.$ ,  $\beta_l = -0.8$ ,  $\beta = -1.4$ ,  $\beta_c = -0.4$ .  $\beta_c$  is the neighbor coupling between molecule 2. and 3. This is the closest we have gotten to the structure seen in the Childs' article fig. 3 A). The article are plotting the transmission as a function of momentum whereas our replication are represented by the transmission as a function of the energy seen in fig. 3 C).

The replication of the molecule does not match their model perfectly. However, we will not dwell any more upon replicating the transmission as the main interest is in their approach and not their exact molecule. If one were to map their theoretical molecule onto a synthesizable one, it would corresponds to something like a linear chain with cyclobutadiene as side chain. For a chemical point of view the ring strain of cyclobutadiene as well as the long side chain compared to the size of the ring would make the molecule very unstable.[22] In the article by Childs' et. al. they also seem to be using positive values for beta which generally known should be negative. The molecule suggested by Childs' et. al. would therefore be very difficult to synthesize in a stable form. However, they managed to get a  $\pi/4$  phase difference at a transmission of 1. This was obtained by adding a cyclic side chain to a linear conjugated molecular junction as well as tuning the parameters of the Hückel Hamiltonian. This approach are used in the next section to come up with some general trends on how the phase changes with the structure and parameters of different molecules.

### 3.4 CHANGING THE PHASE OF LINEAR CONJUGATED SYSTEMS

As the goal is a phase of  $\pi/4$  one need to look for something else than multiples of  $\pi/2$ . Inspired by the key elements in the article presented above the following are done:[21]

- Change of the parameters  $\alpha_l$ ,  $\alpha$ ,  $\beta$  and  $\beta_l$ .
- Add a cyclic side chain to the linear conjugated system.

When investigating  $\alpha$ ,  $\alpha_l$ ,  $\beta$ , and  $\beta_l$  all occurrences of the parameters are changed in the Green's function. Firstly, the impact of the  $\alpha$  are examined for linear conjugated systems. As the wide band approximation are used, the  $\alpha_l$  is not part of our equations and the impact will therefore not be studied.

#### 3.4.1 Impact of $\alpha$

Fig. 4 show the influence of  $\alpha$  on the phase for a linear-5 system. The right of the figure is the phase as a function of  $\alpha$ . Each colored graph corresponds to the phase of a transmission peak. Arbitrary of  $\alpha$  the phase of each peak does not change. This indicate that the phase value of a transmission peak is

not effected by  $\alpha$ . As a result, all 5 graphs are constant as shown in 4 B).

Changing  $\alpha$  is however shifting the transmission graph with respect to the energy as seen in fig. 4 A). In A) top the transmission graph is plotted for 7 different values of  $\alpha$  ranging from 0 to 0.65. In A) bottom the corresponding phase graphs are plotted. As seen in the top figure the change of  $\alpha$  is directly proportional with the shift of the transmission graph as a function of energy. When alpha is shifted by 0.65 the transmission graph is likewise shifted by 0.65 with respect to the energy as seen in fig. 4 A). Knowing that  $\alpha$  shifts the transmission but the value of the phase at a transmission peak, must indicate, that the phase graph is also shifted by the same amount as the transmission graph. When alpha is shifted by 0.65, then both the transmission- and the phase graph is shifted by 0.65 with respect to the energy axis.

Based on the fact that the transmission and phase are equally shifted when changing  $\alpha$  the phase at the Fermi energy can be chosen. If one want a phase which is  $2\epsilon$  away from the Fermi energy, the energy difference is simply added to  $\alpha$ . Given that linear conjugated systems with  $n$  atoms has  $n$  transmission peaks, there are  $n$  different phases to be shifted between. For now, we assume that the alpha-values for every linear molecule shift the transmission and phase equally for all linear systems. This gives an opportunity for getting phase-values different from  $\pi/2$  at transmission peak at the Fermi energy. In the rest of the investigation of the phase change for linear conjugated systems, we lock  $\alpha$  and  $\alpha_l$  to 0 and change the  $\beta$  and  $\beta_l$  parameters.

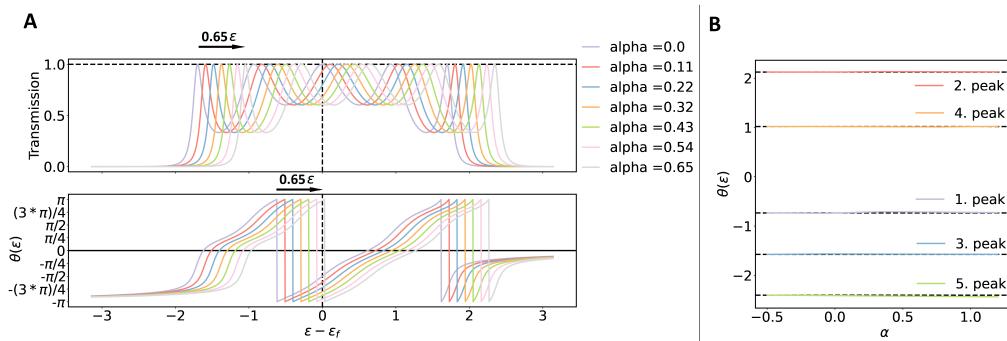


Figure 4: A) 7 different plots of the transmission and the phase as a function of energy at 7 different  $\alpha$  values.

The  $\alpha$  is ranging from 0 to 0.65. The calculated shifting in the peaks with respect to the energy are calculated for the same range as alpha which are shown to be directly proportional. B) Phase as a function of change in  $\alpha$  within a 5 atom linear conjugated molecular system. All the functions are constant indicating there is no change.

### 3.4.2 Impact of $\beta$ and $\beta_l$

The beta values are chosen in the range from  $-0.5$  to  $-1.4$ . Outside those intervals the linear conjugated system will not behave according to nature and to the things we want to investigate. When  $\beta_l$  is getting very negative, the peaks around the middle will fuse to 1 making the molecular system theoretically act like a system with fewer atoms. In the limit of  $\beta_l$  near 0 the phases will go to  $\pi/2$  phases which we are trying to avoid.

Linear molecules has symmetric transmission peaks around the Fermi energy as seen in fig. 5. In fig. 5 A) the transmission and phase for a linear-5 junction is plotted as a function of the energy. The transmission and phase is plotted for 6 different values of  $\beta$ . Changing the beta values does not break the symmetry of the transmission graphs. Due to this symmetry the transmission peaks can be thought of as pairs of 2. Each time a peak within a pair is changed the other is changed with the same absolute

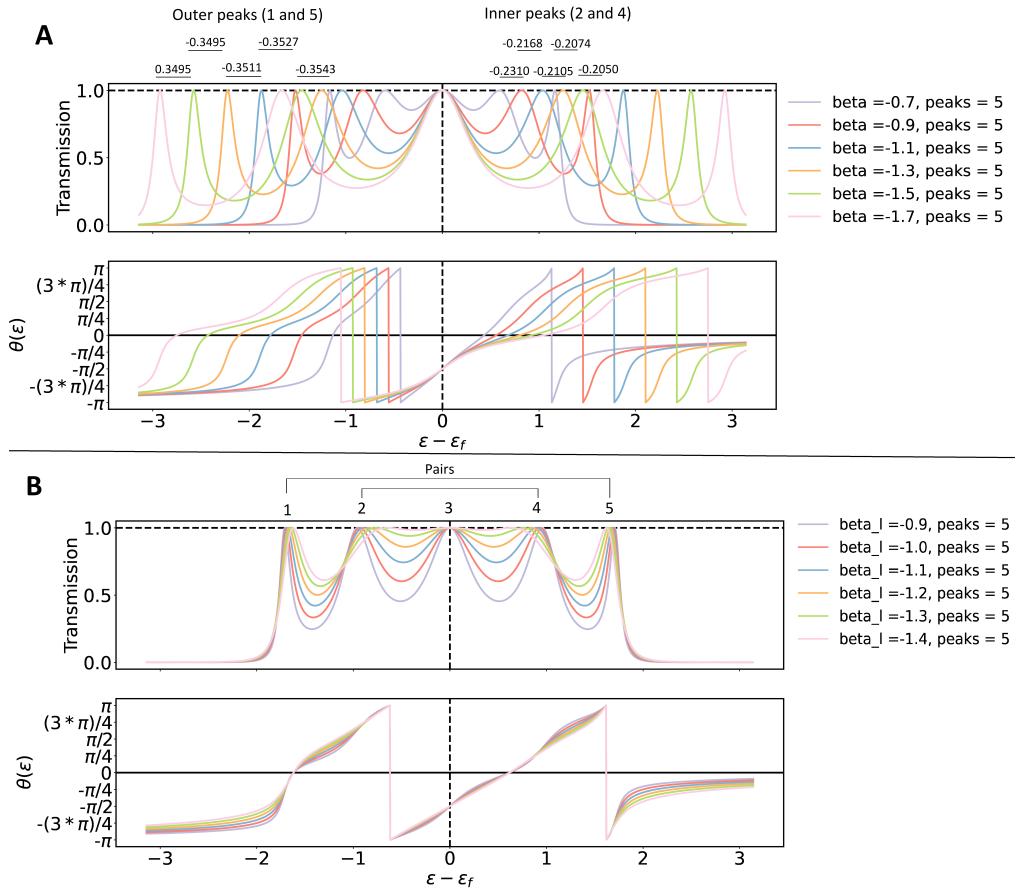


Figure 5: A) Transmission and phase as a function of energy (energy-Fermi energy) at different  $\beta$  values.  $\beta$  is ranging from  $-0.7$  to  $-1.7$ . It also displays the distances of the peaks between each change of beta for outer peaks (left) and inner peaks(right). B) Transmission and phase as a function of energy for  $\beta_l$  ranging from  $-0.9$  to  $-1.4$ . The pairs of the peaks are also displayed for linear 5 systems. Here the pairs are (1 and 5), (2 and 4) and 3 is left out due to an odd number.

value with respect to the energy. The peaks are paired as seen in fig. 5 B). For the 5-linear case peak 1 and 5 is a pair along with 2 and 4 which leaves out peak number 3 due to the number of peaks being odd. Each peak within a pair occur at the same absolute value of the energy. This also applies for even molecules except that no peak is left out when paired.

$\beta$  is the strength of the coupling between each atom in the molecule, and  $\beta_l$  is the strength of the coupling between the molecule and the electrodes. We lock  $\beta_l$  to -1 and decrease  $\beta$ , that is making the absolute value bigger which results in a stronger coupling.  $\beta$  can change the positions of the transmission peaks. As discussed above, both peaks within a pair is changed with the same absolute value. When  $\beta$  is decreased the peaks are pushed symmetrical away from the middle as seen in fig. 5 A).  $\beta$  is also slightly narrowing the peaks which is investigated in appendix A. When decreasing  $\beta$  the outer transmission peaks change more than the inner transmission peaks. As seen in fig. 5 A) the change in the outer peaks (peak 1 and 5) are calculated for every change in beta shown to the left. The change in the inner peaks (peak 2 and 4) are shown to the right. The outer peaks (1 and 5) for a 5-linear systems move about —0.35— with respect to the energy each time  $\beta$  is changed by 0.2 seen in fig . 5 A) left. This is arbitrary of what the initial value of  $\beta$  was before it was changed.

For the inner transmission peaks (peak 2 and 4) the change is not following the same pattern. Seen in fig. 5 A) right the inner peaks change differently depending on the starting value of  $\beta$ . When beta changes from -0.7 to -0.9 the change of the inner transmission peaks is  $|0.23|$  with respect to the energy. This is compared to when beta changes from -1.5 to -1.7 then the change in the inner transmission peak is around  $|0.205|$  with respect to the energy.

For linear molecules with 6 atoms we see the same behavior of as for 5-linear systems when changing  $\beta$  (See appendix H). The outer peaks has a constant change of around  $|0.36|$  when beta is changed 0.2. The inner peaks starts with a change of  $|0.27|$  when  $\beta$  is changing from -0.7 to -0.9 and a change of  $|0.25|$  when  $\beta$  is changing from -0.7 to -0.9. The change in the outer peaks is a constant and the change in the inner peaks is dependent of the initial value of  $\beta$ . The relation of the change in the inner peaks to the  $\beta$  will not be further studied in this project.

Due to the fact that the outer peaks change faster than the inner peaks when  $\beta$  is changed, the tails from the peaks are getting less fused together. Along with the slightly narrowing of the peaks when changing  $\beta$  this results in the peaks becoming more distinct from each other. Therefore, the gaps between the dips and peaks in the transmission graph is becoming greater as seen in fig. 5 A).

When inspecting the impact of  $\beta_l$ , the value of  $\beta$  is locked at -1. A change in  $\beta_l$  mainly broadens the transmission peaks. However,  $\beta_l$  also change the graph a tiny amount with respect to the energy seen in fig. 5 B). As  $\beta_l$  is broadening each peak they become less distinct and more fused

together. This is opposite as for changing  $\beta$ . Since both beta parameters are broadening and changing the transmission graph with respect to the energy, each to a different degree, we need to take a look at their ratio in order to understand their relation. This is done when investigating the phase. A short summary of the transmission graph dependence to a change in  $\beta$  and  $\beta_l$  is provided below.

- When  $|\beta|$  increases:
  - The position of each transmission peak goes to larger absolute energies. The positions of the peaks are pushed away from the Fermi energy.
  - Each peak is slightly narrowing and therefore becomes more distinct.
- When  $|\beta_l|$  increases:
  - The peaks are broadened and becoming less distinct.
  - There is a slight change in the peak position.

The phase change with respect to  $\beta$  and  $\beta_l$  is examined. From now on, the phase at a transmission peak is referred to as the phase. Changing  $\beta$  change the position of the phase just like for the transmission

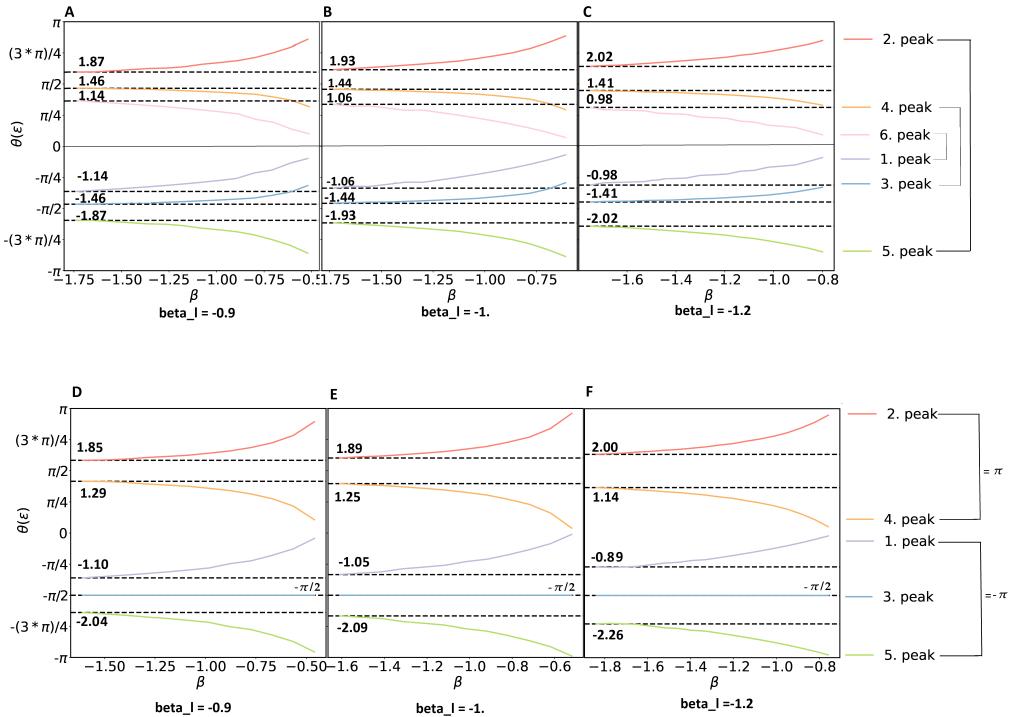


Figure 6: The phase as a function of  $\beta$  for 6 atoms (top) and 5 atoms (bottom) linear conjugated systems. The phase as a function of  $\beta$  is different depending on the choice of  $\beta_l$ . The  $\beta_l$  values plotted are: -0.9 (A and D), -1.0 (B and E) and -1.2 (C and F). The peaks are paired which for odd molecules leaves a transmission peak out and thereby 1 phase out. The pairs for linear 5 is (1 and 5), (2 and 4) and 3 are left out. The pairs for linear 6 is (1 and 6) (2 and 5) and (3 and 4).

graph. In fig. 5 top the phase is plotted as a function of the energy. When beta is decreased, the phase graph is pushed away from the middle alike the transmission graph. The phase is not changing with the same rate as the transmission peaks. Therefore we see a change in the phase at the transmission peaks when changing  $\beta$ . In fig. 5 bottom the impact of  $\beta_l$  on the phase graph is shown.  $\beta_l$  changes the phase graph with respect to the y-axis. For negative energies: the value of the phase are increasing when  $\beta_l$  is decreasing. For positive energies: the values of the phase are decreasing when  $\beta_l$  is decreasing. When changing the value of  $\beta_l$  the change in phase, is different from the change in the transmission just like when  $\beta$  was changed. Therefore, both  $\beta$  and  $\beta_l$  is responsible for phase change. This raise the question of what the exact numerical change of the phase is, when you change the beta parameters. Does every phase of the transmission peaks change with the same amount? Can we understand the relation and find some general trends for the phase change in conjugated linear systems? In order to answer those questions, we need to take a closer look at the change of phase at the transmission peaks and see if we can comprehend the connections between  $\beta$ ,  $\beta_l$  and the phase.

Since there are n peaks for linear conjugated systems with n atoms, there is also n phases. The phases of conjugated linear systems can be thought of as pairs of 2 just like the transmission peaks. For odd molecules, this leaves 1 phase out. As stated above,  $\beta$  can change the phase at a transmission peak. Fig. 6 shows the phase as a function of  $\beta$ . Where  $\beta_l$  is locked at -0.9 (A) and D)), at -1.0(B) and E)), and -1.1(C) and F)). Each coloured graph represent the phase at a transmission peak.

For even numbered of linear molecules the value of the phases within a pair is equal but opposite. In other words, the absolute value of the phase within a pair is the same as seen in fig. 6 top. This is arbitrary of the change in  $\beta$ . However, this only applies for even numbered of linear systems. Thus, when one phase within a pair is increased, the other is decreased with the same amount following the relation:

$$\text{phase}_1 + \text{phase}_2 = 0 \quad (19)$$

$\text{phase}_1$   $\text{phase}_2$  is the two phases within a pair. Consequently, this makes the phase as a function of beta symmetric around  $\theta = 0$  for even molecules.

As seen in fig. 6 A)  $\beta_l$  is locked at -0.9. The impact of  $\beta$  is examined in the range of -0.5 to -1.75. For a linear system with 6 molecules the phase at transmission peak 1 and 6 has opposite but equal values( $\pm 1.14$ ) which is the same for 2 and 5( $\pm 1.46$ ) along with 3 and 4( $\pm 1.87$ ). Adding the values within a pair all give 0.

$\beta$  also changes the phase at a transmission peak for odd numbered of molecules. The phase of odd numbered linear systems can likewise be divided into pairs of 2. Due to the odd number this leaves the middle transmission peak out. As seen in fig. 6 D) the phase of the middle transmission peak which doesn't have a partner is a constant. It's value is an integer of  $\pi/2$ . The integer is determined

by the length of the linear conjugated system just as we saw in the beginning in fig. 2 top. For linear 5 systems, the middle peak has a value of  $-\pi$  seen in fig. 6 D), E) and F). Unlike for even systems, the phases within a pair does not have the same absolute value. The phases for odd molecules are connected by the following equation:

$$\text{phase}_2 = -\text{phase}_1 \pm \pi \Leftrightarrow \text{phase}_2 + \text{phase}_1 = \pm\pi \quad (20)$$

(every other is plus and every other is minus).  $\text{phase}_1$  and  $\text{phase}_2$  is the two phases within a pair. For linear conjugated systems at  $\beta_l = -1.2$  with 5 atoms, the pairs are 1 =  $-0.89$  and 5 =  $-2.26$  as well as 2 =  $2.00$  and 4 =  $1.14$  as seen in fig. 5 F). When the phase of transmission peak 1 and 5 as well as 2 and 4 are added, it yields a result of  $-\pi$  and  $\pi$ , respectively.

As for even systems, the slope of the phases as a function of  $\beta$  within the pairs are equal but opposite. When a phase within a pair is increasing, the other is correspondingly decreasing with the same amount.

None of the phase slopes shown in fig. 6 is the same. However, the slope of the phase within a pair has the same absolute value. All the phase slopes are functions of  $\beta$ . This must indicate that the influence of  $\beta$  is not equal on every change phase. Nevertheless, all the slopes are stabilizing at around the same value of  $\beta$ . This implies there is a interval of  $\beta$  for which the phase doesn't change. We will refer to this value of  $\beta$ , where there is no significant change in the phase, as the stability point. At the stability point, the phase change are not significant even though the transmission graph and  $\beta$  are changing.

As stated above, both  $\beta$  and  $\beta_l$  have an effect on the width of the transmission peaks. Their interrelationship are investigated in terms of the change in phase.  $\beta_l$  can change the stability point of  $\beta$ . As seen in fig. 6 D) when  $\beta_l$  is locked at -0.9 the stability point of  $\beta$  is around -1.5. This is opposed to F) where  $\beta_l$  is locked at -1.2 and the stability point of  $\beta$  is around -1.7. Consequently,  $\beta_l$  is changing the interval of  $\beta$  where a change in the phase occurs. Looking at the bottom in fig. 6(for 5 atom (odd) linear molecule): When  $\beta_l$  is -0.9 (A), the change of phase occurs in the interval where  $\beta$  is going from -0.5 to -1.5. When  $\beta_l$  is -1.0(B), the change of phase occurs in the interval where  $\beta$  is going from around -0.6 to -1.6 when  $\beta_l$  is -1.2(C), then the change of phase occurs in the interval where  $\beta$  is going from -0.8 to -1.8.

From the results above it looks like there is a tendency for when the stability point of  $\beta$  is obtained. The stability point is occurring when beta is sufficiently high compared to  $\beta_l$ . At this point there is no significant change in the phase when changing  $\beta$ . When  $\beta$  is small compared to  $\beta_l$ , there is a large change in phase when changing  $\beta$ . On the basis of the 5 linear molecule, the ratio between  $\beta$  and  $\beta_l$  at the stability point should be around 1.67. This result raises a ton of questions; does the stability point occur at the same ratio between  $\beta$  and  $\beta_l$  for every molecule? Or is there different stability points? And in that case, what is the ratio determined by, and how do we find it? We are not able to answer all

of the questions in this project. Anyhow, there is a stability point for all the molecules examined so far. However, the ratio to where this occur, is not the same. Further, the ratio at the stability point is not necessarily the same within the same molecule either. This can be seen when looking at fig. 6 A) B) C) for linear-6 molecules. For every value of  $\beta_l$  there is a different stability point. Nonetheless, one thing can be stated. The stability point for all examined molecules have a value of  $\beta$  which is sufficiently large compared to  $\beta_l$ . From the impact analysis of  $\beta$  and  $\beta_l$  we managed to find some tendencies of the change in phase. The change occurs because  $\beta$  and  $\beta_l$  does not change the transmission- and phase graph equally. The trends for the phase change found in linear conjugated systems is summarized above:

1. For  $n$  atoms in a conjugated linear molecular junction with  $\alpha, \alpha_l = 0$  and  $\beta, \beta_l = -1$ , there are  $n$  transmission peaks and hence  $n$  different obtainable phases.
2. The phase at the Fermi energy have a cyclic pattern. The phase is increasing by  $\pi/2$  when the number of atoms are increased in the linear chain.
3. The phases can be thought of as pairs of 2 (like the transmission)
4. For even molecules, the value of the two phase within a pair are equal but opposite. This results in a symmetry around  $\theta = 0$ .
5. For odd molecules, if you add the values of the two phases within a pair you'll get  $\pm\pi$ . The phase without a partner is an integer of  $\pi/2$  following the same relation as in section 3.2.
6. For alpha values ( $\alpha$ ):
  - You are able to shift the phase and transmission equally with respect to the energy when changing  $\alpha$ . This makes it possible to change the phase and transmission at the Fermi energy.
7. For beta values ( $\beta$ ):
  - A change in  $\beta$  will result in a change in the phase. The slope of the phase change within a pair is equal but opposite of each other.
  - A stability point occurs when the slope of the phase is going to 0. This happens when the ratio between  $\beta$  and  $\beta_l$  is sufficiently high.
8. For beta values ( $\beta_l$ ):
  - A change in  $\beta_l$  changes the stability point of  $\beta$ . The ratio of the beta values determines the slope of the phase when plotting it against  $\beta$ .

With the gained knowledge we are now able to change the phase and the transmission at the Fermi energy by changing the parameters. However, there are still many unanswered questions regarding the phase, and we are therefore not able to fully control the exact value of the phase. Based on the results, it's not possible to predict what values of the phase is present, but we are able to tune the phase by tuning the parameters.

In order to get a better understanding of the phase we now look at linear conjugated systems with cyclic chains. The objective of the following part is to look at how the phase changes when a side chain is added. This is compared to the clean linear molecules. Gaining insight into this knowledge will get us 1 step closer to making a quantum phase gate.

### 3.5 THE PHASE OF CYCLIC MOLECULES CONNECTED TO LINEAR CHAINS

Before moving on to linear conjugated systems with cyclic side chains, a further look will be taken at the article by Childs' et. al. As mentioned before, they are using cyclobutadiene for their  $\pi/4$  phase gate.[21] Even though their approach and results are of great interest, the molecule in their molecular junction has extensive ring strain. From a chemical point of view, their phase gate would be nearly impossible to experimentally synthesize. However, their idea of taking a linear conjugated system and adding a cyclic side chain is interesting. We will primarily focus on the change of phase when adding cyclic side chains of 5, 6, 7, and 8 aromatic rings onto 1-, 3- and 5-atoms linear conjugated systems. This is done at initial conditions of  $\alpha, \alpha_l = 0$ ,  $\beta = -1$  and  $\beta_l = -1$ . As seen in fig. 7 the grey atoms are representing the linear chains, the gold atoms are the electrodes and, the purple atom is representing an arbitrary cyclic side chain. The choice of odd number linear systems is due to maintaining some of the symmetry when adding a cyclic side chains. When Childs' et. al. were making their molecule, they changed the coupling between the atoms connecting the linear molecule and the cyclic side chain to  $-0.4$ . We will also implement this in our project. In fig. 7 the

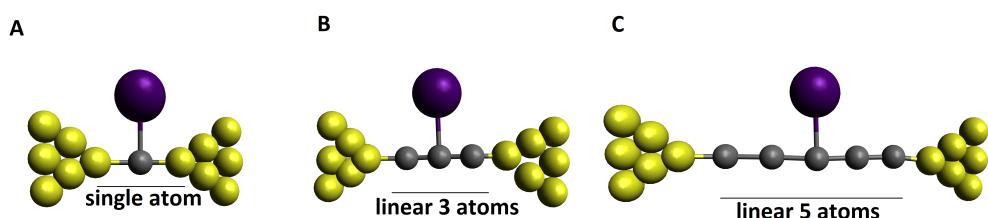


Figure 7: Model of a molecular junction with cyclic side chains connected to a single atom (A), linear conjugated systems with 3 atoms(B), and a linear conjugated systems with 5 atoms(C). The purple atom is representing the cyclic side chain constituent of either 5,6,7 or 8 atoms.

changed coupling would be on the first atom for (A), the second atom for (B) and the third atom for (C).

### 3.5.1 Cyclic molecules connected to 1 atom

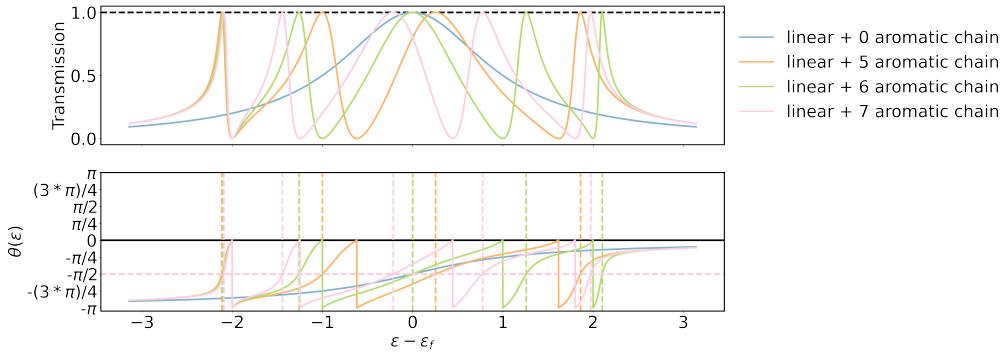


Figure 8: Transmission (top) and phase (bottom) as a function of energy for linear conjugated systems of 1 atom (blue) with a cyclic chain of 5 (orange), 6 (green) and 7 (light red) atoms.

The phase of cyclic molecules connected to 1 atom is seen in fig. 8. In the bottom, the phase is plotted as a function of energy. This is done for a single-atom-linear-chain (blue) and a 1-linear chain with 5 (orange), 6 (green) and 7 (light red) atom aromatic chains are seen. Even though the figure seems a bit messy, there is a clear connection of the phases for the different molecules. As seen by the horizontal light red dotted line in the bottom figure they all have the same phase of  $-\pi/2$ . In this case all the phases of different molecules is similar to a 1 molecular "chain". That is independent of the beta or alpha settings along with the number of transmission peaks.

### 3.5.2 Cyclic molecules connected to 3 and 5 atoms

Straightaway, we are going to look at 3- and 5- linear systems with cyclic side chains. The 6- and 8- atoms aromatic molecules connected to 3- and 5- atoms linear chains has a symmetric transmission graph around the Fermi energy. This can be seen in fig. 9. The light purple graphs correspond to the pure 3 linear chain, the blue graphs correspond to the aromatic chain and the red ones are the linear chains with the aromatic side chains.

There is a pattern of the number of transmission peaks when you add a linear and an aromatic molecule together. A 3-Linear molecule and 5-Linear molecule has 3 and 5 transmission peaks, respectively. This is compared to a benzene ring which has 4 transmission peaks and an aromatic ring with 8 atoms has 5 transmission peaks. As seen in 9 A) and B) the red graphs is representing the 3-linear chains

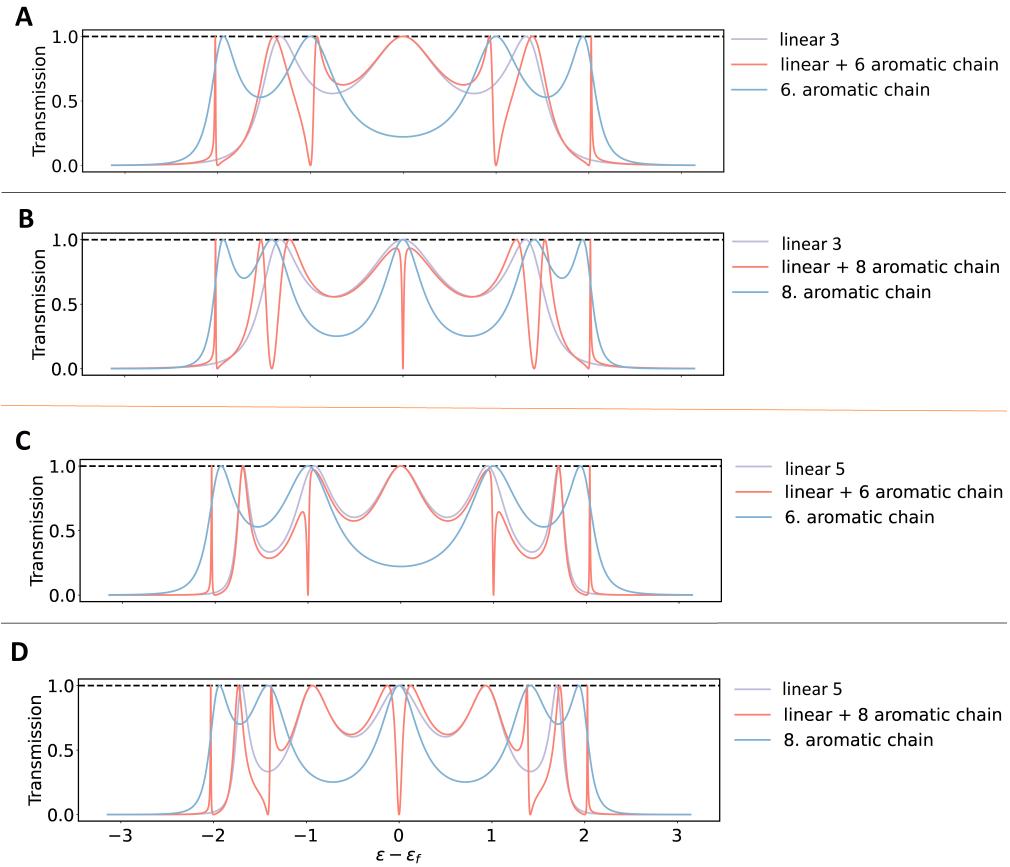


Figure 9: 3(A)(B)- and 5(C)(D) atom linear conjugated systems with aromatic side chains of 6 (A)(C)- and 8(B)(D)- atoms. The graphs represent the transmission as a function of energy. The light purple graphs correspond to the pure 3 linear chain, the blue graphs show the aromatic chain and the red ones are the linear chains with the aromatic side chains.

with cyclic side chains. For a benzene side chain (A) the number of transmission peaks are equal to 7. This is exactly the number of transmission peaks of its constituents (3+4). Likewise, for a side chain with 8 atoms (B) the transmission peaks are 8. This is equal to the number of peaks for the linear 3 chain(3 peaks) added to the number of peaks for an aromatic 8 molecule(5 peaks). The same tendency is seen for 5-linear systems(C + D).

There are some important relations between the linear systems with cyclic side chains and the pure linear chains. As for the linear chain  $\alpha$  can shift the transmission peaks. When you change the alpha parameter, you will see a shift in peak position with respect to the energy. Moreover, the shifting in the energy is directly proportional with the change in alpha seen in appendix D.

Subsequently, it becomes very fascinating when looking at the phase of the linear molecules with cyclic side chains. All the phases of linear conjugated systems with cyclic side chains show the same tendency as for odd linear conjugated systems! That is following eq. 20. Thus, the transmission peaks (and thereby the phases) can be thought of as pairs of 2 (see fig 10). In the case of 3-linear

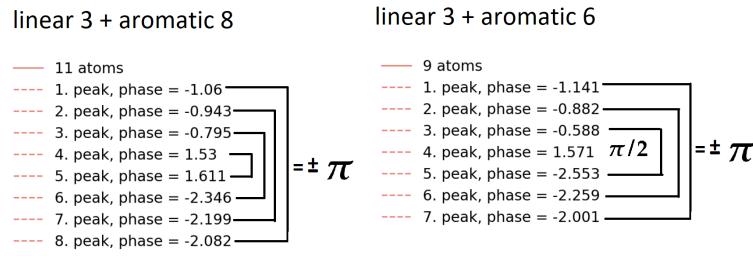


Figure 10: The paired number of peaks along with the corresponding phases for linear-3 chains with a cyclic side chain of 8(left) and 6(right) atoms.

with benzene there are 7 transmission peaks. They are paired as followed: (1 and 7), (2 and 6), (3 and 5) and then 4 is the peak left out due to an odd number. The 4th peak has a phase of  $\pi/2$ . This is exactly the same as for linear-3 systems with initial conditions of  $\alpha, \alpha_l = 0$ . and  $\beta, \beta_l = -1$ . at the Fermi energy (fig. 2). Further, the pairs are connected with each other like odd molecules and meets the equation 20. This tells us that when adding the phases within a pair, it becomes  $\pm\pi$ . As seen in fig. 10 left, 3-Linear with an 8 atom aromatic side chain has 8 transmission peaks. Again there is a connection between the phases when you divide them into pairs of 2. However, even though the number of transmission peaks is an even number, the pairs behave like an odd numbered linear conjugated systems. This mean they do also meet equation 20. This also applies for linear 5-, 6- and 8 aromatic side chains (see appendix F). However, if we detect an odd number of peaks for linear-5 then the phase of the peak left out is  $-\pi/2$ . This is the same for linear-5 at the Fermi energy. Remarkably, when adding cyclic side chains to odd number of linear conjugated systems, many of the phase characteristics are preserved! The most significant ones are:

- The number of transmission peaks of a linear chain with a cyclic side chain is equal to the number of transmission peaks for its constituents.
- The phase at the Fermi energy for an odd linear chain is preserved when adding a cyclic side chain with an even number of transmission peaks.
- The alpha parameter shifts the transmission and phase equally with respect to the energy axis. The change in alpha is directly proportional with the shift in energy.
- The phases of linear molecules with cyclic side chains can be thought of as pairs of two. When adding the phases within a pair, they will meet equation. 20.

Seeing that some of the tendencies found for linear conjugated systems can be applied to more advanced molecules set a new milestone for understanding the phase. Nonetheless, it also raises a whole new area of questions to be answered.

One could ask why all the molecules we have looked at, except linear conjugated systems with even numbers of atoms, show the same behavior? Why is the behavior for simple odd numbered linear systems so dominating? And why is it specifically even linear systems which does not meet this behavior? A test of the pi-relation to the phase of even-linear systems was done by adding the phases, subtracting the phases, multiplying the phases and finding some integer of the normalization constant of the eigen vectors to the phases (see appendix B and C). However, no obvious integer of  $\pi$  was found in the phase. Why is there a relation of  $\pi$  for all molecules except linear conjugated systems with an even number of atoms?

Another question to be asked is why it makes such a big difference when you add cyclic side chains to a linear-1 chain as opposed to adding it to a linear-3 or 5 chain? Regardless of what you added to the linear-1 chain, we saw no other phases than  $-\pi/2$ . Why do we see this degeneracy which is not like any other molecule studied? Nor did the other studied molecules preserved the value of the phase when you added a disturbance to the system.

The number of transmission peaks for a linear chain with cyclic side chains is equal to the number of transmission peaks of its constituents. This pattern also applies for the number of phases. An explanation for this could be that the McO basis for the constituent molecules form a new basis for the composite molecule. Even though we have not investigated the specific relation between the change in phase and the addition of cyclic side chains, we can still on the basis of our gained knowledge, come up with a suggestion of a  $\pi/4$  phase gate. Firstly we will recap the so far known requirements for a  $\pi/4$  phase gate candidate system.

### 3.6 TOWARDS A CANDIDATE FOR A $\pi/4$ PHASE GATE

A  $\pi/4$  phase gate is build out of 2 molecules. We will use a linear molecule as the first and a linear molecules with a cyclic side chain as the second. The phase difference should be  $\pi/4$  between the two chosen molecules. Each molecule has it's own pair of electrodes and do not interact. On the basis of this, the same theory as stated in the theory section is used. The criteria for a quantum phase gate which have to be meet are (pi on 4 phase gate):

- The system we are looking for needs to have a transmission of 1 at the Fermi energy for both the molecules.
- At the transmission peak the phase difference need to be  $\pi/4$ .
- The molecule used need to be stable and somewhat synthesizable from a chemical point of view.

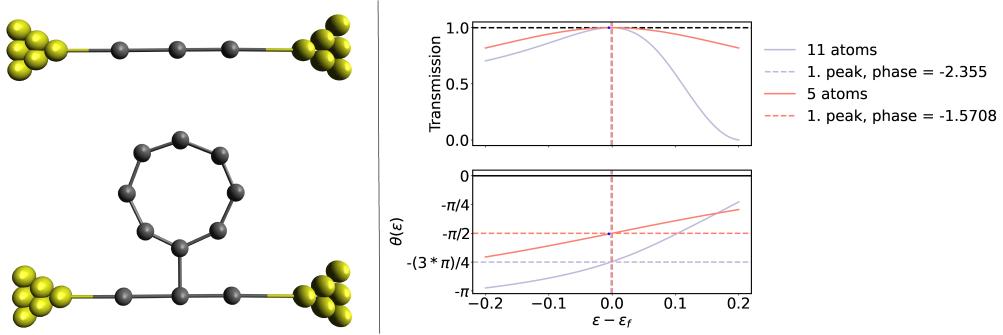


Figure 11: The final version of the  $\pi/4$  phase gate candidate. Plot of the transmission and phase as a function of the energy around the Fermi energy. The energy interval is ranging from -0.2 to 0.2. The red graph is for linear-5 and the purple graph is for the linear chain with the 8-cyclic side chain. The stippled line is at the Fermi energy.

The linear conjugated systems with cyclic side chains offers a lot of different phases. We will start from a molecule which has a phase close to  $\pm\pi/4$  or  $\pm-3*\pi/4$ . We can use  $-3*\pi/4$  because we are simply looking for a phase gate with a difference of  $\pi/4$ . Since all the linear molecules have a phase which is an integer of  $\pi/2$ , we can obtain a phase difference by having the cyclic side chain to have  $\pm\pi/4$  or  $\pm3*\pi/4$ . We want to use the gained knowledge in order to see how precise we can hit a phase of  $\pi/4$ .

When taking a look at the phases in fig. 10, we observe that the linear conjugated system with an 8 aromatic chain has a phase of -2.346 which is very close to  $-3*\pi/4 \approx -2.3562$ . Our starting point will then be a 3-linear chain with an 8 aromatic side chain. Our initial starting values of the parameters are:  $\alpha, \alpha_l = 0$ . and  $\beta, \beta_l = -1$ . and  $\beta_c = -0.4$ .  $\beta_c$  is the coupling between atom 2 in the linear chain and the coupling atom in the aromatic-8 chain.

A script was coded in order to look for a value equal to  $3*\pi/4$  down to the 3rd decimal. This was implemented on the 3-linear chain with the 8 aromatic side chain. The parameters which were tuned was  $\beta, \beta_l$  and  $\beta_c$ . When the wanted phase was found  $\alpha$  was tuned in order to set the peak at the Fermi energy. The final proposal for the candidate  $\pi/4$  phase gate is seen in fig. 11. The parameters ended up being:

- For the linear-3 chain  $\alpha_l = 0$ ,  $\alpha = 0$ ,  $\beta_l = -1$ ,  $\beta = -1$ .
- For the linear-3 chain + 8 aromatic:  $\alpha_l = 0$ ,  $\alpha = -1.2$ ,  $\beta_l = -1$ ,  $\beta = -1$ ,  $\beta_c = -0.444$ .

The figure 11 left) is a model of the  $\pi/4$  phase gate candidate. right) shows a close up of the 2 transmission- and phase graphs as a function of energy. The phases shown on the bottom of the graph is the phases at the Fermi energy. The red graphs is the phase of the 5-linear chain and the purple is the phase of the 5-linear +8-cyclic system. The energy interval is sat very small. It is ranging from

-0.2 to 0.2 in order to clarify the phase difference. The vertical stippled line is at the Fermi energy. The phase difference is not perfectly  $\pi/4$ . It is wrong at the 3rd decimal.

In order to implement a phase gate, it need to have a much more precise phase difference of  $\pi/4$ . However, we do not yet have the sufficient knowledge to make the small corrections to our phase. It could also be, that a whole other structure of molecule was more suited for the  $\pi/4$  phase gate. We have only studied a small part of all the molecules available, and the probability of finding a better molecule is high. A whole other approach is to look at the calculations and work out a mathematical expression of the phase dependence. This project has mainly focused on the larger changes and more universal tendencies of the phase for different kinds of linear systems. We have looked at what impact the parameters have on the phase and the transmission. However we have not glanced upon why the parameters effect the phase neither what sets the phase of the particular peak?

The electronic transport is calculated using Green's function with LCOA theory for describing the electronic structure. Even though the Hückel theory is a nice approximation when working with conjugated systems, a more precise approach would be to express the electronic structure by using density function theory (DFT) which among other is dependent of the electron density. It would be very interesting to investigate if the trends found for linear systems and linear systems with cyclic side chains is unchanged with a theory with fewer approximations.

There is still a lot more to investigate and an interesting start would be to see what happens when not all alpha or beta parameters were changed simultaneously. What would happen if only a single atom within the molecule was changed? This would correspond to replacing 1 atom in the molecular chain with another different from the rest in order to see what would happen to the phase. Another approach would be to dig into the equations and try to come up with expressions for some of the relations found in order to develop a ground solid theory for the phase tendencies.

# 4

---

## CONCLUSION

---

The field of single molecular junctions is at great development since it can be used for many purposes like quantum gates and thermal insulators. However, the phase of the transmitted wave function through a junction is still a great mystery. Therefore, its phase characteristic need to be studied more exhaustively. It is however known that interference effects observed in molecules indicate that phase coherence is maintained across it. Knowledge of the phase is important if we want to build a phase gate as we want absolute control and prediction of the function of the gate. The question is, what relation the phase has to the atoms and geometry of the molecular junction and which, if any, is the most dominating one.

The molecular junctions studied in this project was theoretically programmed in python using Green's function with LCOA theory. We looked at linear conjugated systems and linear conjugated systems with aromatic rings of (5,6,7,8) as side chains. We tried to find some tendencies when changing the parameters of the extended Hückel Hamiltonian. The objective of this procedure was to come up with a  $\pi/4$  phase candidate.

Based on the results found from studying the phase of our theoretical single molecular junction model we found that it was possible to change the phase by adjusting the different parameters and geometry of the molecule. We found that the  $\alpha$  parameter does not change the phase at a transmission peak, but it is able to shift the whole graph of both the transmission and the phase with respect to the energy. For linear conjugated systems, the number of different transmission peaks and thereby phases is equal to the number of atoms. As  $\alpha$  is shifting the graph, you can tune it in order to set the wanted transmission peak at the Fermi energy. Further the project found that when changing the  $\beta$  parameters the peaks of the transmission graphs was narrowing and broadening differently depending on which  $\beta$  value you adjusted. More importantly, there is a dependence between  $\beta$  and  $\beta_l$  which need to be investigated further. When we studied the linear systems with cyclic side chains, we found a connection to the odd linear systems. The impact of  $\alpha$  and the tendencies in the phases was the same as for odd systems. Lastly, a  $\pi/4$  phase gate candidate was proposed based on the gained knowledge.

Even though the goal of this project was to find a  $\pi/4$  phase gate candidate, the objective was also to

get a better understanding of the phase of the transmitted wave function. The latter has been fulfilled, but it has also raised thousands of new question which need to be answered in order to make an even better candidate for a  $\pi/4$  phase gate. The question that needs to be answered is what sets the phase of the particular transmission?

Molecular electronics will hardly replace the silicon based computers, but it can help contribute with other functionalities or other ways of calculating different task which seems nearly impossible right now even with the fastest computers yet produced. Inserting and manipulating molecules in junctions in order to build quantum gates is indeed a pure form of components and is absolutely a very elegant thought.

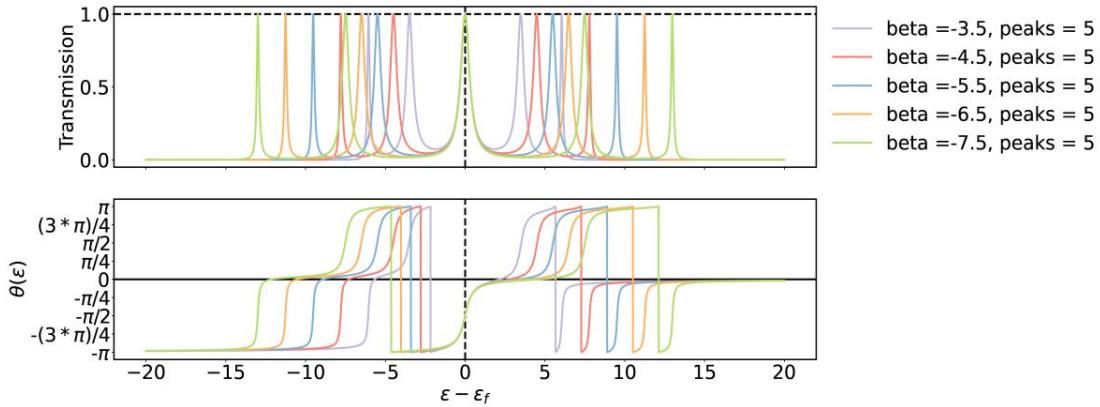
A INVESTIGATION OF NARROWING

## Investigation of the narrowing of the peaks

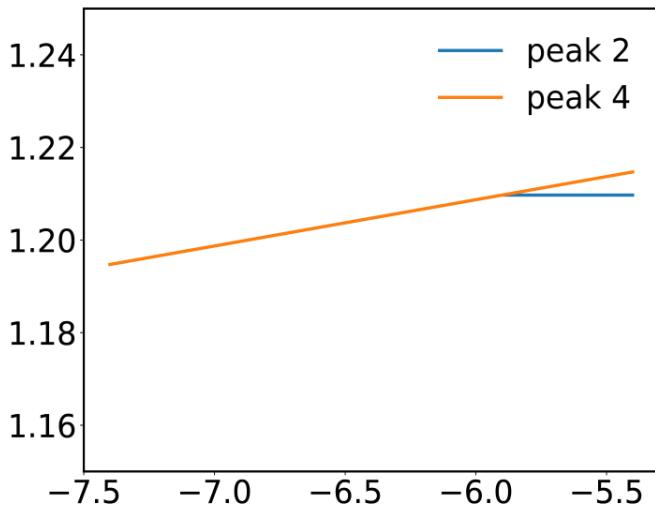
In order to find out if it is narrowing the peak or if the change in peaks widths are only depending of the gap between each peak are being increased and thereby the tails of each peak are less and less fused with the other peaks. We know that the tails of the peaks are fusing together, but is it responsible for all the change? Is there a narrowing somewhere?

We are looking in an interval which cannot be mapped onto a molecule since the beta values are so strong.

We start by plotting the transmission range in order to see if the tails are separated



Then we use a script made by Andreas Juul Bay smidt in order to calculate the width of the peaks.



We have taking the plot in the interval of beta to be -5.5 to -7.5 - the slope is linear and the y-axis is in terms of energy

The blue and the orange curve should be precisely the same. Them being not the same is an artifact due to the choice of energy

B INVESTIGATION PI IN EVEN MOLECULES - MAPLE

```

restart
with(Gym):
with(LinearAlgebra):
with(Stuff)
[Columns, Divergence, FlowCurve, FlowCurveSpecific, JacobianFunction, MGramSchmidt,
NormalizeColumns, Rotation, Rows, SumList, TangentialCurveIntegral, fillplot, fillplot3d]

```

(1)

## ▼ Greens function

**Eigen energy matrix**

$$E := \begin{bmatrix} \varepsilon & 0 \\ 0 & \varepsilon \end{bmatrix} = \begin{bmatrix} \varepsilon & 0 \\ 0 & \varepsilon \end{bmatrix}$$

**Hamiltonian hückel matrix**

$$H := \begin{bmatrix} \alpha & \beta \\ \beta & \alpha \end{bmatrix} = \begin{bmatrix} \alpha & \beta \\ \beta & \alpha \end{bmatrix}$$

**Coupling matrix:**

$$\Gamma_L := \begin{bmatrix} 2 \cdot a & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 2a & 0 \\ 0 & 0 \end{bmatrix}$$

$$\Gamma_R := \begin{bmatrix} 0 & 0 \\ 0 & 2 \cdot a \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 2a \end{bmatrix}$$

**Self energy matrix:**

$$\Sigma := \frac{i \cdot (\Gamma_L + \Gamma_R)}{2} = \begin{bmatrix} Ia & 0 \\ 0 & Ia \end{bmatrix}$$

**Pertubated Hamiltonian matrix:**

$$V := H - \Sigma = \begin{bmatrix} \alpha - Ia & \beta \\ \beta & \alpha - Ia \end{bmatrix}$$

**Greens function:**

$$k := E - V = \begin{bmatrix} \varepsilon - \alpha + Ia & -\beta \\ -\beta & \varepsilon - \alpha + Ia \end{bmatrix}$$

$$Eigenvectors\left(\frac{1}{k}\right) = \begin{bmatrix} \frac{1}{Ia - \alpha - \beta + \varepsilon} \\ \frac{1}{Ia - \alpha + \beta + \varepsilon} \end{bmatrix}, \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

We have not found an expression for the eigenvalues of a linear 2 molecule: - we will go on with this result in "HOMO and LUMO for 2 atom linear chain"

$$G_r := \text{MatrixInverse}(E - V) =$$

$$\left[ \begin{array}{l} \left[ -\frac{\varepsilon - \alpha + Ia}{2Ia\alpha - 2Ia\varepsilon + a^2 - \alpha^2 + 2\alpha\varepsilon + \beta^2 - \varepsilon^2}, -\frac{\beta}{2Ia\alpha - 2Ia\varepsilon + a^2 - \alpha^2 + 2\alpha\varepsilon + \beta^2 - \varepsilon^2} \right], \\ \left[ -\frac{\beta}{2Ia\alpha - 2Ia\varepsilon + a^2 - \alpha^2 + 2\alpha\varepsilon + \beta^2 - \varepsilon^2}, -\frac{\varepsilon - \alpha + Ia}{2Ia\alpha - 2Ia\varepsilon + a^2 - \alpha^2 + 2\alpha\varepsilon + \beta^2 - \varepsilon^2} \right] \end{array} \right]$$

$$G_a := \text{HermitianTranspose}(G_r) =$$

$$\left[ \begin{array}{l} \left[ -\left( \frac{\varepsilon - \alpha + Ia}{2Ia\alpha - 2Ia\varepsilon + a^2 - \alpha^2 + 2\alpha\varepsilon + \beta^2 - \varepsilon^2} \right), -\left( \frac{\beta}{2Ia\alpha - 2Ia\varepsilon + a^2 - \alpha^2 + 2\alpha\varepsilon + \beta^2 - \varepsilon^2} \right) \right], \\ \left[ -\left( \frac{\beta}{2Ia\alpha - 2Ia\varepsilon + a^2 - \alpha^2 + 2\alpha\varepsilon + \beta^2 - \varepsilon^2} \right), -\left( \frac{\varepsilon - \alpha + Ia}{2Ia\alpha - 2Ia\varepsilon + a^2 - \alpha^2 + 2\alpha\varepsilon + \beta^2 - \varepsilon^2} \right) \right] \end{array} \right]$$

Eigenvectors + values of greens function:

$$\text{Eigenvectors}(G_r) = \begin{bmatrix} \frac{1}{Ia - \alpha - \beta + \varepsilon} \\ \frac{1}{Ia - \alpha + \beta + \varepsilon} \end{bmatrix}, \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

$$\text{Eigenvectors}(G_a) =$$

$$\left[ \begin{array}{l} \left[ \left( \frac{\beta}{-\varepsilon^2 + (-2Ia + 2\alpha)\varepsilon + 2Ia\alpha + a^2 + \beta^2 - \alpha^2} \right) - \left( \frac{\varepsilon - \alpha + Ia}{-\varepsilon^2 + (-2Ia + 2\alpha)\varepsilon + 2Ia\alpha + a^2 + \beta^2 - \alpha^2} \right) \right], \\ \left[ -\left( \frac{\beta}{-\varepsilon^2 + (-2Ia + 2\alpha)\varepsilon + 2Ia\alpha + a^2 + \beta^2 - \alpha^2} \right) - \left( \frac{\varepsilon - \alpha + Ia}{-\varepsilon^2 + (-2Ia + 2\alpha)\varepsilon + 2Ia\alpha + a^2 + \beta^2 - \alpha^2} \right) \right] \end{array} \right], \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}$$

$$\begin{aligned}
C_r &:= \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \\
C_{r2} &:= \text{MatrixInverse}(C_r) = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \\
C_a &:= \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \\
C_{a2} &:= \text{MatrixInverse}(C_a) = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix} \\
\text{HermitianTranspose}(C_r) &= \begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix} \\
\text{MatrixInverse}(\text{HermitianTranspose}(C_r)) &= \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \\
G_{r2} &:= \text{MatrixMatrixMultiply}(C_{r2}, \text{MatrixMatrixMultiply}(G_r, C_r)) = \xrightarrow{\text{simplify symbolic}} \\
&\left[ \left[ \frac{-Ia + \alpha + \beta - \varepsilon}{-\varepsilon^2 + (-2Ia + 2\alpha)\varepsilon + 2Ia\alpha + a^2 + \beta^2 - \alpha^2}, 0 \right], \right. \\
&\quad \left. \left[ 0, \frac{-Ia + \alpha - \beta - \varepsilon}{-\varepsilon^2 + (-2Ia + 2\alpha)\varepsilon + 2Ia\alpha + a^2 + \beta^2 - \alpha^2} \right] \right] \\
G_{a2} &:= \text{MatrixMatrixMultiply}(C_{r2}, \text{MatrixMatrixMultiply}(G_a, C_r)) = \xrightarrow{\text{simplify}} \\
&\left[ \left[ \left( \frac{\beta}{-\varepsilon^2 + (-2Ia + 2\alpha)\varepsilon + 2Ia\alpha + a^2 + \beta^2 - \alpha^2} \right) - \right. \right. \\
&\quad \left( \frac{\varepsilon - \alpha + Ia}{-\varepsilon^2 + (-2Ia + 2\alpha)\varepsilon + 2Ia\alpha + a^2 + \beta^2 - \alpha^2} \right), 0 \Big], \\
&\quad \left. \left[ 0, -\left( \frac{\beta}{-\varepsilon^2 + (-2Ia + 2\alpha)\varepsilon + 2Ia\alpha + a^2 + \beta^2 - \alpha^2} \right) - \right. \right. \\
&\quad \left. \left( \frac{\varepsilon - \alpha + Ia}{-\varepsilon^2 + (-2Ia + 2\alpha)\varepsilon + 2Ia\alpha + a^2 + \beta^2 - \alpha^2} \right) \right] \Big] \\
&\xrightarrow{\text{assuming integer}} \\
&\left[ \left[ \frac{-Ia - \alpha - \beta + \varepsilon}{\varepsilon^2 + (-2Ia - 2\alpha)\varepsilon + 2Ia\alpha - a^2 - \beta^2 + \alpha^2}, 0 \right], \right]
\end{aligned}$$

$$\left[ 0, \frac{-Ia - \alpha + \beta + \varepsilon}{\varepsilon^2 + (-2Ia - 2\alpha)\varepsilon + 2Ia\alpha - a^2 - \beta^2 + \alpha^2} \right]$$

► Transmission

► Coupling

► Phase

► Trying to find which graph the phase is following

▼ HOMO and LUMO for 2 atom linear chain

$$\text{Eigenvectors}\left(\frac{1}{k}\right) = \begin{bmatrix} \frac{1}{Ia - \alpha - \beta + \varepsilon} \\ \frac{1}{Ia - \alpha + \beta + \varepsilon} \end{bmatrix}, \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$$

The first is the eigenvalues, the second is the eigenvectors.

The normalization constant is  $\frac{1}{\sqrt{2}}$

Finding phase for linear 2 - taken from python calculations:

1. phase

$m := -1.32359345$

$m := -1.32359345$  (6.1)

2. phase

$n := 1.32359345$

$n := 1.32359345$  (6.2)

The difference

$n \cdot 2$

$2.64718690$  (6.3)

Energy

The first energy

$mm := -1.59984154$

$mm := -1.59984154$  (6.4)

The second energy  
 $nn := 1.59984154$

$$nn := 1.59984154 \quad (6.5)$$

$$\alpha = 0$$

$$\beta = -1.65$$

Multiplying with the normalization constant:

$$\frac{1}{\sqrt{2}} \cdot n$$

$$0.9313836081 \quad (6.6)$$

We see, that when multiplied with the eigenvalue, we still don't get a phase of pi.  
Further, the phases are symmetric around the y-axis when changing beta, you don't change the normalization constant, but you change the eigenvalues. Now the eigenvalues are investigated.

Multiplying with the eigenvalues

The eigenvalue:

$$\frac{1}{Ia - \alpha - \beta + \varepsilon}$$

$$k := \frac{1}{1.65 - 1.59984154} = 19.93681624 \quad (6.7)$$

$$k \cdot m = -0.4072793808 \quad (6.8)$$

$$l := \frac{1}{-1.65 - 1.59984154} = -0.3077073106$$

$$l \cdot m = \frac{0.4072793808}{0.4072793808 \cdot 1} = \frac{\sqrt{2}}{\sqrt{2}} = 0.2879900121 \quad (6.9)$$

The energy():

$$\frac{1}{Ia - \alpha + \beta + \varepsilon}$$

$$v := \frac{1}{-1.65 - 1.59984154} = -0.3077073106$$

$$v \cdot m = 0.4072793808 \quad (6.10)$$

We don't see an obvious relation if we use the eigenvalues instead.

## ► HOMO and LUMO for 6 atom linear chain

C INVESTIGATING PI EVEN MOLECULES

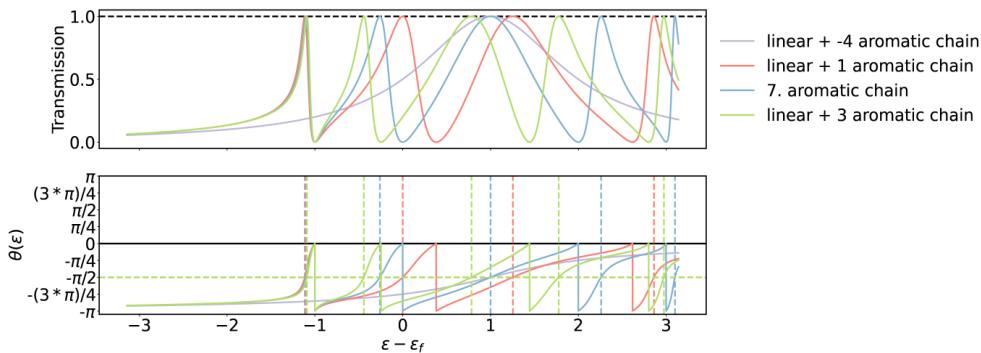


D INVESTIGATING ALPHA FOR CYCLIC MOLECULES

For linear-1 - when alpha is changed with 1, then the transmission graphs are also shifted by 1.

Phase and energy of the transmission peaks before:

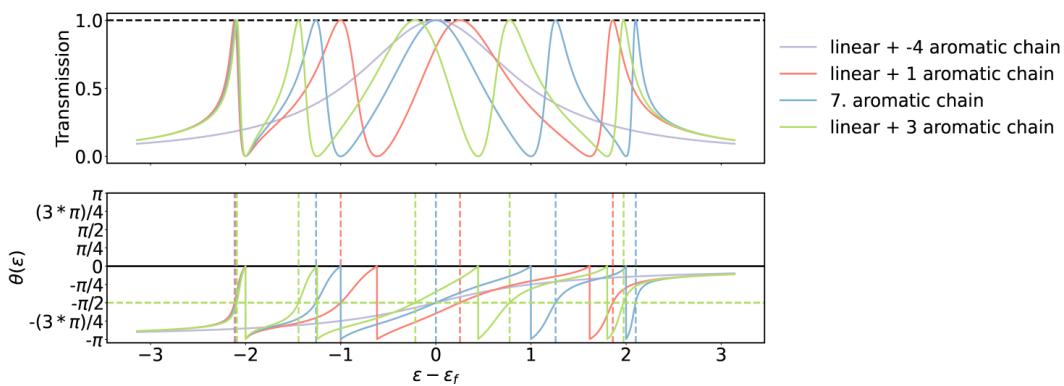
Linear 1	phase = [-1.57071678]	grid = [0.]
Aromatic 5	phase = [-1.57565833 -1.57111449 -1.57089805 -1.57109132]	grid = [-2.11520555 -1.00007955 0.25404455 1.86076835]
Aromatic 6	phase = [-1.57198146 -1.57046913 -1.57079633 -1.57112352 -1.56961119]	grid = [-2.10107015 -1.25922855 0. 1.25922855 2.10107015]
Aromatic 7	phase = [-1.56476707 -1.57321917 -1.57091015 -1.57122859 -1.5704514 ]	grid = [-2.09086125 -1.44298875 -0.21635015 0.77626905 1.97385155]



Phase and energy of the transmission peaks before:

Linear 1	phase = [-1.57071678]	grid = [1.00007955]
Aromatic 5	phase = [-1.56794359 -1.57079633 -1.57145551 -1.57355731]	grid = [-1.11473335 0. 1.25373145 2.86045525]
Aromatic 6	phase = [-1.57748699 -1.57245392 -1.57065711 -1.57311199 -1.5751485 ]	grid = [-1.10138325 -0.25954165 1.00007955 2.25891545 3.10075705]

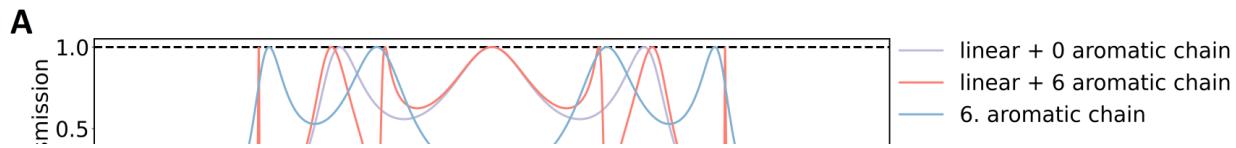
Aromatic 7	phase = [-1.5706246 -1.56895902 -1.57154791 -1.56935842 -1.57384657]	grid = [-1.09117435 -0.44251655 0.78333675 1.77674125 2.97353845]
------------	--	---

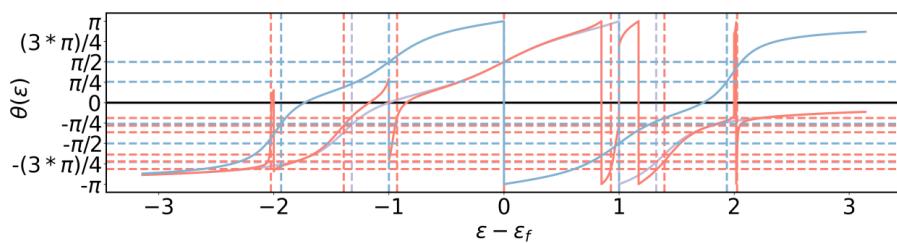


For linear-3 - when alpha is changed with 1, then the transmission graphs are also shifted by 1.

Phase and energy of the transmission peaks before:

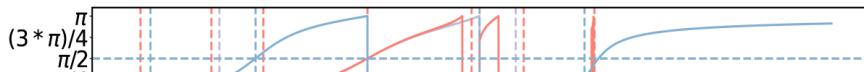
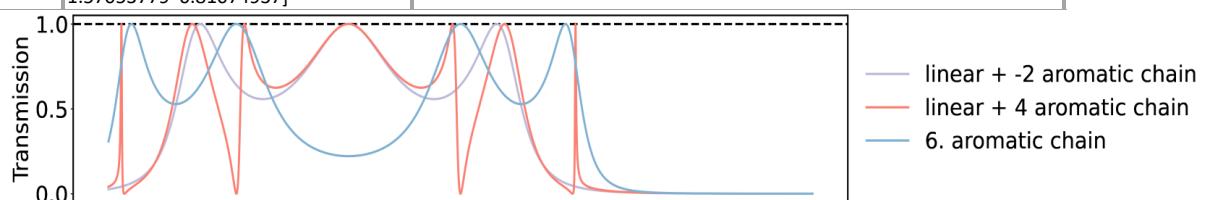
Linear 3	phase = [-0.84791087 1.57079633 -2.29368179]	grid = [-1.32283785 0. 1.32283785]
Linear 3 + Aromatic 6	phase = [-1.14095714 -0.88243789 -0.58824901 1.57079633 -2.55334365 -2.25915476 -2.00063551]	grid = [-2.02646665 -1.39351485 -0.92940255 0. 0.92940255 2.02646665]
Aromatic 6	phase = [-0.81074937 1.57053779 -1.57053779 0.81074937]	grid = [-1.93615715 -1.00007955 1.00007955 1.93615715]

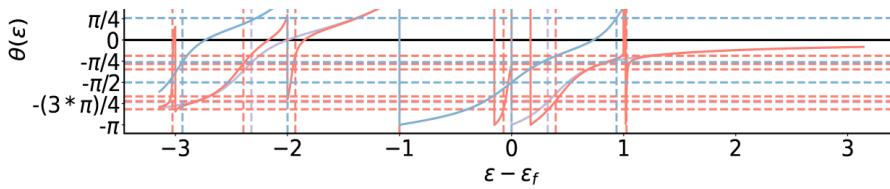




**Phase and energy of the transmission peaks after:**

Linear 3	phase = [-0.84791087 1.57079633 -2.29368179] grid = [-2.32252475 -1.00007955 0.32315095]
Linear 3 + aromatic 6	phase = [-1.14095714 -0.88243789 -0.58824901 1.57079633 -2.55334365 -2.25915476 -2.00063551] grid = [-3.02615355 -2.39320175 -1.92908945 -1.00007955 -0.07106965 0.39304265 1.02599445]
Aromatic 6	phase = [-0.81074937 1.57053779 -1.57053779 0.81074937] grid = [-2.93662935 -1.99976645 0. 0.93647025]

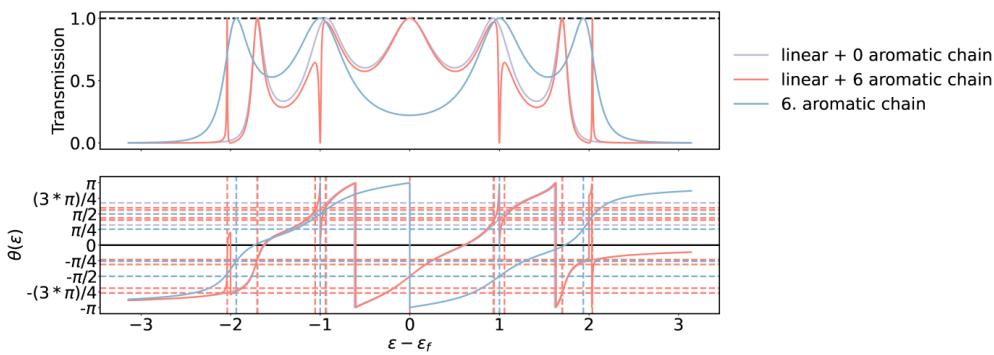




For linear-5 - when alpha is changed with 1, then the transmission graphs are also shifted by 1.

Phase and energy of the transmission peaks before:

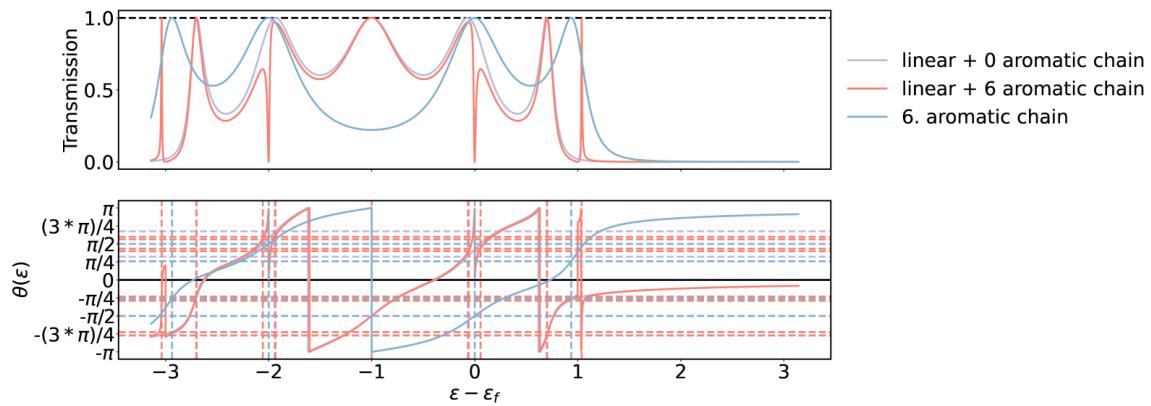
Linear 5	phase = [-0.72780651 2.12760748 -1.57079633 1.01398517 -2.41378614]	grid = [-1.69821125 -0.93097315 0. 0.93097315 1.69821125]
Linear 5 + aromatic 6	phase = [-0.97417164 -0.73104394 1.77002483 1.87997152 -1.57079633 1.26162114 1.37156782 -2.41054871 -2.16742102]	grid = [-2.03824615 -1.70292305 -1.05740645 -0.94039675 0. 0.94039675 1.05740645 1.70292305 2.03824615]
Aromatic 6	phase = [-0.81074937 1.57053779 -1.57053779 0.81074937]	grid = [-1.93615715 -1.00007955 1.00007955 1.93615715]



Phase and energy of the transmission peaks after:

Linear 5	phase = [-0.72780651 2.12760748 -1.57079633 1.01398517 -2.41378614]	grid = [-2.69789815 -1.93144535 -1.00007955 -0.06871375 0.69773905]
----------	---	---

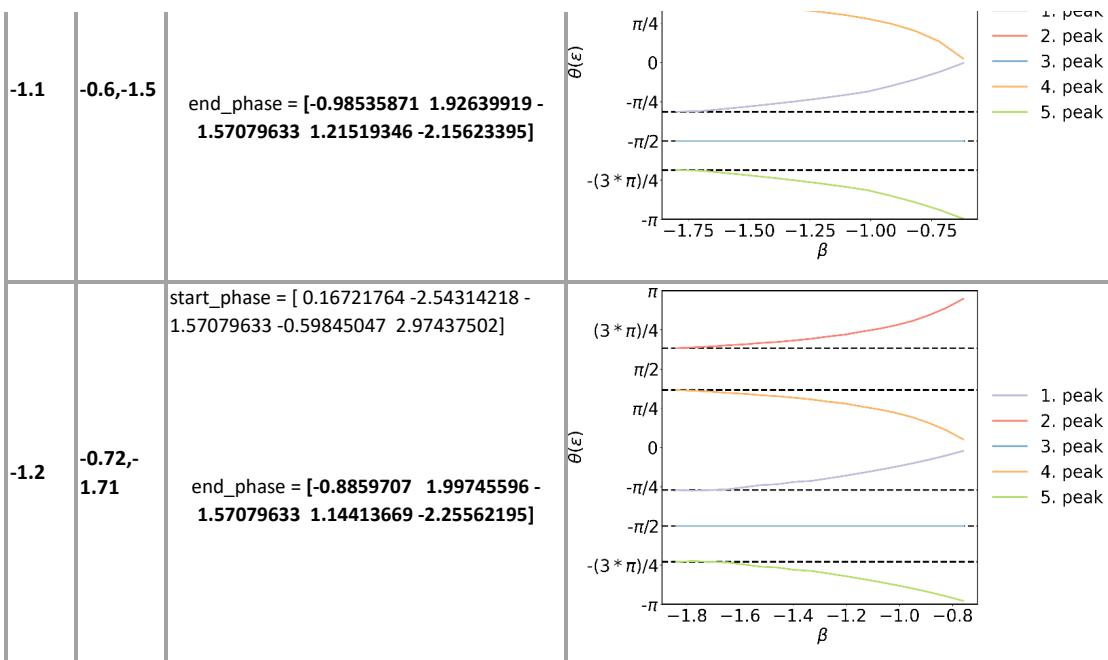
Linear 5 + aromatic 6	phase = [-0.97417164 -0.73104394 1.77002483 1.87997152 -1.57079633 1.26162114 1.37156782 -2.41054871 - 2.16742102] grid = [-3.03793305 -2.70260995 -2.05709335 -1.94008365 -1.00007955 - 0.06007545 0.05693425 0.70245085 1.03777395]
Aromatic 6	phase = [-0.81074937 1.57053779 - 1.57053779 0.81074937] grid = [-2.93662935 -1.99976645 0. 0.93647025]



E PHASE AS A FUNCTION OF BETA FOR 5 -LINEAR

## Values for phase as a function og beta - start and end phase for changing beta

Beta_I	Range of beta	Equilibrium	
-0.9	-0.46-1.61	<p>end_phase = [-1.10174428 1.84966165 -1.57079633 1.29193101 -2.03984837]</p>	
-1	-0.52,-1.61	<p>start_phase = [-0.03596579 3.01895484 -1.57079633 0.12263782 -3.10562687] end_phase = [-1.04844843 1.89302102 -1.57079633 1.24857163 -2.09314422]</p>	
		<p>start_phase = [-0.01240651 3.06266198 -1.57079633 0.07893067 -3.12918614]</p>	

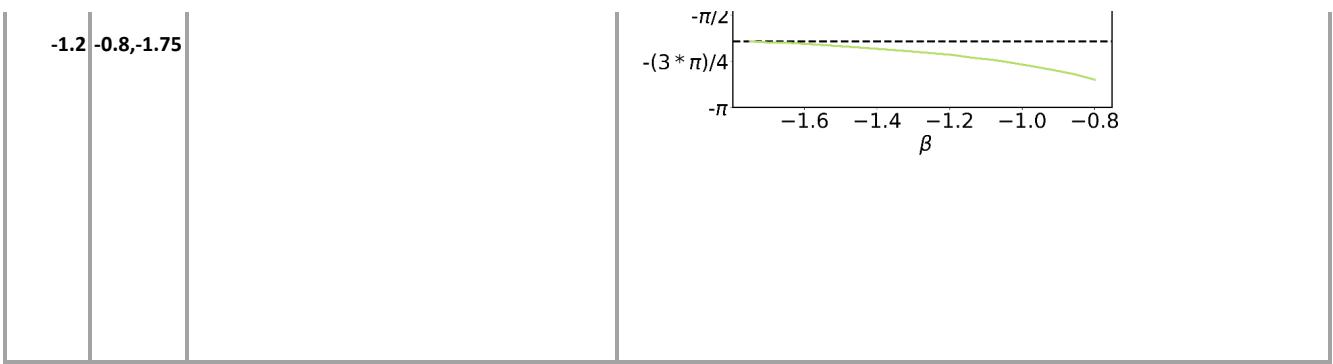


## F PHASE AS A FUNCTION OF BETA FOR 6 - LINEAR

### Transmission and phase as a function of energy - Changing beta\_I keeping beta at -1.

Beta_I Even (6 molecules)	Range of I Equilibrium	
-0.9	-2.27	<pre>start_phase = [-0.3096504  2.70083756 - 0.99436161 0.99436161 -2.70083756 0.3096504 ] end_phase = [-1.14237897  1.8704016 - 1.46172562 1.46172562 -1.8704016 1.14237897] phase[max_ind]-start_phase=[-0.83272857 - 0.83043596 -0.467364  0.467364  0.83043596 0.83272857]</pre>
		<pre>start_phase = [-0.21881082  2.78505972 - 0.92270177 0.92270177 -2.78505972 0.21881082] end_phase = [-1.05871353  1.9338445 - 1.43984649 1.43984649 -1.9338445 1.05871353]</pre>

	<pre> phase[max_ind]-start_phase=[-0.8399027 - 0.85121523 -0.51714472 0.51714472 0.85121523 0.8399027 ] </pre> <p>-1 -0.62,-1.7</p>	
-1.1	<pre> start_phase = [-0.20588964 2.82307902 - 0.88689486 0.88689486 -2.82307902 0.20588964] end_phase = [-0.93488399 2.02197335 - 1.39890645 1.39890645 -2.02197335 0.93488399] phase[max_ind]-start_phase=[-0.72899435 - 0.80110567 -0.51201158 0.51201158 0.80110567 0.72899435] </pre> <p>-1.1 -0.72,-1.6</p>	
	<pre> start_phase = [-0.28624291 2.66902774 - 1.03609957 1.03609957 -2.66902774 0.28624291] end_phase = [-0.98020402 2.01635649 - 1.40827284 1.40827284 -2.01635649 0.98020402] phase[max_ind]-start_phase=[-0.69396111 - 0.65267126 -0.37217326 0.37217326 0.65267126 0.69396111] </pre>	



G SHIFT IN TRANSMISSION FOR 5 - LINEAR

## Transmission and phase as a function of energy - Changing beta keeping beta\_l at -1.

Beta interval	Peak movement	Graph
Changing beta from -0.7 to -1.7	<pre> start_trans = [-1.16768551 -0.59248646  0.                0.59248646  1.16768551] end_trans = [-2.92471432 -1.6611623  0.                1.6611623  2.92471432] end_trans-start_trans = [-1.75702881 -                            1.06867584 0.      1.06867584 1.75702881] start_phase = [-0.40618318 2.45231677 -                1.57079633 0.68927589 -2.73540947] end_phase = [-1.07813736 1.87931259 -                1.57079633 1.26228007 -2.0634553 ] end_phase-start_phase = [-0.67195418 -                            0.57300418 0.      0.57300418 0.67195418] max_phase_start = [-0.43532825 1.12996754                      3.14159265] max_phase_end = [-1.05138844 2.74869712                      3.14159265] max_phase_end-phase_start = [-0.61606019                                1.61872958 0.      ] </pre>	<p>Legend for top plot:</p> <ul style="list-style-type: none"> <li>beta = -0.7, peaks = 5</li> <li>beta = -0.9, peaks = 5</li> <li>beta = -1.1, peaks = 5</li> <li>beta = -1.3, peaks = 5</li> <li>beta = -1.5, peaks = 5</li> <li>beta = -1.7, peaks = 5</li> </ul>
Changing beta from -0.7 to -0.9	<pre> start_trans = [-1.16685483 -0.591086  0.                0.591086  1.16685483] end_trans = [-1.52111368 -0.82202193 0.                0.82202193 1.52111368] end_trans-start_trans = [-0.35425885 -                            0.23093593 0.      0.23093593 0.35425885] start_phase = [-0.39521147 2.45917425 -                1.57079633 0.6824184 -2.74638118] end_phase = [-0.63126034 2.20297866 -                1.57079633 0.938614 -2.51033231] end_phase-start_phase = [-0.23604887 -                            0.2561956 0.      0.2561956 0.23604887] </pre>	<p>Legend for top plot:</p> <ul style="list-style-type: none"> <li>beta = -0.7, peaks = 5</li> <li>beta = -0.8, peaks = 5</li> <li>beta = -0.9, peaks = 5</li> </ul>

	<pre> max_phase_start = [-0.43320124  1.13229299 3.14159265] max_phase_end = [-0.55652416  1.45591749 3.14159265] max_phase_end-phase_start = [-0.12332293 0.3236245  0.      ] </pre>	
Changing beta from -0.9 to -1.1	<pre> start_trans = [-1.52111368 -0.82202193  0. 0.82202193  1.52111368] end_trans = [-1.87380154 -1.03881892  0. 1.03881892  1.87380154] end_trans-start_trans = [-0.35268786 - 0.21679699  0.      0.21679699  0.35268786] start_phase = [-0.63126034  2.20297866 - 1.57079633  0.938614 -2.51033231] end_phase = [-0.7965338  2.06539472 - 1.57079633  1.07619794 -2.34505885] end_phase-start_phase = [-1.65273462e-01 - 1.37583940e-01  2.22044605e-16 1.37583940e-01 1.65273462e-01] max_phase_start = [-0.55652416  1.45591749 3.14159265] max_phase_end = [-0.67984709  1.77954198 3.14159265] max_phase_end-phase_start = [-0.12332293 0.3236245  0.      ] </pre>	<p>The figure consists of two vertically stacked plots. The top plot shows Transmission on the y-axis (ranging from 0.0 to 1.0) against <math>\epsilon - \epsilon_r</math> on the x-axis (ranging from -3 to 3). Three curves are shown: a blue curve for <math>\beta = -0.9</math> with 5 peaks, a red curve for <math>\beta = -1.0</math> with 5 peaks, and a cyan curve for <math>\beta = -1.1</math> with 5 peaks. A vertical dashed line is at <math>\epsilon - \epsilon_r = 0</math>. The bottom plot shows <math>\theta(\epsilon)</math> on the y-axis (ranging from <math>-(3\pi)/4</math> to <math>(3\pi)/4</math>) against <math>\epsilon - \epsilon_r</math> on the x-axis (ranging from -3 to 3). The same three curves are shown, corresponding to the same beta values.</p>
	<pre> start_trans = [-1.87380154 -1.03881892  0. 1.03881892  1.87380154] end_trans = [-2.22491841 -1.24933195  0. 1.24933195  2.22491841] end_trans-start_trans = [-0.35111687 - 0.21051302  0.      0.21051302  0.35111687] start_phase = [-0.7965338  2.06539472 - 1.57079633  1.07619794 -2.34505885] </pre>	<p>The figure consists of two vertically stacked plots. The top plot shows Transmission on the y-axis (ranging from 0.0 to 1.0) against <math>\epsilon - \epsilon_r</math> on the x-axis (ranging from -3 to 3). Three curves are shown: a blue curve for <math>\beta = -1.1</math> with 5 peaks, a red curve for <math>\beta = -1.2</math> with 5 peaks, and a cyan curve for <math>\beta = -1.3</math> with 5 peaks. A vertical dashed line is at <math>\epsilon - \epsilon_r = 0</math>. The bottom plot shows <math>\theta(\epsilon)</math> on the y-axis (ranging from <math>-(3\pi)/4</math> to <math>(3\pi)/4</math>) against <math>\epsilon - \epsilon_r</math> on the x-axis (ranging from -3 to 3). The same three curves are shown, corresponding to the same beta values.</p>

Changing beta from -1.1 to -1.3	<pre> end_phase = [-0.9148415  1.97927491 - 1.57079633  1.16231775 -2.22675115] end_phase-start_phase = [-1.18307698e-01 - 8.61198084e-02 -2.22044605e-16 8.61198084e-02 1.18307698e-01] max_phase_start = [-0.67984709  1.77954198 3.14159265] max_phase_end = [-0.80395551  2.10316648 3.14159265] max_phase_end-phase_start = [-0.12410842 0.3236245  0.      ] </pre>	
Changing beta from -1.3 to -1.5	<pre> start_trans = [-2.22491841 -1.24933195  0. 1.24933195  2.22491841] end_trans = [-2.57446429 -1.45670298  0. 1.45670298  2.57446429] end_trans-start_trans = [-0.34954588 - 0.20737104  0.      0.20737104  0.34954588] start_phase = [-0.9148415  1.97927491 - 1.57079633  1.16231775 -2.22675115] end_phase = [-0.99746914  1.91935351 - 1.57079633  1.22223914 -2.14412351] end_phase-start_phase = [-0.08262764 - 0.0599214  0.      0.0599214  0.08262764] max_phase_start = [-0.80395551  2.10316648 3.14159265] max_phase_end = [-0.92727844  2.42679097 3.14159265] max_phase_end-phase_start = [-0.12332293 0.3236245  0.      ] </pre>	
	<pre> start_trans = [-2.57446429 -1.45670298  0. 1.45670298  2.57446429] end_trans = [-2.92401016 -1.66171753  0. 1.66171753  2.92401016] </pre>	

Changing beta from -1.5 to -1.7	<pre> end_trans-start_trans = [-0.34954588 -0.20501455 0. 0.20501455 0.34954588] start_phase = [-0.99746914 1.91935351 -1.57079633 1.22223914 -2.14412351] end_phase = [-1.06954579 1.87699846 -1.57079633 1.26459419 -2.07204687] end_phase-start_phase = [-0.07207664 -0.04235505 0. 0.04235505 0.07207664] max_phase_start = [-0.92727844 2.42679097 3.14159265] max_phase_end = [-1.05138687 2.75041547 3.14159265] max_phase_end-phase_start = [-0.12410842 0.3236245 0. ] </pre>	
Changing beta from -1.4 to -1.6	<pre> start_trans = [-2.39980589 -1.3531322 0. 1.3531322 2.39980589] end_trans = [-2.66068853 -1.50714725 0. 1.50714725 2.66068853] end_trans-start_trans = [-0.26088263 -0.15401505 0. 0.15401505 0.26088263] start_phase = [-0.95915622 1.94763474 -1.57079633 1.19395792 -2.18243643] end_phase = [-1.00215477 1.91158501 -1.57079633 1.23000764 -2.13943789] end_phase-start_phase = [-4.29985444e-02 -3.60497285e-02 1.11022302e-15 3.60497285e-02 4.29985444e-02] max_phase_start = [-0.86594175 2.26464983 3.14159265] max_phase_end = [-0.96023667 2.50667348 3.14159265] max_phase_end-phase_start = [-0.09429493 0.24202365 0. ] </pre>	

## Transmission and phase as a function of energy - Changing beta\_I keeping beta at -1.

Beta_I interval	Peak movement	Graph
Changing beta_I from -0.9 to -1.3	<pre> start_trans = [-1.70830976 -0.95709351 0. 0.95709351 1.70830976] end_trans = [-1.62030116 -0.63963392 0. 0.63963392 1.62030116] end_trans-start_trans = [ 0.0880086 0.31745959 0. -0.31745959 -0.0880086 ] start_phase = [-0.86574144 2.00078206 - 1.57079633 1.14081059 -2.27585122] end_phase = [-0.01647123 3.08155058 - 1.57079633 0.06004208 -3.12512143] end_phase-start_phase = [ 8.49270212e-01 1.08076851e+00 -6.66133815e-16 - 1.08076851e+00 -8.49270212e-01] max_phase_start = [-0.62077494 1.617158 3.14159265] max_phase_end = [-0.62077494 1.617158 3.14159265] max_phase_end-phase_start = [0. 0. 0.] </pre>	<p>The top plot shows Transmission (y-axis, 0.0 to 1.0) versus <math>\epsilon - \epsilon_r</math> (x-axis, -3 to 3). Six curves are shown for <math>\beta_I = -0.9, -1.0, -1.1, -1.2, -1.3, -1.4</math>, each with 5 peaks. The bottom plot shows phase <math>\theta(\epsilon)</math> (y-axis, -pi to pi) versus <math>\epsilon - \epsilon_r</math> (x-axis, -3 to 3) for the same <math>\beta_I</math> values.</p>
	<pre> start_trans = [-1.70884731 -0.95634181 0. 0.95634181 1.70884731] end_trans = [-1.69785036 -0.93120592 0. 0.93120592 1.69785036] end_trans-start_trans = [ 0.02513588 0.02513588 0. -0.02513588 - 0.02513588 ] </pre>	<p>The top plot shows Transmission (y-axis, 0.0 to 1.0) versus <math>\epsilon - \epsilon_r</math> (x-axis, -3 to 3) for <math>\beta_I = -0.9, -0.95, -1.0</math>. The bottom plot shows phase <math>\theta(\epsilon)</math> (y-axis, -pi to pi) versus <math>\epsilon - \epsilon_r</math> (x-axis, -3 to 3) for the same <math>\beta_I</math> values.</p>

Changing beta_l from -0.9 to -1.0	<pre> start_phase = [-0.87390687 2.00478748 - 1.57079633 1.13680517 -2.26768578] end_phase = [-0.72328099 2.12656741 - 1.57079633 1.01502525 -2.41831166] end_phase-start_phase = [ 0.15062588 0.12177993 0. -0.12177993 -0.15062588] max_phase_start = [-0.61857838 1.61772973 3.14159265] max_phase_end = [-0.61857838 1.61772973 3.14159265] max_phase_end-phase_start = [0. 0. 0.] </pre>	
Changing beta_l from -1.0 to -1.1	<pre> start_trans = [-1.69785036 -0.93120592 0. 0.93120592 1.69785036] end_trans = [-1.68371143 -0.89428759 0. 0.89428759 1.68371143] start_phase = [-0.72328099 2.12656741 - 1.57079633 1.01502525 -2.41831166] end_phase = [-0.5608571 2.27881786 - 1.57079633 0.8627748 -2.58073556] end_phase-start_phase = [ 1.62423895e-01 1.52250452e-01 -6.66133815e-16 - 1.52250452e-01 -1.62423895e-01] max_phase_start = [-0.61857838 1.61772973 3.14159265] max_phase_end = [-0.61857838 1.61772973 3.14159265] max_phase_end-phase_start = [0. 0. 0.] </pre>	
	<pre> start_trans = [-1.68371143 -0.89428759 0. 0.89428759 1.68371143] end_trans = [-1.66564501 -0.84165934 0. 0.84165934 1.66564501] </pre>	

	<pre> C111_U_d111-S111_U_d111 = 1.001000042 0.05262826 0. -0.05262826 - 0.018066471 start_phase = [-0.5608571 2.27881786 - 1.57079633 0.8627748 -2.58073556] end_phase = [-0.38334741 2.46856775 - 1.57079633 0.6730249 -2.75824524] 1.1 to -1.2 end_phase-start_phase = [ 1.77509684e-01 1.89749895e-01 4.44089210e-16 - 1.89749895e-01 -1.77509684e-01] max_phase_start = [-0.61857838 1.61772973 3.14159265] max_phase_end = [-0.61857838 1.61772973 3.14159265] max_phase_end-phase_start = [0. 0. 0.] </pre>	
Changing beta_l from - 1.1 to -1.2	<pre> start_trans = [-1.66564501 -0.84165934 0. 0.84165934 1.66564501] end_trans = [-1.64443661 -0.76232421 0. 0.76232421 1.64443661] end_trans-start_trans = [ 0.0212084 0.07933513 0. -0.07933513 -0.0212084 ] start_phase = [-0.38334741 2.46856775 - 1.57079633 0.6730249 -2.75824524] end_phase = [-0.201388 2.72385576 - 1.57079633 0.41773689 -2.94020465] end_phase-start_phase = [ 0.18195941 0.25528801 0. -0.25528801 -0.18195941] max_phase_start = [-0.61857838 1.61772973 3.14159265] max_phase_end = [-0.61857838 1.61772973 3.14159265] max_phase_end-phase_start = [0. 0. 0.] </pre>	
Changing beta_l from - 1.2 to -1.3	<pre> start_trans = [-1.64443661 -0.76232421 0. 0.76232421 1.64443661] </pre>	

<pre> end_trans = [-1.62165722 -0.64057227 0. 0.64057227 1.62165722] end_trans-start_trans = [ 0.022277959 <b>0.12175193 0. -0.12175193 -</b> <b>0.022277959</b> start_phase = [-0.201388 2.72385576 - 1.57079633 0.41773689 -2.94020465] Changing beta_l from -1.3 to -1.4 end_phase = [-0.02638809 3.07892617 - 1.57079633 0.06266648 -3.11520456] end_phase-start_phase = [ 1.74999911e-01 3.55070405e-01 -4.44089210e-16 - 3.55070405e-01 -1.74999911e-01] max_phase_start = [-0.61857838 1.61772973 3.14159265] max_phase_end = [-0.61857838 1.61772973 3.14159265] max_phase_end-phase_start = [0. 0. 0.] </pre>	<p>Top plot: Transmission vs energy (<math>\epsilon - \epsilon_f</math>). The plot shows two sharp peaks at approximately <math>\epsilon - \epsilon_f = \pm 1.5</math>. A legend indicates <math>\beta_l = -1.4</math>, peaks = 5.</p> <p>Bottom plot: Phase shift <math>\theta(\epsilon)</math> vs energy (<math>\epsilon - \epsilon_f</math>). The plot shows a step-like transition across the energy range, with values ranging from <math>-(3\pi/4)</math> to <math>(3\pi/4)</math>.</p>
<pre> start_trans = [-1.62030116 -0.63963392 0. 0.63963392 1.62030116] end_trans = [-1.5731537 0. 1.5731537] start_phase = [-0.01647123 3.08155058 - 1.57079633 0.06004208 -3.12512143] end_phase = [ 0.30441993 -1.57079633 2.83717272] max_phase_start = [-0.62077494 1.617158 3.14159265] max_phase_end = [-0.62077494 1.617158 3.14159265] </pre>	<p>Top plot: Transmission vs energy (<math>\epsilon - \epsilon_f</math>). The plot shows two broad peaks at approximately <math>\epsilon - \epsilon_f = \pm 1.5</math> for different beta_l values. A legend indicates four cases: beta_l = -1.4, peaks = 5; beta_l = -1.45, peaks = 5; beta_l = -1.5, peaks = 5; beta_l = -1.6, peaks = 3.</p> <p>Bottom plot: Phase shift <math>\theta(\epsilon)</math> vs energy (<math>\epsilon - \epsilon_f</math>). The plot shows a step-like transition across the energy range, with values ranging from <math>-(3\pi/4)</math> to <math>(3\pi/4)</math>.</p>

H SHIFT IN TRANSMISSION FOR 6 - LINEAR

## Transmission and phase as a function of energy - 6 molecules - Changing beta keeping beta\_l at -1.

Beta interval	Peak movement	Graph
Changing beta from -0.7 to -1.7	<pre> start_trans = [-1.23174305 -0.78804855 -0.24697685 0.24697685 0.78804855 1.23174305] end_trans = [-3.04971255 -2.08693475 -0.73778935 0.73778935 2.08693475 3.04971255] end_trans-start_trans = [1.8179695 -1.2988862 -0.4908125 0.4908125 1.2988862 1.8179695] start_phase = [-0.36317589 2.59292168 -1.09353122 1.09353122 -2.59292168 0.36317589] end_phase = [-1.05217851 1.94917156 -1.43216219 1.43216219 -1.94917156 1.05217851] end_phase-start_phase = [-0.68900262 -0.64375011 -0.33863096 0.33863096 0.64375011 0.68900262] max_phase_start = [-0.70009495 0.69930965 3.14159265] max_phase_end = [-1.70056715 1.69978185 3.14159265] max_phase_end-phase_start = [-1.0004722 1.0004722 0.    ] </pre>	
	<pre> start_trans = [-1.23174305 -0.78804855 -0.24697685 0.24697685 0.78804855 1.23174305] end_trans = [-1.59769285 -1.05819175 -0.35848945 0.35848945 1.05819175 1.59769285] </pre>	

<p>Changing beta from -0.7 to -0.9</p> <pre> end_trans-start_trans = [-0.3659498 -0.2701432 -0.1115126 0.1115126 0.2701432 0.3659498] start_phase = [-0.36317589 2.59292168 -1.09353122 1.09353122 -2.59292168 0.36317589] end_phase = [-0.61647375 2.32715235 -1.26036119 1.26036119 -2.32715235 0.61647375] end_phase-start_phase = [-0.25329786 -0.26576933 -0.16682996 0.16682996 0.26576933 0.25329786] max_phase_start = [-0.70009495 0.69930965 3.14159265] max_phase_end = [-0.90034645 0.89956115 3.14159265] max_phase_end-phase_start = [-0.2002515 0.2002515 0. ] </pre>	
<p>Changing beta from -0.9 to -1.1</p> <pre> start_trans = [-1.59769285 -1.05819175 -0.35848945 0.35848945 1.05819175 1.59769285] end_trans = [-1.96128675 -1.32048195 -0.45822255 0.45822255 1.32048195 1.96128675] end_trans-start_trans = [-0.3635939 -0.2622902 -0.0997331 0.0997331 0.2622902 0.3635939] start_phase = [-0.61647375 2.32715235 -1.26036119 1.26036119 -2.32715235 0.61647375] end_phase = [-0.76928658 2.17069696 -1.3383187 1.3383187 -2.17069696 0.76928658] </pre>	

```

end_phase-start_phase = [-0.15281283 -
0.15645538 -0.07795751 0.07795751
0.15645538 0.15281283]
max_phase_start = [-0.90034645
0.89956115 3.14159265]
max_phase_end = [-1.10059795
1.09981265 3.14159265]
max_phase_end-phase_start = [-0.2002515
0.2002515 0.]

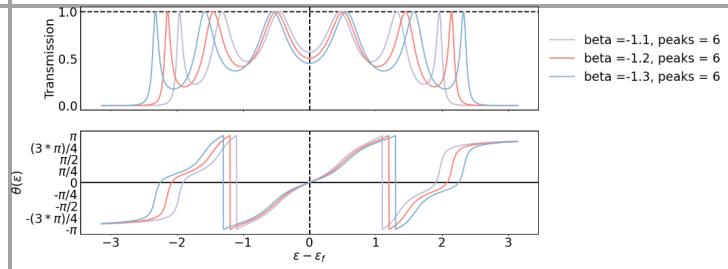
```

Changing beta from -1.1 to -1.3

```

start_trans = [-1.96128675 -1.32048195 -
0.45822255 0.45822255 1.32048195
1.96128675]
end_trans = [-2.32488065 -1.57806035 -
0.55245855 0.55245855 1.57806035
2.32488065]
end_trans-start_trans = [-0.3635939 -
0.2575784 -0.094236 0.094236
0.2575784 0.3635939]
start_phase = [-0.76928658 2.17069696 -
1.3383187 1.3383187 -2.17069696
0.76928658]
end_phase = [-0.89377979 2.07108629 -
1.37956384 1.37956384 -2.07108629
0.89377979]
end_phase-start_phase = [-0.12449322 -
0.09961067 -0.04124515 0.04124515
0.09961067 0.12449322]
max_phase_start = [-1.10059795
1.09981265 3.14159265]
max_phase_end = [-1.30006415
1.29927885 3.14159265]
max_phase_end-phase_start = [-0.1994662
0.1994662 0.]

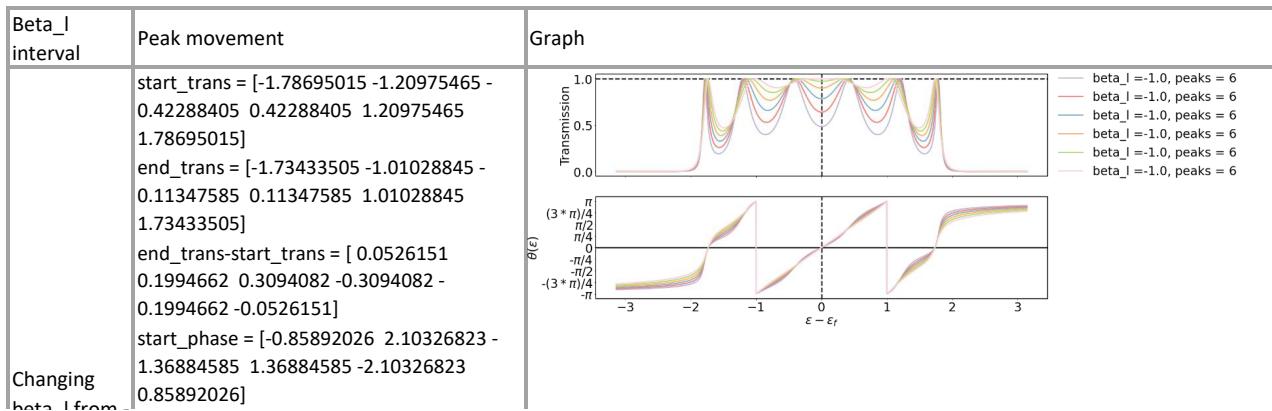
```



<pre> start_trans = [-2.32488065 -1.57806035 - 0.55245855 0.55245855 1.57806035 2.32488065] end_trans = [-2.68768925 -1.83328285 - 0.64590925 0.64590925 1.83328285 2.68768925] end_trans-start_trans = [-0.3628086 - 0.2552225 -0.0934507 0.0934507 0.2552225 0.3628086] start_phase = [-0.89377979 2.07108629 - 1.37956384 1.37956384 -2.07108629 0.89377979] end_phase = [-0.9859828 2.00083732 - 1.41092879 1.41092879 -2.00083732 0.9859828 ] end_phase-start_phase = [-0.09220301 - 0.07024897 -0.03136495 0.03136495 0.07024897 0.09220301] max_phase_start = [-1.30006415 1.29927885 3.14159265] max_phase_end = [-1.50031565 1.49953035 3.14159265] max_phase_end-phase_start = [-0.2002515 0.2002515 0. ] </pre>	

Changing beta from -1.5 to -1.7	<pre> start_phase = [-0.9859828  2.00083732 - 1.41092879  1.41092879 -2.00083732 0.9859828] end_phase = [-1.05217851  1.94917156 - 1.43216219  1.43216219 -1.94917156 1.05217851] end_phase-start_phase = [-0.0661957 - 0.05166576 -0.02123339  0.02123339 0.05166576  0.0661957] max_phase_start = [-1.50031565 1.49953035  3.14159265] max_phase_end = [-1.70056715 1.69978185  3.14159265] max_phase_end-phase_start = [-0.2002515 0.2002515  0.] </pre>
---------------------------------	---

### Transmission and phase as a function of energy - 6 molecules - Changing beta\_I keeping beta at -1.



beta_l from -0.9 to -1.3	<pre> end_phase = [-0.02757718 3.10022195 - 0.34118238 0.34118238 -3.10022195 0.02757718] end_phase-start_phase = [ 0.83134307 0.99695372 1.02766347 -1.02766347 - 0.99695372 -0.83134307] max_phase_start = [-1.00007955 0.99929425 3.14159265] max_phase_end = [-1.00007955 0.99929425 3.14159265] max_phase_end-phase_start = [0. 0. 0.] </pre>	
Changing beta_l from -0.9 to -1.0	<pre> start_trans = [-1.78695015 -1.20975465 - 0.42288405 0.42288405 1.20975465 1.78695015] end_trans = [-1.77988245 -1.19012215 - 0.40874865 0.40874865 1.19012215 1.77988245] end_trans-start_trans = [ 0.0070677 0.0196325 0.0141354 -0.0141354 - 0.0196325 -0.0070677] start_phase = [-0.85892026 2.10326823 - 1.36884585 1.36884585 -2.10326823 0.85892026] end_phase = [-0.70520803 2.23927471 - 1.3034983 1.3034983 -2.23927471 0.70520803] end_phase-start_phase = [ 0.15371223 0.13600648 0.06534755 -0.06534755 - 0.13600648 -0.15371223] max_phase_start = [-1.00007955 0.99929425 3.14159265] max_phase_end = [-1.00007955 0.99929425 3.14159265] max_phase_end-phase_start = [0. 0. 0.] </pre>	<p>The figure consists of two vertically stacked plots sharing a common x-axis representing the energy difference <math>\epsilon - \epsilon_f</math> from -3 to 3.</p> <p>The top plot shows Transmission on the y-axis (0.0 to 1.0). It displays three curves for different values of <math>\beta_l</math>, all showing six sharp peaks symmetric about <math>\epsilon - \epsilon_f = 0</math>. A vertical dashed line is at <math>\epsilon - \epsilon_f = 0</math>.</p> <p>The bottom plot shows <math>\theta(\epsilon)</math> on the y-axis (<math>-(3*m)/4\pi</math> to <math>(3*m)/4\pi</math>) on the y-axis. It also displays three curves for different values of <math>\beta_l</math>, showing a step-like behavior with jumps at specific energy differences.</p>

<pre> start_trans = [-1.77988245 -1.19012215 - 0.40874865 0.40874865 1.19012215 1.77988245] end_trans = [-1.77045885 -1.16185135 - 0.38676025 0.38676025 1.16185135 1.77045885] end_trans-start_trans = [ 0.0094236 0.0282708 0.0219884 -0.0219884 - 0.0282708 -0.0094236] start_phase = [-0.70520803 2.23927471 - 1.3034983 1.3034983 -2.23927471 0.70520803] end_phase = [-0.5333023 2.40628467 - 1.21543961 1.21543961 -2.40628467 0.5333023 ] end_phase-start_phase = [ 0.17190572 0.16700996 0.08805868 -0.08805868 - 0.16700996 -0.17190572] max_phase_start = [-1.00007955 0.99929425 3.14159265] max_phase_end = [-1.00007955 0.99929425 3.14159265] max_phase_end-phase_start = [0. 0. 0.] </pre>	
<pre> start_trans = [-1.77045885 -1.16185135 - 0.38676025 0.38676025 1.16185135 1.77045885] end_trans = [-1.75946465 -1.12337165 - 0.35142175 0.35142175 1.12337165 1.75946465] end_trans-start_trans = [ 0.0109942 0.0384797 0.0353385 -0.0353385 - 0.0384797 -0.0109942] </pre>	

<p>Changing beta_I from -1.1 to -1.2</p> <pre> start_phase = [-0.5333023  2.40628467 -                1.21543961 1.21543961 -2.40628467                0.5333023 ] end_phase = [-0.360707  2.60469326 -               1.08870306 1.08870306 -2.60469326               0.360707 ] end_phase-start_phase = [ 0.17259531                            0.19840859 0.12673655 -0.12673655 -                            0.19840859 -0.17259531] max_phase_start = [-1.00007955                      0.99929425 3.14159265] max_phase_end = [-1.00007955                      0.99929425 3.14159265] max_phase_end-phase_start = [0. 0. 0.] </pre>	
<p>Changing beta_I from -1.2 to -1.3</p> <pre> start_trans = [-1.75946465 -1.12337165 -                0.35142175 0.35142175 1.12337165                1.75946465] end_trans = [-1.74689985 -1.07311245 -               0.28545655 0.28545655 1.07311245               1.74689985] end_trans-start_trans = [ 0.0125648                            0.0502592 0.0659652 -0.0659652 -                            0.0502592 -0.0125648] start_phase = [-0.360707  2.60469326 -                1.08870306 1.08870306 -2.60469326                0.360707 ] end_phase = [-0.18622102 2.8362177 -               0.87138736 0.87138736 -2.8362177               0.18622102] end_phase-start_phase = [ 0.17448598                            0.23152444 0.21731571 -0.21731571 -                            0.23152444 -0.17448598] max_phase_start = [-1.00007955                      0.99929425 3.14159265] </pre>	

```

max_phase_end = [-1.00007955
0.99929425 3.14159265]
max_phase_end-phase_start = [0. 0. 0.]

```

```

start_trans = [-1.74689985 -1.07311245 -
0.28545655 0.28545655 1.07311245
1.74689985]
end_trans = [-1.73433505 -1.01028845 -
0.11347585 0.11347585 1.01028845
1.73433505]
end_trans-start_trans = [ 0.0125648
0.062824 0.1719807 -0.1719807 -0.062824
-0.0125648]
start_phase = [-0.18622102 2.8362177 -
0.87138736 0.87138736 -2.8362177
0.18622102]

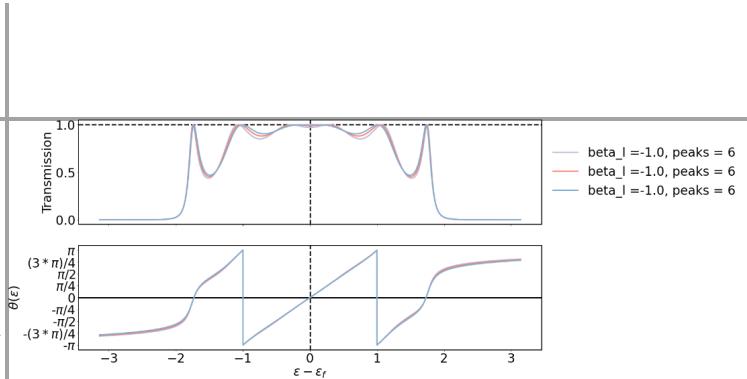
```

Changing  
beta\_l from -  
1.3 to -1.4

```

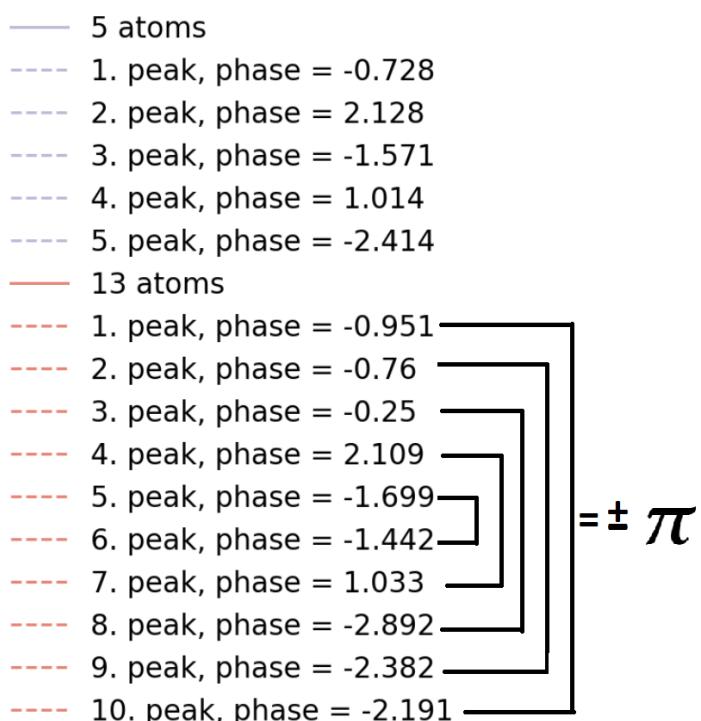
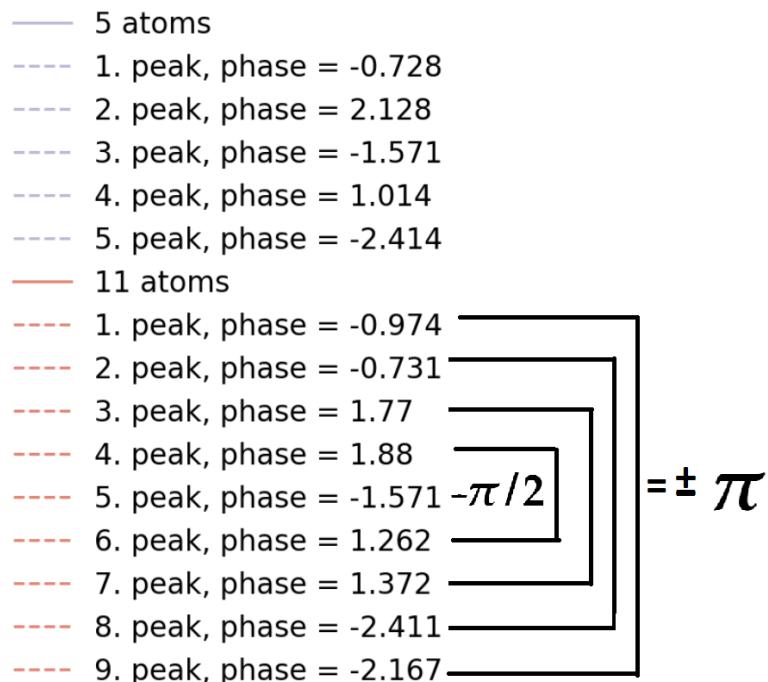
end_phase = [-0.02757718 3.10022195 -
0.34118238 0.34118238 -3.10022195
0.02757718]
end_phase-start_phase = [ 0.15864383
0.26400425 0.53020497 -0.53020497 -
0.26400425 -0.15864383]
max_phase_start = [-1.00007955
0.99929425 3.14159265]
max_phase_end = [-1.00007955
0.99929425 3.14159265]
max_phase_end-phase_start = [0. 0. 0.]

```



I PHASE OF CYCLIC SYSTEMS

Phases of linear 5 conjugated systems with cyclic side chains.



---

## B I B L I O G R A P H Y

---

- [1] J.-P. Deschamps, E. Valderrama, and L. Terés, *Digital Systems*. Cham: Springer International Publishing, 2017, ISBN: 978-3-319-41197-2 978-3-319-41198-9. DOI: [10.1007/978-3-319-41198-9](https://doi.org/10.1007/978-3-319-41198-9). [Online]. Available: <http://link.springer.com/10.1007/978-3-319-41198-9> (visited on 06/13/2021).
- [2] K. Mølmer, *Kvantemekanik: Atomernes vilde verden*, Dansk. Aarhus Universitetsforlag, 2010, ISBN: ISBN 978 87 7934 452 5.
- [3] O. “Let’s talk about quantum computing in drug discovery,” *Chemical & Engineering News*, [Online]. Available: <https://cen.acs.org/business/informatics/Lets-talk-quantum-computing-drug/98/i35> (visited on 06/13/2021).
- [4] R. P. Feynman, “Simulating physics with computers,” p. 22,
- [5] C. R. Arroyo, R. Frisenda, K. Moth-Poulsen, J. S. Seldenthuis, T. Bjørnholm, and H. S. van der Zant, “Quantum interference effects at room temperature in OPV-based single-molecule junctions,” *Nanoscale Research Letters*, vol. 8, no. 1, p. 234, Dec. 2013, ISSN: 1556-276X. DOI: [10.1186/1556-276X-8-234](https://doi.org/10.1186/1556-276X-8-234). [Online]. Available: <https://nanoscalereslett.springeropen.com/articles/10.1186/1556-276X-8-234> (visited on 02/19/2021).
- [6] S. Debnath, N. M. Linke, C. Figgatt, K. A. Landsman, K. Wright, and C. Monroe, “Demonstration of a small programmable quantum computer with atomic qubits,” *Nature*, vol. 536, no. 7614, pp. 63–66, Aug. 2016, ISSN: 0028-0836, 1476-4687. DOI: [10.1038/nature18648](https://doi.org/10.1038/nature18648). [Online]. Available: <http://www.nature.com/articles/nature18648> (visited on 06/10/2021).
- [7] M. Thoss and F. Evers, “Perspective: Theory of quantum transport in molecular junctions,” *The Journal of Chemical Physics*, vol. 148, no. 3, p. 030901, Jan. 21, 2018, ISSN: 0021-9606, 1089-7690. DOI: [10.1063/1.5003306](https://doi.org/10.1063/1.5003306). [Online]. Available: <http://aip.scitation.org/doi/10.1063/1.5003306> (visited on 05/14/2021).
- [8] G. C. Solomon, “Challenging The Limits Of Molecular Quantum Interference Effects,” *Part B*, p. 9, 2018.

- [9] J. C. Cuevas and E. Scheer, *Molecular Electronics: An Introduction to Theory and Experiment*. WORLD SCIENTIFIC, Jun. 2010, ISBN: 978-981-4282-58-1 978-981-4282-59-8. DOI: [10 . 1142 / 7434](https://doi.org/10.1142/7434). [Online]. Available: [http : / / www . worldscientific . com / worldscibooks / 10 . 1142 / 7434](http://www.worldscientific.com/worldscibooks/10.1142/7434) (visited on 02/23/2021).
- [10] R. W. Field, “MIT5\_61F17\_lecturenote26,” 2017.
- [11] (Jun. 15, 2015). “4.13C: Hückel MO Theory,” Chemistry LibreTexts, [Online]. Available: [https : / / chem . libretexts . org / Bookshelves / Inorganic\\_Chemistry / Map % 3A \\_ Inorganic\\_Chemistry \\_ \(Housecroft\) / 04 % 3A \\_ Experimental \\_ techniques / 4.13 % 3A \\_ Computational \\_ Methods / 4.13C % 3A \\_ Huckel \\_ MO \\_ Theory](https://chem.libretexts.org/Bookshelves/Inorganic_Chemistry/Map%3A_Inorganic_Chemistry_(Housecroft)/04%3A_Experimental_techniques/4.13%3A_Computational_Methods/4.13C%3A_Huckel_MO_Theory) (visited on 06/12/2021).
- [12] S. H. Simon, *The Oxford Solid State Basics*. 2016, ISBN: 978-0-19-968077-1.
- [13] M. Galperin, S. Toledo, and A. Nitzan, “Numerical computation of tunneling fluxes,” *The Journal of Chemical Physics*, vol. 117, no. 23, pp. 10817–10826, Dec. 15, 2002, ISSN: 0021-9606, 1089-7690. DOI: [10 . 1063 / 1 . 1522404](https://doi.org/10.1063/1.1522404). [Online]. Available: [http : / / aip . scitation . org / doi / 10 . 1063 / 1 . 1522404](http://aip.scitation.org/doi/10.1063/1.1522404) (visited on 03/24/2021).
- [14] S. R. Garcia and R. A. Horn, *A Second Course in Linear Algebra*: 1st ed. Cambridge University Press, May 11, 2017, ISBN: 978-1-107-10381-8 978-1-316-21841-9. DOI: [10 . 1017 / 9781316218419](https://doi.org/10.1017/9781316218419). [Online]. Available: [https : / / www . cambridge . org / core / product / identifier / 9781316218419 / type / book](https://www.cambridge.org/core/product/identifier/9781316218419/type/book) (visited on 04/22/2021).
- [15] S. Datta, *Electronic Transport in Mesoscopic Systems*, 1st ed. Cambridge University Press, Sep. 14, 1995, ISBN: 978-0-521-41604-7 978-0-521-59943-6 978-0-511-80577-6. DOI: [10 . 1017 / CBO9780511805776](https://doi.org/10.1017/CBO9780511805776). [Online]. Available: [https : / / www . cambridge . org / core / product / identifier / 9780511805776 / type / book](https://www.cambridge.org/core/product/identifier/9780511805776/type/book) (visited on 03/10/2021).
- [16] S. Gunasekaran, J. E. Greenwald, and L. Venkataraman, “Visualizing Quantum Interference in Molecular Junctions,” *Nano Lett.*, p. 6, 2020.
- [17] S. Datta, *Quantum Transport: Atom to Transistor*. Cambridge: Cambridge University Press, 2005, ISBN: 978-1-139-16431-3. DOI: [10 . 1017 / CBO9781139164313](https://doi.org/10.1017/CBO9781139164313). [Online]. Available: [http : / / ebooks . cambridge . org / ref / id / CBO9781139164313](http://ebooks.cambridge.org/ref/id/CBO9781139164313) (visited on 05/15/2021).
- [18] G. C. Solomon, D. Q. Andrews, T. Hansen, R. H. Goldsmith, M. R. Wasielewski, R. P. Van Duyne, and M. A. Ratner, “Understanding quantum interference in coherent molecular conduction,” *The Journal of Chemical Physics*, vol. 129, no. 5, p. 054701, Aug. 7, 2008,

- ISSN: 0021-9606, 1089-7690. DOI: [10.1063/1.2958275](https://doi.org/10.1063/1.2958275). [Online]. Available: <http://aip.scitation.org/doi/10.1063/1.2958275> (visited on 02/19/2021).
- [19] O. Christensen, R. D. Schlosser, and S. G. Stenspli, “Predicting Quantum Interference via Transmission Phase,” p. 25,
- [20] Y. Xue, S. Datta, and M. A. Ratner, “First-Principles Based Matrix-Green’s Function Approach to Molecular Electronic Devices: General Formalism,” *Chemical Physics*, vol. 281, no. 2-3, pp. 151–170, Aug. 2002, ISSN: 03010104. DOI: [10.1016/S0301-0104\(02\)00446-9](https://doi.org/10.1016/S0301-0104(02)00446-9). arXiv: [cond-mat/0112136](https://arxiv.org/abs/cond-mat/0112136). [Online]. Available: <http://arxiv.org/abs/cond-mat/0112136> (visited on 06/15/2021).
- [21] A. M. Childs, “Universal Computation by Quantum Walk,” *Physical Review Letters*, vol. 102, no. 18, p. 180501, May 4, 2009, ISSN: 0031-9007, 1079-7114. DOI: [10.1103/PhysRevLett.102.180501](https://doi.org/10.1103/PhysRevLett.102.180501). [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevLett.102.180501> (visited on 03/10/2021).
- [22] (May 3, 2015). “4.3: Stability of Cycloalkanes - Ring Strain,” Chemistry LibreTexts, [Online]. Available: [https://chem.libretexts.org/Bookshelves/Organic\\_Chemistry/Map%3A\\_Organic\\_Chemistry\\_\(McMurry\)/04%3A\\_Organic\\_Compounds\\_-\\_Cycloalkanes\\_and\\_their\\_Stereochemistry/4.03%3A\\_Stability\\_of\\_Cycloalkanes--Ring\\_Strain](https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Map%3A_Organic_Chemistry_(McMurry)/04%3A_Organic_Compounds_-_Cycloalkanes_and_their_Stereochemistry/4.03%3A_Stability_of_Cycloalkanes--Ring_Strain) (visited on 05/16/2021).