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QUANTUM DYNAMICS OF ELECTRONS IN ATOMS NEAR GRAPHENE MULTILAYERS

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Abstract

This thesis is divided into two parts: the study on graphene-based transistors and the study on graphene-based atom chips.

For the first part, we explore the tunnelling current characteristics of graphene-based field-effect transistors by means of theoretical investigation and computer simulations for various device parameters such as the misalignment angle between graphene layers, the Fermi energies of the graphene electrodes, the hBN barrier thickness, and the device temperature. We focus more on understanding the tunnelling mechanism and what gives rise to it rather than the form of the tunnelling current characteristics itself. We have found that the misalignment between graphene layers gives rise to a lower tunnelling current because a larger momentum change is required for electron tunnellings. We have found that the tunnelling current does not vary monotonically with the applied gate voltage, i.e. does not follow Ohm's law, due to a complicated competition among the availability of electronic states, the density of states, and the conservation of momentum. For a device with perfectly aligned graphene layers, we have found that the increasing density of states dominantly determines the magnitude of the tunnelling current: the higher the density of states, the higher the tunnelling current. We have found that increasing hBN barrier thickness decreases the tunnelling current due to the decay nature of the electron wavefunctions. We have found that a resonant tunnelling occurs when the electrostatic energy difference between graphene layers is approximately equal to the energy associated with the sum of the inverse square of the scattering length scale and the square of the difference in momenta between the two Dirac points of the graphene layers, $q_c^2 + |\Delta \mathbf{K}|^2$. Lastly, we have found that the tunnelling current increases with increasing temperature due to the non-zero occupation of electrons in a higher density of states above and below the Fermi levels, giving rise to an increase in the like-band tunnellings.

For the second part, with the knowledge of the electronic properties of graphene and hBN gathered in the first part, we have found that graphene multilayers

yield a weaker Casimir-Polder potential and a longer Johnson noise lifetime than metal slabs, showing the performance advantages of graphene-based atom chips over the present generation of atom chips. The theoretical formalism for calculating the Casimir-Polder potential and the Johnson noise lifetime has been developed and can be used for future work.

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Chapter 1

Introduction

The quantum dynamics of simple models of atoms near metallic bodies is well understood nowadays. However, for novel two-dimensional materials such as graphene and hexagonal boron-nitride, the work to understand the physics of complex structures consisting of these materials such as graphene-based transistors and atom chips, as well as how to make use of them are still in their pioneering stage, despite the fact that the basic properties of these materials alone are well explored and understood [1, 3, 21, 41, 78, 107, 121, 122].

For graphene-based transistors, the theories for the tunnelling-current characteristics as a function of the bias voltage between two graphene layers have been sufficiently established [40], but there are still areas for exploration such as how the devices behave over a range of temperatures, what internal properties of electrons in graphene govern what phenomena, etc. Moreover, we still need to overcome the experimental limitations of the device fabrication.

For graphene-based atom chips, the work on device design such as the shape of the wires and the layouts of the substrates has been around for a few years [38, 39]. The general theories involving the Casimir-Polder potential and Johnson noise of an atom near planar interfaces under different frameworks were developed long ago but only recently have we used these theories

to specifically investigate the Casimir-Polder potential and Johnson noise in atom chips [54, 68], let alone in novel graphene-based atom chips.

The structure of this thesis is as follows:

Chapter 2 An introduction to the electronic properties of graphene. We will show an application of the tight-binding model to derive the peculiar electronic properties of graphene such as the Dirac-like behaviour and chirality.

Chapter 3 A description of graphene-based transistors and the derivation of tunnelling current associated with the devices. We mainly investigate the direct-current characteristics of the devices as a function of the bias voltage and the effect of the misalignment of graphene electrodes on the tunnelling-current characteristics. We also discuss the contributions to the tunnelling current from each electronic band in graphene.

Chapter 4 Here, we investigate the variation of the tunnelling currents with the barrier thickness and temperature of the graphene-based transistors. This is a small chapter; since at the time of conducting the research on this topic, the topic has lost its popularity.

Chapter 5 In this chapter, we look into the optical properties of graphene and introduce a numerical method called “transfer-matrix method” for calculating the reflection coefficients. We test our method on various configurations of planar structures.

Chapter 6 This chapter is one of the most significant chapters in this thesis. We derive an analytical expression for the Casimir-Polder potential then use it, in conjunction with the transfer-matrix method, to investigate the Casimir-

Polder potential produced by metal slabs and graphene-multilayers.

Chapter 7 The other key result of this thesis: we develop the theoretical formalism for calculating the thermal spin flip rate (Johnson noise); we then explore the Johnson noise lifetimes for ultra-cold ^{87}Rb atoms near thin metal slabs and graphene-multilayers and discuss the performance advantages of graphene-based atom chips.

Chapter 8 Here, we discuss the future work on investigating the Casimir-Polder potential and Johnson noise lifetime for different two-dimensional multilayers other than graphene and the effect of the tunnelling current in gated graphene-based heterostructures on the trap potential profiles of the atom chips.

Chapter 2

Graphene

Graphene is a two-dimensional material that has peculiar and outstanding properties. It is one-atom thick and its electronic energy-wavevector spectrum is linear, exhibiting similar properties to massless Dirac fermions [78, 86]. It also has a high carrier mobility [7, 77] and is very transparent [46]. In terms of its physical properties, graphene is very strong and highly flexible [64]; it has been demonstrated that a monolayer graphene membrane is impermeable to standard liquids and gases, including helium [16]. Its thermal conductivity is also high [5]. One fascinating property, of direct relevance to micro-fabricated graphene-based atom chips, is that it can withstand high current densities ($\sim 1 \times 10^{12} \text{ A m}^{-2}$, i.e. up to $\sim 700 \text{ A m}^{-1}$, taking the thickness of graphene to be 0.335 nm) [9, 55, 83]. Regarding magnetism and its spin transport, graphene does not show sizeable spin-orbit interaction [43] and also has a very long spin relaxation length at room temperature [105].

Having all these properties together in a single material makes graphene uniquely interesting: technologies and fundamental research in flexible electronics, efficient field-effect transistors [11, 12, 26, 40, 85], transparent protective coating and atom chips can all benefit from its properties [37].

How is graphene produced? Since there are many methods for graphene

production, we will only list them without going into the details. The first method is called dry exfoliation. The initial method of dry exfoliation for producing graphene is micromechanical exfoliation, also known as *sticky tape method* [74,98]. The others are anodic bonding [82,101] and photoexfoliation [29,81,94]. Liquid-phase exfoliation exploits ultrasound vibration or kitchen blenders to extract individual graphene layers from graphite [51,52,73,92]. The third type is electrochemical exfoliation [69]. The last graphene production method is direct growth or deposit on substrates [33,57,67,90,100,111,112,114].

2.1 The Crystal Structure of Monolayer Graphene

Before we explore the properties of graphene, we first need a basic knowledge of carbon, the sixth element of the periodic table. A carbon atom is made up of six protons, six electrons and six to eight neutrons. In the atomic ground state, the six electrons are in the configuration $1s^2 2s^2 2p^2$. However, in the excited state, it is favourable to excite one more electron from the 2s orbital to the 2p orbital, i.e. to be in the $1s^2 2s^1 2p^3$ configuration. This results in four equivalent quantum-mechanical states, $|2s\rangle$, $|2p_x\rangle$, $|2p_y\rangle$, and $|2p_z\rangle$. A quantum-mechanical superposition of $|2s\rangle$ with n $|2p_j\rangle$ states is called sp^n hybridisation. We will briefly consider the sp^2 hybridisation as it is related to graphene.

In the case of graphene, the planar sp^2 hybridisation is formed as a result of a superposition of the 2s orbital and two 2p orbitals, namely, $|2p_x\rangle$ and $|2p_y\rangle$ [96]. These three hybridised orbitals are oriented in the xy -plane and have mutual 120° angles (see Figure 2.1). These electrons form strong covalent σ bonds with the adjacent carbon atoms (see Figure 2.2). The remaining unhybridised $2p_z$ orbital is perpendicular to the plane and, when combined with the $2p_z$ orbitals of the adjacent atoms, forms a π orbital. The combination of all π orbitals forms a sea of electrons. It is the electrons from the π orbitals that

are responsible for the electronic properties of graphene at low energies.

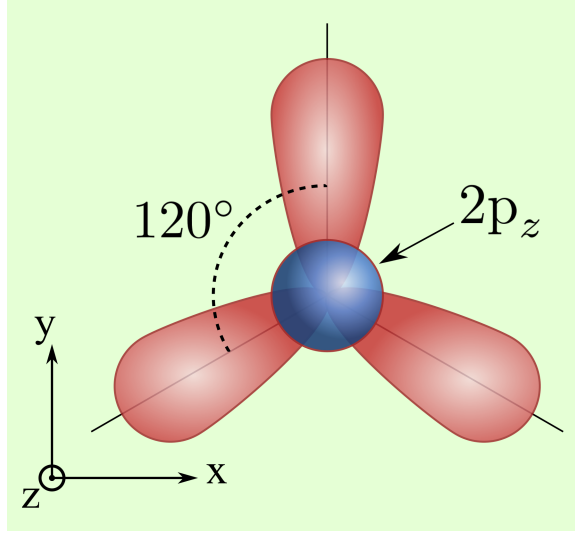


Figure 2.1: Schematic diagram of the sp^2 hybridisation structure. A superposition of the $2s$, $2p_x$ and $2p_y$ orbitals forms three hybridised orbitals (shaded red) that are oriented at 120° to each other in the xy -plane. The remaining unhybridised $2p$ orbital is the $2p_z$ orbital (shaded blue), which is perpendicular to the plane.

2.1.1 The real space structure

Monolayer graphene is a two-dimensional structure of carbon atoms arranged in a hexagonal pattern as shown in Figure 2.2a. In order to describe the crystal structure of graphene, we will first introduce a lattice basis and the associated primitive lattice vectors. A Cartesian coordinate system with the x - and y -axis in the plane of the graphene crystal and the z -axis perpendicular to the graphene plane will be used throughout this chapter. The basis of the Bravais lattice of graphene consists of two carbon atoms, labelled A and B , and the primitive lattice vectors are

$$\mathbf{a}_1 = \left(\frac{a}{2}, \frac{\sqrt{3}a}{2} \right), \quad \mathbf{a}_2 = \left(\frac{a}{2}, -\frac{\sqrt{3}a}{2} \right), \quad (2.1)$$

where $a = |\mathbf{a}_1| = |\mathbf{a}_2| = 2.46 \text{ \AA}$ is the lattice constant (see Figure 2.2b) [96].

The shortest distance between two carbon atoms is the carbon-carbon bond length $a_{CC} = a/\sqrt{3} = 1.42 \text{ \AA}$. Note that it is not possible to connect atomic

positions A and B with a lattice vector $\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2$, where n_1 and n_2 are integers, implying that the honeycomb structure shown in Figure 2.2a is not a Bravais lattice.

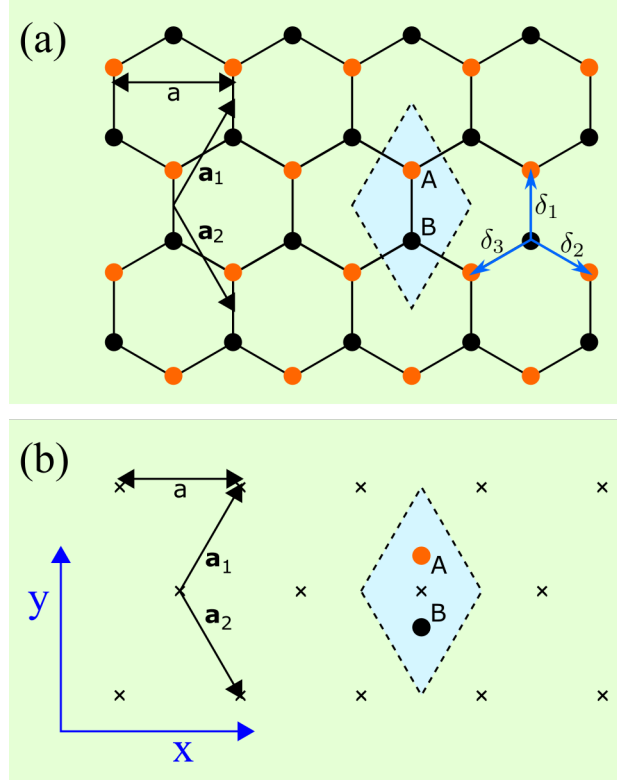


Figure 2.2: (a) Schematic illustration of the crystal structure of monolayer graphene in real space where the orange and black circles represent A and B lattice sites respectively, each accommodating one carbon atom, and straight lines indicate σ bonds between them. Vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ are primitive lattice vectors of length equal to the lattice constant, a . A unit cell, indicated by a blue rhombus, consists of two carbon atoms from A and B sites, forming a basis for the Bravais lattice. The nearest neighbours of an atom on the B sublattice are specified by position vectors δ_1 , δ_2 , and δ_3 whose length is $1.42 \text{ \AA}$. (b) Crosses indicate lattice points of the hexagonal Bravais lattice. A whole blue rhombus, representing a unit cell, is placed on top of a cross to show the relationship between the crystal structure and the Bravais lattice.

2.1.2 The reciprocal lattice of graphene

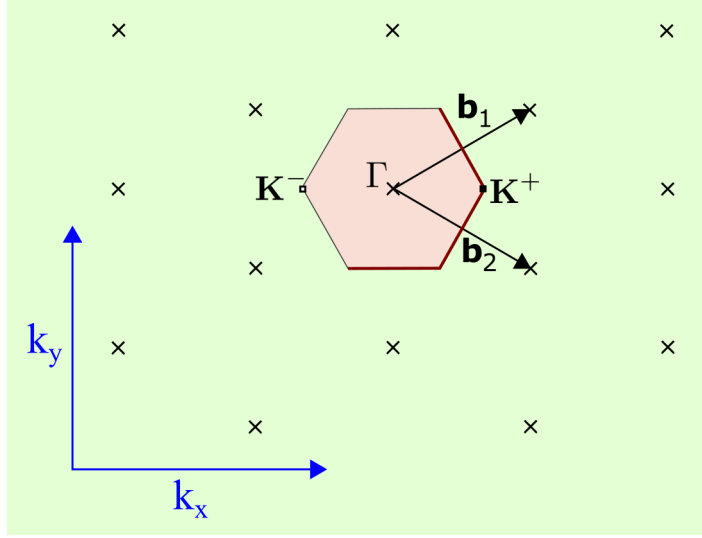


Figure 2.3: Reciprocal lattice of graphene: crosses indicate the lattice points; vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ are the primitive lattice vectors. The pink hexagon with the thick part of the border (shaded dark red) represents the first Brillouin zone defined in a strict manner; no equivalent points are doubly counted. Γ , and K^+ (black square) and K^- (white square) are its centre, and two inequivalent corners, respectively.

The reciprocal lattice, which is defined with respect to the hexagonal Bravais lattice, is depicted with crosses in Figure 2.3. The primitive reciprocal lattice vectors are given by

$$\mathbf{b}_1 = \left(\frac{2\pi}{a}, \frac{2\pi}{\sqrt{3}a} \right) \quad \text{and} \quad \mathbf{b}_2 = \left(\frac{2\pi}{a}, \frac{-2\pi}{\sqrt{3}a} \right). \quad (2.2)$$

The pink hexagon and the thick part of its border represent the first Brillouin zone, which is a set of points that may not be connected to one another by any combinations of the reciprocal lattice vectors. Physically, these points represent distinguishable lattice excitations. The long-wavelength excitations, which are not of interest in our scope of research, are located in the vicinity of the Γ point, in the first Brillouin zone. The six corners of the first Brillouin zone are where the conduction and valence bands meet (see Figure 2.5). Owing to the massless behaviour of the electrons in graphene in the vicinity of these

points – they obey Dirac’s relativistic wave equation – these points have been given a special name called Dirac points. Despite the fact that there are six Dirac points, only two of them, represented by $\mathbf{K}^\pm = (\pm 4\pi/3a, 0)$, are inequivalent. These crystallographic points are of importance for the electronic properties of graphene. This will be discussed in detail in the following section. To prevent any possible confusion in the future, we will end this section by emphasising that the inequivalence of the two corners of the Brillouin zone has nothing to do with the fact that the basis of the crystalline lattice consists of two spatially inequivalent atoms. It is the form of the Bravais lattice (described by the lattice vectors) that intrinsically give rises to the form of the Brillouin zone.

2.2 Electronic Band Structure of Monolayer Graphene

2.2.1 General tight-binding model

We start by considering the tight-binding model for a system with n atomic orbitals ϕ_j in the unit cell, labelled by index $j = 1, \dots, n$. It is assumed that the system is infinitely large; the system has translational invariance. Under this assumption, the model may be described using n Bloch functions $\Phi_j(\mathbf{k}, \mathbf{r})$ that depend on the wave vector $\mathbf{k}$ and position vector $\mathbf{r}$. They are given by [96]

$$\Phi_j(\mathbf{k}, \mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{i=1}^N e^{i\mathbf{k} \cdot \mathbf{R}_{j,i}} \phi_j(\mathbf{r} - \mathbf{R}_{j,i}), \quad (2.3)$$

where the sum is over N different unit cells, labelled by index $i = 1, \dots, N$, and $\mathbf{R}_{j,i}$ denotes the position of the j -th orbital in the i -th unit cell. To illustrate the form of a Bloch function graphically, let us consider a fictitious one-dimensional lattice in Figure 2.4: the red dots represent the positions of the atoms in the lattice with single-atom electronic wavefunctions, ϕ_j , depicted

by a blue curve in Figure 2.4a. The exponential term in Equation (2.3), which acts as an envelope (dashed red curve in Figure 2.4), modulates the single-atom wavefunctions, resulting in a deformed wavefunction, which is technically the tight-binding, Bloch function (solid blue curve in Figure 2.4b) describing an energy eigenstate of an electron in the whole lattice. These n Bloch functions, for a given $\mathbf{k}$, form an orthonormal basis which can be used to describe any electronic wavefunctions for the system.

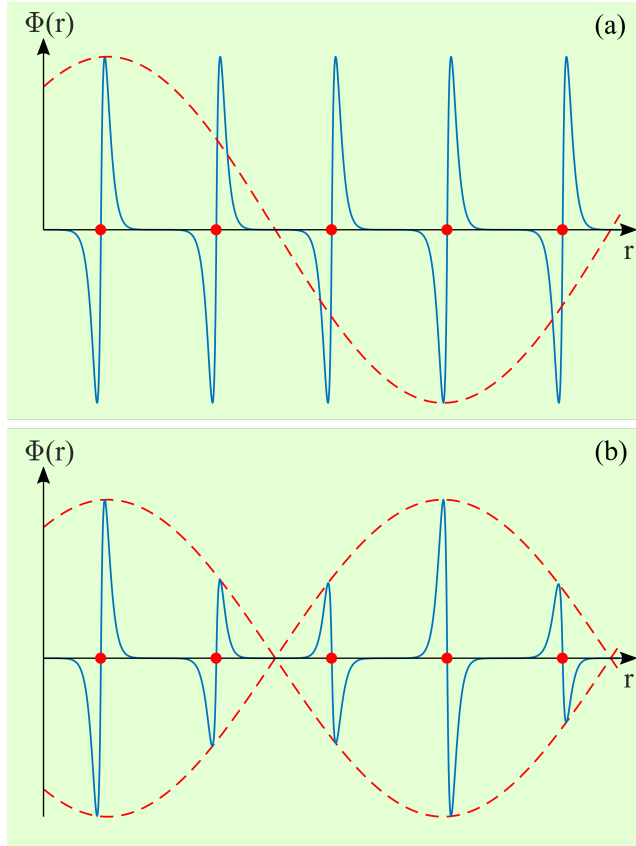


Figure 2.4: Illustration of a tight-binding, Bloch function (solid blue curve in (b)), single-particle orbitals (solid blue curve in (a)), and a phase factor (dashed red curves in (a) and (b)) in Equation (2.3), versus position, $\mathbf{r}$, of a one-dimensional crystal. The red dots represent the lattice points. The single-particle electronic wavefunctions of the whole crystal are modulated by the phase factor, $e^{i\mathbf{k} \cdot \mathbf{R}_{j,i}}$, yielding the tight-binding, Bloch function, which describes an electronic state of the crystal.

Following from the above statement, a wavefunction of an electron in the

system (e.g. a crystal) is given by,

$$\Psi_j(\mathbf{k}, \mathbf{r}) = \sum_{l=1}^n c_{j,l}(\mathbf{k}) \Phi_l(\mathbf{k}, \mathbf{r}), \quad (2.4)$$

where $c_{j,l}(\mathbf{k})$ are coefficients of the expansion.

These wavefunctions are the eigenfunctions of the Hamiltonian; therefore, the one-electron energy $E_j(\mathbf{k})$ of the j -th band is given by

$$E_j(\mathbf{k}) = \frac{\langle \Psi_j | \mathcal{H} | \Psi_j \rangle}{\langle \Psi_j | \Psi_j \rangle}, \quad (2.5)$$

where $\mathcal{H}$ is the Hamiltonian. Substituting the expansion of the wavefunction (2.4) into the energy gives

$$E_j(\mathbf{k}) = \frac{\sum_{i,l}^n c_{ji}^* c_{jl} \langle \Phi_j | \mathcal{H} | \Phi_j \rangle}{\sum_{i,l}^n c_{ji}^* c_{jl} \langle \Phi_j | \Phi_j \rangle}, \quad (2.6)$$

$$= \frac{\sum_{i,l}^n c_{ji}^* c_{jl} H_{il}}{\sum_{i,l}^n c_{ji}^* c_{jl} S_{il}}, \quad (2.7)$$

where the transfer integral matrix elements and overlap integral matrix elements are rewritten as

$$H_{il} = \langle \Phi_j | \mathcal{H} | \Phi_j \rangle, \quad S_{il} = \langle \Phi_j | \Phi_j \rangle. \quad (2.8)$$

In order to find the readily solvable relationship of the energy, transfer integral matrix and overlap integral matrix, we calculate the derivative of $E_j(\mathbf{k})$ with respect to the coefficient c_{jm}^* and set it to 0, which eventually yields

$$\sum_{l=1}^n H_{ml} c_{jl} = E_j \sum_{l=1}^n S_{ml} c_{jl}. \quad (2.9)$$

By inspection, this can be written as a matrix equation as follows:

$$H \Psi_j = E_j S \Psi_j, \quad (2.10)$$

where Ψ_j is a vector representation of the electronic state given in (2.4). This is equivalent to the homogeneous system

$$(H - E_j S)\Psi_j = 0. \quad (2.11)$$

A linear system of equations has nontrivial solutions if and only if the determinant vanishes, so the solutions of equation (2.11), i.e. the energies E_j , are given by

$$\det(H - E_j S) = 0. \quad (2.12)$$

Note that the number of solutions is equal to the number of different atomic orbitals per unit cell and that $E_j = E_j(\mathbf{k})$.

2.2.2 The tight-binding model of monolayer graphene

We first need to figure out how many atomic orbitals per unit cell there are for monolayer graphene. In our model, we will take into account only one $2p_z$ orbital per atomic site. Because there are two carbon atoms per unit cell (see Figure 2.2), the basis of our quantum system consists of two Bloch functions, namely, Φ_A and Φ_B . Now that we have our building blocks, the transfer integral matrix elements and overlap integral matrix elements can be determined.

Diagonal matrix elements

The diagonal matrix element, H_{AA} , can be written as

$$H_{AA} = \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^N e^{i\mathbf{k} \cdot (\mathbf{R}_{A,j} - \mathbf{R}_{A,i})} \langle \phi_A(\mathbf{r} - \mathbf{R}_{A,i}) | \mathcal{H} | \phi_A(\mathbf{r} - \mathbf{R}_{A,j}) \rangle, \quad (2.13)$$

$$\approx \frac{1}{N} \sum_{i=1}^N \langle \phi_A(\mathbf{r} - \mathbf{R}_{A,i}) | \mathcal{H} | \phi_A(\mathbf{r} - \mathbf{R}_{A,i}) \rangle \quad (2.14)$$

where $\mathbf{k} = (k_x, k_y)$ is the wave vector in the graphene plane. Although Equation (2.13) includes a double summation over all the A sites of the lattice, we have approximated it by assuming that the contribution that arises from the same site $j = i$ within every unit cell is dominant. Since the system is translationally invariant, it follows that the matrix element $\langle \phi_A | \mathcal{H} | \phi_A \rangle$ has the same value on every site A and can be set to equal the energy of the $2p_z$ orbital, ϵ_{2p} . This gives

$$H_{AA} \approx \frac{1}{N} \sum_{i=1}^N \epsilon_{2p} = \epsilon_{2p}. \quad (2.15)$$

It can easily be seen that $H_{BB} = H_{AA}$ due to the identical form of the A and B sublattices. The diagonal elements of the overlap integral matrix can be calculated in a similar way under the same assumption. Basically, it is the overlap of a $2p_z$ orbital with itself at the same position in space, which is equal to unity: $S_{AA} = S_{BB} = 1$.

Off-diagonal matrix elements

The off-diagonal matrix elements describe the processes of hopping between the different sublattices, i.e. between the A and B sublattices. It is more complicated to determine the off-diagonal matrix elements than the diagonal ones. We begin by substituting the expression for the Bloch function given in Equation (2.3) into the definition of the transfer integral, Equation (2.8); therefore, we have

$$H_{AB} = \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^N e^{i\mathbf{k} \cdot (\mathbf{R}_{B,j} - \mathbf{R}_{A,i})} \langle \phi_A(\mathbf{r} - \mathbf{R}_{A,i}) | \mathcal{H} | \phi_A(\mathbf{r} - \mathbf{R}_{B,j}) \rangle. \quad (2.16)$$

Let us assume that the dominant contribution in the sum arises from hopping between the nearest neighbours only. Referring back to Figure 2.2, an individual B atom has three neighbouring A atoms; therefore, the approximation of the off-diagonal matrix element (2.16) is given by

$$H_{AB} \approx \frac{1}{N} \sum_{l=1}^3 \sum_{j=1}^N e^{i\mathbf{k} \cdot (\mathbf{R}_{B,j} - \mathbf{R}_{A,l})} \langle \phi_A(\mathbf{r} - \mathbf{R}_{A,l}) | \mathcal{H} | \phi_A(\mathbf{r} - \mathbf{R}_{B,j}) \rangle. \quad (2.17)$$

Owing to the symmetry of the system, the matrix element between neighbouring atoms is independent of indices l and j . Thus, we set it equal to a hopping parameter, $t = \langle \phi_A(\mathbf{r} - \mathbf{R}_{A,l}) | \mathcal{H} | \phi_A(\mathbf{r} - \mathbf{R}_{B,j}) \rangle$. As t is negative [96], we will express it in terms of a positive parameter $\gamma_0 = -t$. The off-diagonal matrix element now becomes

$$H_{AB} \approx -\frac{1}{N} \sum_{l=1}^3 \sum_{j=1}^N e^{i\mathbf{k} \cdot (\mathbf{R}_{B,j} - \mathbf{R}_{A,l})} \gamma_0, \quad (2.18)$$

$$= -\frac{\gamma_0}{N} \sum_{l=1}^3 \sum_{j=1}^N e^{i\mathbf{k} \cdot (\boldsymbol{\delta}_l)} \equiv -\gamma_0 f(\mathbf{k}), \quad (2.19)$$

$$f(\mathbf{k}) = \sum_{l=1}^3 e^{i\mathbf{k} \cdot (\boldsymbol{\delta}_l)}, \quad (2.20)$$

where the position vector of atom A_l relative to the B_j atom is denoted $\boldsymbol{\delta}_l = \mathbf{R}_{B,j} - \mathbf{R}_{A,l}$. The position vectors connecting the B atom under consideration to its three neighbours are as follows:

$$\boldsymbol{\delta}_1 = \left(0, \frac{a}{\sqrt{3}}\right), \quad \boldsymbol{\delta}_2 = \left(\frac{a}{2}, -\frac{a}{2\sqrt{3}}\right), \quad \boldsymbol{\delta}_3 = \left(-\frac{a}{2}, -\frac{a}{2\sqrt{3}}\right). \quad (2.21)$$

As mentioned before, $|\boldsymbol{\delta}_1| = |\boldsymbol{\delta}_2| = |\boldsymbol{\delta}_3| = a/\sqrt{3}$ is the carbon-carbon bond length. Then, the function $f(\mathbf{k})$ describing the nearest-neighbour hopping can be evaluated:

$$f(\mathbf{k}) = \sum_{l=1}^3 e^{i\mathbf{k} \cdot (\boldsymbol{\delta}_l)}, \quad (2.22)$$

$$= e^{ik_y a/\sqrt{3}} + 2e^{-ik_y a/2\sqrt{3}} \cos\left(\frac{k_x a}{2}\right). \quad (2.23)$$

The other off-diagonal matrix element H_{BA} is the complex conjugate of H_{AB} . Thus, it is given by

$$H_{BA} \approx -\gamma_0 f^*(\mathbf{k}). \quad (2.24)$$

It follows that

$$S_{AB} = s_0 f(\mathbf{k}) \quad \text{and} \quad S_{BA} = s_0 f^*(\mathbf{k}), \quad (2.25)$$

where the parameter $s_0 = \langle \phi_A(\mathbf{r} - \mathbf{R}_{A,l}) | \phi_A(\mathbf{r} - \mathbf{R}_{B,j}) \rangle$. Here, l and j are defined in the same way as in (2.17).

2.2.3 The electronic bands of monolayer graphene

Putting all ingredients together, the transfer integral matrix and the overlap integral matrix can be written as:

$$H = \begin{pmatrix} \epsilon_{2p} & -\gamma_0 f(\mathbf{k}) \\ -\gamma_0 f^*(\mathbf{k}) & \epsilon_{2p} \end{pmatrix}, \quad S = \begin{pmatrix} 1 & s_0 f(\mathbf{k}) \\ s_0 f^*(\mathbf{k}) & 1 \end{pmatrix}. \quad (2.26)$$

Solving the secular equation (2.12) yields the energy:

$$E_{\pm} = \frac{\epsilon_{2p} \pm \gamma_0 |f(\mathbf{k})|}{1 \mp s_0 |f(\mathbf{k})|}. \quad (2.27)$$

The parameter values $\gamma_0 = 3.033 \text{ eV}$, $s_0 = 0.129$, $\epsilon_{2p} = 0$ are quoted in [96], in order to reproduce the ab-initio calculation of the graphite energy bands [32, 91]. Having $\epsilon_{2p} = 0$ means the zero of energy is set to equal to the energy of the $2p_z$ orbital. The band structure consists of two bands, namely, the conduction band (E_+) and the valence band (E_-) (see Figure 2.5). A feature of the band structure worth noting is that there is no gap between the conduction and valence bands. The bands cross at six points called K points. Near these points, the energy dispersion is linear; thus, the low-energy electronic properties of monolayer graphene maybe described by a Dirac-like Hamiltonian; this gives rise to another term for the K points, namely **Dirac points**. Most

material presented in later chapters in this thesis will involve this feature.

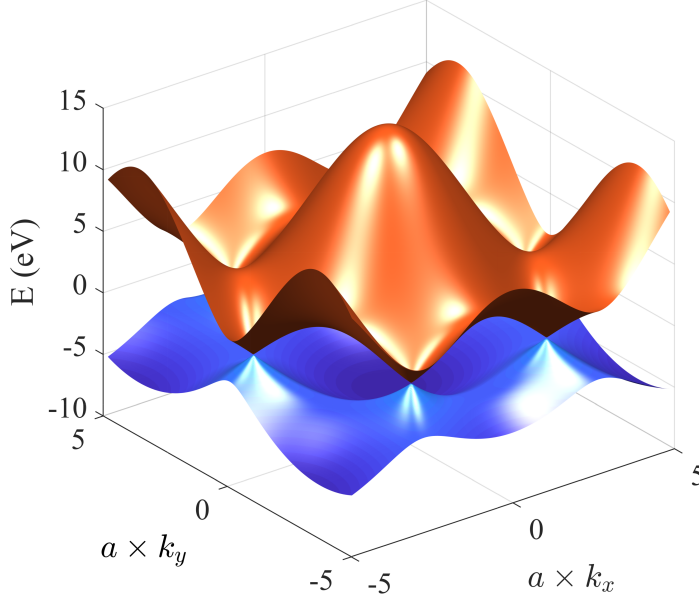


Figure 2.5: The energy band structure of an electron in monolayer graphene, versus $a \times k_x$ and $a \times k_y$, where $a = 2.46 \text{ \AA}$ is the lattice constant, in the vicinity of the first Brillouin zone calculated by using the tight-binding model. The six corners of the first Brillouin zone (see Figure 2.3) are where the conduction band (shaded orange) and the valence band (shaded blue) touch.

Massless chiral electrons in monolayer graphene

In this section, we will study the electronic properties near Dirac points, $K^\pm$ as shown in Figure 2.6. These two points out of six are chosen as they are non-equivalent points. For future reference, we will use an index $\xi = \pm 1$ to specify the K^ξ point in consideration. Note that the K points are often called **valleys** and two non-equivalent K points arise from the lattice geometry of graphene. In [78], it has been shown that

$$f(\mathbf{K}^\xi) = 0. \quad (2.28)$$

This indicates that there are two different sets of Schrödinger equations: one describing the electronic states specified by $\mathbf{K}^+$, the other by $\mathbf{K}^-$.

To approximate the function $f(\mathbf{k})$ near Dirac points, we introduce a wavevector

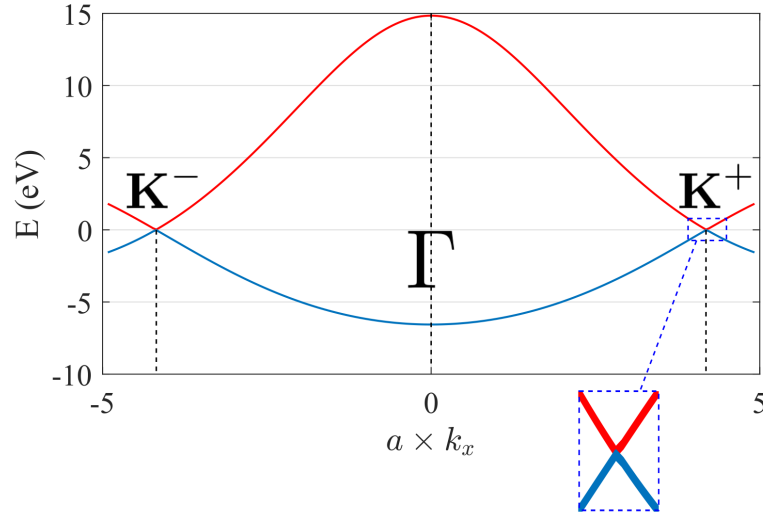


Figure 2.6: Energy dispersion relation, calculated versus k_x , along the $k_y = 0$ plane. The points Γ , K^+ and K^- , which are, respectively, the centre of the Brillouin zone, and the two inequivalent points where the conduction and valence bands meet, are also shown. The inset shows the linear dispersion relation in the vicinity of the Dirac points.

$\mathbf{q}$ that is measured relative to $\mathbf{K}^\xi$,

$$\mathbf{q} = \mathbf{k} - \mathbf{K}^\xi. \quad (2.29)$$

The approximation of the coupling between the A and B sublattices near Dirac points is now given by,

$$f(\mathbf{k}) \approx -\frac{\sqrt{3}a}{2}(\xi q_x - i q_y), \quad (2.30)$$

where $\mathbf{q} = (q_x, q_y)$.

This approximation is only valid for $qa \ll 1$, where $q = |\mathbf{q}|$. It follows that the transfer integral matrix for the energy in the vicinity of point K^ξ may be written as:

$$H^\xi = \hbar v_F \begin{pmatrix} 0 & \xi q_x - i q_y \\ \xi q_x + i q_y & 0 \end{pmatrix}, \quad (2.31)$$

where $v_F = \sqrt{3}a\gamma_0/(2\hbar) \approx 1 \times 10^6 \text{ m s}^{-1}$ is called “Fermi velocity”.

The energy eigenvalues and eigenstates of H^ξ are given by

$$E_\pm = \pm \hbar v_F q, \quad \Psi_\pm = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm \xi e^{i\xi\varphi} \end{pmatrix} e^{i\mathbf{q}\cdot\mathbf{r}}, \quad (2.32)$$

where φ is the polar angle of the wavevector, $\mathbf{q} = q(\cos \varphi, \sin \varphi)$, in the graphene plane and $\pm$ refers to the conduction and valence bands, respectively.

We can see that, for one $\mathbf{q}$ -state, there are four different corresponding wavefunctions reflecting the two-fold valley degeneracy and two energy bands (conduction and valence bands).

Energy density of states

The allowed wavevectors, $\mathbf{k} = (k_x, k_y)$, of a particle in a two-dimensional box of sides L_x and L_y are well-known to satisfy the following conditions:

$$k_x L_x = \pi n_x, \quad \text{and} \quad k_y L_y = \pi n_y, \quad (2.33)$$

where n_x and n_y are integers. This implies that the k-space area taken up by each allowed k-state is $\pi^2/L_x L_y$, and its reciprocal, A/π^2 , determines the density of states in k-space, where $A = L_x L_y$ is the area of the box in real space. The number of k-states $N(k)$, contained in the annulus of a given magnitude of wavevector $|\mathbf{k}|$ and thickness dk , can be calculated by multiplying the k-state density by the area of the annulus:

$$N(k) = 2\pi k \left[\frac{A}{\pi^2} \right] dk. \quad (2.34)$$

For a given energy band, the k-states described above correspond to the states contained in the annulus of radius E and thickness dE :

$$D(E)dE = 2\pi k \left[\frac{A}{\pi^2} \right] dk, \quad (2.35)$$

where $D(E)$ is the energy density of states. Using the linear dispersion relation, $E = \pm \hbar v_F k$, which describes the energy bands near the Dirac point, we then obtain the expression for energy density of states per area A [34]:

$$D_{\text{area}}(E) = \frac{2|E|}{\hbar^2 v_F^2 \pi}. \quad (2.36)$$

It is noted that the expression above does not account for the two-fold valley degeneracy.

Pseudospin and chirality in graphene

In this section, we will investigate the significance of having two components in the energy eigenstates.

In the vicinity of the K_ξ points, the two components of the energy eigenstates give rise to another degree of freedom [78], called “pseudospin”. Since the column vector Ψ (2.4) is the linear superposition of the Bloch functions, each component of Ψ corresponds to the relative probability amplitude of the Bloch function of the A and B sublattices.

A pure Bloch function associated to sublattice A can be thought of as a pseudospin ‘up’ state (pointing upwards out of the graphene sheet), $|\uparrow\rangle = (1, 0)$. In this state, all electrons can only be found on the A sublattice.

On the other hand, the electronic density solely on the B sublattice can be thought of as a pseudospin ‘down’ state (pointing downwards out of the graphene plane), $|\downarrow\rangle = (0, 1)$.

The orientation of the pseudospin is also related to the direction of the electronic wavevector $\mathbf{q}$. This property is called “chirality”. This arises from the

fact that the amplitudes on the A or B sublattice of the eigenstates depend on the polar angle φ .

Using Pauli spin matrices, we can rewrite the effective Hamiltonian (2.31) as

$$H^\xi = \hbar v_F \boldsymbol{\sigma} \cdot \hat{\mathbf{n}}, \quad (2.37)$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is a pseudospin vector and $\hat{\mathbf{n}} = (\xi \cos \varphi, \sin \varphi, 0)$ is a unit vector associated with the direction of $\mathbf{q}$. Note that the pseudospin here is analogous to the Dirac spinor that arises in the massless Dirac equation. The dot product of $\boldsymbol{\sigma}$ and $\hat{\mathbf{n}}$ indicating the link between the directions of the pseudospin and wavevector is called the chiral operator which has ± 1 as its eigenvalues. The expectation value of the pseudospin operator $\langle \boldsymbol{\sigma} \rangle = (\langle \sigma_x \rangle, \langle \sigma_y \rangle, \langle \sigma_z \rangle)$ with respect to the eigenstate $\Psi_\pm$ can be calculated as follows:

$$\begin{aligned} \langle \sigma_x \rangle_\pm &= \langle \Psi_\pm(\varphi) | \sigma_x | \Psi_\pm(\varphi) \rangle, \\ &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & \pm \xi e^{-i\xi\varphi} \end{pmatrix} e^{-i\mathbf{q}\cdot\mathbf{r}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm \xi e^{i\xi\varphi} \end{pmatrix} e^{i\mathbf{q}\cdot\mathbf{r}}, \\ &= \frac{1}{2} \begin{pmatrix} 1 & \pm \xi e^{-i\xi\varphi} \end{pmatrix} \cdot \begin{pmatrix} \pm \xi e^{i\xi(\varphi)} \\ 1 \end{pmatrix}, \\ &= \pm \frac{1}{2} \xi (e^{i\xi\varphi} + e^{-i\xi\varphi}), \\ &= \pm \xi \cos \varphi. \end{aligned} \quad (2.38)$$

The calculations for $\langle \sigma_y \rangle$ and $\langle \sigma_z \rangle$ can proceed in a similar way, yielding $\langle \sigma_y \rangle_\pm = \pm \sin \varphi$ and $\langle \sigma_z \rangle_\pm = 0$. The final result is given by

$$\langle \boldsymbol{\sigma} \rangle_\pm = \pm (\xi \cos \varphi, \sin \varphi, 0), \quad (2.39)$$

where $\pm$ denote the conduction and valence bands, respectively. As $\mathbf{q} = q(\cos \varphi, \sin \varphi, 0)$, we can see that for K^+ point, the pseudospin in the conduction band, $\langle \boldsymbol{\sigma} \rangle_+ = (\cos \varphi, \sin \varphi, 0)$, is parallel to the wavevector $\mathbf{q}$, i.e. the chirality is positive. In contrast to the pseudospin in the conduction band, the pseudospin in the valence band $\langle \boldsymbol{\sigma} \rangle_-$ is anti-parallel to $\mathbf{q}$, i.e. the chirality is negative.

Klein tunnelling

There must be a reason why the degree of freedom arising from the fact that the eigenfunctions have two components is called pseudospin. In fact, there is. Let us consider the probability of a chiral electron scattering in a direction φ , where $\varphi = 0$ defines the forward direction. The probability can be calculated from the overlap of the eigenstates $w(\varphi) = \left| \langle \Psi_{\pm}(\varphi) | \Psi_{\pm}(0) \rangle \right|^2$. Using the effective eigenstates for low energy approximation and considering only the chiral part of the wavefunction, we have $w(\varphi) = \cos^2(\varphi/2)$. This function is anisotropic and, for backscattering, $\varphi = \pi$, this function is zero. This means Dirac-like electrons cannot scatter into a state with opposite momentum because it requires a reversal of pseudospin: But since pseudospin must be conserved, backscattering is forbidden [1] [23]. On the other hand, the probability of scattering into the same momentum state is 1, regardless of the nature of the scattering potential as long as it does not break the symmetry of the A and B sublattices. Note that the interpretation of the wavevector $\mathbf{k}$ in (2.4) is not obvious; however, it is not the momentum that can be interpreted in the same way as in the momentum of free particles and its direction is not necessarily in the same direction of propagation associated with the Fermi velocity v_F .

2.3 Chapter summary

We have outlined the production of graphene and its possible uses. We derived and discussed, mainly, its electronic transport properties. The experimental

results reported in [86] confirm the massless properties of graphene's electrons predicted by the theories. In the next Chapter, we will discuss more on graphene-based field-effect transistors.

Chapter 3

Graphene-based Transistors

3.1 Van der Waals Heterostructures

Van der Waals (vdW) heterostructures are made of multiple layers of two-dimensional materials. They are called vdW heterostructures because each of these 2D layered material is weakly bound to neighbouring layers via vdW forces. The weak vdW interactions found in these materials allow us to isolate or combine these 2D atomic layers to create a wide range of vdW heterostructures with novel properties without the constraints of lattice matching and processing compatibility [42, 66, 71].

What makes vdW heterostructures special, in terms of their applications, is their quantum properties such as: spin and valley dynamics, which can be used in spin-based memories; electron tunnelling between layers [58] for application in tunnelling field-effect transistors [12, 40, 80, 110], resonant tunnelling spectroscopy [106], and optoelectronics [120]; unfamiliar quantum phase transitions [87]. It is possible that vdW heterostructures might yield repulsive Casimir-Polder forces [79].

3.2 The heterostructure of graphene-based resonant tunnelling transistors

The schematic structure of our device is shown in Fig 3.1. The graphene heterostructure is formed by sandwiching a thin layer of hexagonal boron-nitride between two atomically-thin graphene layers [11] [78] [108]. This structure is then mounted to a base made of a thick layer of hBN on top of an oxidised Si substrate of thickness of 300 nm to allow for the visual detection of the graphene flakes [8] [45]. The thickness of the hBN barrier is 1.4 nm throughout this thesis unless stated otherwise. The active tunnelling area, A , is the spatial overlap between the top and bottom graphene electrodes. To form a working electrical circuit with the device, gold contacts are attached to the edge region of the graphene that is not part of the active tunnelling region and conducting wires are connected to allow for voltage controls over the device. A gate voltage, V_g , is applied between the doped silicon wafer and the bottom graphene electrode to change the chemical potential μ_b in the bottom graphene electrode, whilst a bias voltage, V_b , is applied between the bottom and top graphene electrodes to change the Dirac points of both electrodes. Another voltage, V_t , can be applied to fine-tune the chemical potential μ_t in the top graphene electrode.

3.3 Modelling

3.3.1 Derivation of tunnelling current

We will be looking into the tunnelling process of electrons in a structure comprising a hexagonal boron nitride sheet sandwiched between two monolayer-graphene sheets.

The Bardeen-transfer-Hamiltonian approach will be adopted to find the ex-

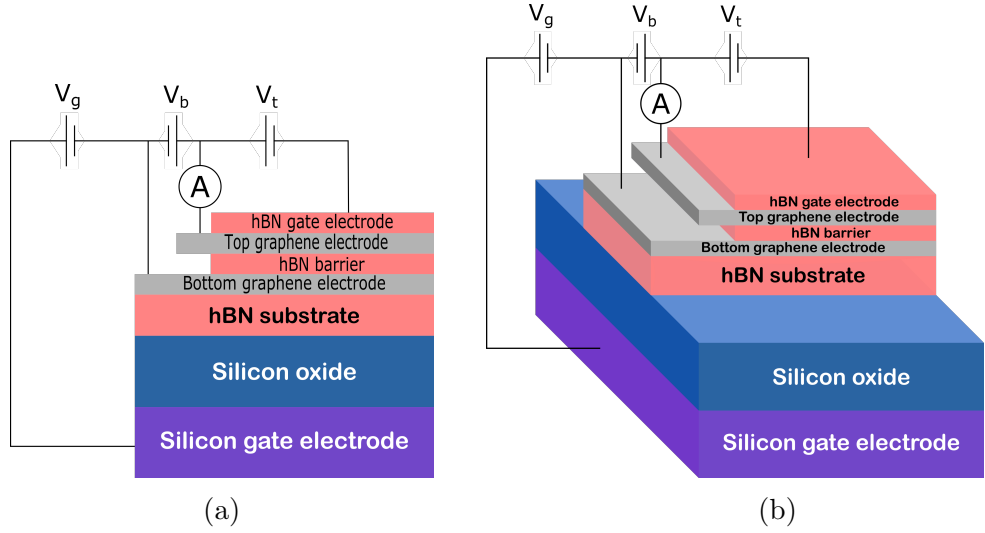


Figure 3.1: (a) The side view and (b) 3D view of the schematic structure of our device. The graphene heterostructure is formed by sandwiching a thin layer of hexagonal boron-nitride between two atomically-thin graphene layers. The thickness of the hBN layer between the bottom and top graphene electrodes is 1.4 nm throughout this thesis unless stated otherwise. A bias voltage V_b can be applied to allow electrons to tunnel between the two graphene layers.

pression of the tunnelling current in our device (see Figure 3.1b) [6]. Along with the Fermi's golden rule, the tunnelling current through the barrier is given by [31, 36, 119]

$$I = g_S g_V e \sum_{\mathbf{k}_B, \mathbf{k}_T} \frac{1}{\tau_{B \rightarrow T}} f_B(E_B) [1 - f_T(E_T)] - \frac{1}{\tau_{T \rightarrow B}} f_T(E_T) [1 - f_B(E_B)], \quad (3.1)$$

where $g_S = 2$ is the spin degeneracy and $g_V = 2$ is the valley degeneracy. Here, the labels B and T denote the bottom and top electrodes, respectively. $\frac{1}{\tau_{B \rightarrow T}}$ and $\frac{1}{\tau_{T \rightarrow B}}$ are the tunnelling rates for electrons tunnelling from the bottom to top electrodes and from the top to bottom electrodes, respectively. The function $f(E) = [1 + e^{(E - \mu)/k_B T}]^{-1}$ is the Fermi occupation factor; $E_{B,T} = s_{B,T} \hbar v_F k_{B,T}$, where $s_{B,T} = 1(-1)$ for electrons in conduction (valence) band, is the energy in consideration measured with respect to its corresponding Dirac points; $\mu_{B,T}$ are the chemical potentials in each electrode, and T and k_B are the temperature of the device and the Boltzmann constant, respectively.

In order to get the total tunnelling current, all states described by different wavefunctions accounting for different spins and valleys within the first Brillouin zone must be considered. To prevent over-counting, in 3.1, only one of the two valleys, $K^\pm$, is considered; the summation is over all $\mathbf{k}$ -states specified by the in-plane wavevector $\mathbf{k}_{B,T}$ measured relative to the chosen nearest Dirac point specified by $\mathbf{K}_{B,T}^\pm$. The tunnelling rates are given by [35]

$$\frac{1}{\tau_{B \rightarrow T}} = \frac{2\pi}{\hbar} |M_{BT}|^2 \delta(E_B - E_T) = \frac{1}{\tau_{T \rightarrow B}}, \quad (3.2)$$

where

$$M_{BT} = \frac{\hbar^2}{2m} \int dS \left(\Psi_B^* \frac{d\Psi_T}{dz} - \Psi_T \frac{d\Psi_B^*}{dz} \right) \quad (3.3)$$

is the matrix element for the transition between electrodes with m being the free electron mass, and $\Psi_B(\mathbf{r}, z)$ and $\Psi_T(\mathbf{r}, z)$ are the energy eigenfunctions in the bottom and top electrodes, respectively, and $\mathbf{r}$ and z are the in-plane position vector and the coordinate in the tunnelling direction normal to the graphene plane, respectively. The surface integral in Equation (3.4) is evaluated over a flat surface located half way between the bottom and top graphene layers. Equivalently, the matrix element may be expressed as

$$M_{BT} = \int dV \left(\Psi_T^*(\mathbf{r}, z) V_S(\mathbf{r}, z) \Psi_B(\mathbf{r}, z) \right), \quad (3.4)$$

where $V_S(\mathbf{r}, z)$ is the scattering potential that provides momentum change for tunnelling between the states with different in-plane wavevectors. Here, the volume integral is evaluated over the volume of the barrier between the electrodes. The current thus becomes

$$I = g_S g_V \frac{2\pi e}{\hbar} \sum_{\mathbf{k}_B, \mathbf{k}_T} |M_{BT}|^2 \left[f_B(E_B) - f_T(E_T) \right] \delta(E_B - E_T). \quad (3.5)$$

The tight-binding model may be applied here. For graphene, there are two

identical atoms, labelled α and β , per unit cell constituting two basis functions, $\Phi_{\alpha,\mathbf{k}}$ and $\Phi_{\beta,\mathbf{k}}$, for a given $\mathbf{k}$. For a state specified by wavevector $\mathbf{k}$, the wavefunction can be written in terms of the aforementioned basis functions as

$$\Psi_{\mathbf{k}}(\mathbf{r}, z) = \chi_{\alpha}\Phi_{\alpha,\mathbf{k}}(\mathbf{r}, z) + \chi_{\beta}\Phi_{\beta,\mathbf{k}}(\mathbf{r}, z), \quad (3.6)$$

where $\Phi_{j,\mathbf{k}}$ is of the Bloch form:

$$\Phi_{j,\mathbf{k}}(\mathbf{r}, z) = \frac{1}{\sqrt{A}}\exp(i\mathbf{k} \cdot \mathbf{r})\phi_{j,\mathbf{k}}(\mathbf{r}, z). \quad (3.7)$$

Here, $\phi_{j,\mathbf{k}}(\mathbf{r}, z)$ is the cell-periodic part of the Bloch function in graphene and A is the effective tunnelling area—that is, theoretically, the overlapping area of the two graphene sheets. As the name of the model suggests, these periodic functions are localised around the basis atoms of each graphene electrode. However, in the plane located half way between the two electrodes, these functions spread out. From this fact, we can further assume that the cell-periodic parts are separable into the radial-dependent functions and z -dependent functions. This allows us to approximate the radial-dependence of the tunnelling matrix element into numerical constants and to assume, for the z -dependence, the usual decaying form $2\kappa e^{-\kappa b}/D$, where b is the separation between the electrodes and κ is the decay constant of the wavefunctions in the barrier and D is a normalisation constant comparable to the inter-planar separation in graphite.

The coefficients, χ_{α} and χ_{β} , have appeared previously when we discussed the electronic properties of monolayer graphene. As a reminder, they are given by

$$\begin{bmatrix} \chi_{\alpha} \\ \chi_{\beta} \end{bmatrix} = \begin{bmatrix} 1 \\ s\xi e^{i\xi\varphi} \end{bmatrix}, \quad (3.8)$$

where $s = +1$ is taken for the electrons in the conduction band, $s = -1$ for the valence band, $\xi = +1$ for K^+ valley, $\xi = -1$ for K^- valley and φ is the

polar angle of the wavevector is the graphene plane.

The transfer integral matrix elements can now be calculated component by component; they are given here without showing the calculating steps as [35]

$$M_{BT} = \frac{\hbar^2 \kappa}{mAD} e^{-\kappa b} g_\theta(\varphi_B, \varphi_T) \int dS e^{\mathbf{\Delta K} \cdot \mathbf{r}} e^{i(\mathbf{k}_T - \mathbf{k}_B) \cdot \mathbf{r}}, \quad (3.9)$$

where

$$g_\theta(\varphi_B, \varphi_T) = \gamma(\theta) \left[(1 + s_B s_T \xi_B \xi_T e^{i(\xi_T \varphi_T - \xi_B \varphi_B)}) + (s_T \xi_T e^{i\xi_T \varphi_T} + s_B \xi_B e^{-i\xi_B \varphi_B}) \right]. \quad (3.10)$$

Here, $\mathbf{\Delta K}$ is the relative displacement in $\mathbf{k}$ -space (see Figure 3.5) associated with the polar rotation, θ , of the two graphene layers such that the wavevector of an electron in the top layer measured relative to the Dirac point of the bottom layer is $\mathbf{k}_T + \mathbf{\Delta K}$. The spatial overlap, $\gamma(\theta)$, of the cell-periodic part of the Bloch states in the xy plane is evaluated over the area of all unit cells, S , and may be expressed as

$$\gamma(\theta) = \frac{1}{dS_C} \int_S dS \phi_T^*(\mathbf{r}) \phi_B(\mathbf{r}), \quad (3.11)$$

where dS_C is the area of a unit cell and ϕ_T takes the same form as ϕ_B but rotated by θ in spatial space relative to ϕ_B . This function was calculated by in [40] and it is shown graphically in Figure 3.2.

We can also derive the matrix element using the scattering potential method [11] which is equivalent to the Bardeen transfer Hamiltonian method. For the scattering potential method, the matrix element is given by

$$M_{BT} = \frac{\hbar^2 \kappa}{mAD} e^{-\kappa b} g_\theta(\varphi_B, \varphi_T) V_S(\mathbf{q}), \quad (3.12)$$

where $V_S(\mathbf{q}) = V_0/(q^2 + q_c^2)$ is the a scattering potential with V_0 and q_c to be determined to fit the experimental data. Throughout this thesis, the calcula-

tions related to the tunnelling current of the graphene-based devices are based on this method and the expression of the tunnelling current for computational purposes is as follows:

$$I = \int_E C(E) dE, \quad (3.13)$$

where E are electron energies between the chemical potentials of the bottom and top graphene electrodes. Here, $C(E) = dI/dE$ is a current contribution distribution defined as a function of electron energy as follows:

$$\left. \frac{dI}{dE} \right|_E = \int_{\varphi_B} \int_{\varphi_T} |M_{BT}|^2 d\varphi_B d\varphi_T \left[f_B(E_B) - f_T(E_T) \right] D(E_B) D(E_T), \quad (3.14)$$

where the function is evaluated at an energy E , which can be set to equal E_B if the bottom Dirac cone is chosen as a reference point and $D_{\text{area}}(E)$ is the energy density of states as given in Equation (2.36). Note that the current contribution distribution is a key quantity for analysing tunnelling currents.

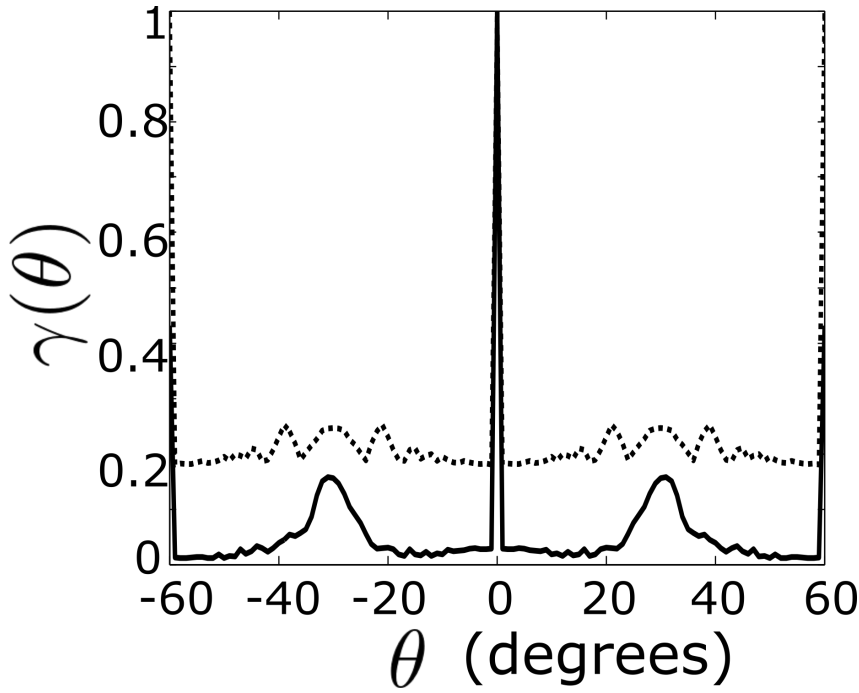


Figure 3.2: The spatial overlap, $\gamma(\theta)$, of the normalised cell-periodic part of the Bloch states. The solid curve is the exact calculation by density functional theory by [40], whereas the dashed curve is the approximation based on the assumption that the cell-periodic part of the Bloch states is of the Gaussian form.

3.4 Electrostatics of the graphene-hBN-graphene devices

We can study the electrostatics of the device by considering the diagram shown in Figure 3.3. There are three voltages that can be applied to the device: a bottom gate voltage, V_g , can be applied across the silicon oxide substrate and the bottom graphene electrode, a bias voltage, V_b , across the two graphene electrodes, and a top gate voltage, V_t , across the top graphene electrode and hBN substrate attached on top of the top graphene electrode. The function of these voltages is to increase or decrease the area charge carrier densities, n_B and n_T , in the bottom and top graphene sheets, respectively. Unlike an ordinary perfect conducting plate, the density of states close to the Dirac point is low in monolayer graphene resulting in weak electric field screening [75]. Therefore,

when the bottom gate voltage, V_g , is applied, an electric field, F_g , not only is induced between the silicon oxide substrate and the bottom graphene sheet but also penetrates through the bottom graphene sheet shifting the chemical potential of the bottom graphene electrode and, at the same time, the Dirac point of the top graphene electrode. The top gate voltage, V_t , works in a similar manner to V_g . The applied voltage, V_b , is the most important among the three in the sense that it governs the chemical potential difference between the two graphene electrodes which determines the magnitude of the tunnelling current of the device.

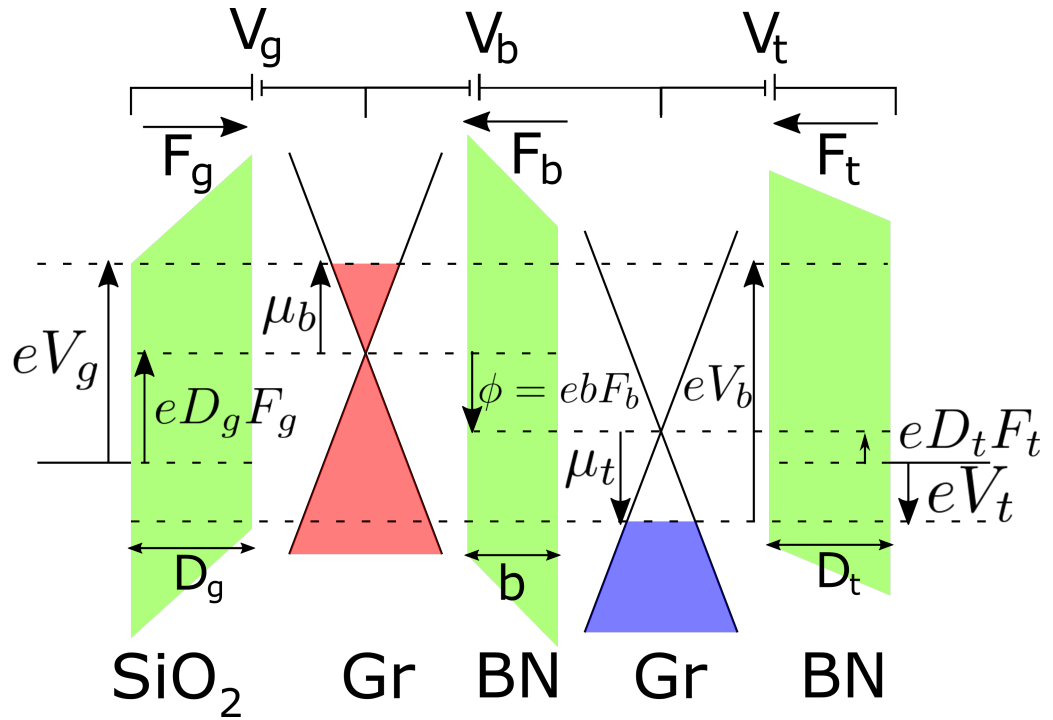


Figure 3.3: Electrostatic diagram of the device, showing the energy differences due to 3 applied voltages, V_g , V_b , V_t , and the band diagrams of graphene. The filled states of the bottom(top) electrode is shaded red(blue). The thickness of the hBN barrier sandwiched between the two electrodes is b .

According to Gauss's law, the relationship between an electric field density, $\mathbf{F}$ and charge density, ρ , is:

$$\oint \mathbf{F} \cdot d\mathbf{A} = \frac{\rho}{\epsilon_0 \epsilon_r} = \frac{ne}{\epsilon_0 \epsilon_r}, \quad (3.15)$$

where n is the number of charges per unit area and is defined to be positive

for holes and negative for electrons, e is the elementary electric charge, ϵ_0 is the permittivity of free space and ϵ_r is the relative permittivity of the medium the electric field permeates.

It is easy to see that

$$\epsilon_{BN}F_b - \epsilon_{Si}F_g = en_b, \quad (3.16)$$

and

$$\epsilon_{BN}F_t - \epsilon_{BN}F_b = en_t. \quad (3.17)$$

We can also deduce from the diagram in Figure 3.3 that

$$eV_b = \mu_b(n_b) - \mu_t(n_t) - ebF_b. \quad (3.18)$$

Here, $\epsilon_{BN} = 3.25$ is the relative permittivity of hBN, and $\epsilon_{Si} = 3.9$ is the relative permittivity of the silicon oxide substrate and b is the thickness of the hBN barrier. From the diagram, F_g is positive, while F_b and F_t are negative. For energies within the linear dispersion regime of graphene, the Fermi level (the chemical potential) in the two electrodes is defined as:

$$\mu(n) = -\text{sgn}(n)\sqrt{\pi|n|\hbar^2v_F^2}, \quad (3.19)$$

where $\text{sgn}(n) = +1$ for $n > 0$ and -1 for $n < 0$. Solving (3.16), (3.17), (3.18), and 3.19 simultaneously yields the quantities we are interested such as μ_b and μ_t .

3.5 DC characteristics of the graphene-hBN-graphene devices

In this section, we will give a review of the general behaviour of the current-bias voltage curves of our graphene-hBN-graphene devices and investigate how the device parameters affect the magnitude and shape of the $I(V_b)$ characteristics

and which parameters control the key features.

3.5.1 Rotationally aligned graphene electrodes

In this section, we will explore what happens when we vary the bias voltage applied to the device in which the two graphene electrodes are rotationally aligned.

As a starting point, we will investigate the $I(V_b)$ characteristics for the $V_g = 0$ case at the temperature of 2 K (see Figure 3.4).

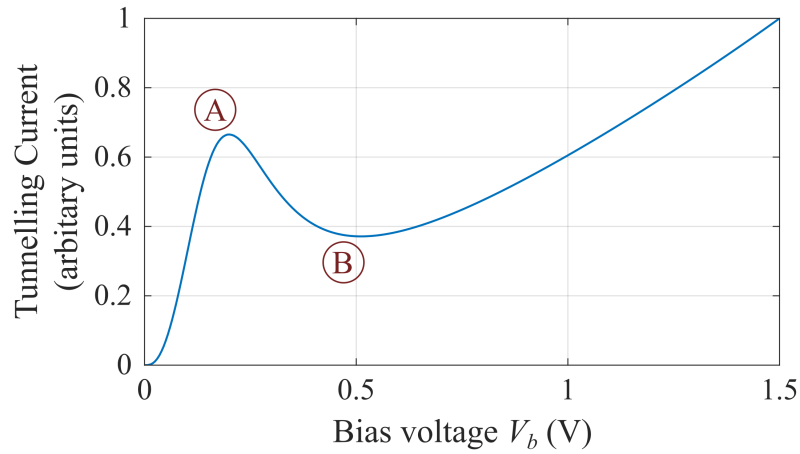


Figure 3.4: The $I(V_b)$ curve of the graphene-based transistor. The two graphene layers are aligned and the gate voltage is 0 V. Temperature is 2 K.

When $V_b = 0$, the chemical potentials in both graphene electrodes are equal and the Dirac cones are neutrally aligned, therefore, the tunnelling current is zero. As the bias voltage is increased up to a certain value (labelled A in Figure 3.4), the tunnel increases and reaches its peak. Thus, the characteristics of the device over the range of bias voltage up to the peak A can be thought of, although not in a strict manner, as those of Ohmic resistors.

After a particular V_b which gives rise to the peak of the tunnelling current, the tunnelling current decreases as the bias voltage is increased. The tunnelling current keeps decreasing until it reaches a certain value (labelled B in Figure 3.4) then it rises again.

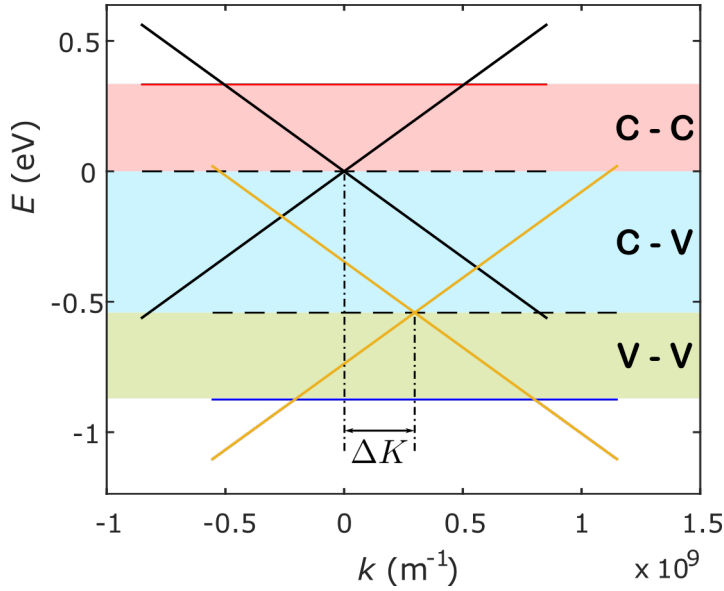


Figure 3.5: Simplified E-k dispersion diagram for the purpose of future reference. The Dirac cone for the bottom graphene electrode is drawn by solid black lines with a black dashed line drawn at the corresponding intersection as its energy neutral level. The Dirac cone for the top graphene electrode is drawn by solid yellow lines with a black dashed line drawn at the corresponding intersection as its energy neutral level. The red(blue) line indicates the chemical potential of the bottom(top) layer. The region shaded pink indicates the tunnelling between conduction bands (denoted by C-C). The region shaded blue indicates the tunnelling between a conduction band and a valence band (denoted by C-V). And the region shaded green indicates the tunnelling between valence bands (denoted by V-V). The centres of the two Dirac cones are misplaced by ΔK with respect to each other in the horizontal axis due to a rotational misalignment of the graphene flakes in real space.

Three different regimes of tunnelling may be distinguished as shown in Figure 3.5: tunnelling between states in one conduction band and states in another conduction band (C-C), tunnelling between states in a conduction band and states in a valence band (C-V), tunnelling between states in one valence band and states in another valence band (V-V).

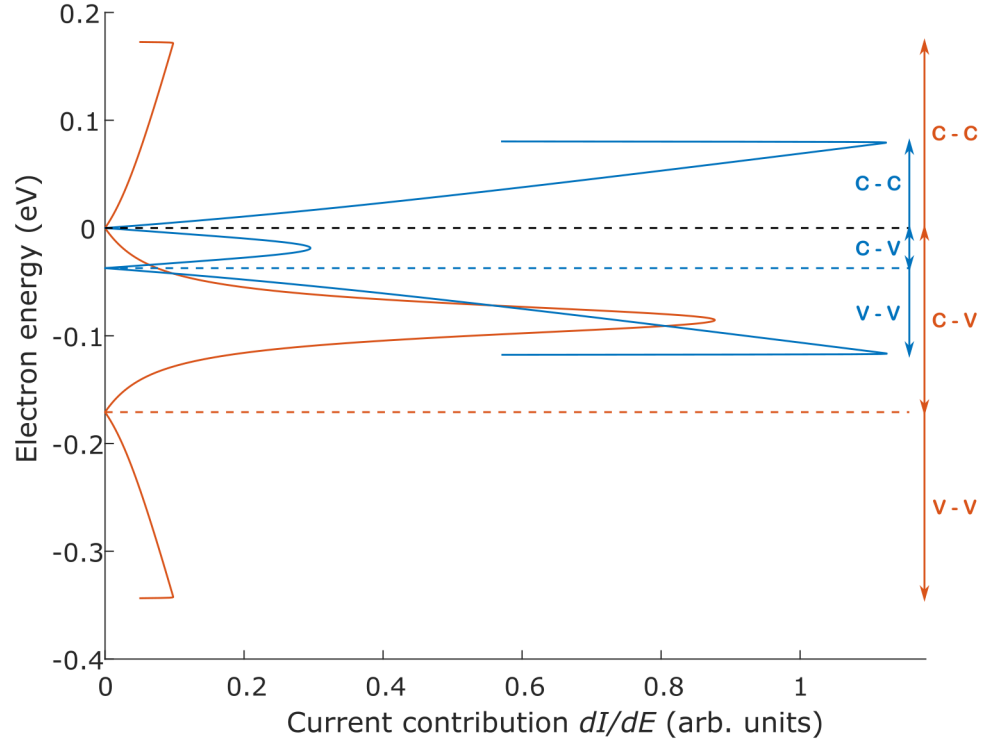


Figure 3.6: Current contribution dI/dE as a function of electron energy E on the vertical axis. The area under the curve is the tunnelling current at a particular V_b . The blue (orange) curve is the current contribution distribution at the $I(V_b)$ curve peak (trough) (point A (B)) as depicted in Figure 3.4). Black, orange and blue dashed lines indicate the Dirac points separating three different regimes of electron tunnelling (see Figure 3.5). We can see that the like band tunnellings are weaker when the tunnelling current reaches its trough. This is because elastic scattering process cannot provide large enough momentum change for tunnelling. While the tunnelling between unlike bands become bigger due to the increase in size of the energy range, hence the increase in the density of states.

We can now look into a plot of a quantity, dI/dE , versus E in which the area enclosed by the curve and the y -axis is the tunnelling current (see Figure 3.6). The blue curve is the dI/dE variation associated with the current peak, labelled A in Figure 3.4. The top end indicates the chemical potential of the bottom graphene electrode, while the bottom end indicates the chemical potential of the top graphene electrode. The zero on the energy E -axis (indicated by the black dashed line) marks the Dirac point of the bottom $E-k$ cone. From the top end to the zero of the electron energy is the region of C-C tunnelling. The bell-shaped curve in the middle is the region of C-V tunnelling

and the last region is the V-V tunnelling which starts from the Dirac point of the top cone (indicated by the blue dashed line) to the bottom end of the blue curve. The orange curve is the dI/dE plot associated with the trough of the tunnelling current (point B) and a similar description as that of a blue curve is implied.

It can be seen that, for the peak of the tunnelling current, the main contribution comes from the like band tunnellings, whereas for the trough of the tunnelling current, the contribution from the C-V tunnelling dominates. Since the density of states of monolayer graphene is proportional to the electron energy, having a large contribution from the like band tunnelling should yield a high tunnelling current.

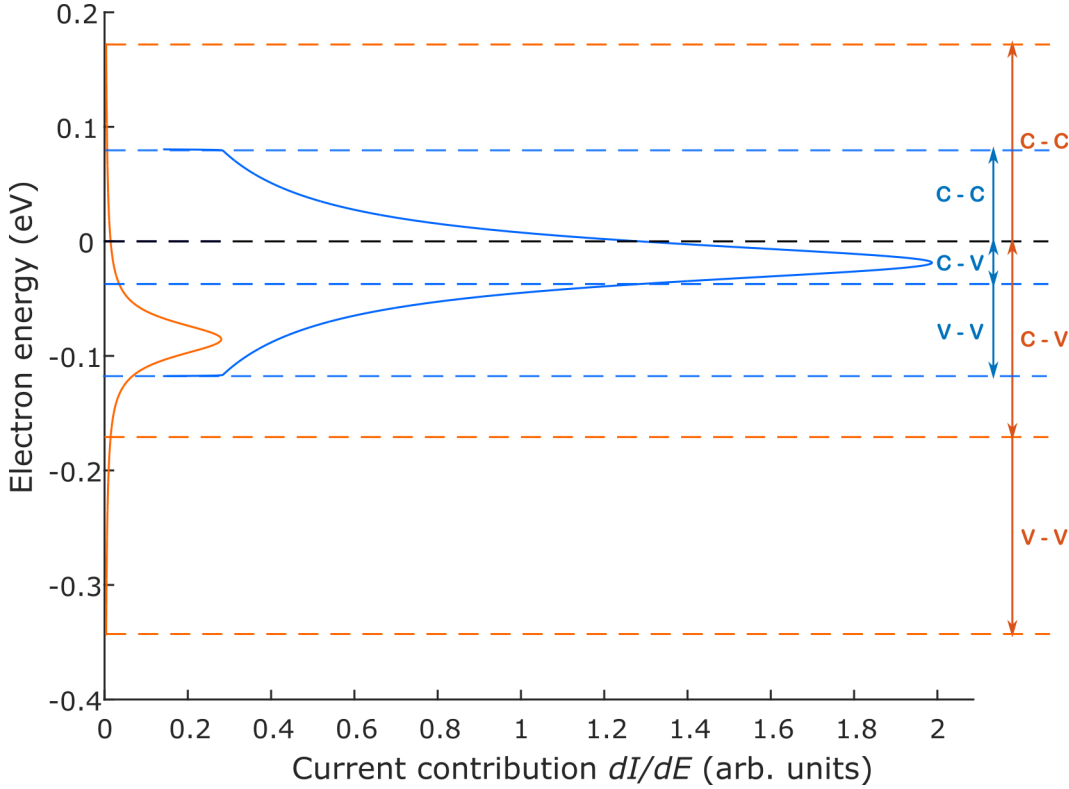


Figure 3.7: The diagram shows the current contribution dI/dE in which the density of states is set to unity in order to make a comparison with the diagram in Figure 3.6. The blue(orange) curve is the current contribution distribution at the peak(trough) (point A(B) as depicted in Figure 3.4). Due to the linear relation of the density of states of monolayer graphene to electron energy, like band tunnellings are affected greatly by the presence of such feature.

We can see how the density of states affect the shapes of the dI/dE curves in

Figure 3.7. Even with the effect of the density of states taken out, i.e. density of states is set to unity, the orange curve is flatter than the blue curve, hence the smaller area under the curve. The only factor that can determine when the tunnelling current reaches its peak or trough after we remove the effect of the density of states is the conservation of momentum which gives rise to the resonant tunnelling condition. At some point, the momentum mismatch between two electronic states is favourably compensated by the momentum provided by the scattering potential allowing for resonant tunnelling in the elastic scattering regime. Mathematically, the resonant tunnelling condition involves two quantities: ebF_b and $\hbar v_F q_c$. Interestingly, the sharp current peak of the blue curve, in Figure 3.7, which occurs due to the fact that the resonant tunnelling condition is satisfied, is lowered greatly owing to the very low density of states near the Dirac point as shown in Figure 3.6. Thus, it is safe to say that the Dirac-like behaviour of electrons in monolayer graphene plays an important role in charge transport through the device.

3.6 Small misalignment in graphene electrodes

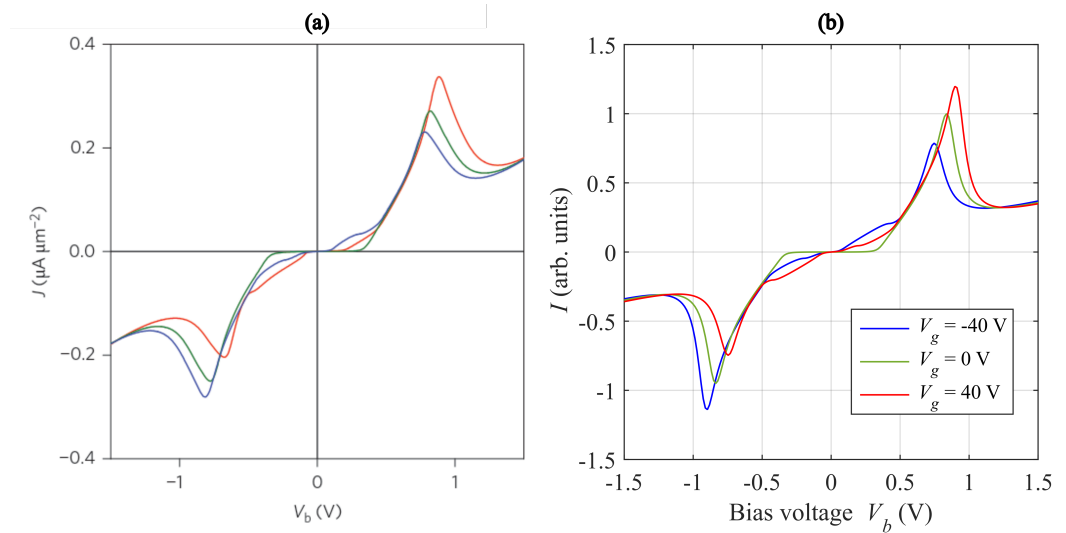


Figure 3.8: Comparison of current-bias voltage characteristics: (a) experimental measurement, adapted from [80] and (b) theoretical simulations, at three different values of V_g : 40 V (red), 0 V (green), -40 V (blue). Device characteristics: temperature 2 K, hBN barrier thickness 1.4 nm, $\theta \approx 1.8^\circ$, $q_c^{-1} = 15$ nm.

In the device fabrication process, aligning two graphene flakes perfectly is difficult [93]. Consequently, it is worth investigating the $I(V_b)$ characteristics of devices with very small rotational misalignment, i.e. $\theta < 2^\circ$. It is apparent that the effect of a rotational misalignment in real space in two graphene flakes is equivalent to a rotational misalignment in $\mathbf{k}$ -space, hence the shift of the $E - k$ cones. Figure 3.8 shows $I(V_b)$ curves obtained in (a) the experiment reported in [80] and (b) via my theoretical simulations, for three different values of bottom gate voltages, V_g . Here, the red curve is for $V_g = 40$ V, the green curve is for $V_g = 0$ V, and the blue curve is for -40 V. Starting from the $I(V_b)$ curve, for 0 V, the curve is symmetric as expected but, in contrast with the $I(V_b)$ curve of the aligned device, there is a fairly big flat region in which the tunnelling current is zero or close to zero. This region exists because the momentum change provided by the scattering potential is not enough to allow any elastic scattering. Beyond this region, the general characteristics follow those of aligned devices. As for the red and blue curves, the chemical potentials of the two graphene layers are not zero when the bias voltage is zero. Compared with the green curve, the peaks of the red and blue ones are higher and the regions of zero tunnelling current are smaller. The positions of the peaks for $V_g \neq 0$ also shift with respect to that for $V_g = 0$. Generally, the theoretical simulations agree well with the experimental measurements.

3.6.1 Discussion of the tunnelling process

A part of the $I(V_b)$ curve for $V_g = 0$ in Figure 3.8 is plotted as the solid black curve in Figure 3.9 for 0.6 V $< V_b < 1.0$ V. Here, we pay particular attention to the three types of tunnelling as a function of V_b . At low bias voltage, the contributions from C-C and V-V tunnellings (see red and blue curves) dominate. This is expected because the two Dirac cones are also most energetically aligned leaving only a small region of C-V tunnelling (expressed by a green curve in Figure 3.9). Figure 3.10(a) shows the band diagram for

the event in which the blue and red curves reach their peaks. The sides of the two Dirac cones do not touch and the reason for this is not apparent by just looking at the band diagram. However, we can see that the trend of the like band tunnellings follow the characteristics of the scattering potential function, $V_S(\mathbf{q})$. This function takes into account all the differences of the wave vectors among all pairs of states related to tunnelling. Thus, we can conclude that the scattering length scale, q_c , influences like band tunnellings more than unlike band tunnellings. In comparison with the peaks of the current from like band tunnellings, the total current reaches its peak at higher bias voltage. The sides of the two Dirac cones shown in Figure 3.10(b) get closer but still do not touch. At this particular value of V_b , the contribution from unlike band tunnelling starts to show its significance (see green curve in Figure 3.11). This must be due to the increase in the states available for C-V tunnelling and the reduction in the separation of initial and final states in $\mathbf{k}$ -space. It is surprising that when the two Dirac cones tangentially touch (see Figure 3.10(c)), the tunnelling current is slightly lower than its peak, as indicated by a black dash-dotted line in Figure 3.9. The effect of the conservation of momentum on the $I(V_b)$ curves is more complicated than the band diagram shows. However, by setting other terms except $V_S(\mathbf{q})$ in the tunnelling matrix element, M_{BT} as given in (3.12), to unity to focus on the effect of the momentum mismatch, the plot of this modified tunnelling current can tell us why the current drops slightly; elastic scattering for like band tunnellings is less favourable (see the solid orange curve in Figure 3.9). All in all, it can be said that the characteristics of the tunnelling current are determined in a complicated manner mainly by the competition between the density of states and the conservation of momentum.

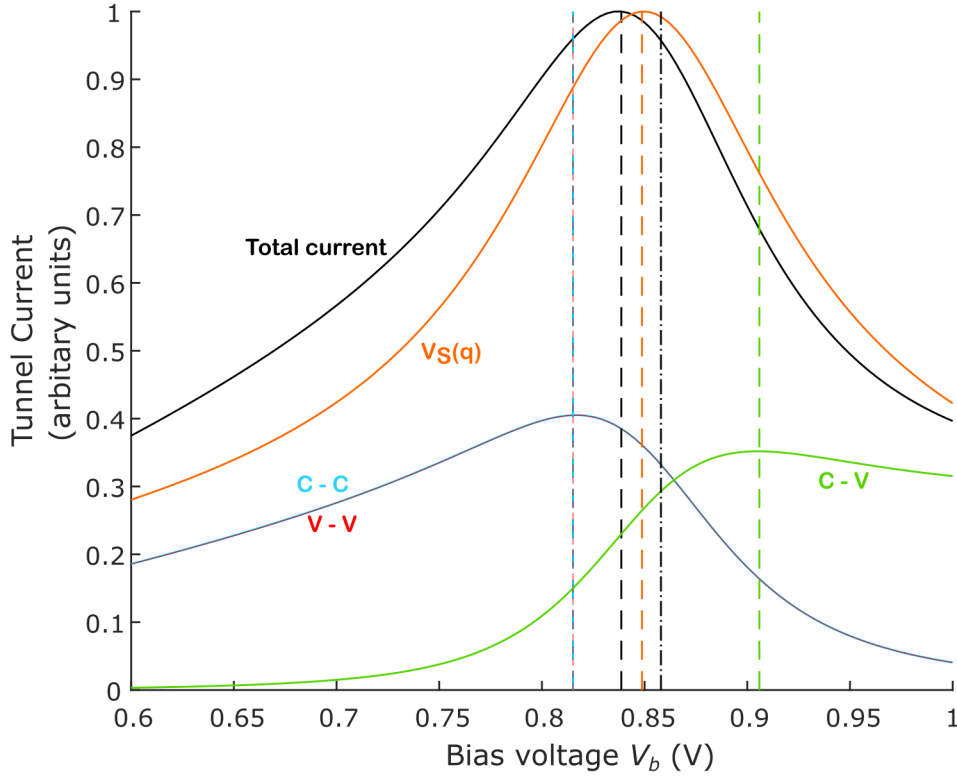


Figure 3.9: Tunnelling current contribution plots: solid black curve is the tunnelling current; solid red, green and blue curves, normalised to the maximum value of the black curve, are the current contributions from tunnelling between valence and valence bands (V-V), conduction and valence bands (C-V), conduction and conduction bands (C-C); solid orange curve is the plot of the normalised scattering potential term solely, $V_S(\mathbf{q})$. Dashed lines indicate the peaks of the curves of corresponding colours. Black dash-dotted line indicates the value of V_b at which the two cones tangentially touch (see Figure 3.10c). Before the current peak, C-V tunnelling barely contributes to the total current. However, the C-V contribution increases sharply near the resonant condition. Device characteristics: $V_g = 0$ V, temperature 2 K, hBN barrier thickness 1.4 nm, $\theta \approx 1.8^\circ$, $q_c^{-1} = 15$ nm.

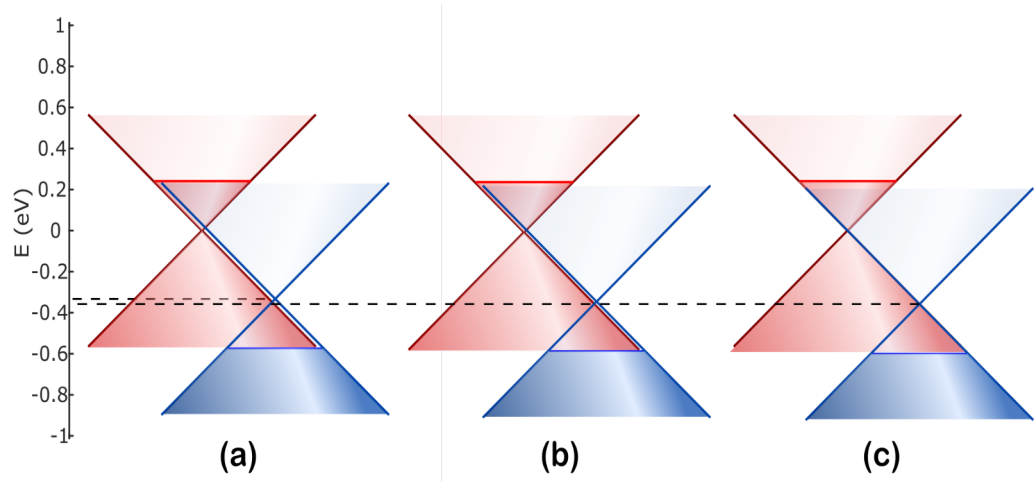


Figure 3.10: Band diagrams depicting (a) an event in which the like-band tunnelling reaches its peak as shown in Figure 3.9 as red and blue curves. The sides of the two cones do not touch yet; (b) an event in which the tunnelling current reaches its peak shown in Figure 3.9. The sides of the two cones almost touch. The contribution from the C-V tunnelling has increased drastically due to the increase in the number of electronic states between the Dirac points of the bottom and top layers; (c) an event in which the two cones tangentially touch as indicated by the black dash-dotted line in Figure 3.9. The tunnelling current drops since the scattering potential cannot well provide a large $\mathbf{k}$ change for the transitions between like bands;

Red and blue cones, with their corresponding chemical potential shown as red and blue horizontal lines, represent the band diagrams for the bottom and top layers, respectively. Black dashed lines show the levels of the Dirac points of the top cones.

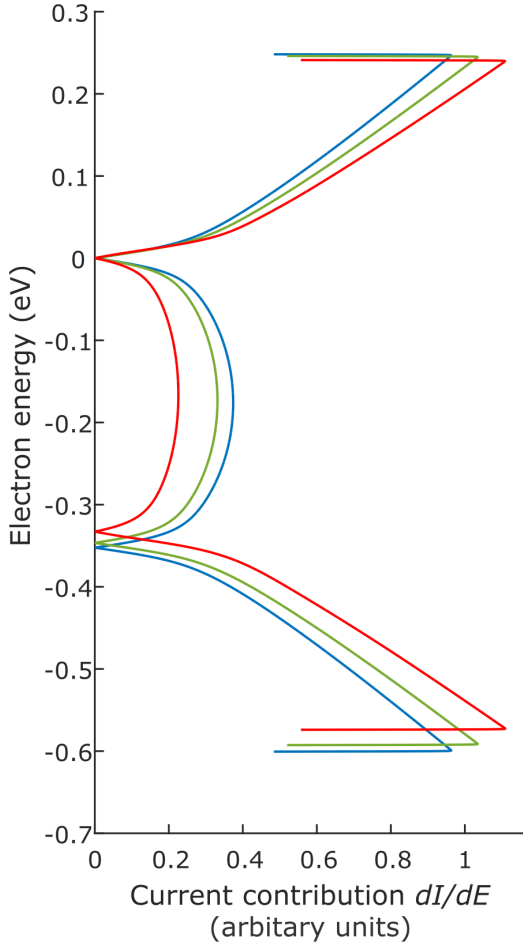


Figure 3.11

Current contribution distribution as a function of electron energy with respect to the neutral point of the bottom cone for three different V_b : red curve for the event, in which the like band tunnelling reaches their maximum, as depicted in Figure 3.10(a), green curve for the event, in which the total tunnelling current is at its peak, as depicted in Figure 3.10(b), and blue curve for the event, in which the scattering potential term, $V_s(\mathbf{q})$, reaches its maximum, as depicted in Figure 3.10(c). The total area under each of these curves with respect to the energy E -axis yields the tunnelling current at the corresponding V_b . The values of the curves are normalised with respect to the highest value among them.

Chapter 4

Variation of tunnelling current with Barrier Thickness and Temperature

4.1 Investigation on the effect of the barrier thickness

In our model, there are two places that are affected by the barrier thickness, b : the first one is the electrostatics of the device and the other is the component of the electron wavefunction in the tunnelling direction. In this chapter, we will investigate how these quantities which contain the information of the barrier thickness affects the $I(V_b)$ characteristics.

The decay term of the wavefunction in the tunnelling direction given in (3.9) is of exponential form which will affect the magnitude of the tunnelling current greatly when the barrier thickness changes. As we can see that the exponent is negative, the tunnelling current is expected to increase as the barrier thickness decreases (see Figure 4.1).

It is obvious from basic electrostatics that for a given applied bias voltage, devices with a thinner barrier will have a higher capacitance; the device holds more charge, hence more available states are occupied. This should result in higher tunnelling rate.

From Figure 4.2, we can see that the electrostatic energy difference $\phi_b = ebF_b$ increases more slowly with increasing bias voltage as the barrier thickness goes down. The black dashed line in the figure is the value of $\hbar v_F q_c$, indicating the energy associated with the elastic scattering processes due to the disorder potential in the device system or the nature of the interaction of graphene electrons with impurities in the layers; this energy is associated with the scattering length scale in the scattering potential term, $V_S(\mathbf{q})$, which is chosen to match experimental data [40].

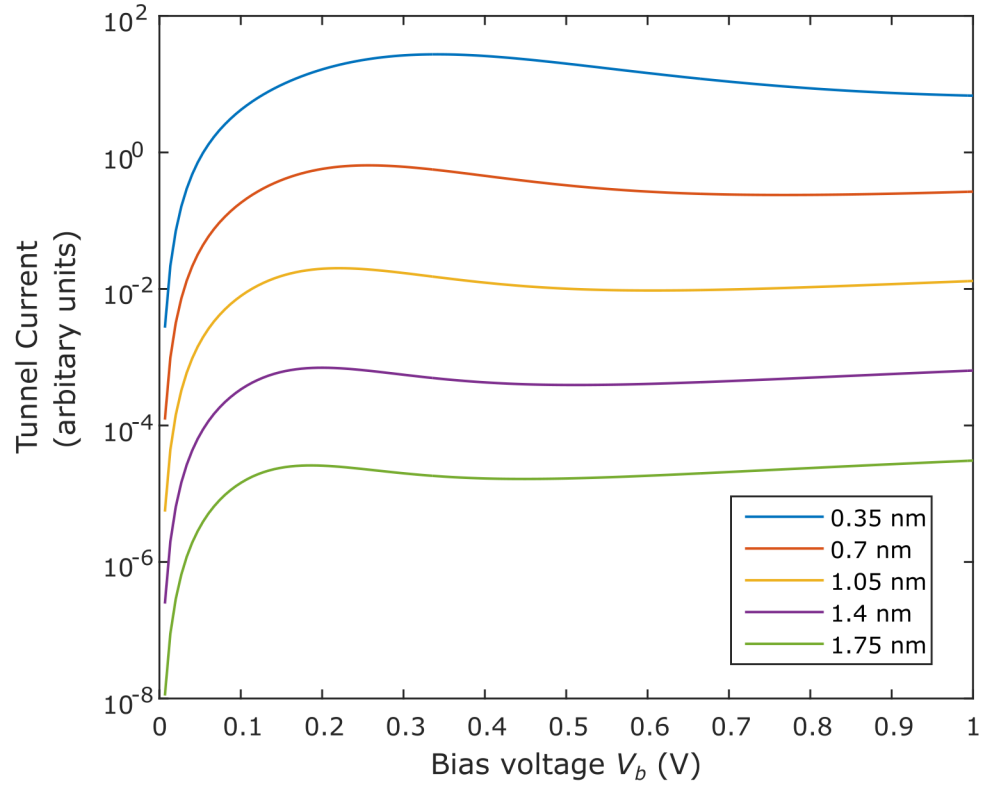


Figure 4.1: $I(V_b)$ curves plotted for five different values of barrier thickness: 0.35 nm, 0.7 nm, 1.05 nm, 1.4 nm, and 1.75 nm. The current axis is on a logarithmic scale, while the bias voltage axis is linear. The magnitude of the current increases as the barrier thickness increases because of an increasing capacitance and an increase in the overlap of the electron wavefunctions in the tunnelling direction.

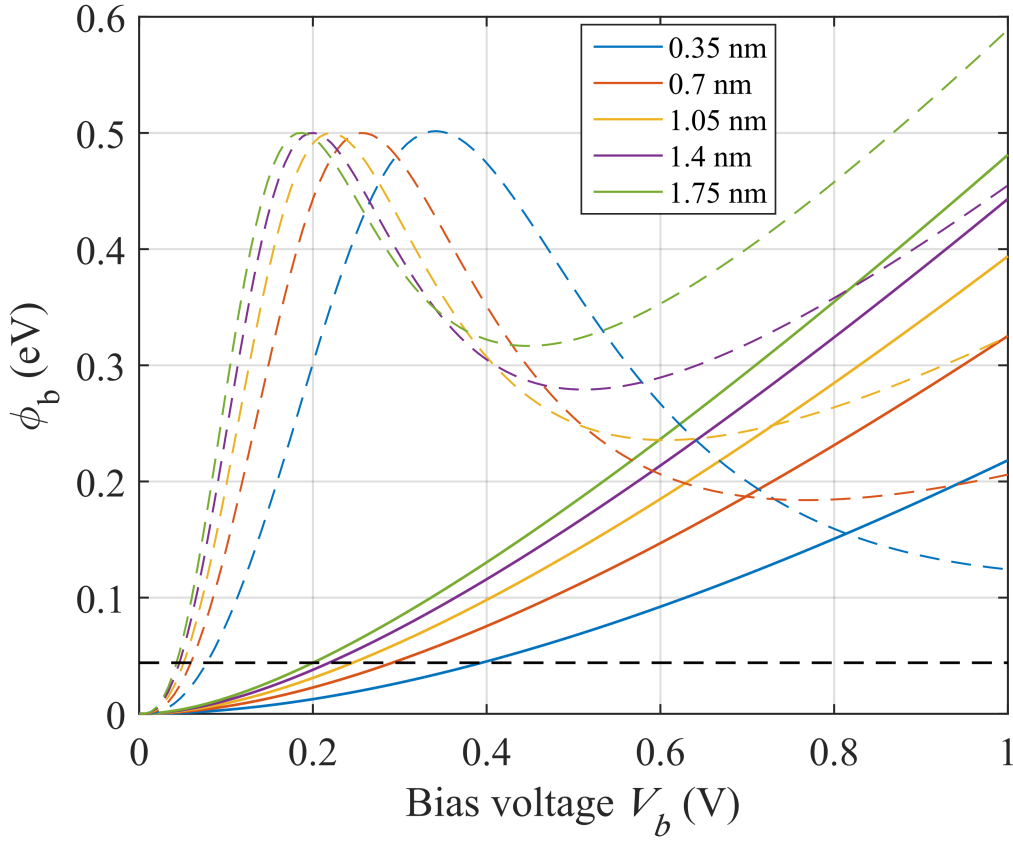


Figure 4.2: Solid lines show the electrostatic energy difference between two aligned graphene layers (see Figs. 3.1 and 3.3 for schematic diagrams of the device) as a function of the bias voltage, V_b , for different barrier thicknesses. Coloured dashed lines are corresponding dimensionless $I(V_b)$ curves normalised to the maximum value among them only for the purpose of showing the positions of current peaks. The black dashed line indicates the energy of $\hbar v_F q_c$ (left scale). The significance of this particular value of energy is that it determines where the current peak is; the peak occurs just before ϕ_b reaches this value. At higher ϕ_b , the scattering potential cannot supply the large momentum change needed for elastic tunnelling. The current peak is shifted to higher bias voltage for thinner barrier thickness as ϕ_b increases more slowly with increasing bias voltage.

4.2 Resonant tunnelling condition

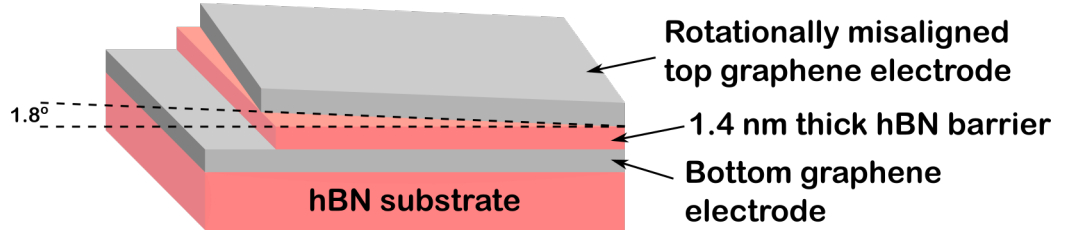


Figure 4.3: Simplified schematic diagram of a graphene-based transistor of which the top graphene layer is rotationally misaligned by 1.8° with respect to the bottom graphene layer. The spatial misalignment gives rise to a momentum change of $\Delta\mathbf{K}$ between the Dirac points of the two graphene layers in the momentum space which changes the resonant tunnelling condition, hence the position of current peaks. Other parameters of the device: hBN barrier thickness = 1.4 nm, $T = 2$ K, hBN substrate thickness = 300 nm.

We want a simple expression for the resonant tunnelling condition which can estimate where the current peak occurs. Based on our previous analysis, it is reasonable to investigate the resonant condition based on the following parameters: barrier thickness, misalignment angle, gate and bias voltages. A simplified schematic diagram of the device used as a model for this section is shown in Figure 4.3: the misalignment angle between the two graphene layers is 1.8° , barrier thickness = 1.4 nm, $T = 2$ K, thickness of hBN substrate is 300 nm. Solid lines plotted in Figure 4.4 are the electrostatic energy difference, $\phi_b = ebF_b$, as a function of bias voltage, V_b , of the device for three values of V_g . We can see that the bias voltage at which the electrostatic energy difference intersects with the black-dashed line, indicating the energy equal to $\hbar v_F \sqrt{q_c^2 + |\Delta\mathbf{K}|^2}$, is close to that at which the current reaches its peak. This means that the quantity, $\hbar v_F \sqrt{q_c^2 + |\Delta\mathbf{K}|^2}$, is a good indicator for the current peak position. It can be said that the resonant tunnelling occurs when the following condition is satisfied:

$$\phi_b \sim \hbar v_F \sqrt{q_c^2 + |\Delta\mathbf{K}|^2}. \quad (4.1)$$

Here, the left-hand side of the equation contains the effect of barrier thickness

and bias and gate voltages, while the right-hand side contains the information about the scattering potential and the misalignment of graphene electrodes. Now that we have acquired the expression for resonant tunnelling condition, we can re-investigate the effect of the barrier thickness. If we keep the right-hand side of (4.1) fixed and consider the electrostatic potential energy across the hBN barrier region, it can be seen that, from a basic electrostatics, decreasing the barrier thickness will require higher bias voltage across the barrier to reach the same electrostatic energy difference.

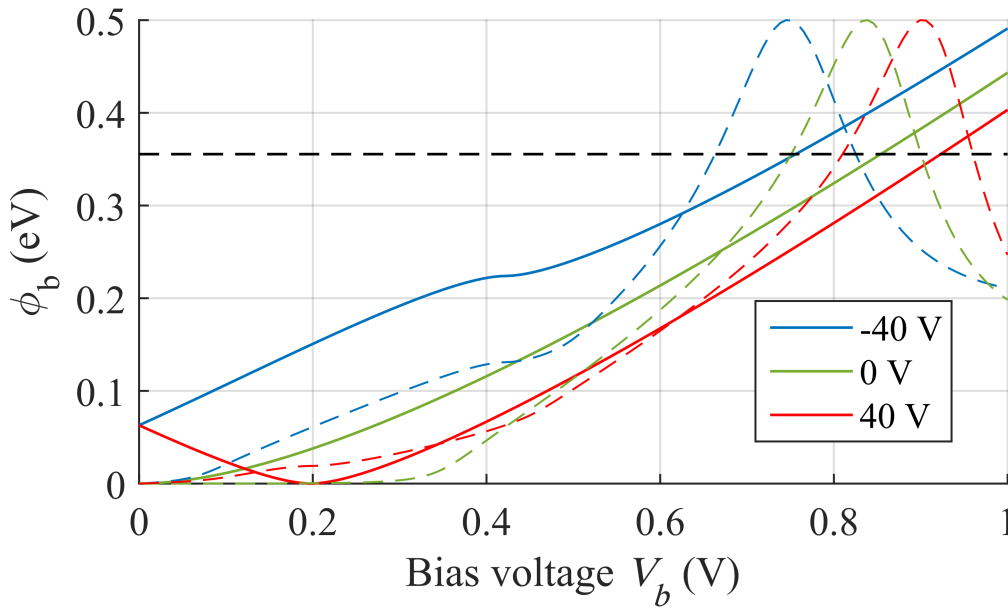


Figure 4.4: Solid lines show the electrostatic energy difference, ϕ_b , as a function of the bias voltage, V_b , for three different bottom gate voltages, V_g : -40 V, 0 V, and 40 V for a device with $\theta = 1.8^\circ$ and barrier thickness = 1.4 nm as shown in Figure 4.3. Coloured dashed lines are corresponding dimensionless $I(V_b)$ curves. The black dashed line indicates the energy of $\hbar v_F \sqrt{q_c^2 + |\Delta \mathbf{K}|^2}$. For all the gate voltages, the tunnelling current reaches its peak when $\phi_b \sim \hbar v_F \sqrt{q_c^2 + |\Delta \mathbf{K}|^2}$.

4.3 Investigation of the effect of temperature on tunnelling current

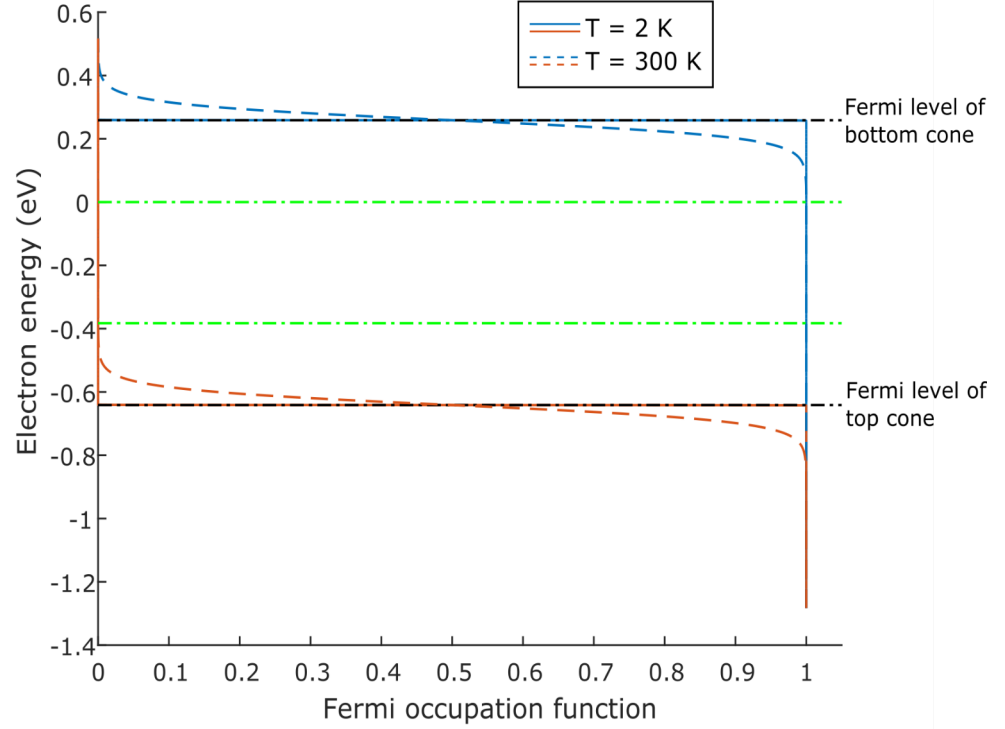


Figure 4.5: Fermi functions plotted for two different temperatures of bottom (blue) and top (orange) graphene layers: 2 K (solid curves) and 300 K (dashed curves). Black dash-dotted lines indicate the chemical potentials of the graphene electrodes. Green dash-dotted lines indicate the Dirac points, where that of the bottom cone centred at $E = 0$. The electron occupation spreads out near the chemical potentials at $T = 300$ K compared to that at $T = 2$ K, resulting in an increase in tunnelling current. Device characteristics: $\theta = 0^\circ$, barrier thickness = 1.4 nm, $V_g = 0$, $V_b = 0.19$ V.

There is one last parameter that appears in the expression of tunnelling current, which we have yet investigated it in detail; it is temperature. As temperature appears in the Fermi-Dirac distribution only, we expect its effect on electron tunnelling to be more apparent for electron energies close to the chemical potentials; we expect the tunnelling current to increase when the temperature increases since, at higher temperature, more electronic states of energies beyond the chemical potential are occupied in contrast with the electron occupations beyond the chemical potential at very low temperature, for

example, $T = 2$ K, which sharply drops to almost zero (see Figure 4.5).

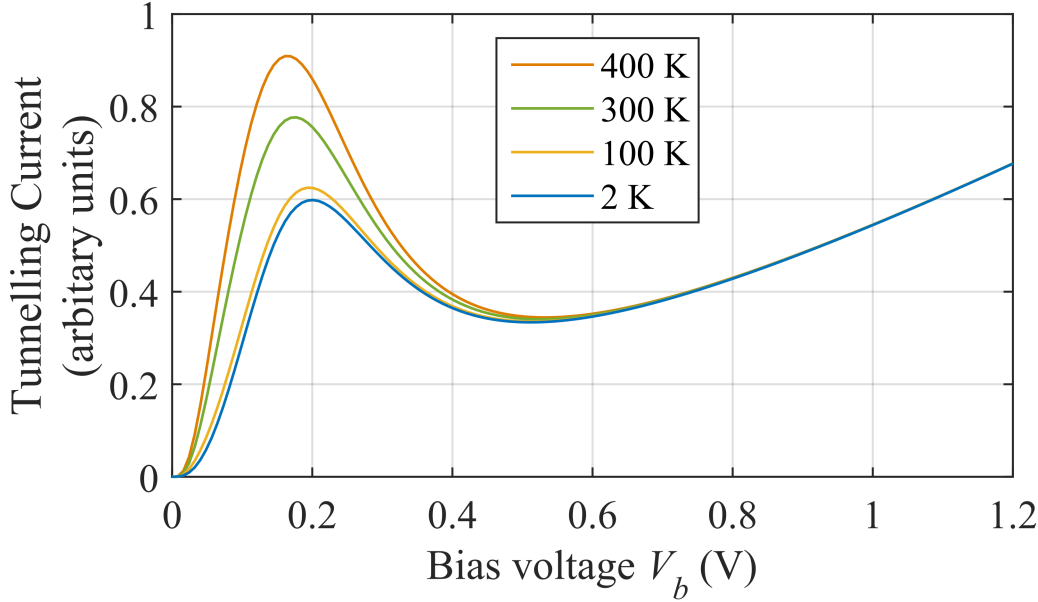


Figure 4.6: $I(V_b)$ characteristics calculated for various temperatures. The magnitude of tunnelling current curves, for V_b approximately below 0.7 V, increases as temperature increases as a result of more electrons gaining thermal energy, which in turn allows them to occupy high energy states beyond the chemical potential level. For $V_b > 0.7$ V, all $I(V_b)$ characteristics have similar behaviours as the effect of conservation of in-plane momentum dominates over the effect of increasing temperature and density of states. Device characteristics: $\theta = 0^\circ$, barrier thickness = 1.4 nm, $V_g = 0$.

Figure 4.6 shows the $I(V_b)$ curves for $T = 2$ K, 100 K, 300 K, and 400 K. We can see that their $I(V_b)$ characteristics for $V_b < 0.7$ V and for $V_b > 0.7$ V are different: the magnitude of the tunnelling current at low bias voltage increases as the temperature increases, whereas, at high bias voltage, all $I(V_b)$ curves keep increasing to the same high value. The reason for the increase in the magnitude of the tunnelling currents as temperature increases can be seen from the dI/dE diagrams plotted at $V_b = 0.19$ V and $V_b = 1.2$ V in Figure 4.7 and Figure 4.8, respectively.

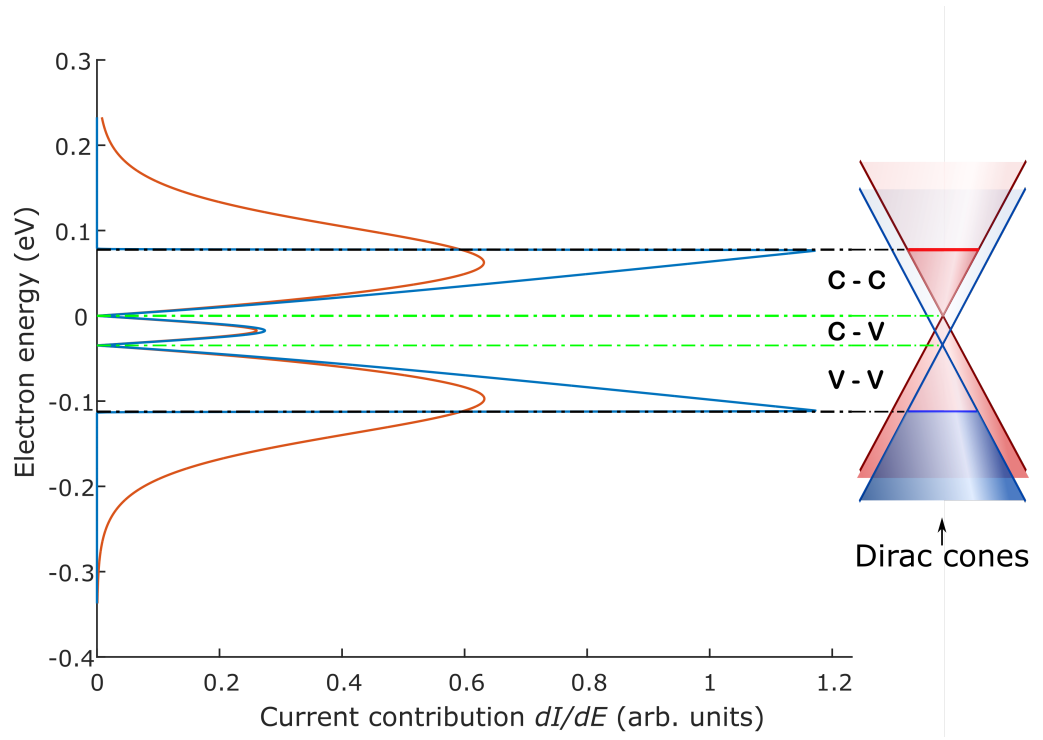


Figure 4.7: Current contribution distribution, dI/dE , as a function of electron energy E plotted at $V_b = 0.19$ V for $T = 2$ K (solid blue) and $T = 300$ K (solid orange). Green dashed lines indicate the Dirac points of the bottom and top cones which are shown on the right by red and blue cones, respectively. Above, between, and below these lines are three different tunnelling regimes: between the conduction bands (C-C), between the conduction and valence bands (C-V), and between the valence bands (V-V). Black dash-dotted lines indicate the chemical potentials. The Dirac cones at the right side are aligned with the energy axis to help understanding the tunnelling between bands better. In comparison with the current contribution, dI/dE , at $T = 2$ K, the current contribution at $T = 300$ K from the C-V tunnelling regime is slightly smaller. On the other hand, the current contribution from the C-C and V-V tunnelling regimes (although not visually apparent) are bigger when the temperature increases. This implies that the main contributions that give rise to a high tunnelling current in low V_b are those from C-C and V-V tunnellings.

In Figure 4.7, the unlike-band contribution (C-V) is barely affected by the change in temperature since the Fermi function, for electron energies in the C-V tunnelling regime at high temperatures, drops slightly (see Figure 4.5); on the other hand, the like-band contributions increase significantly when $T = 300$ K as compared to $T = 2$ K because of the non-trivial spread of the Fermi function beyond the chemical potentials and the increase in the density of states. This implies that the dominating factors that give rise to a higher tunnelling current

in low V_b are the increase in the availability of states associated with the increase in temperature and the increase in the number of states associated with the C-C and V-V transition regimes.

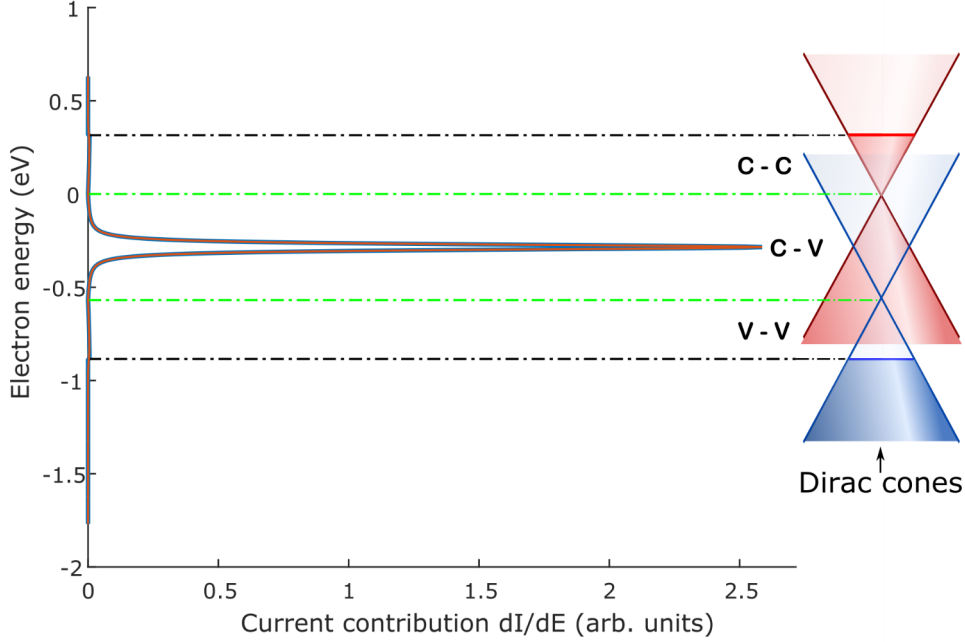


Figure 4.8: Current contribution distribution, dI/dE , as a function of electron energy E plotted at $V_b = 1.2$ V for $T = 2$ K (solid blue) and $T = 300$ K (solid orange). The blue curve is deliberately made thicker to allow for visualising the overlap between the two curves. Green dashed lines indicate the Dirac points of the bottom and top cones which are shown on the right by red and blue cones, respectively. Above, between, and below these lines are three different tunnelling regimes: between the conduction bands (C-C), between the conduction and valence bands (C-V), and between the valence bands (V-V). Black dash-dotted lines indicate the chemical potentials. At this V_b , the momentum difference between two states in general is very large while the scattering potential can only provide little momentum change. For this reason, elastic scattering is not favoured and only the states at vicinity of the intersection energy of the two Dirac cones can tunnel. However, the total current is higher because of the increase in the density of states. The decrease in tunnelling rate due to the requirement of large momentum changes dominates the increase in tunnelling rate due to a high density of states at high electron energies. In contrast with the case at low bias voltage such as shown in Figure 4.7, the current contribution, dI/dE , here in the like-band tunnelling regime are barely affected by the change in temperature.

As for Figure 4.8, the two Dirac cones (shown on the right of the figure) are so far apart with regard to their electrostatic energy difference that most tunnelling processes cannot be assisted by elastic scattering except for the states

around the intersection energy of the two cones which is far from the chemical potential levels. However, we can see that the dI/dE peaks in the C-V tunnelling region are higher than those at $V_b = 0.19$ V as shown in Figure 4.7 as a result of a linear behaviour of the energy density of states which increases as electron energy increases, thus the increase in tunnelling current (see Figure 4.6 for $V_b > 0.7$ V). In the C-C and V-V tunnelling regimes in Figure 4.8, the dI/dE curves flat out to zero even though there are more electronic states available. The only reason for this must be that the momentum changes required for tunnelling are far too large. We did not investigate further the cases for very high temperature as graphene might break down and loses its properties as described in this thesis [63, 70, 115].

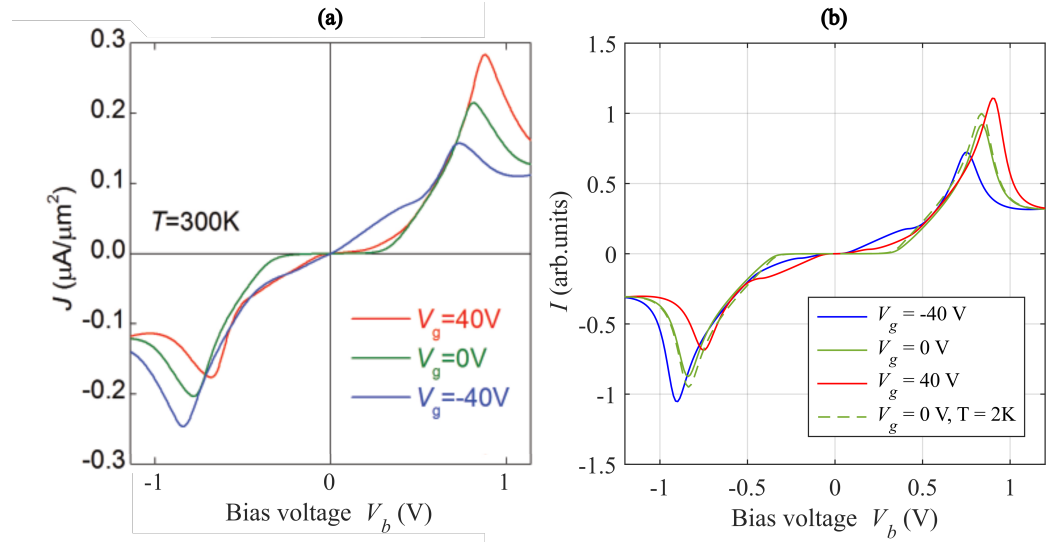


Figure 4.9: Solid curves show (a) experimental and (b) theoretical measurements of the current-bias voltage characteristics of the device at $T = 300$ K, for three different V_g : (red) 40 V, (green) 0 V and (blue) -40 V. Figure (a) is adapted from Supplementary Figure 7 in [80]. Dashed green curve, whose maximum value is set to 1, is added for the magnitude comparison between very low and high temperatures. In general, the experimental results show smaller peak-to-valley ratios. Device parameters: $\theta = 1.8^\circ$, barrier thickness $= 1.4$ nm.

Figure 4.9 shows (a) experimental measurements and (b) theoretical simulations of $I(V_b)$ characteristics for a device with $\theta = 1.8^\circ$ at $T = 300$ K (solid curves), for three gate voltages, V_g . Figure 4.9(a) is adapted from Figure 7 of

the Supplementary material in [80]. For $V_g = 0$ V, the magnitude of the calculated tunnelling current at $T = 300$ K is slightly smaller than that at $T = 2$ K. This is not the case for the device with $\theta = 0^\circ$. In general, the experimental results show smaller peak-to-valley ratios than the simulations.

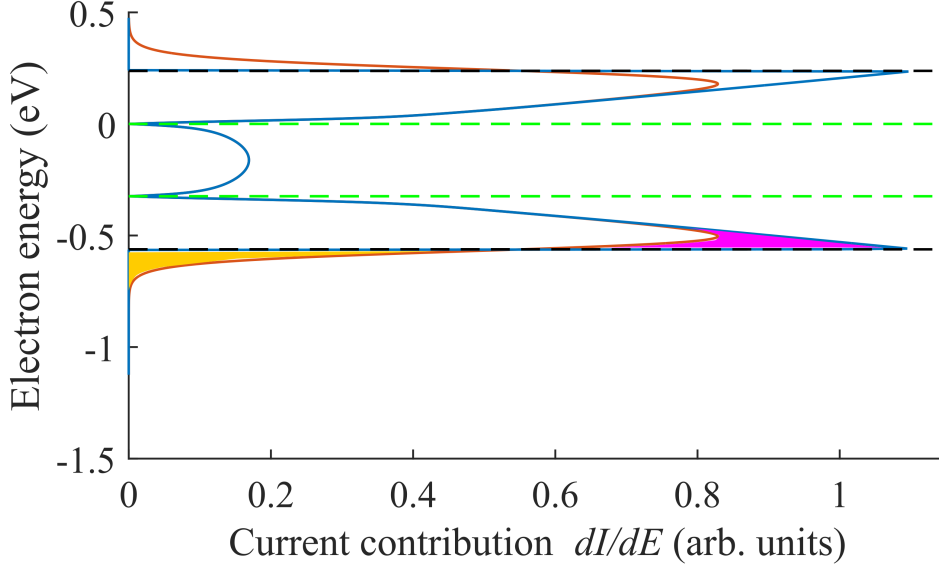


Figure 4.10: Current contribution distribution, dI/dE , as a function of electron energy E plotted at $V_b = 0.8$ V and $V_g = 0$ V for $T = 2$ K (solid blue) and $T = 300$ K (solid orange). See Fig. 4.7 for the description of green dashed and black dash-dotted lines. Compared to Fig. 4.7, the tunnelling current gain (yellow shaded area) due to the spread-out of the Fermi function at $T = 300$ K near the chemical energy levels is slightly smaller than the current loss (pink shaded area), resulting in a decrease in the total tunnelling current. This shows the domination of the effect of requiring bigger momentum changes due to misalignment over the availability of states gained owing to high temperatures.

To explain why the tunnelling current decreases as the temperature increases, we have plotted the current contribution distribution, dI/dE (see Fig. 4.10). We can see that, unlike the $\theta = 0^\circ$ case, the current gained due to having more states for tunnelling as T increases from 2 K to 300 K (indicated by yellow shaded area) is slightly smaller than the current loss due to the reduction in the electron occupation (indicated by pink shaded area). Since the misalignment of the graphene sheets is related to the misalignment of the momentum space, the requirement for bigger momentum changes for tunnelling must be

the reason why the variation of the $I(V_b)$ characteristics associated with temperature for the device with misaligned graphene sheets is opposite to that with aligned graphene sheets.

That our model only includes the effects of temperature through the form of the Fermi function means that it has some limitations: it is less accurate since thermal effects such as phonon scattering processes can occur at high temperatures. Nevertheless, our model shows nicely why the peak-to-valley ratio is maintained at high temperatures: the effect of momentum conservation suppresses the tunnelling rates, limiting electron tunnelling processes even though available states for tunnelling transitions are available.

4.4 Conclusions

In chapters 3 and 4, we studied the current-bias voltage, $I(V_b)$, characteristics of graphene-based transistors as well as how parameters such as gate and bias voltages (V_g and V_b , respectively), misalignment of graphene electrodes, hBN barrier thickness and temperature affect the $I(V_b)$ characteristics. We identified that a gate voltage shifts the Dirac points of graphene electrodes and tunnelling current peaks. We also found that a small rotational misalignment of graphene electrodes gives rise to a region in V_b in which the tunnelling current is or close to zero, as a result of a larger momentum change required for tunnelling as compared to a smaller momentum change required in the case of no rotational misalignment. We found an expression for resonant tunnelling condition which is related to the barrier thickness, scattering potential and the rotational misalignment of the graphene electrodes. We identified how the change of the barrier thickness shifts the position of current peaks and the magnitude of the tunnelling current. We studied the tunnelling current in regards to the competition among the increasing availability of states associated with increasing temperature, the increasing density of states associated

with increasing electron energies and the conservation of momentum associated with increasing bias voltage, V_b . We have identified that, at low V_b , the effects of the increasing availability of states in the like-band tunnelling regimes and the increasing density of states dominate over the effect of the momentum change requirement for tunnelling, resulting in an increase in the magnitude of I as temperature increases, whereas, at high bias voltage, the effect of a large momentum change required for transitions in the like-band tunnelling regimes dominate other factors, which suppresses the dI/dE in those regimes, thus negating the effect of varying temperatures.

Chapter 5

Electromagnetic Properties of Graphene

In the context of micro-fabricated atom chips, electromagnetic properties of the current-carry wires play a crucial role in determining the Casimir-Polder interaction and Johnson noise, which governs the stability and longevity of trapped atom clouds [30, 38, 97]. Knowing the optical conductivity of materials allows us to further calculate the reflection coefficients which are the core parameters in the Green's function. In this chapter, we lay the foundations for calculating optical properties of graphene besides the electronic properties laid out in Chapter 2 and present a numerical method for calculating electromagnetic scattering coefficients of graphene-based planar structures.

5.1 Optical Conductivity of Graphene

The relevant information on the physics governing the electromagnetic interactions between a solid, e.g. graphene, and external electromagnetic radiation is contained in the solid's optical conductivity. Optical conductivity can be split into two distinct contributions: one describes how the solid's electrons respond to electromagnetic waves by transiting to higher energy states within the same energy bands where the momenta are not conserved (intraband-transitions);

the other accounts for the response of the electrons to electromagnetic waves by undergoing vertical transitions from the valence band to the conduction band where the momenta are conserved (interband- transitions). Mathematically, we can separate them into two contributions to the conductivity as

$$\sigma(\omega) = \sigma_{\text{intra}}(\omega) + \sigma_{\text{inter}}(\omega), \quad (5.1)$$

where $\sigma_{\text{intra}}(\omega)$ and $\sigma_{\text{inter}}(\omega)$ are the conductivity due to intraband- and interband- transitions, respectively, ω is the angular frequency of the electromagnetic field to which the solid is exposed.

An exact description of the conductivity of graphene in the framework of Dirac model which considers both nonzero mass gap and chemical potential can be found in [62]. In some asymptotic regimes, this model was shown to be similar to a simpler model, namely Kubo's formula, which is for ungapped graphene.

In this thesis, we only use Kubo's formula for all calculations of the conductivity of graphene. Kubo's formula [46, 48, 49, 102] provides graphene's optical conductivity as follows:

$$\sigma_{\text{intra}}(\omega) = \frac{\sigma_0}{\pi} \frac{4}{\hbar\gamma - i\hbar\omega} \left[E_F + 2k_B T \ln \left(1 + e^{-E_F/k_B T} \right) \right], \quad (5.2)$$

$$\sigma_{\text{inter}}(\omega) = \sigma_0 \left[G(\hbar\omega/2) + i \frac{4\hbar\omega}{\pi} \int_0^\infty dE \frac{G(E) - G(\hbar\omega/2)}{(\hbar\omega)^2 - 4E^2} \right], \quad (5.3)$$

with

$$G(x) = \frac{\sinh \left(\frac{x}{k_B T} \right)}{\cosh \left(\frac{E_F}{k_B T} \right) + \cosh \left(\frac{x}{k_B T} \right)}, \quad (5.4)$$

where $\sigma_0 = e^2/(4\hbar)$ is termed the universal alternating-current conductivity of

graphene, $\hbar$ is the reduced Planck's constant, k_B is the Boltzmann's constant, γ is the relaxation rate of graphene's electrons which associates with the relaxation time in the Drude model, E_F is the Fermi energy and T is temperature of graphene in Kelvin.

Figure 5.1 shows the calculated optical conductivity of doped monolayer graphene with $E_F = 0.1 \text{ eV}$ and $\gamma = 4 \text{ THz}$ as a function of electromagnetic radiation frequency in the THz regime at absolute zero temperature. Note that both the doping level and relaxation rate considered here fall within the range found in [2, 4, 46, 47, 109]); they represent an average graphene, i.e. graphene with an average level of impurities. The energies of photons in this frequency range are low compared to the Fermi energy of the graphene sheet ($0 - 0.1E_F$). Therefore, following from Pauli's exclusion principle, these low energy photons cannot promote electrons in the valence band to the conduction band due to the fact that all electronic states of energies below the Fermi energy in the conduction band are occupied; for this reason, graphene's optical conductivity is dominated by the term describing intraband transitions as expressed in (5.2).

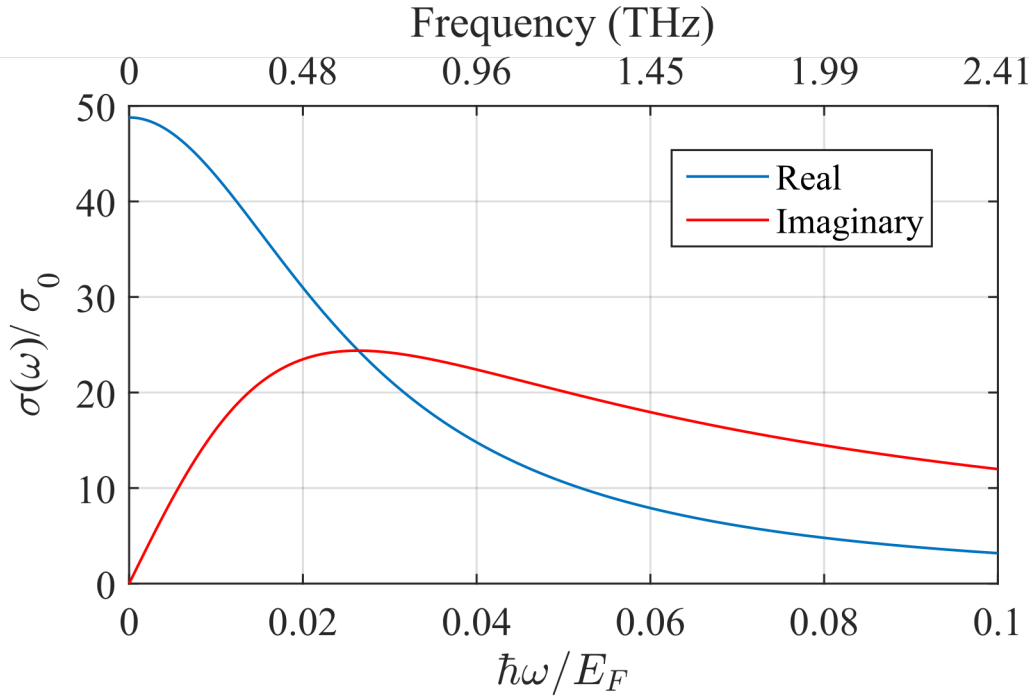


Figure 5.1: Real part (blue) and imaginary part (red) of graphene's optical conductivity modelled by Kubo's formula, as a function of electromagnetic wave frequency in the THz regime (top scale). The frequency axis corresponds to electron's energies between $0-0.1E_F$ (bottom scale). The main contribution is from intraband transitions of graphene's electrons, whereas the contribution from interband transitions is negligible due to Pauli blocking. The graphene considered here is an average graphene with the chemical potential and electron relaxation rate in a typical range particularly found in [2, 4, 46, 47, 109]). Parameters: $E_F = 0.1 \text{ eV}$, $\gamma = 4 \text{ THz}$ and $T = 300 \text{ K}$.

Figure 5.2 shows the optical conductivity of the same monolayer graphene as a function of electromagnetic radiation frequency in the mid-IR regime ($0 - 84.5 \text{ THz}$) at two different temperatures, $T = 0 \text{ K}$ and $T = 300 \text{ K}$, in order to allow interband transitions to occur noticeably and to see the effect of thermal excitations. Let us consider the $T = 0 \text{ K}$ case, which can be split into two regimes: $\hbar\omega < 2E_F$ and $\hbar\omega > 2E_F$. In the first regime, the real part of the conductivity is dominated by the term describing intraband transitions, which decreases with radiation frequency, ω as it has ω in the denominator. On the other hand, the contribution from the term describing interband transitions is zero. The real part has a sudden rise at $\hbar\omega = 2E_F$, which is due to the contribution from the integral term in the expression for σ_{inter} as written in (5.3) and it plateaus at the value of σ_0 in the second regime. As for the imaginary

part, it diverges to negative infinity for $\hbar\omega = 2E_F$ due to the singularity of the integral term in (5.3). For the $T = 300$ K case, we know from the Fermi-Dirac statistics that the states of energies less than E_F are not fully occupied and the states of energies higher than E_F are slightly occupied; therefore, the real part of the term describing interband transitions starts increasing at some point before $\hbar\omega = 2E_F$, while it is smaller than σ_0 at the region just after $\hbar\omega > 2E_F$ and eventually converges to σ_0 at high frequency regime. In contrast with the $T = 0$ K case, the imaginary part of the conductivity for the $T = 300$ K case, for $\hbar\omega = 2E_F$, is finite.

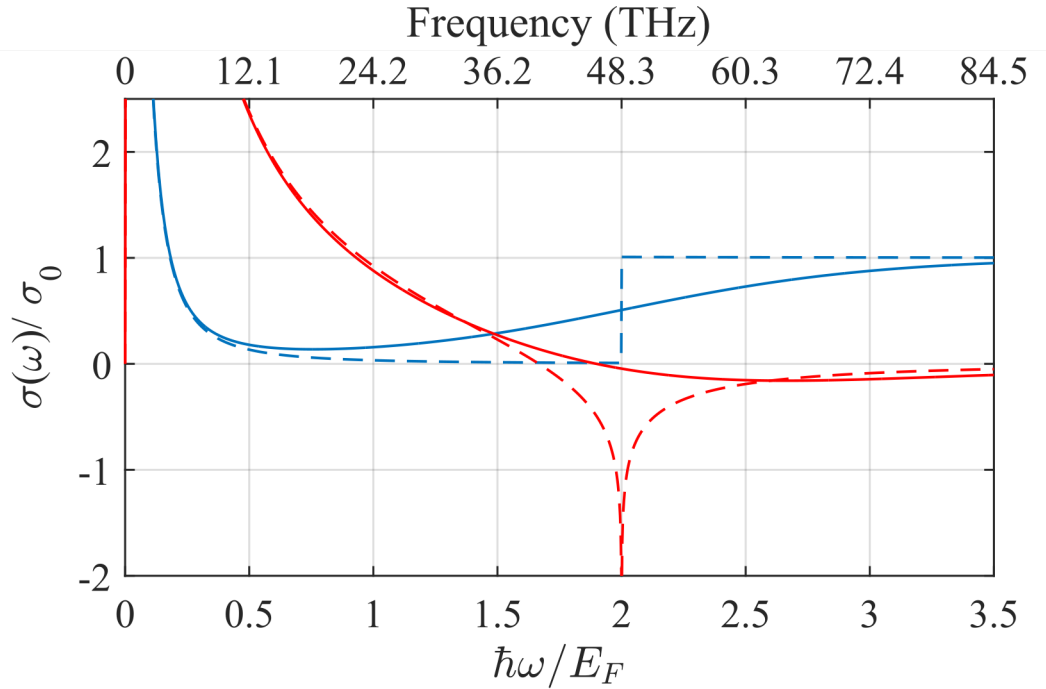


Figure 5.2: Real part (blue) and imaginary part (red) of graphene's optical conductivity obtained via Kubo's formula, as a function of electromagnetic wave frequency in the mid-IR regime for $T = 0$ K (dashed curves) and $T = 300$ K (solid curves). For $\hbar\omega > 2E_F$, the contribution from interband transitions totally dominates in the real part. For $T = 300$ K, some interband transitions are allowed due to the fact that the electronic states of energies below the Fermi level, E_F , are not fully occupied as opposed to the case for $T = 0$ K. Note that the real part converges to the universal AC conductivity of graphene, σ_0 , whereas the imaginary part vanishes for $\hbar\omega \gg 2E_F$. Note that, in the limit $\omega \rightarrow \infty$, the real and imaginary parts approach 1 and 0, respectively. Parameters: $E_F = 0.1$ eV, $\gamma = 4$ THz.

5.2 Transfer-Matrix Method

In this section, we will introduce a method to efficiently calculate the electromagnetic scattering coefficients that are necessary for the calculation of Green's tensor in the chapters ahead. One way to do this is to use a transfer-matrix method [118]. The concept of the transfer-matrix method is to find an effective matrix that can relate the amplitude of the electromagnetic wave incident on a structure, especially, a multi-layered planar system, with that of the transmitted wave. After we have obtained such a relation, we can calculate the effective reflection coefficients as well as the effective transmission and absorption coefficients. There are two basic building blocks for this method, namely, transmission matrices and propagation matrices: A transmission matrix describes the change of the wave amplitudes when the wave travels across an interface between two media, whereas a propagation matrix captures the phase change when the wave propagates through a medium.

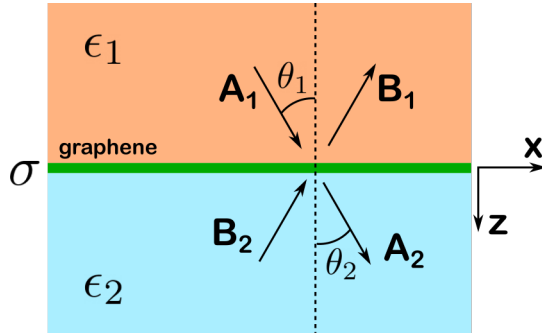


Figure 5.3: A schematic diagram of electromagnetic scattering in a structure composed of a single graphene sheet (green) sandwiched by two semi-infinite dielectric media of relative permittivities, ϵ_1 (orange) and ϵ_2 (blue). The graphene sheet is located at the plane defined by $z = 0$ and its electromagnetic properties are encompassed by a conductivity, σ . Arrows, all lying in a plane called the plane of incidence, which coincides with the x - z plane, indicate electromagnetic waves with their z -components travelling towards the positive z -direction (denoted by A_1 and A_2) and the negative z -direction (denoted by B_1 and B_2). θ_1 and θ_2 are the incident and refracted angles, respectively.

We start with the derivation of the transmission matrices. Let us consider an event as depicted in Figure 5.3: electromagnetic waves of frequency, ω , scatter in a planar structure consisting of a monolayer graphene, cladded by

two semi-infinite dielectric media of relative permittivities, ϵ_1 and ϵ_2 . The graphene sheet is located at the plane defined by $z = 0$ and is assumed to be mathematically thin such that the medium 1 (characterised by a relative permittivity, ϵ_1) occupies the region defined by $z < 0$ and the medium 2 (characterised by a relative permittivity, ϵ_2) occupies the region defined by $z > 0$. Let us further assume that the waves are plane waves, that their $\mathbf{B}$ -field only has a y -component, and that their $\mathbf{E}$ -field is parallel to the plane of incidence, which coincides with the x - z plane (commonly known as transverse magnetic waves or p-polarised waves). Therefore, the $\mathbf{B}$ -fields can be written as

$$\mathbf{B}_y^{(j)}(\mathbf{r}, t) = (A_j e^{ik_{j,z}z} + B_j e^{-ik_{j,z}z}) e^{i(k_{j,x}x - \omega t)} \hat{\mathbf{y}}, \quad (5.5)$$

where $j = 1, 2$ are for the waves in medium 1 and medium 2, respectively, A_j and B_j are the amplitudes of the waves propagating in the positive and negative z -directions, respectively, subscripts, x, y , and z denote the components associated with the coordinate axes, t is time, $\hat{\mathbf{y}}$ is a unit vector pointing in the positive y -direction (out of the page) and the relation between the z - and x - components of the wavevector is given by

$$k_{j,z}^2 = \epsilon_j \frac{\omega^2}{c^2} - k_{j,x}^2. \quad (5.6)$$

In dielectric media, the relation between $\mathbf{B}$ - and $\mathbf{E}$ - fields is given by the following Maxwell's equation,

$$\nabla \times \mathbf{B} = -i \frac{\epsilon \omega}{c^2} \mathbf{E}, \quad (5.7)$$

where c is the speed of light in vacuum. Using the equation given above, the x -component of the $\mathbf{E}$ -fields is found to be

$$\mathbf{E}_x^{(j)}(\mathbf{r}, \mathbf{t}) = \frac{k_{j,z}c^2}{\omega\epsilon_j}(A_j e^{ik_{j,z}z} - B_j e^{-ik_{j,z}z})e^{i(k_{j,x}x - \omega t)}\hat{\mathbf{x}}, \quad (5.8)$$

where $\hat{\mathbf{x}}$ is a unit vector pointing in the positive x -direction.

In order to find the relations between the amplitudes of the waves in medium 1 and medium 2, we need to invoke the boundary conditions at the interface between the two dielectric media for the parallel components of $\mathbf{E}$ - and $\mathbf{B}$ -fields; they are given below

$$\hat{\mathbf{n}} \times (\mathbf{E}^{(1)} - \mathbf{E}^{(2)}) = 0, \quad (5.9)$$

$$\hat{\mathbf{n}} \times (\mathbf{B}^{(1)} - \mathbf{B}^{(2)}) = \mu_0 \mathbf{J}_s, \quad (5.10)$$

where $\hat{\mathbf{n}}$ is a normal unit vector pointing from medium 2 into medium 1 (equivalent to $-\hat{\mathbf{z}}$), μ_0 is the permeability of vacuum, $\mathbf{J}_s$ are the free surface current densities at the boundary, which is the graphene sheet in this case. Writing out only the relevant components and using the generalised Ohm's law, $\mathbf{J} = \sigma \mathbf{E}$, we obtain

$$E_x^{(1)}(z=0) = E_x^{(2)}(z=0), \quad (5.11)$$

$$B_y^{(1)}(z=0) - B_y^{(2)}(z=0) = \mu_0 \sigma E_x^{(1)}(z=0), \quad (5.12)$$

where σ is the optical conductivity of the 2D material at the interface (graphene). Substituting (5.5) and (5.8) into the above boundary conditions, yields

$$A_1 - B_1 = \frac{\epsilon_1 k_{2,z}}{\epsilon_2 k_{1,z}}(A_2 - B_2), \quad (5.13)$$

$$A_1 + B_1 = (A_2 + B_2) + \frac{\sigma k_{2,z}}{\omega \epsilon_0 \epsilon_2}(A_2 - B_2). \quad (5.14)$$

Converting (5.13) and (5.14) into a matrix equation yields

$$\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} \eta_p & -\eta_p \\ 1 + \xi_p & 1 - \xi_p \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \quad (5.15)$$

where the following functions have been introduced to simplify our notation,

$$\eta_p = \frac{\epsilon_1 k_{2,z}}{\epsilon_2 k_{1,z}} \quad \text{and} \quad \xi_p = \frac{\sigma k_{2,z}}{\omega \epsilon_0 \epsilon_2}. \quad (5.16)$$

Multiplying (5.15) by the inverse of the leftmost matrix of (5.15), we obtain a transfer-matrix equation

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 + \eta_p + \xi_p & 1 - \eta_p - \xi_p \\ 1 - \eta_p + \xi_p & 1 + \eta_p - \xi_p \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \quad (5.17)$$

$$= \mathbf{T}_p \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \quad (5.18)$$

where

$$\mathbf{T}_p = \frac{1}{2} \begin{pmatrix} 1 + \eta_p + \xi_p & 1 - \eta_p - \xi_p \\ 1 - \eta_p + \xi_p & 1 + \eta_p - \xi_p \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}. \quad (5.19)$$

Here, $\mathbf{T}_p$ is a transmission matrix, which relates the amplitudes of the incident and transmitted p-polarised electromagnetic waves across an interface between two dielectric media; it contains the information of the dielectric constants of both media, the incident and refracted angles of the waves, the frequency of the waves, and the optical conductivity of the 2D material at the interface.

By following the same procedure, a transmission matrix for s-polarised waves (transverse electric waves) is found to be

$$\mathbf{T}_s = \frac{1}{2} \begin{pmatrix} 1 + \eta_s + \xi_s & 1 - \eta_s + \xi_s \\ 1 - \eta_s - \xi_s & 1 + \eta_s - \xi_s \end{pmatrix} \begin{pmatrix} A_2 \\ B_2 \end{pmatrix}, \quad (5.20)$$

where

$$\eta_s = \frac{k_{2,z}}{k_{1,z}} \quad \text{and} \quad \xi_s = \frac{\sigma\mu_0\omega}{k_{1,z}}. \quad (5.21)$$

We now consider the propagation matrix, which can easily be derived by recalling the fact that an electromagnetic wave, with the z -component, k_z , of its wavevector, propagating through a distance, d , in the z -direction in a uniform medium only changes its phase by $k_z d$. Hence, the propagation matrix is given by

$$\mathbf{P}(d) = \begin{pmatrix} e^{-ik_z d} & 0 \\ 0 & e^{ik_z d} \end{pmatrix}. \quad (5.22)$$

Now that we have obtained explicit forms for both transmission and propagation matrices, we can construct a transfer-matrix by performing a series of matrix multiplications in an order such that the matrix associated with the first chronological event will be placed at the leftmost position and the matrix associated with the second event will be placed on the right of the first matrix and so on.

For example, the effective transfer matrix that is built for a two-sided graphene structure consisting of a dielectric slab (with thickness, d , and relative permittivity, ϵ_d), sandwiched between two graphene sheets, with the whole structure suspended in a homogeneous medium as depicted in Figure 5.4, is given by

$$\mathbf{M} = \mathbf{T}_{\text{gr},1} \mathbf{P}(d) \mathbf{T}_{\text{gr},2}, \quad (5.23)$$

where $\mathbf{T}_{\text{gr},1}$ is the transmission matrix describing an electromagnetic wave crossing the graphene interface from the homogeneous medium to the dielectric slab, $\mathbf{P}(d)$ is the propagation matrix associated with the propagation of the wave through distance, d , along the dielectric slab, and $\mathbf{T}_{\text{gr},2}$ accounts for an electromagnetic wave crossing the graphene interface from the dielectric slab to the homogeneous medium. Keep in mind that a notation $\mathbf{M}$ will be used to refer to a transfer-matrix which is a resulting product of constituent

transmission and propagation matrices from now on, unless otherwise stated, and subscripts, s and p , for s-polarisation and p-polarisation, respectively, will be omitted where it is convenient.

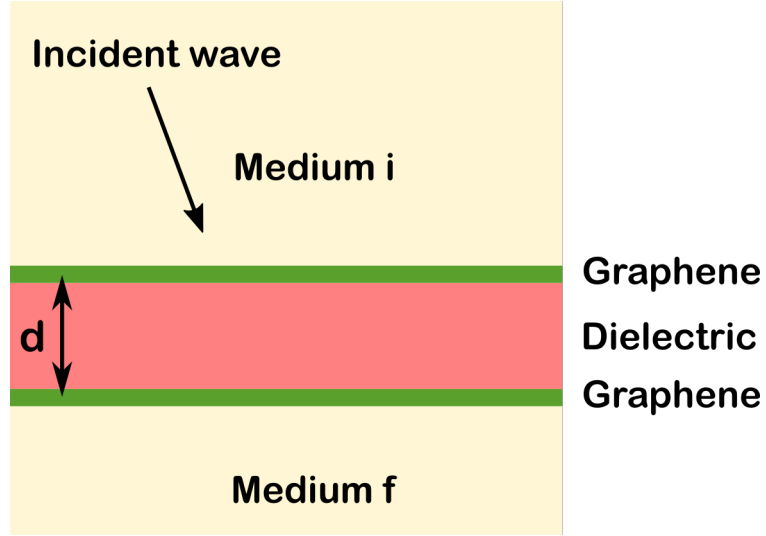


Figure 5.4: Pictorial representation of an electromagnetic wave incident on a structure consisting of a slab of a dielectric medium (with thickness, d , and relative permittivity, ϵ_d) sandwiched between two layers of graphene, suspended in a homogeneous medium. The wave encounters the top graphene sheet first, and after that, propagates through the dielectric slab then transmits past the bottom graphene sheet.

Recalling that the relation between the wave amplitudes in the media above and below the structure under consideration is embedded in the transfer-matrix, the expressions for the scattering coefficients can be straightforwardly obtained from the elements of our transfer-matrix, $\mathbf{M} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}$; in particular, via

$$r = \frac{M_{21}^{i \rightarrow f}}{M_{11}^{i \rightarrow f}} \quad \text{and} \quad t = \frac{1}{M_{11}^{i \rightarrow f}}, \quad (5.24)$$

respectively for the reflection and transmission coefficients. Here, i denotes the medium in which the electromagnetic radiation is propagating before it encounters the structure in consideration, whereas f denotes the medium in which the electromagnetic radiation is propagating after it has exited the structure (see Figure 5.4).

Having obtained these scattering coefficients, we can calculate the reflectance, R , transmittance, T , as well as the absorbance, A ,

$$R_p = |r_p|^2 \quad \text{and} \quad R_s = |r_s|^2, \quad (5.25)$$

$$T_p = \eta_p |t_p|^2 \quad \text{and} \quad T_s = \eta_s |t_s|^2, \quad (5.26)$$

$$A_p = 1 - T_p - R_p \quad \text{and} \quad A_s = 1 - T_s - R_s, \quad (5.27)$$

where η_p and η_s are

$$\eta_p = \frac{\epsilon_i k_{f,z}}{\epsilon_f k_{i,z}} \quad \text{and} \quad \eta_s = \frac{k_{f,z}}{k_{i,z}}. \quad (5.28)$$

Here, we have invoked subscripts, p and s , to avoid ambiguity when considering the two distinct wave polarisations.

5.3 Results and Validity of the Transfer-Matrix Method

Here, we will apply the transfer-matrix method to a few graphene-based structures and compare the obtained results with our common knowledge in optics.

5.3.1 Single graphene layer

The very first question we should ask is: what is the behaviour of the transmittance, reflectance, and absorbance of a single graphene sheet embedded in vacuum as a function of the frequency of the incident electromagnetic wave? We can see in Figure 5.5 that the transmittance increases, while the reflectance and absorbance decrease as the energy of the incident photon increases. The absorbance converges to the value of 2.3% which is the “universal” frequency-independent absorption of monolayer graphene. We have seen in Figure 5.1

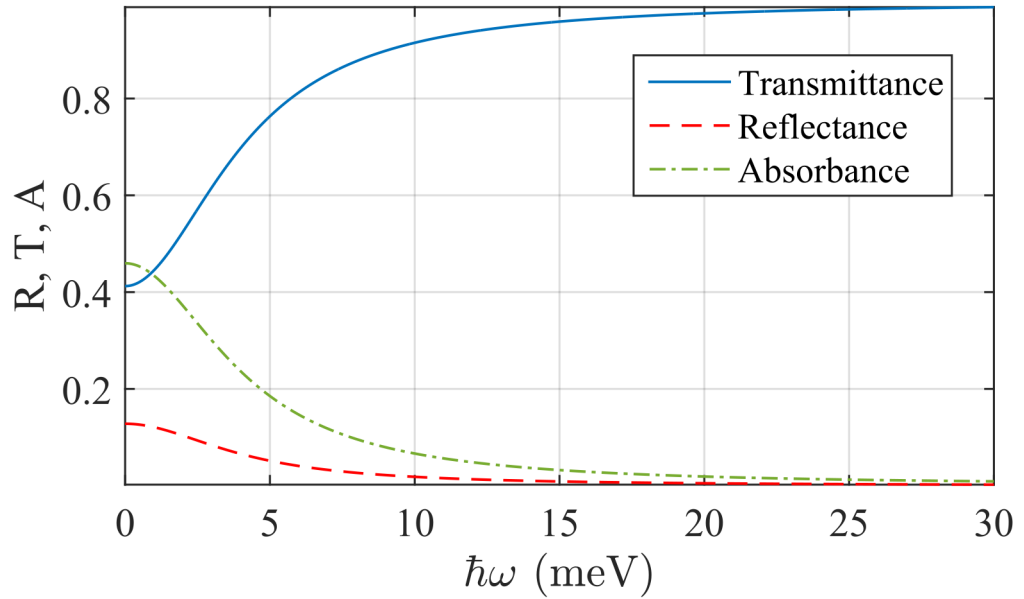


Figure 5.5: Transmittance, reflectance and absorbance of electromagnetic waves at normal incident through a single graphene layer suspended in a vacuum, calculated as a function of the frequency of the incident wave. Here, graphene's conductivity is modelled by Kubo's formula [46, 48, 49, 102], with $E_F = 0.1$ eV, $\gamma = 4$ THz and $T = 300$ K. As the frequency of the electromagnetic wave increases, the absorbance converges to the frequency-independent value of 2.3% for an isolated monolayer graphene. The reflectance also follows a similar tendency as the absorbance, whereas the transmittance increases to almost 1 at high frequency, making the graphene layer appear almost transparent. This is the reason that we need a 300-nm-thick oxidised silicon substrate underneath the graphene sheet to enable optical imaging of the graphene-based transistors in chapter 3.

that, for very low energy photons, the optical conductivity decreases as the frequency of the incident photons increases. Therefore, graphene's optical properties become more like those of a vacuum, which has zero optical conductivity. That graphene has high transmittance (low visibility) is consistent with many experiments, including our graphene-based transistors in the preceding chapters, in which we need some substrates, for example, 300-nm-thick SiO₂ wafer, to enhance graphene's visibility [8, 11]. It is safe to say that the electromagnetic scattering coefficients obtained from transfer-matrix method behave as expected from the characteristics of graphene's optical conductivity.

5.3.2 Total internal reflection

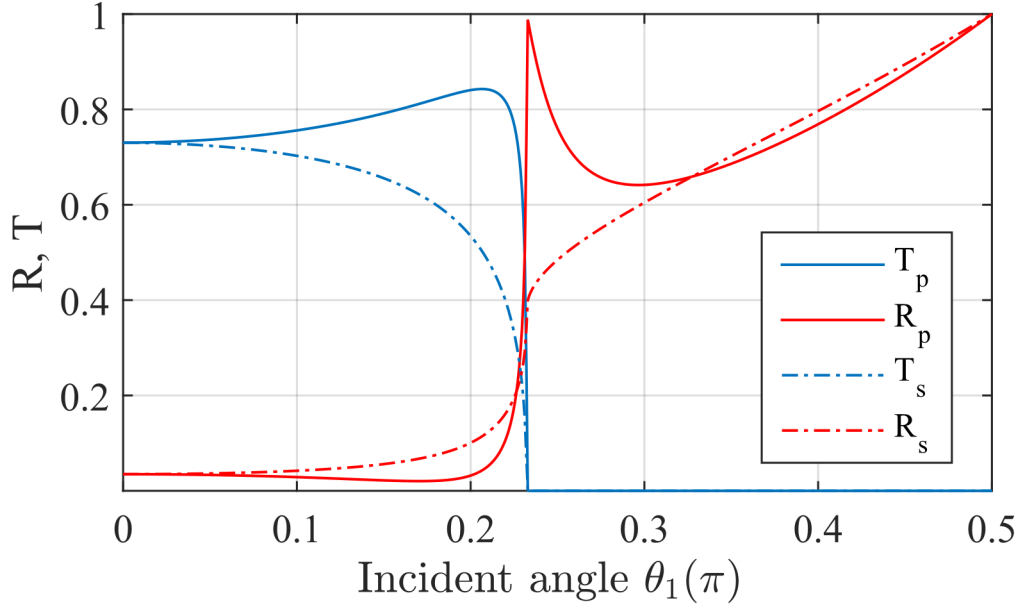


Figure 5.6: Transmittance and reflectance of electromagnetic radiation incident on a structure depicted in Figure 5.3, with $\epsilon_1 = 2.25$ and $\epsilon_2 = 1$, calculated as a function of incident angle, for p-polarisation (solid curves) and s-polarisation (dash-dotted curves). The reflectance of both polarisations undergo an abrupt increase to almost 1 at the critical angle of approximately 0.23π , which can be compared to total internal reflection when an electromagnetic wave encounters an interface from a dielectric medium of higher permittivity to that of a lower permittivity. Parameters: $E_F = 0.1$ eV, $\gamma = 4$ THz, $T = 300$ K and $\omega = 2\pi \times 1$ THz.

We know from basic optics that when light propagates from a dense medium to a less dense medium, passing a certain incident angle, total internal reflection occurs. Therefore, it is interesting to investigate the effect of changing the angle of the incident electromagnetic wave. We will calculate the transmittance and reflectance of a structure consisting of a single graphene sheet sandwiched between two semi-infinite dielectric media with relative permittivities, $\epsilon_1 = 2.25$ and $\epsilon_2 = 1$ as depicted in Figure 5.3 for $\omega = 2\pi \times 1$ THz and $T = 300$ K. Using Snell's law of refraction, the critical angle of the structure is equal to 0.23π . It can be seen from Figure 5.6 that the transmittances calculated for both polarisations fall to zero at the critical angle as expected. The difference from the case without the graphene sheet is that the reflectances are not unity;

there is minor absorption due to the non-zero conductivity of graphene (see Figure 5.7). One interesting characteristic of the absorbances for p- and s-polarisations, arising due to the difference in the signs of ϵ_p and ϵ_s in the transmission matrix element, is that the absorbances approach two different values: one for the p-polarisation approaching 0, the other 0.04.

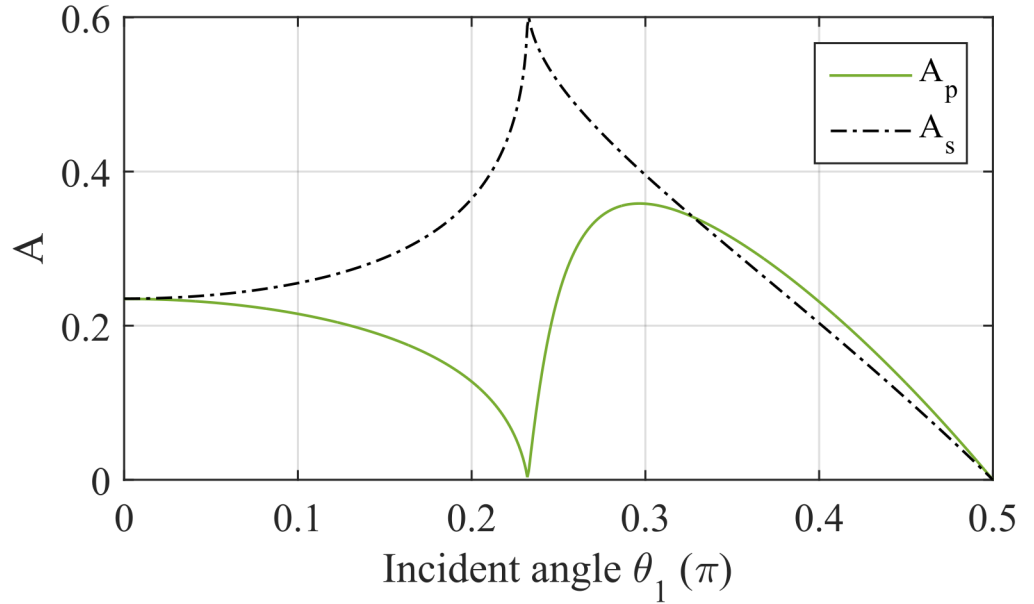


Figure 5.7: Absorbances for the system considered in Figure 5.6. At normal incident angle ($\theta_1 = 0$), the absorbances for both polarisations start from approximately the same value but they approach two different values at the critical angle and then go to zero. That the absorbance curves go in opposite directions before the critical angle is due to the difference in the signs of ϵ_p and ϵ_s in the transmission matrix element T_{21} .

5.3.3 Fabry-Pérot resonator

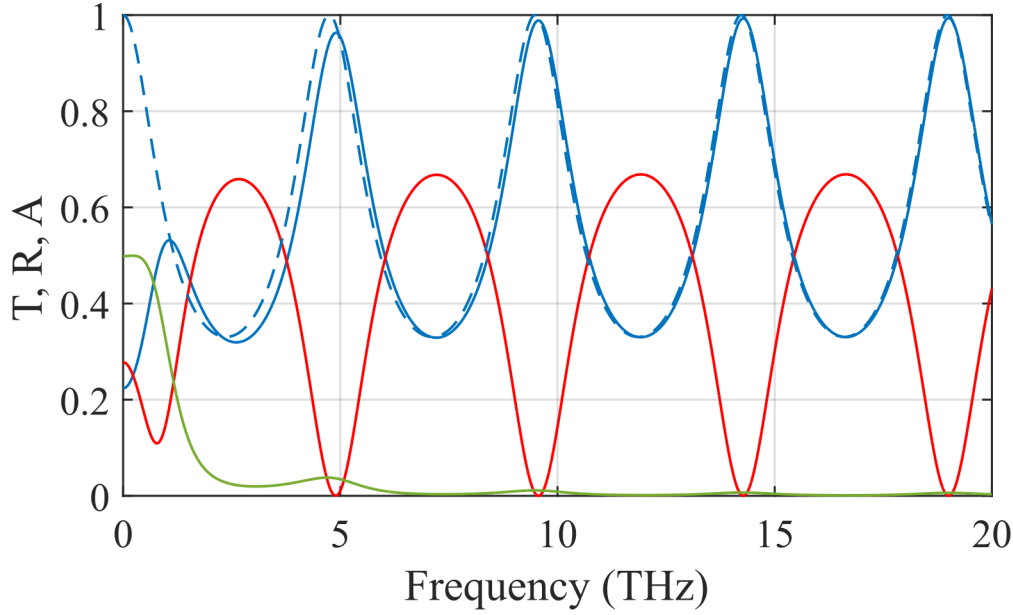


Figure 5.8: Transmittance (solid blue curve), reflectance (solid red curve) and absorbance (solid green curve) of p-polarised electromagnetic radiation at normal incident on a double-layer graphene structure (as depicted in Figure 5.4), suspended in a vacuum and calculated as a function of the frequency of the incident wave in the terahertz regime. The transmittance of the same structure but without graphene sheets – which can be considered as a Fabry-Pérot resonator – is added as a comparison (dashed blue curve). It can be seen that, compared to the typical Fabry-Pérot transmission resonance peaks of the sole dielectric slab, the positions and heights of the transmission resonance peaks of the two-layer graphene structure are shifted to the right and are lower, respectively, due to the high conductivity of graphene at the lower end of the frequency range shown. When the frequency increases, the behaviour of the two-sided graphene structure tends towards that of the sole dielectric slab as a result of the negligible graphene conductivity at high frequencies. Structural parameters: $d = 10 \mu\text{m}$, $\epsilon_d = 10$, $E_F = 0.1 \text{ eV}$, $\gamma = 4 \text{ THz}$ and $T = 300 \text{ K}$.

An interesting phenomenon in optics is Fabry-Pérot resonances, which happen when light propagates through an optical cavity with partially reflective surfaces on either side: light waves can pass through the Fabry-Pérot resonator only when they are in resonance with it. Therefore, we expect the transmittance to modulate with the frequency of the incident electromagnetic wave. Our graphene-based resonator consists of a dielectric slab of thickness, $d = 10 \mu\text{m}$, and relative permittivity, $\epsilon_d = 10$, sandwiched between two

graphene sheets which act as the partially reflective surfaces. The whole structure is at temperature, $T = 300$ K and suspended in vacuum, as depicted in Figure 5.4. The reason for choosing a high value of relative permittivity for the dielectric slab is to enhance the resonance effect so that we can see sharp transmittance peaks. A typical Fabry-Pérot resonator of the same structure, but without the graphene sheets, will be used to compare the characteristics of the transmittances. We can see in Figure 5.8 that the positions and heights of the transmission resonance peaks of the two-sided graphene resonator (solid blue curve) are shifted to the right and are lower, respectively, than those of the typical Fabry-Pérot resonator (dashed blue curve). The characteristics of the transmittance of the two-sided graphene resonator tend towards those of the typical Fabry-Pérot resonator at high frequencies as the graphene's optical conductivity gets very low for high energy photons. Another interesting feature due to the presence of the graphene sheets is the appearance of a significant percentage of absorption at low frequencies.

5.3.4 Periodic graphene layers

The last thing we will investigate in this chapter is the emergence of photonic band gaps, caused by Bragg scattering, in so-called photonic crystals [27, 59, 113]. Here, we expect a forbidden range of electromagnetic wave frequencies where the transmittance is close to zero for graphene-based periodic structures. The structure that we consider is the same structure considered in page 44 in [46], which consists of 50 graphene layers, each separated by a dielectric slab with relative permittivity, $\epsilon_d = 4$, and thickness, $d = 30 \mu\text{m}$, the whole structure being embedded in vacuum. We could have added more layers of graphene, but 50 layers should suffice in terms of results and also give acceptable simulation time. We set the Fermi energy of graphene, E_F , to 0.5 eV and we also set the damping constant, γ , to zero to get rid of absorption effects. The analytic expression for the photonic band structure of a 1D

periodically infinite structure for electromagnetic waves at normal incident is given by [88, 118]

$$\cos(q_B d) = \cos(k_z d) - \frac{i\xi}{2} \sin(k_z d), \quad (5.29)$$

where q_B is Bloch wavevector, k_z is the z -component of the wavevector in the dielectric slab, $\xi = \xi_p, \xi_s$ for p-polarisation and s-polarisation, respectively.

We can see in the top panel of Figure 5.9 that there is a photonic band gap spanning in the 2.5 - 3 THz region in which the propagation of the electromagnetic wave is forbidden. Although the reflectance is 1, as in the case of total internal reflection, this phenomenon is different because it originates from destructive interference of the scattered electromagnetic waves inside the structure, which follows from the absence of the plane wave solutions of Maxwell's equations. The bottom panel shows the transmittance and reflectance of the 50-layer-graphene structure. The plot exhibits two features. Firstly, the transmittance curve exhibits oscillations, which are the manifestation of multiple of Fabry-Pérot resonances. Secondly, the transmittance falls to zero in the same frequency range as that of the photonic band gap. We can see that all the characteristics we expected appear in the transmittance plot, which confirms the validity and potential of the transfer-matrix method.

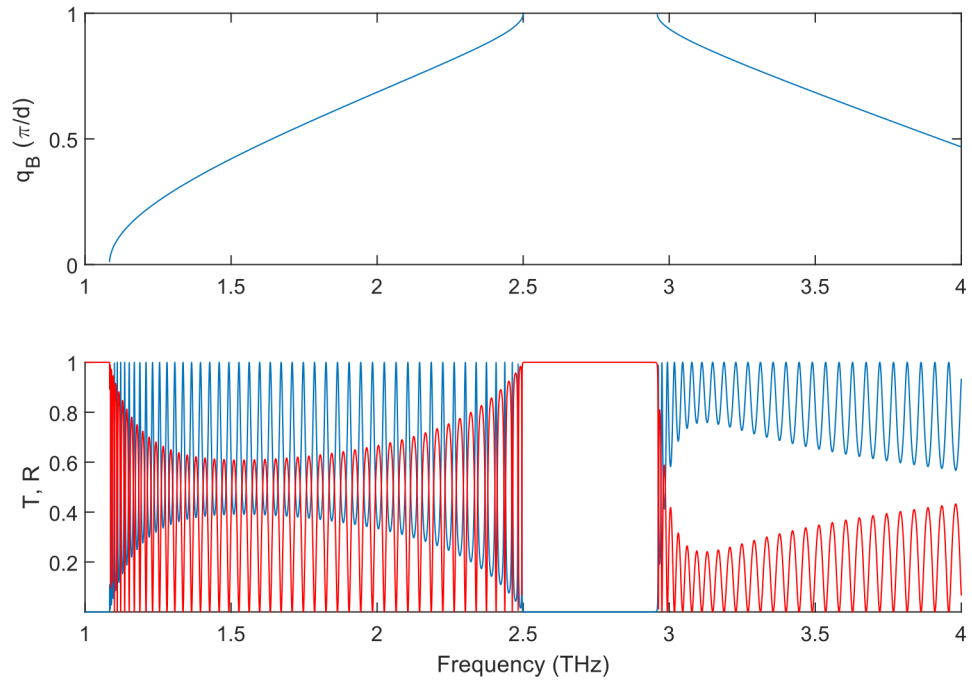


Figure 5.9: Top panel: Photonic band-structure, in the first Brillouin zone, calculated for a graphene-based photonic crystal composed of an infinite number of graphene layers, each separated by a dielectric slab with relative permittivity, ϵ_d , and thickness, d , embedded in vacuum (q_B stands for Bloch's momentum); in the 2.5 - 3 THz region, electromagnetic wave propagation is forbidden. Bottom panel: Transmittance (blue), reflectance (red) of p-polarised electromagnetic radiation at normal incident on 50 graphene layers, each separated by a dielectric slab with relative permittivity, ϵ_d , and thickness, d , embedded in vacuum; the modulation of the transmittance curve shows the manifold of Fabry-Pérot resonances; the transmittance is zero in the frequency range where there is a photonic band gap. Structural parameters: $d = 30 \mu\text{m}$, $\epsilon_d = 4$, $E_F = 0.5 \text{ eV}$, $\hbar\gamma = 0 \text{ meV}$ and $T = 0 \text{ K}$.

5.4 Chapter Summary

We have laid out the theoretical foundations (both analytical and numerical) for finding the optical conductivity of monolayer graphene and for calculating the electromagnetic scattering coefficients of graphene-based planar structures. Simulations have been presented to confirm the validity and versatility of the transfer-matrix method. In the remaining chapters, this method will be heavily used to investigate the effect of the multilayer on nearby atoms.

Chapter 6

Casimir-Polder Attraction

6.1 Dispersion Forces

6.1.1 The concept of nothing in quantum physics

There are various concepts for the state of nothing but here we will look into the concept that many physicists nowadays are fond of. First of all, the term that physicists commonly use for **nothing** is **vacuum**. The vacuum of quantum physics is a region of space from which matter and radiation have been removed as completely as possible. Quantum theory proposes that, in the quantum vacuum – the energy ground-state of space, there are fluctuations of virtual particles and photons: they, purely randomly on their own, come into existence for a very short moment at any instant. The coming into existence and the vanishing of virtual particles and photons cannot be observed directly [13].

6.1.2 Fluctuations of virtual photons

What we might exploit here to find the evidence that virtual photons exist is that virtual photons, once created, obey the same physical laws as real photons. Both real and virtual photons are electromagnetic waves. A boundary condition such as a perfectly conducting mirror restricts the behaviour of electromagnetic waves: A node must be formed on the mirror surface. The

exciting consequence start from here onward. When we place two mirrors into the quantum vacuum, nodes must be formed on each mirror surface allowing for only virtual photons of certain discrete wavelengths to exist between them, see Figure 6.1. On the other hand, arbitrary wavelengths are allowed for virtual photons outside the mirrors. That the space between the mirrors allows for fewer different types of photons than does the space on the outside, creates a net imbalance of forces originating from the process in which the photons, actually present at any given instant of time, hit the mirror surfaces. As a result, there is a net attractive force between the two mirrors. This effect was first described by Hendrik Casimir [19].

6.1.3 Fluctuations of virtual particles

Let us consider two small particles such as atoms, each containing equal amounts of positive and negative electric charges. In quantum physics, the distribution of charges in each atom is not uniform and is asymmetric: There are fluctuations of real charges due to interaction with virtual photons created in accordance with Heisenberg's Uncertainty Principle. As a result, the two atoms interact with each other via non-vanishing electromagnetic forces. In this case, the resulting net force between them is attractive. Why the net force is attractive can be understood by realising that the fluctuations of real charges on both atoms are coupled together; when the charges inside one atom are distributed in a way that the negative charges lean towards the other atom in an instant of time, i.e. the charges form an electric dipole, the positive charges of the second atom are more likely to lean towards the negative charges of the first atom. The attractive force between two neutral particles is commonly known as the van der Waals (vdW) force.

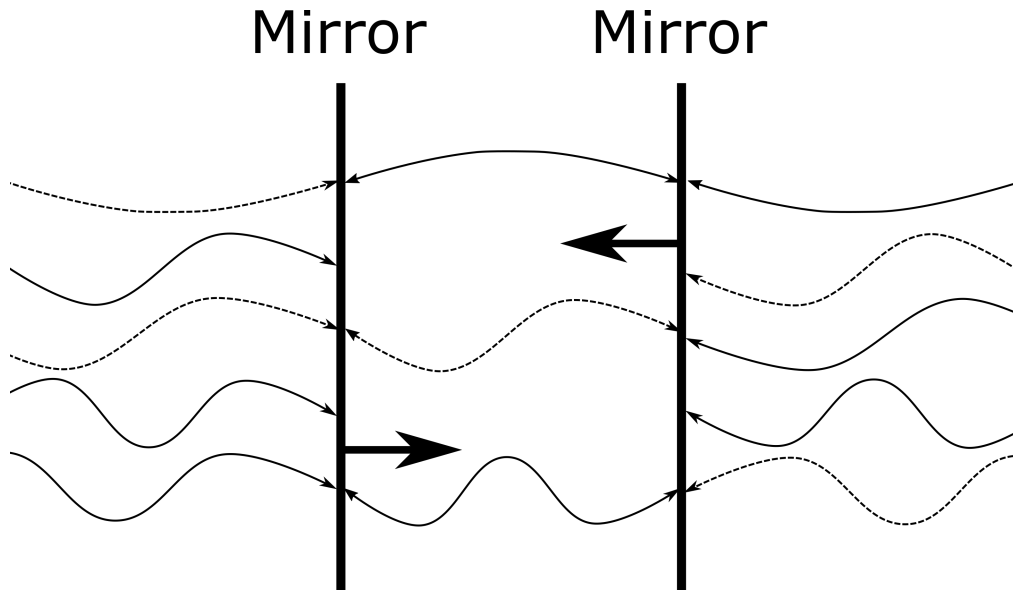


Figure 6.1: A schematic diagram showing the attractive Casimir force between two parallel mirrors in vacuum: The dashed waves represent allowed virtual photons, while the solid waves represent the virtual photons randomly present at a given instant of time as a result of quantum fluctuations.

6.1.4 The link between charges and field

We can now see that virtual photons are the manifestation of quantum fluctuations of an electromagnetic field, while randomly fluctuating electric dipoles in neutral ensembles of charged particles are the manifestation of quantum fluctuations of charges. To put it elegantly, fluctuating charges give rise to fluctuating fields and vice versa.

We did not mention the fluctuation of charges in the case of the Casimir force before. However, if we look closely how the mirrors can impose such boundary conditions for electromagnetic fields, the sources of the fluctuating charges must be inside the mirrors. The random motion of charges inside the mirrors induces an electric field which, in turn, cancels out the electric field of virtual photons on the surface. As for the case of the vdW force, virtual photons act on the charges inside an ensemble of particles giving rise to fluctuating charges which, in turn, give rise to fluctuating fields, which act on the other charges. Effective Lorentz forces due to quantum fluctuations of charges and electromagnetic fields which act between well-separated neutral,

unpolarised and unmagnetised atoms or bodies in the absence of any applied electromagnetic fields, such as Casimir and vdW forces, are known as **dispersion forces** [13, 14].

6.2 Casimir-Polder Forces

Dispersion forces between atoms and bodies are commonly referred to as Casimir-Polder (CP) forces [20]. The historical reason behind this name is that the calculation of the dispersion force on an atom in the presence of magnetoelectric bodies was first done by Casimir and Polder. Their approach is that they considered the shift of the ground-state energy due to the atom-field interaction under the assumption that both atom and field were prepared in their ground-state; in other words, the atom and field interact with each other via virtual photons only. The position-dependent part of this energy shift is taken to define the CP potential

$$U(\mathbf{r}_A) = \Delta E(\mathbf{r}_A), \quad (6.1)$$

where $\mathbf{r}_A$ is the position of the centre of mass of the atom with respect to the body.

In order to advance their concept further to use in situations, such as atom chip systems, in which the atoms are not in their ground-state and can emit real thermal photons to excite the field, we need to account for the dependence of temperature in our analysis.

In this section, we are going to present the expression of the thermal CP potential derived by using the perturbation theory. The method used relies on Born-Oppenheimer approximation, assuming that the fast internal, electronic motion effectively decouples from the slow centre-of-mass motion [14].

Following the normal routine in the perturbation theory, we start by defining

the energy eigenstate in which the uncoupled system, with the Hamiltonian $\hat{H} = \hat{H}_A + \hat{H}_F$, where $\hat{H}_A$ and $\hat{H}_F$ are the atom and field Hamiltonians, respectively, was initially prepared.

The initial energy eigenstate of the uncoupled system can be described by a density matrix

$$\hat{\rho} = \sum_{\psi} p_{\psi} |\psi\rangle \langle \psi|, \quad (6.2)$$

where p_{ψ} are the probabilities of finding the uncoupled system, initially, in the states $|\psi\rangle$.

The energy shift is now an average and is given by [14]

$$\langle \Delta E \rangle \approx \sum_{\psi} p_{\psi} \langle \psi | \hat{H}_{AF} | \psi \rangle + \sum_{\psi} p_{\psi} \sum_{I \neq \psi} \frac{\langle \psi | \hat{H}_{AF} | I \rangle \langle I | \hat{H}_{AF} | \psi \rangle}{E_{\psi} - E_I}, \quad (6.3)$$

where $\hat{H}_{AF}$ is the atom-field Hamiltonian.

For an atom in an incoherent superposition of internal-energy eigenstates,

$$\hat{\sigma} = \sum_n p_n |n\rangle \langle n|, \quad (6.4)$$

with the field being in a thermal state $\hat{\rho}_T$ of uniform temperature T , the uncoupled atom-field system reads $\hat{\rho} = \hat{\sigma} \otimes \hat{\rho}_T$.

Lastly, the non-resonant (nres) component of the CP potential, which is our only interest, for an atom in an isotropic state $\hat{\alpha}$ is given by [14, 15]

$$U_n^{\text{nres}}(\mathbf{r}_A) = \mu_0 k_B T \sum_{j=0}^{\infty} \xi_j^2 \alpha_n(i\xi_j) \text{tr } \mathbf{G}^{(1)}(\mathbf{r}_A, \mathbf{r}_A, i\xi_j), \quad (6.5)$$

where $\xi_j = 2\pi k_B T j / \hbar$, $j = 0, 1, 2, \dots$, are commonly known as the Matsubara frequencies [76], α_n is the isotropic atomic polarisability, k_B is the Boltzmann constant,

$$\mathbf{G}^{(1)}(\mathbf{r}_A, \mathbf{r}_A, i\xi) = \frac{1}{8\pi} \int_{\xi/c}^{\infty} d\kappa^{\perp} e^{-2\kappa^{\perp} z_0} \left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} r_s - \frac{c^2}{\xi^2} \begin{pmatrix} \kappa^{\perp 2} & 0 & 0 \\ 0 & \kappa^{\perp 2} & 0 \\ 0 & 0 & 2k^{\parallel 2} \end{pmatrix} r_p \right] \quad (6.6)$$

is the scattering part of the Green's tensor, where z_0 is the distance between the surface and the centre of mass of the atom (see Figure 6.2),

$$k^{\parallel} = \sqrt{\kappa^{\perp 2} - \frac{\xi^2}{c^2}}. \quad (6.7)$$

The prime on the Matsubara sum (6.5) indicates that the $j = 0$ term carries half-weight and tr denotes the trace operator. More details on the Green's function can be found in the next chapter.

6.3 Numerical Results for the Casimir-Polder Potential in various layered planar media

Now that we are equipped with the necessary tools, we can investigate the characteristics of the Casimir-Polder potential in various planar stratified media. The schematic diagram of the system of planar stratified media of interest is shown in Figure 6.2: the planar structure consists of N thin conducting layers (black horizontal lines, labelled $1, 2, 3, \dots, N-2, N-1, N$ and dielectric slabs, each with thickness d (coloured pink); the x - and y -dimensions of all layers are infinite; an atom (blue circle) is trapped in free space at distance z_0 above layer 1. The reason we are interested in such planar systems is that the systems can be thought of as simplified models for atom chips; it is crucial to know the limitations in trapping distance due to the Casimir-Polder attraction. Note that in all considered cases, the systems are in thermal equilibrium at $T = 300 \text{ K}$.

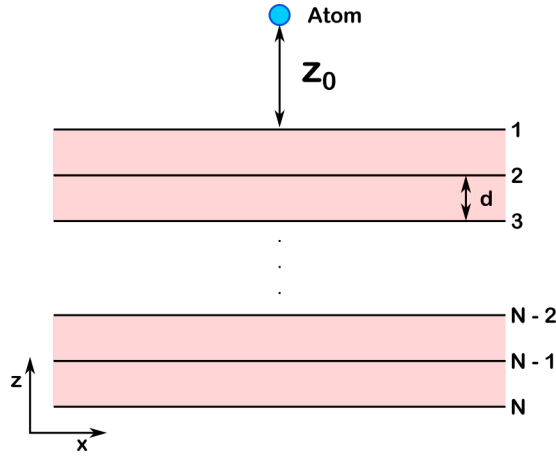


Figure 6.2: Schematic diagram of the planar structure and nearby atom: the planar structure consists of N thin conducting layers (black horizontal lines, labelled 1, 2, 3, ..., $N - 2$, $N - 1$, N and dielectric slabs, each with thickness d (coloured pink); the x - and y -dimensions of all layers are infinite; an atom (blue circle), subjected to the Casimir-Polder attraction associated with the presence of the planar structure, is trapped in free space at distance z_0 above layer 1

6.3.1 Single-material system

We start with investigating the Casimir-Polder potential of a single graphene sheet influencing a hydrogenic atom such as ^7Li and ^{87}Rb for the $n = 1$ case in (6.5). The reason for comparing two different elements is that we want to investigate the effect of the atomic polarisability. We only consider the atomic polarisability of the form

$$\alpha_1(i\xi_j) = \frac{\alpha_0 \omega_T^2}{\omega_T^2 + \xi_j^2}, \quad (6.8)$$

where $\alpha_0 = 2.70 \times 10^{-39} \text{ Fm}^2$ and $5.27 \times 10^{-39} \text{ Fm}^2$ is the static polarisability for ^7Li and ^{87}Rb atoms, respectively [99]. Here, the atomic transition frequency, $\omega_T = 2.8 \times 10^{15} \text{ s}^{-1}$, taken at the wavelength of 671 nm for ^7Li and $2.4 \times 10^{15} \text{ s}^{-1}$, the characteristic transition frequency of the D2 line transition at the wavelength of 780 nm for ^{87}Rb [103, 116].

Following the transfer-matrix method outlined in Chapter 5, we calculate the

reflection coefficients of various systems with graphene's parameters $E_F = 0.1$ eV, $\gamma = 4$ THz, $T = 300$ K.

The calculated results are shown in Figure 6.3. The Casimir-Polder potential is distance-dependent: the attraction between the graphene layer and the atom is stronger when the separation is smaller and it increases rapidly below the sub-micron distance. Additionally, the attraction is stronger for the ^{87}Rb atom than the ^7Li atom as rubidium has higher polarisability.

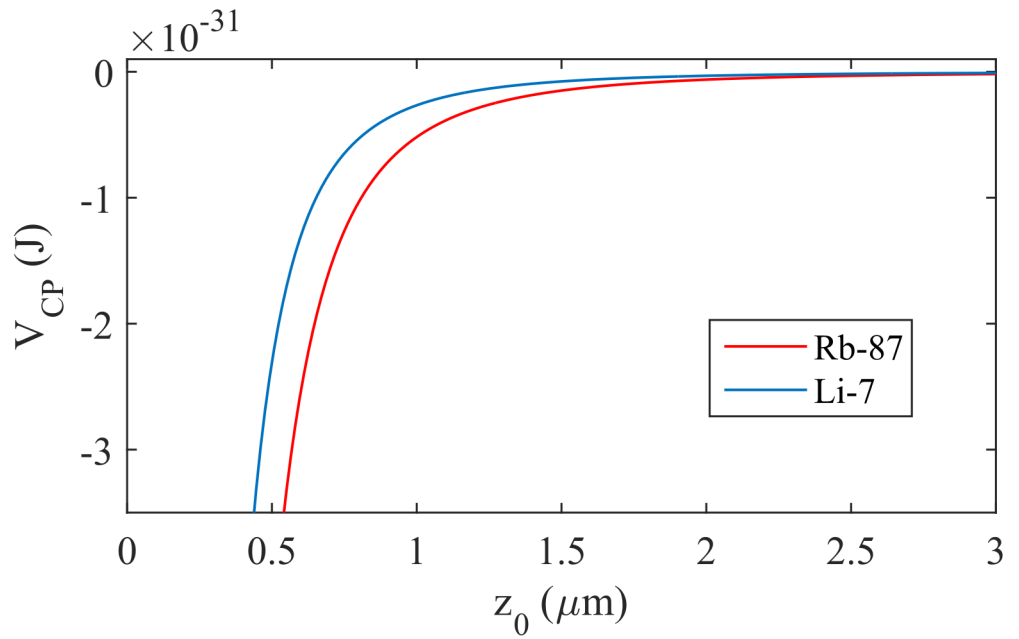


Figure 6.3: Casimir-Polder potential, calculated versus distance, z_0 , from a single graphene layer in free space for a ^{87}Rb atom (red curve) and a ^7Li atom (blue curve) in thermal equilibrium. The Casimir-Polder potential for the ^{87}Rb atom is more negative than that of the ^7Li atom as rubidium has higher polarisability. Parameters: $E_F = 0.1$ eV, $\gamma = 4$ THz, $T = 300$ K.

Next we compare the Casimir-Polder attraction calculated for an ^{87}Rb atom versus the separation distance, from four different layers of single material: a 125 nm-thick gold plate, a 125 nm-thick sapphire plate, a monolayer graphene, and a monolayer hBN.

The generalised Fresnel reflection coefficients of a plate of finite thickness, d , are given by [13]

$$r_s = \frac{[\mu^2(i\xi)\kappa_1^{\perp 2} - \kappa_1^{\perp 2}] \tanh(\kappa_1^{\perp} d)}{2\mu(i\xi)\kappa_1^{\perp} \kappa_1^{\perp} + [\mu^2(i\xi)\kappa_1^{\perp 2} + \kappa_1^{\perp 2}] \tanh(\kappa_1^{\perp} d)}, \quad (6.9)$$

$$r_p = \frac{[\epsilon^2(i\xi)\kappa_1^{\perp 2} - \kappa_1^{\perp 2}] \tanh(\kappa_1^{\perp} d)}{2\epsilon(i\xi)\kappa_1^{\perp} \kappa_1^{\perp} + [\epsilon^2(i\xi)\kappa_1^{\perp 2} + \kappa_1^{\perp 2}] \tanh(\kappa_1^{\perp} d)}, \quad (6.10)$$

where $\kappa_1^{\perp} = \sqrt{(\epsilon(i\xi)\mu(i\xi)\xi^2/c^2) + k^2}$, $\epsilon(i\xi)$ and $\mu(i\xi)$ are the frequency-dependent permittivity and permeability of the plate.

The permittivity of gold follows from the Drude-Sommerfeld free-electron model and is given by [89]

$$\epsilon_{\text{gold}}(\xi) = 1 - \frac{\omega_p^2}{\xi^2 + i\Gamma\xi}, \quad (6.11)$$

where $\omega_p = 1.38 \times 10^{16} \text{ s}^{-1}$ is the plasma frequency and $\Gamma = 1.075 \times 10^{14} \text{ s}^{-1}$ is the electron relaxation rate.

$$\epsilon_{\text{sapphire}}(\xi) = \eta + \frac{\omega_p^2}{\omega_T^2 - \xi^2 - i\Gamma\xi}, \quad (6.12)$$

where $\eta = 2.71$, $\omega_p = 2.12 \times 10^{14} \text{ s}^{-1}$, $\omega_T = 1.08 \times 10^{14} \text{ s}^{-1}$, $\Gamma = 2.31 \times 10^{12} \text{ s}^{-1}$.

The reflection coefficients of the hBN single layer are obtained using the transfer-matrix method, where the optical conductivity of ultra-thin hBN slab is given by [18, 44, 65, 84]

$$\sigma_{\text{hBN}}(\xi) = \epsilon_0 \xi d [\epsilon_{\perp, \text{hBN}}(\xi) - \epsilon_{\perp}(\infty)], \quad (6.13)$$

where the frequency-dependent dielectric constant of hBN is given by

$$\epsilon_{\perp, \text{hBN}}(\xi) = \epsilon_{\perp}(\infty) + \frac{s_{\nu} \omega_{\nu}^2}{\omega_{\nu}^2 - i\gamma_{\nu} \xi - \xi^2}, \quad (6.14)$$

where $\omega_\nu = 2.58 \times 10^{14} \text{ s}^{-1}$, $\gamma = 1.319 \times 10^{12} \text{ s}^{-1}$, $s_\nu = 1.83$, $\epsilon_\perp(\infty) = 4.87$ were calculated from first principles [18, 109], and $d = 0.335 \text{ nm}$.

The plot of the Casimir-Polder potential for a ^{87}Rb atom trapped above the aforementioned layers is shown in Figure 6.4. The thick gold slab yields stronger Casimir-Polder attraction, as expected from the larger reflection coefficients compared to those of single-layer materials. The Casimir-Polder potential of a single hBN layer is far weaker than that of a single graphene layer for sub-micron atom-surface distances even though their crystal structures are very similar because hBN is an insulator.

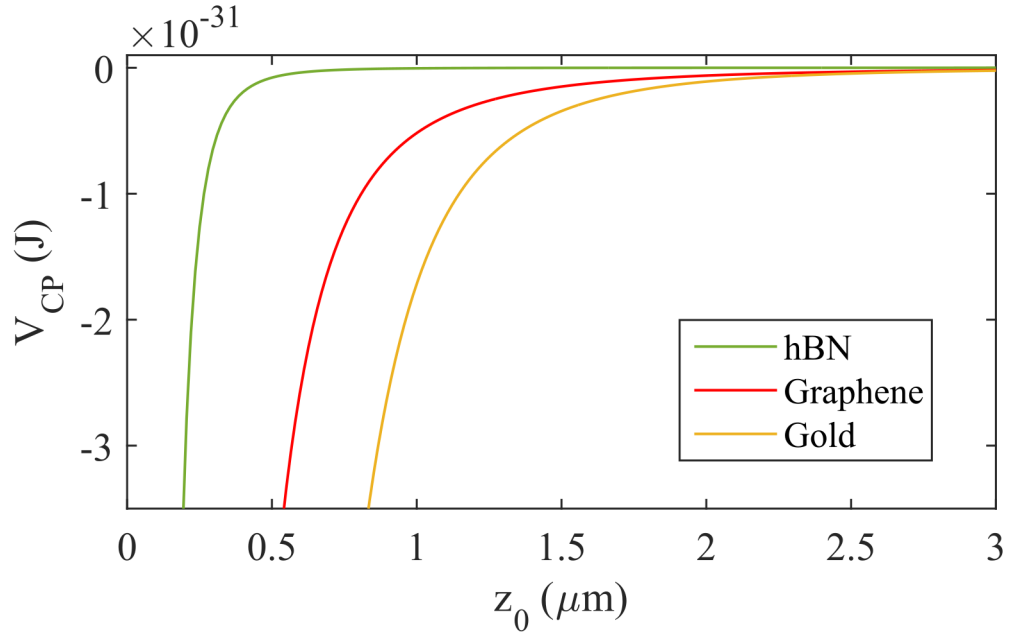


Figure 6.4: Casimir-Polder potential calculated for a ^{87}Rb atom near a 125 nm-thick gold plate (yellow curve), a monolayer of graphene (red curve), and a monolayer of hBN (green curve) in vacuum in thermal equilibrium at $T = 300 \text{ K}$ as a function of the distance from the surface. Different models are used for calculating the dielectric constant of the materials: the Drude-Sommerfeld free-electron model is used for gold ($\omega_p = 1.38 \times 10^{16} \text{ s}^{-1}$, $\Gamma = 1.075 \times 10^{14} \text{ s}^{-1}$); Kubo's formula for graphene ($E_F = 0.1 \text{ eV}$, $\gamma = 4 \text{ THz}$); the four-parameter semi-quantum model for hBN ($\omega_\nu = 2.58 \times 10^{14} \text{ s}^{-1}$, $\gamma = 1.319 \times 10^{12} \text{ s}^{-1}$, $s_\nu = 1.83$).

Figure 6.5 shows the associated acceleration experienced by a ^{87}Rb atom in

the presence of Casimir-Polder potential versus the separation distance. For all the layers, in the sub-micron regime, the acceleration is the same order of magnitude as that of the gravitational acceleration, whereas, in the sub-nano regime, the Casimir-Polder acceleration gets stronger very quickly. We can see that, for a single graphene layer, moving half a micron closer, from $1\text{ }\mu\text{m}$ to $0.5\text{ }\mu\text{m}$, the acceleration is about 10 times stronger. At the distance just above $0.5\text{ }\mu\text{m}$, the Casimir-Polder acceleration is of the same magnitude as that of the gravitational acceleration. In order to negate the effect of the Casimir-Polder attraction in graphene-based atom chips, we may arrange the trap in such a way that the gravitational pull is in the opposite direction to the direction of the Casimir-Polder attraction ensuring that trapping at the distance about $0.5\text{ }\mu\text{m}$ can be achieved.

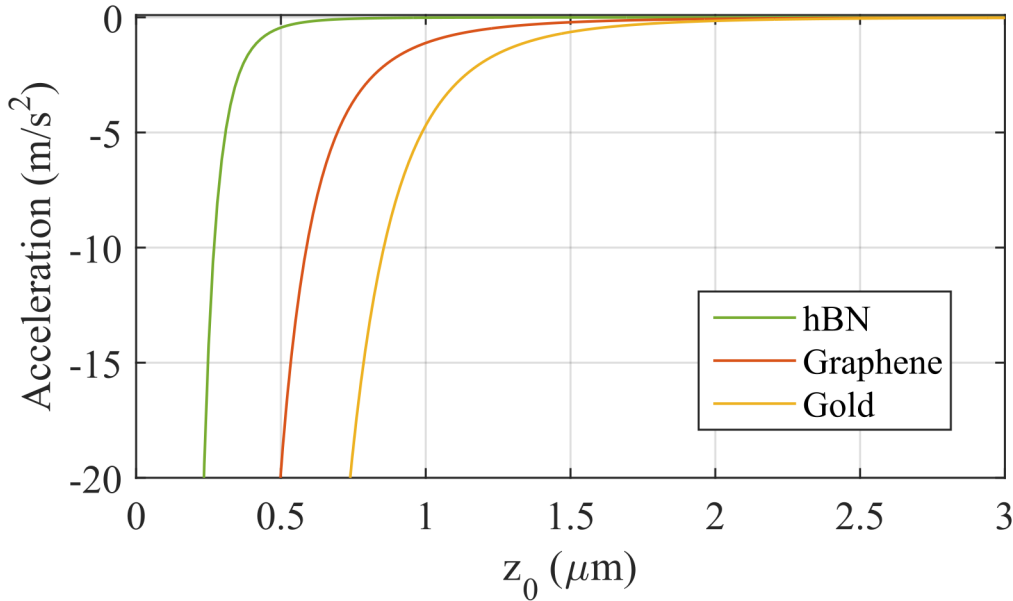


Figure 6.5: The associated acceleration due to the Casimir-Polder potential for a ^{87}Rb atom, calculated from the potential energy profiles shown in Figure 6.4.

6.3.2 Graphene-encased structures

We investigate the Casimir-Polder potential near a more complicated structure consisting of an hBN slab of thickness, d , sandwiched between two layers of

graphene. We use two samples of hBN slabs: the first is a very thin slab of thickness, $d = 1.4 \text{ nm}$, characterised by a frequency-dependent dielectric constant according to the four-parameter semi-quantum model as described in the previous section, the second is a thicker slab of thickness, $d = 0.5 \text{ }\mu\text{m}$, characterised by a dielectric constant, $\epsilon_{\text{hBN}} = 3.25$ [28]. The reflection coefficients are obtained using the transfer-matrix method. The results of our Casimir-Polder potential versus distance calculations are shown in Figure 6.6. The calculated Casimir-Polder potential for the first structure is fairly close to that of a single layer of graphene. This seems reasonable as the Casimir-Polder attraction of the monolayer hBN is extremely weak (Figure 6.4). That the Casimir-Polder attraction is still relatively weak for the combination of monolayer graphene and hBN shows the possible robustness of graphene-based atom chips. For the second structure with a thicker hBN slab, the characteristics of the Casimir-Polder potential go towards those of thick metallic plates.

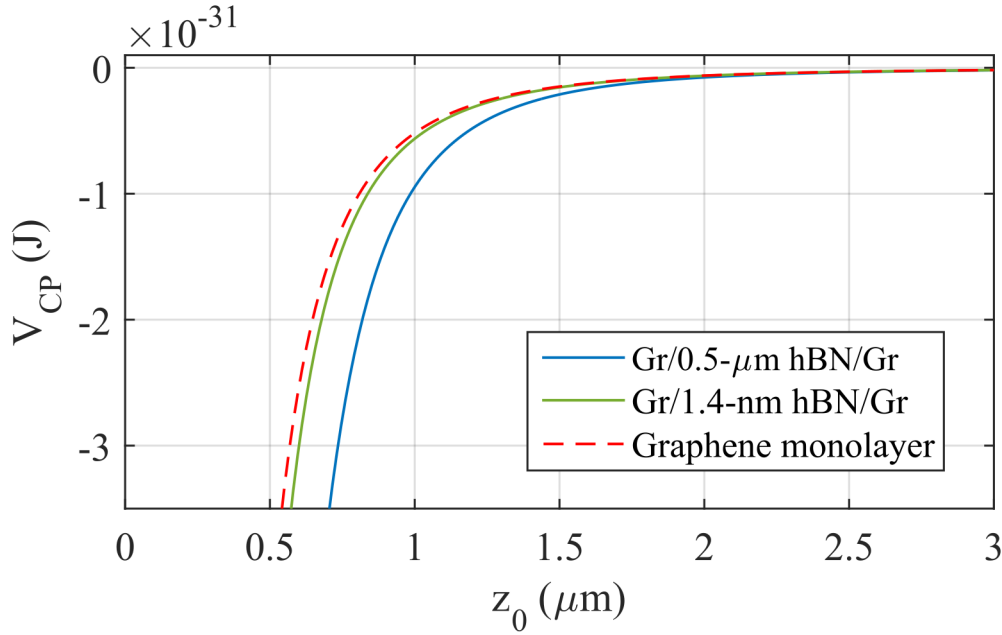


Figure 6.6: Casimir-Polder potential calculated for a ^{87}Rb atom near three different structures in vacuum in thermal equilibrium at $T = 300\text{ K}$ as a function of the distance from the surface: (green curve) a two-sided graphene structure, in which the two graphene layers enclose an hBN dielectric slab with thickness, $d = 1.4\text{ nm}$, characterised by a frequency-dependent dielectric constant according to the four-parameter semi-quantum model, (blue curve) a two-sided graphene structure, enclosing a slab of hBN with thickness, $d = 0.5\text{ }\mu\text{m}$, characterised by a dielectric constant, $\epsilon_{\text{hBN}} = 3.25$, and (dashed red curve) a monolayer graphene. Parameters: (for graphene) $E_F = 0.1\text{ eV}$, $\gamma = 4\text{ THz}$; (for hBN) $\omega_\nu = 2.58 \times 10^{14}\text{ s}^{-1}$, $\gamma = 1.319 \times 10^{12}\text{ s}^{-1}$, $s_\nu = 1.83$.

Next, we investigate the Casimir-Polder potential versus the hBN thickness enclosed by two graphene layers, where the permittivity of the hBN follows from three different models: the first is a single slab of constant relative permittivity, $\epsilon_{\text{hBN}} = 3.25$, the second is a single slab characterised by the frequency-dependent dielectric constant according to the four-parameter semi-quantum model, the last is a stack of hBN monolayers. For the last model, the structure is as depicted in Figure 6.2 with graphene as the top- and bottom-most layers and multiple layers of hBN in between, each separated by a layer of vacuum with thickness $= 0.335\text{ nm}$. The remaining layers, from 2 to $N - 1$, are hBN, modelled such that the conductivity of each hBN layer is that of a hBN monolayer of thickness, $= 0.335\text{ nm}$, calculated according to the four-parameter semi-quantum model. Note that the transfer-matrix method for calculating

the reflection coefficients for the structure treats all conductive layers as having zero thickness.

Figure 6.7 shows the Casimir-Polder potential experienced by a ^{87}Rb atom trapped at $z_0 = 1\text{ }\mu\text{m}$, versus the thickness of the whole planar structure. The first two models give similar qualitative results: the Casimir-Polder attraction increases toward the values for bulk materials as the thickness increases. This is expected even though the conductivities are different, the hBN layers are still single slabs. The last model produces a surprisingly different result. The Casimir-Polder Potential reaches its peak at thickness $\sim 0.1\text{ }\mu\text{m}$, then decreases as the thickness decreases. Unfortunately, our computing power did not allow calculations beyond thickness of about $0.6\text{ }\mu\text{m}$, limiting our investigations of the impacts of the crystal structures on the Casimir-Polder potential.

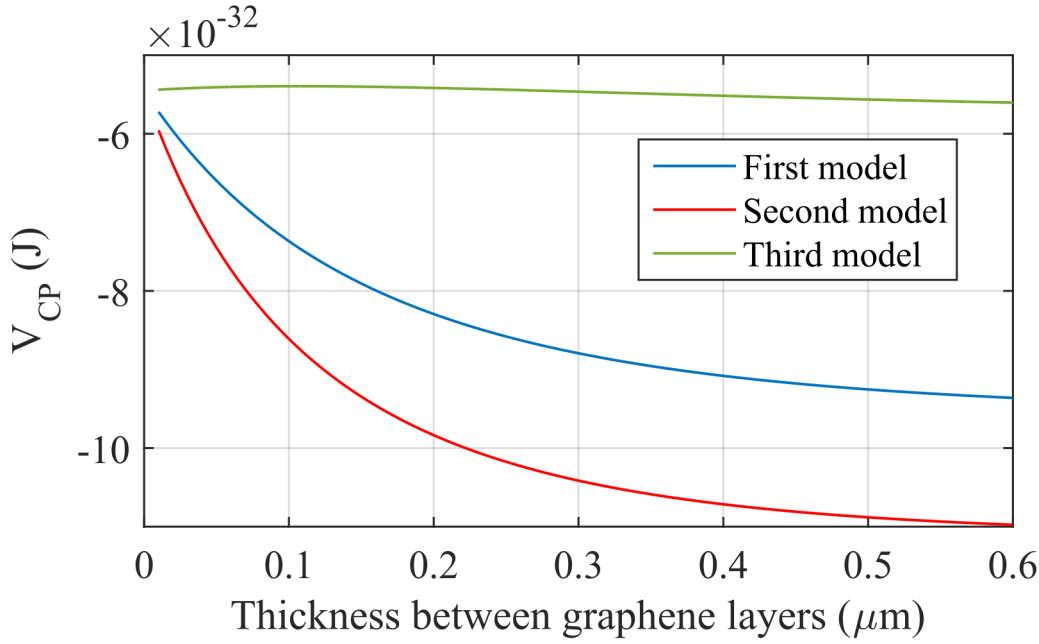


Figure 6.7: Casimir-Polder potential for a ^{87}Rb atom trapped at $z_0 = 1\text{ }\mu\text{m}$ above a two-sided graphene structure as a function of the thickness, d , of the dielectric slab (hBN) sandwiched between the graphene layers. The hBN is modelled using three methods: (red curve) a single slab with constant relative permittivity, $\epsilon_{\text{hBN}} = 3.25$, (green curve) a single slab characterised by a frequency-dependent dielectric constant according to the four-parameter semi-quantum model, (blue curve) a stack of hBN monolayers, each characterised by a frequency-dependent optical conductivity according to the four-parameter semi-quantum model. The first two models produce similar results qualitatively, while the third model shows that the Casimir-Polder potential goes up slightly then decreases as the thickness decreases. Parameters: (for graphene) $E_F = 0.1\text{ eV}$, $\gamma = 4\text{ THz}$, $T = 300\text{ K}$; (for hBN) $\omega_\nu = 2.58 \times 10^{14}\text{ s}^{-1}$, $\gamma = 1.319 \times 10^{12}\text{ s}^{-1}$, $s_\nu = 1.83$.

Figure 6.8 shows the comparison of Casimir-Polder potential, experienced by a ^{87}Rb atom trapped at $z_0 = 1\text{ }\mu\text{m}$ above the surface of three different structures, each with thickness, $d = 0.01 - 0.6\text{ }\mu\text{m}$: (red curve) a two-sided graphene structure with a hBN slab characterised by a constant relative permittivity, $\epsilon_{\text{hBN}} = 3.25$, with thickness d , (golden curve) a gold slab, (black dashed curve) a perfectly conducting metal plate ($r_s = -1, r_p = +1$). We can see that the Casimir-Polder attraction from the two-sided graphene structure is much lower than those from the gold slab and perfectly conducting metal plate. The slight curve at the start for gold must be from the fact that gold with thickness below 125 nm does not behave as bulk gold [97]; therefore, the Drude model does not

hold in that regime.

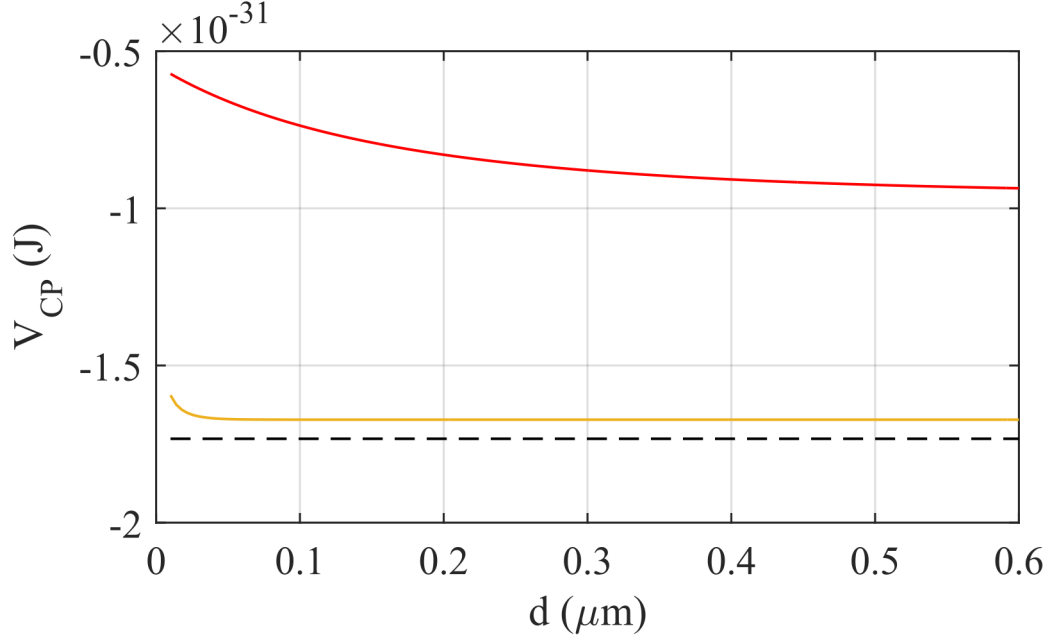


Figure 6.8: Comparison of the Casimir-Polder potential for a ^{87}Rb atom trapped at $z_0 = 1 \mu\text{m}$ above the surface of a two-sided graphene structure, with an hBN slab of thickness, d , characterised by $\epsilon_d = \epsilon_{\text{hBN}} = 3.25$ (red curve), gold slab (golden curve), perfectly conducting metal (black dashed curve) as a function of the thickness, d . Parameters: (for graphene) $E_F = 0.1 \text{ eV}$, $\gamma = 4 \text{ THz}$, $T = 300 \text{ K}$; (for gold) $\omega_p = 1.38 \times 10^{16} \text{ s}^{-1}$, $\Gamma = 1.075 \times 10^{14} \text{ s}^{-1}$.

6.3.3 Gated graphene heterostructure

We have seen that we can change the characteristics of the Casimir-Polder potential by changing the structural parameters, but this is not dynamic in the sense of being able to vary the potential near a single structure. Can we find a way to manipulate the Casimir-Polder attraction by altering the electronic properties of graphene layers?

In the preceding chapter, we showed that, for a Gr/hBN/Gr heterostructure, applying a gate voltage can change the Fermi energy of the layers. Therefore, in this chapter, we will investigate the alteration of the Casimir-Polder potential with variation of the Fermi energy in a gated Gr/hBN/Gr structure consisting of a 1.4 nm-thick monolayer hBN sandwiched between two graphene

monolayers. First of all, to simplify our model, the effect of the tunnel current across the hBN layer will be neglected. Secondly, the size of the 2-dimensional structure is considered large enough that the given Green's tensor is acceptably valid.

Figure 6.9 shows a colour map of the Casimir-Polder potential, felt by a ^{87}Rb atom trapped at $z_0 = 0.3\text{ }\mu\text{m}$, versus the Fermi energies of the top and bottom graphene layers. The Casimir-Polder potential is weakest at the middle corresponding to the case in which both graphene layers are electrically neutral. The Casimir-Polder attraction gets stronger as the magnitudes of the Fermi energies increase.

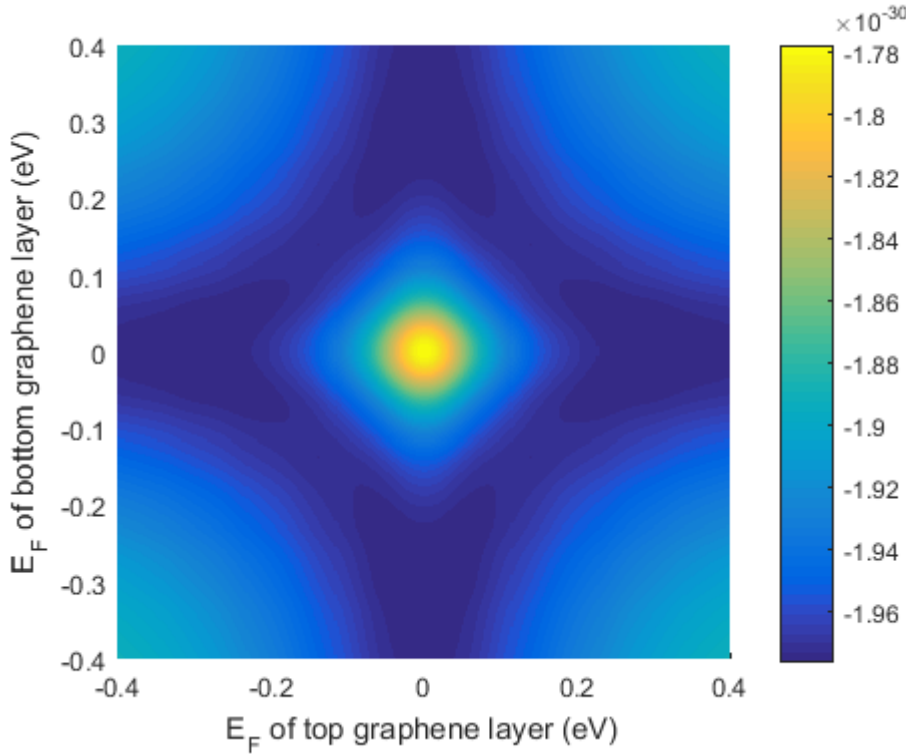


Figure 6.9: Colour map of the Casimir-Polder potential (in joules), experienced by a ^{87}Rb atom trapped at $z_0 = 0.3\text{ }\mu\text{m}$, versus the Fermi energies of the top and bottom graphene layers.

An interesting question involving quantum sensors is how sensitive the depth of a graphene-based atom chip trap is to the change in the Fermi energies. One can imagine the change in the lifetime of the atom cloud trapped in the atom chips when, for example, there are charge impurities in the graphene layers,

while locally change the Fermi energy.

In order to illustrate this, we can model a simple harmonic trap given by,

$$V_{\text{trap}} = \frac{1}{2}m\omega_r^2(z - z_0)^2, \quad (6.15)$$

where m is the mass of the trapped atom, ω_r is the radial trapping frequency, and z_0 is the distance from the trap centre to the surface of the atom chip. We then add the Casimir-Polder potential to the original simple harmonic trap so that when we change the Fermi energies of the graphene layers, we can see how much the trap potential changes.

The parameters of the trap are as follows: $m = 1.44 \times 10^{-25}$ kg [103], $\omega_r = 2\pi \times 50$ kHz, and $z_0 = 0.3 \mu\text{m}$.

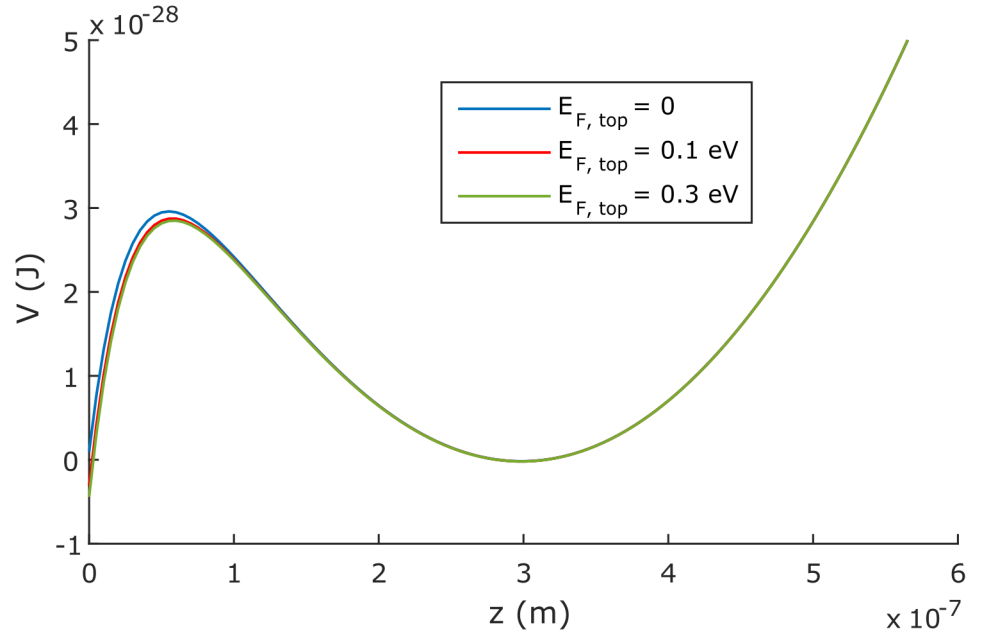


Figure 6.10: The variation of the trap potential with the Fermi energy of the top graphene layer in the atom chip comprising of a 1.4 nm-thick monolayer hBN sandwiched between two graphene monolayers. The total trap potential is the superposition of a simple harmonic trap (see text) and the Casimir-Polder potential experienced by a ^{87}Rb atom. The Fermi energy of the bottom graphene layer remains fixed at 0 eV. Generally, the left side of the simple harmonic trap is deformed by the presence of the Casimir-Polder potential preventing sub-micron trapping. An increase in Fermi energy of the top graphene layer ($E_{F,\text{top}}$) only strengthens the Casimir-Polder attraction slightly. It is hard to tell whether we can make use of this property in quantum sensing.

Figure 6.10 shows the variation of the trap potential with the Fermi energy of the top graphene layer in the atom chip while the Fermi energy of the bottom graphene layer is 0, i.e. at the Dirac point. Now it is clearer since we can see how the Casimir-Polder potential arising from the presence of bodies affects the limit in trapping distance in atom chips (blue curve): the Casimir-Polder potential lowers the height and the width of the left barrier making it easier for the trapped atoms to escape the trap by quantum tunnelling. We also can look at how the change in the Fermi energy of the top graphene layer affects the trap potential. With an increase in the Fermi energy up to 0.3 eV, the left side of the trap is lowered slightly which, in principle, will shorten the lifetime of the trapped atom. We will investigate further the topic of the lifetimes of the atom cloud trapped in atom chips in the next chapter.

Chapter 7

Johnson Noise in atom chips

7.1 Atom chips

In this chapter, we will only summarise briefly on the decades-long journey of atom chip development which is described in detail by Keil et al. [61]. The uses of atom chips are manifold: these devices allow us to trap atoms in sub-micron potential landscapes, which we can make use of in a variety of ways such as sensing very weak electromagnetic fields, as a precise frequency detector, or to explore the properties of pure ensembles of atoms to establish a better understanding of nature.

The basic idea of an atom chip (see Fig. 7.1) is that we create a harmonic magnetic field by first creating a magnetic field from a current-carrying wire then locally cancelling it out by an external bias field. This will create a region of minimum magnetic field near the wire, which can be used to trap atoms, acting as magnetic dipoles. Another offset field is applied in the direction parallel to the current-carrying wire to remove a region of zero magnetic field, preventing Majorana spin-flip transitions [10, 104]. Since the magnetic field is non-uniform, the atom will experience a Stern-Gerlach force and the direction of the force depends on the atom's internal magnetic states. In general, recalling the Stern-Gerlach experiment, there are two states: one of which seeks the

region of increasing field and the other seeks the region of decreasing field. In order for an atom to be trapped, it has to be in the low field seeking state. One problem is that the magnetic state of the atom can be perturbed by thermal photons causing its magnetic moment to flip and go to the high field seeking state, which is unfavourable. Here, the fluctuating thermal photons that cause spin flips are called Johnson noise. In electronic circuits, Johnson noise originates from the wires, and is described here in terms of Green's functions. In the following sections, we will outline and review the necessary theoretical foundation to calculate lifetimes of trapped atoms due to Johnson noise.

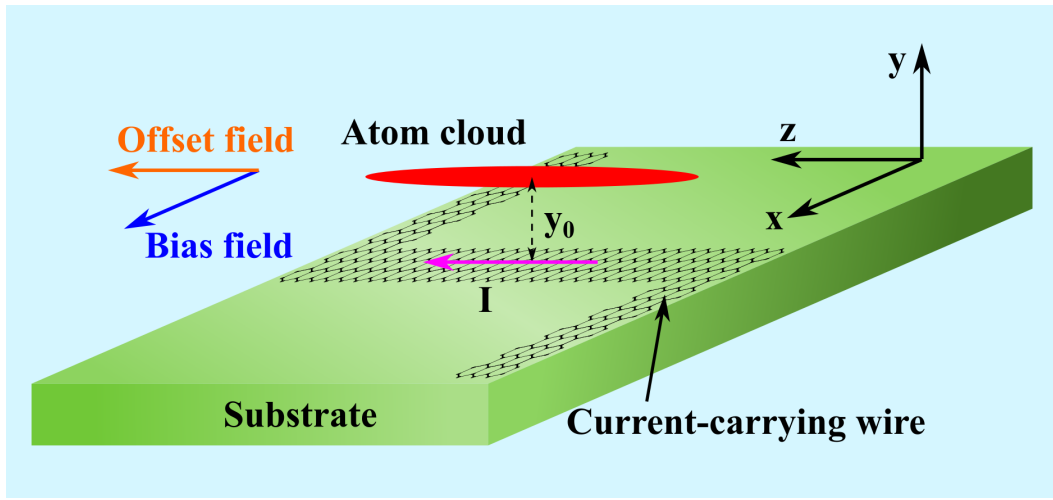


Figure 7.1: Schematic diagram of a micro-fabricated atom chip showing the Z-shaped conducting channel (hexagonal lattice pattern), carrying current, I (pink arrow), above a substrate (green slab). The orientations of the applied magnetic bias field and the offset field are shown by blue and orange arrows respectively. These magnetic fields, together with the one produced by current, I , trap an atomic Bose-Einstein condensate (red) at distance y_0 above the wire.

7.1.1 Dyadic Green's function and dipole fields

An important concept in scattering theory is the Green's function, which was first invented by George Green, a British mathematician and physicist (14 July 1793 - 31 May 1841) [22]. The basic idea of Green's functions is to calculate the fields due to a point source. Before we introduce the general definition of the dyadic Green's function, we first start with the wave equation for the

electric field, at position $\mathbf{r}$, in a homogeneous space, characterised by a relative magnetic permeability μ and a relative permittivity ϵ , as follows

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r}) - k^2 \mathbf{E}(\mathbf{r}) = i\omega\mu_0\mu\mathbf{j}(\mathbf{r}), \quad (7.1)$$

where $\nabla \times$ denotes a curl operator, $k^2 = \epsilon\mu\omega^2/c^2$ is the wave vector determined by the material parameters and the oscillation frequency ω , μ_0 is the permeability of free space, $\mathbf{j}(\mathbf{r}) = j_x(\mathbf{r})\mathbf{n}_x + j_y(\mathbf{r})\mathbf{n}_y + j_z(\mathbf{r})\mathbf{n}_z$ is the current density, where $\mathbf{n}_x, \mathbf{n}_y, \mathbf{n}_z$ are the unit vectors in the x -, y - and z -directions, respectively.

From here, we define Green's functions corresponding to each component of $\mathbf{j}$ explicitly:

$$\nabla \times \nabla \times \mathbf{G}_x(\mathbf{r}, \mathbf{r}') - k^2 \mathbf{G}_x(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')\mathbf{n}_x, \quad (7.2)$$

$$\nabla \times \nabla \times \mathbf{G}_y(\mathbf{r}, \mathbf{r}') - k^2 \mathbf{G}_y(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')\mathbf{n}_y, \quad (7.3)$$

$$\nabla \times \nabla \times \mathbf{G}_z(\mathbf{r}, \mathbf{r}') - k^2 \mathbf{G}_z(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r} - \mathbf{r}')\mathbf{n}_z, \quad (7.4)$$

where $\mathbf{r}'$ is the position of the point source (see Figure 7.2), $\delta(\mathbf{r} - \mathbf{r}')$ is the Dirac delta function.

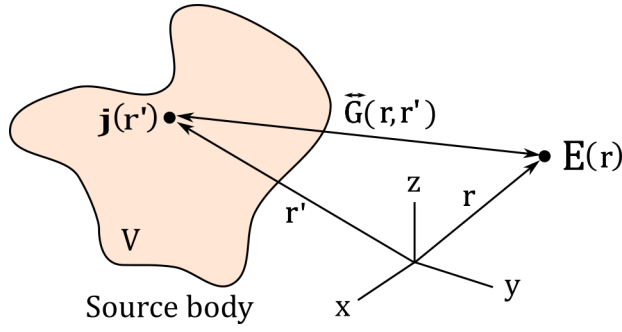


Figure 7.2: Illustration of the dyadic Green's function $\overleftrightarrow{\mathbf{G}}(\mathbf{r}, \mathbf{r}')$. The Green's function forms a relationship between a single point source $\mathbf{j}$ at the source point $\mathbf{r}'$ and the associated electric field $\mathbf{E}$ at the field point $\mathbf{r}$. The total electric field is the superposition of every field corresponding to each point source in the source body of volume V .

These three vectorial Green's functions can be combined into a single tensor giving the general definition of the dyadic Green's function (Green's tensor) for the electric field as

$$\nabla \times \nabla \times \overleftrightarrow{\mathbf{G}}(\mathbf{r}, \mathbf{r}') - k^2 \overleftrightarrow{\mathbf{G}}(\mathbf{r}, \mathbf{r}') = \overleftrightarrow{\mathbf{I}} \delta(\mathbf{r} - \mathbf{r}'), \quad (7.5)$$

where $\overleftrightarrow{\mathbf{I}}$ is the unit dyad (unit tensor). We can see that each column of the tensor $\overleftrightarrow{\mathbf{G}}$ can be mathematically treated individually: the curl operators can be applied to any column of the Green's tensor as if they were to act on a column vector. In addition, each column can be interpreted separately: the first column of the Green's tensor corresponds to the field due to a point source in the x -direction, the second column to the field due to a point source in the y -direction, and the third column is the field due to a point source in the z -direction.

And finally, a particular solution of (7.1) defined by the dyadic Green's function reads

$$\mathbf{E}(\mathbf{r}) = i\omega\mu\mu_0 \int_V \overleftrightarrow{\mathbf{G}}(\mathbf{r}, \mathbf{r}') \mathbf{j}(\mathbf{r}') dV'. \quad (7.6)$$

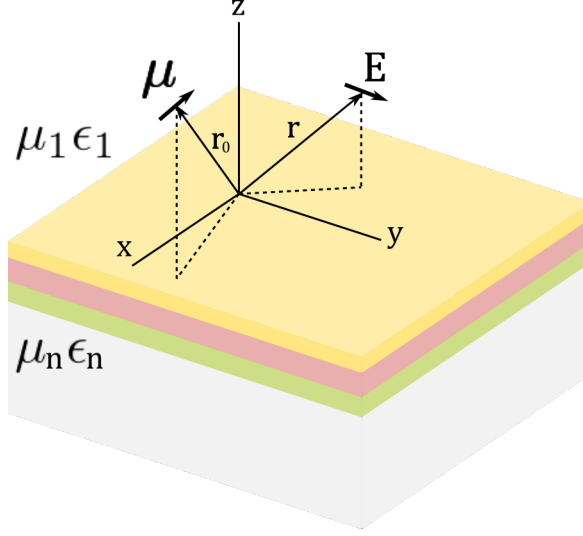


Figure 7.3: Schematic diagram of a dipole near planar interfaces. The dipole (depicted as an arrow labelled $\boldsymbol{\mu}$) is located at $\mathbf{r}_0 = (x_0, y_0, z_0)$ acting as a point source. The surface of the topmost layer (yellow) coincides with the coordinate origin. The other layers are shaded differently and located at $z < 0$. The electromagnetic properties of the upper (vacuum) and lower (substrate) half-spaces are characterised by the permeability μ and permittivity ϵ , designated by the index 1 and n , respectively. An arrow, labelled $\mathbf{E}$, represents the configuration of the electric field at point $\mathbf{r}$.

Now that we have laid out the theoretical foundations, we can start considering the electric fields radiated by an electric dipole by the Green's function approach. At a later stage, we can derive the magnetic dipole fields and the corresponding Green's function from the electric dipole fields that we have considered by very simple substitution.

Let us consider the situation shown in Figure 7.3 where a dipole is located above a layered substrate. We assume that the upper half-space is vacuum while the lower half-space (substrate) is optically denser.

We may take a step back and remove the interfaces in Figure 7.3 and assume that an electric dipole $\boldsymbol{\mu}$, located at $\mathbf{r}_0 = (x_0, y_0, z_0)$, is in a homogeneous, linear and isotropic medium, characterised by ϵ_1 and μ_1 , with an intention to find the primary dyadic Green's function $\overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}_0)$ (sometimes called “free-space Green's function” if the entire space is vacuum).

The associated electric field reads,

$$\mathbf{E}(\mathbf{r}, \omega) = \omega^2 \mu_0 \mu_1 \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}_0, \omega) \boldsymbol{\mu}, \quad (7.7)$$

where ω is the angular frequency of the radiation field, μ_0 is the magnetic permeability of free space.

The explicit form of $\overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}_0, \omega)$ is given by [88]

$$\overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}_0, \omega) = \frac{i}{8\pi^2} \iint_{-\infty}^{\infty} \overleftrightarrow{\mathbf{M}} e^{i[k_x(x-x_0)+k_y(y-y_0)+k_{z1}|z-z_0|]} dk_x dk_y, \quad (7.8)$$

where

$$\overleftrightarrow{\mathbf{M}} = \frac{1}{k_1^2 k_{z1}} \begin{bmatrix} k_1^2 - k_x^2 & -k_x k_y & \mp k_x k_{z1} \\ -k_x k_y & k_1^2 - k_y^2 & \mp k_y k_{z1} \\ \mp k_x k_{z1} & \mp k_y k_{z1} & k_1^2 - k_{z1}^2 \end{bmatrix}, \quad (7.9)$$

where $k_1^2 = \epsilon_1 \mu_1 \omega^2 / c^2 = k_{z1}^2 + (k_x^2 + k_y^2)$. Here, for some terms in the matrix $\overleftrightarrow{\mathbf{M}}$, the upper sign applies for $z > z_0$ and the lower sign for $z < z_0$.

The tensor $\overleftrightarrow{\mathbf{M}}$ can be further decomposed into two parts: an s-polarised part and a p-polarised part

$$\overleftrightarrow{\mathbf{M}}(k_x, k_y) = \overleftrightarrow{\mathbf{M}}^s(k_x, k_y) + \overleftrightarrow{\mathbf{M}}^p(k_x, k_y), \quad (7.10)$$

where

$$\overleftrightarrow{\mathbf{M}}^s(k_x, k_y) = \frac{1}{k_{z1}(k_x^2 + k_y^2)} \begin{bmatrix} k_y^2 & -k_x k_y & 0 \\ -k_x k_y & k_x^2 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (7.11)$$

$$\overleftrightarrow{\mathbf{M}}^p(k_x, k_y) = \frac{1}{k_1(k_x^2 + k_y^2)} \begin{bmatrix} k_x^2 k_{z1} & k_x k_y k_z & \mp k_x(k_x^2 + k_y^2) \\ k_x k_y k_z & k_y^2 k_{z1} & \mp k_y(k_x^2 + k_y^2) \\ \mp k_x(k_x^2 + k_y^2) & \mp k_y(k_x^2 + k_y^2) & (k_x^2 + k_y^2)^2/k_{z1} \end{bmatrix}. \quad (7.12)$$

The reason for performing this decomposition will become clearer when we put back the interfaces to consider the Green's function for the reflected fields.

Let us now consider the situation that we have mentioned earlier: the dipole whose primary field is represented by $\overleftrightarrow{\mathbf{G}}_0$ is located above a planar layered interface at $z_0 > 0$, where the coordinate origin is placed at the surface of the topmost layer. Since we know the primary Green's function that describes the plane waves travelling in space without hindrance, calculating the reflected field in the presence of a planar interface is surprisingly easy: the concept lies in the elementary optics in which we can simply multiply the individual plane waves in $\overleftrightarrow{\mathbf{G}}$ with the corresponding generalised Fresnel reflection coefficients r_s and r_p . The new dyadic Green's function for the reflected electric field is then

$$\overleftrightarrow{\mathbf{G}}_{\text{ref}}(\mathbf{r}, \mathbf{r}_0) = \frac{i}{8\pi^2} \iint_{-\infty}^{\infty} \left[\overleftrightarrow{\mathbf{M}}_{\text{ref}}^s + \overleftrightarrow{\mathbf{M}}_{\text{ref}}^p \right] e^{i[k_x(x-x_0) + k_y(y-y_0) + k_{z1}(z+z_0)]} dk_x dk_y, \quad (7.13)$$

$$\overleftrightarrow{\mathbf{M}}_{\text{ref}}^s = \frac{r_s(k_x, k_y)}{k_{z1}(k_x^2 + k_y^2)} \begin{bmatrix} k_y^2 & -k_x k_y & 0 \\ -k_x k_y & k_x^2 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (7.14)$$

$$\overleftrightarrow{\mathbf{M}}_{\text{ref}}^{\text{p}} = \frac{-r_p(k_x, k_y)}{k_1(k_x^2 + k_y^2)} \begin{bmatrix} k_x^2 k_{z1} & k_x k_y k_z & k_x(k_x^2 + k_y^2) \\ k_x k_y k_z & k_y^2 k_{z1} & k_y(k_x^2 + k_y^2) \\ -k_x(k_x^2 + k_y^2) & -k_y(k_x^2 + k_y^2) & -(k_x^2 + k_y^2)^2/k_{z1} \end{bmatrix}. \quad (7.15)$$

Note that the wave number, k_1 , is determined only by the optical properties of the upper half-space and the radiation frequency in consideration, whereas the longitudinal component, k_{z1} , is subject to the integration variables, k_x and k_y , which run from $-\infty$ to ∞ , hence the wave associated with k_{z1} can be either propagating waves or evanescent waves.

The electric field in the upper half-space due to the electric dipole can now be obtained from the sum of the primary Green's function and the reflected Green's function as

$$\mathbf{E}(\mathbf{r}) = \omega^2 \mu_0 \mu_1 \overleftrightarrow{\mathbf{G}}(\mathbf{r}, \mathbf{r}_0) \boldsymbol{\mu}, \quad (7.16)$$

where $\overleftrightarrow{\mathbf{G}}(\mathbf{r}, \mathbf{r}_0) = \overleftrightarrow{\mathbf{G}}_0(\mathbf{r}, \mathbf{r}_0) + \overleftrightarrow{\mathbf{G}}_{\text{ref}}(\mathbf{r}, \mathbf{r}_0)$.

Manipulated in polar coordinates and evaluated at its origin, $\overleftrightarrow{\mathbf{G}}_{\text{ref}}(\mathbf{r}_0, \mathbf{r}_0)$ assumes the diagonal form [14, 88]

$$\overleftrightarrow{\mathbf{G}}_{\text{ref}}(\mathbf{r}_0, \mathbf{r}_0, \omega) = \frac{i}{8\pi} \int_0^\infty dk_{\parallel} \frac{k_{\parallel}}{k_{z1}} e^{2ik_{z1}z_0} \times \left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} r_s + \frac{c^2}{\omega^2} \begin{pmatrix} -k_{z1}^2 & 0 & 0 \\ 0 & -k_{z1}^2 & 0 \\ 0 & 0 & 2k_{\parallel}^2 \end{pmatrix} r_p \right]. \quad (7.17)$$

Equation (7.17) is equivalent to (6.6) when $\omega = i\xi$.

We have intensively considered the field of an electric dipole; however, our interest lies in the field of a magnetic dipole. Imagine the electric field of a

vertically oriented electric dipole; it is purely p-polarised since its radiating electric field is always parallel to the plane of incidence. What would happen to the electric field if we replaced the electric dipole with a magnetic dipole? From a theoretical point of view, this electric field is dual to the field of the electric dipole, hence the field should be purely s-polarised. Therefore, the magnetic field of a magnetic dipole will look similar to the electric field of a electric dipole, given that these dipoles are oriented in the same direction. In this sense, the field of a magnetic dipole with magnetic moment $\mathbf{m}$ can be derived from the field due to an electric dipole with moment $\boldsymbol{\mu}$ by performing the following substitution [88]

$$[\mathbf{E}, \mathbf{H}, \mu_0\boldsymbol{\mu}, \epsilon_0\epsilon, \boldsymbol{\mu}] \rightarrow [\mathbf{H}, -\mathbf{E}, \epsilon_0\epsilon, \mu_0\boldsymbol{\mu}, \boldsymbol{\mu}\mathbf{m}]. \quad (7.18)$$

Since the s-polarisation and p-polarisation are interchanged when we replace an electric dipole with a magnetic dipole, the Fresnel reflection coefficients r_s and r_p have to be interchanged as well.

7.2 Johnson Noise Losses

We might have come across with the concept that a radiating electric dipole, near planar interfaces, undergoes a spontaneous decay (energy dissipation) at a faster rate than when it is isolated in vacuum. The cause of the faster spontaneous decay rate is the fact that there are now the reflected waves, plane and evanescent, interacting with the dipole [88]. The same principle goes for magnetic dipoles near planar interfaces. These reflected waves are sometimes called “noises”. Johnson noises (thermal noises) originate from the fluctuating nature of charges in dipoles due to their thermal agitations. We will investigate Johnson noise losses of trapped atom clouds in atom chips.

7.2.1 Thermal spin flip rate

We need to look into the loss mechanism before we can calculate the lifetimes of the atoms trapped above a planar interface. Let us consider an alkali atom with magnetic moment, $\mathbf{m}$, located at position, $\mathbf{r}_0$, relative to an origin in the reference frame, in a harmonic magnetic field, $\mathbf{B}(\mathbf{r})$. In general, the magnetic moment of an atom is given by [17, 95, 103]

$$\mathbf{m} = -\mu_B \left(g_S \mathbf{S} + g_L \mathbf{L} - g_I \frac{m_e}{m_{nuc}} \mathbf{I} \right), \quad (7.19)$$

where μ_B is the Bohr magneton, $\mathbf{S}$, $\mathbf{L}$, and $\mathbf{I}$ are electron spin angular momentum, electron angular momentum, and the total nuclear angular momentum, respectively, with their corresponding g-factors g_S , g_L , and g_I , m_e is the electron mass and m_{nuc} is the nuclear mass. Here, we use the convention that the magnitude of the angular momentum, for example, $\mathbf{S}$, is $\sqrt{S(S+1)}\hbar$ and the eigenvalue of the z -component of $\mathbf{S}$, S_z , is $m_S\hbar$. The Hamiltonian describing the interaction between the atom and the magnetic field is then

$$H = -\frac{1}{\hbar} \mathbf{m} \cdot \mathbf{B}. \quad (7.20)$$

For a ground-state alkali atom ($\mathbf{L} = 0$), the rate of magnetic spin flip transitions from an initial hyperfine magnetic state $|i\rangle$ to another state $|f\rangle$ is given by [95]

$$\Gamma = \mu_0 \frac{2(\mu_B g_S)^2}{\hbar^2} \sum_{j,k} \langle f | \hat{\mathbf{S}}_j | i \rangle \langle i | \hat{\mathbf{S}}_k | f \rangle \times \text{Im}[\nabla \times \nabla \times \overleftrightarrow{\mathbf{G}}(\mathbf{r}_0, \mathbf{r}_0, \omega)]_{jk} (\bar{n}_{\text{th}} + 1), \quad (7.21)$$

where the hat symbol over a letter denotes a quantum operator, $\text{Im}[\dots]$ denotes the imaginary part of the function, and the mean thermal occupation number is given by

$$\bar{n}_{\text{th}} = \frac{1}{e^{\hbar\omega/k_B T} - 1}. \quad (7.22)$$

It should be noted that the derivation of this formula is carried out by considering the Heisenberg equations of motion for a quantised magnetic dipole interacting with a fluctuating magnetic field in the rotating wave and Markov approximations.

The angular frequency, ω , that appears in (7.21) is the frequency of radiation due to magnetic spin flips. It will be further discussed in the next section. The Johnson noise lifetime is defined as

$$\tau = \frac{1}{\Gamma}. \quad (7.23)$$

Note that the interaction that induces spin flips is the coupling of the magnetic moment and the *fluctuating* part of the magnetic field, i.e. the magnetic field noises.

7.2.2 Quantum mechanics of ^{87}Rb atom in magnetic field

In this part, we will discuss the treatment of a few terms in (7.21) before carrying out numerical computations.

Let us first recall that the total atomic angular momentum $\mathbf{F}$ is given by

$$\mathbf{F} = \mathbf{J} + \mathbf{I}, \quad (7.24)$$

where $\mathbf{J}$ and $\mathbf{I}$ are the total electron angular momentum ($\mathbf{S} + \mathbf{L}$) and the total nuclear angular momentum, respectively. The coupling between these two angular momenta results in hyperfine splittings. The magnitude of $\mathbf{F}$ can take the values

$$|J - I| \leq F \leq |J + I|. \quad (7.25)$$

For the ^{87}Rb ground-state, $L = 0$, $S = 1/2$, and $I = 3/2$, so F can take values of 1 or 2. In this thesis, we are only interested in the ground-state in which $F = 2$. The m_F quantum number representing the z -component of the total atomic angular momentum can take the values $m_F = -2, -1, 0, 1, 2$, yielding 5 hyperfine states. The notation for the eigenkets representing the states in which F and m_F have fixed values will be $|F, m_F\rangle$.

In atom chips, the offset magnetic field at the centre of the trap is expected to be weak (of order mT); therefore, the energy shift due to the presence of the magnetic field is small compared to the hyperfine splittings. This allows us to use F as a quantum number, to a very good approximation, for the interaction of the magnetic moment and the magnetic field. Equation (7.20) now becomes

$$H = \mu_B g_F \frac{F_z}{\hbar} B_z, \quad (7.26)$$

where we have ignored the components of $\mathbf{B}$ in directions other than the z -direction because, for future calculations of Johnson noise lifetimes, only the z -component of the field is nonzero at the centre of the trap. The hyperfine Landé g-factor is given by [17, 103]

$$g_F \simeq g_J \frac{F(F+1) - I(I+1) + J(J+1)}{2F(F+1)}, \quad (7.27)$$

where

$$g_J \simeq 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)}. \quad (7.28)$$

The angular frequency, ω , of the radiation due to the transition between two hyperfine states, in (7.21), can now be determined from

$$\omega = \mu_B g_F \frac{|\Delta m_F|}{\hbar} B_z. \quad (7.29)$$

For the transition between $|F = 2, m_F = 2\rangle$ and $|F = 2, m_F = 1\rangle$, and taking a typical value of $B_z = 0.8 \times 10^{-4} \text{ T}$, the angular frequency $\omega \simeq 2\pi \times 560 \text{ kHz}$.

The terms $\langle f | \hat{\mathbf{S}}_j | i \rangle$ in (7.21) are next for us to tackle. In order to evaluate them, we need to be able to express the ket $|F, m_F\rangle$ in terms of the direct product of $|I, m_I\rangle$ and $|S, m_S\rangle$. Note that $\{|I, m_I\rangle\}$ form a complete and orthonormal basis, so does $\{|S, m_S\rangle\}$. Let us assume that the coupling between the electron orbital angular momentum and the spin angular momentum is sufficiently weak that the space and spin degrees of freedom of the electron evolve independently of each other, i.e. these momenta commute. Note that $|I, m_I\rangle$ is a joint eigenstate of the observables, $\hat{\mathbf{I}}^2$ and $\hat{\mathbf{I}}_z$, while $|S, m_S\rangle$ is a joint eigenstate of the observables, $\hat{\mathbf{S}}^2$ and $\hat{\mathbf{S}}_z$, such that

$$\hat{\mathbf{I}}^2 |I, m_I\rangle = I(I+1)\hbar^2 |I, m_I\rangle, \quad (7.30)$$

$$\hat{\mathbf{I}}_z |I, m_I\rangle = m_I \hbar |I, m_I\rangle, \quad (7.31)$$

$$\hat{\mathbf{S}}^2 |S, m_S\rangle = S(S+1)\hbar^2 |S, m_S\rangle, \quad (7.32)$$

$$\hat{\mathbf{S}}_z |S, m_S\rangle = m_S \hbar |S, m_S\rangle. \quad (7.33)$$

These four operators commute and their eigenstates also form a complete set; therefore, the Hilbert space to which these four operators belong can be spanned by the direct products of $\{|I, m_I\rangle\}$ and $\{|S, m_S\rangle\}$. Let us now denote the joint eigenstates by $|I, S; m_I, m_S\rangle$, which can be expressed as

$$|I, S; m_I, m_S\rangle = |I, m_I\rangle |S, m_S\rangle. \quad (7.34)$$

Physically, the state described by $|I, S; m_i, m_S\rangle$ is the same as the state described by $|I, m_I\rangle$ and $|S, m_S\rangle$ simultaneously; therefore, the set of the kets $\{|I, S; m_I, m_S\rangle\}$ exhibits the same properties as those of $\{|I, m_I\rangle\}$ and $\{|S, m_S\rangle\}$, that is, the basis $\{|I, S; m_I, m_S\rangle\}$ is complete and orthonormal.

Now the basis $\{|F, m_F\rangle\}$ can be expressed in terms of the basis $\{|I, S; m_i, m_S\rangle\}$ as [117]

$$|F, m_F\rangle = \sum_{m_I=-I}^I \sum_{m_S=-S}^S \langle I, S; m_I, m_S | F, m_F \rangle |I, S; m_I, m_S\rangle. \quad (7.35)$$

The coefficients $\langle I, S; m_I, m_S | F, m_F \rangle$ that connect the $\{|F, m_F\rangle\}$ and $\{|I, S; m_i, m_S\rangle\}$ bases are called the *Clebsch-Gordon coefficients*.

For a spin $\frac{1}{2}$ particle, the Clebsch-Gordon coefficients associated with the coupling of a spin angular momentum $\mathbf{S}$ and the total nuclear angular momentum $\mathbf{I}$ can be readily expressed as

$$\begin{aligned} \left| I \pm \frac{1}{2}, m_F \right\rangle &= \sqrt{\frac{I \mp m_F + \frac{1}{2}}{2I + 1}} \left| I, \frac{1}{2}; m_F + \frac{1}{2}, -\frac{1}{2} \right\rangle \\ &\quad \pm \sqrt{\frac{I \pm m_F + \frac{1}{2}}{2I + 1}} \left| I, \frac{1}{2}; m_F - \frac{1}{2}, \frac{1}{2} \right\rangle. \end{aligned} \quad (7.36)$$

For the ground-state of a ^{87}Rb atom with $I = 3/2$, the $m_F = 2$ and $m_F = 1$ eigenkets can be written as follows

$$|F = 2, m_F = 2\rangle = \left| \frac{3}{2}, \frac{1}{2}; \frac{3}{2}, \frac{1}{2} \right\rangle, \quad (7.37)$$

and

$$|F = 2, m_F = 1\rangle = \frac{1}{2} \left| \frac{3}{2}, \frac{1}{2}; \frac{3}{2}, -\frac{1}{2} \right\rangle + \frac{\sqrt{3}}{2} \left| \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2} \right\rangle. \quad (7.38)$$

We are now in the position to calculate the matrix element $\langle f | \hat{\mathbf{S}}_j | i \rangle$. Let us suppose that a ^{87}Rb atom is initially prepared in the state $|F = 2, m_F = 2\rangle$, behaving as a low field seeking atom. We will use the eigenstates in which the z -component of the spin operator has a fixed value as our base kets; we denote them by $|+\rangle$ and $|-\rangle$ for eigenvalues $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$, respectively. The spin operators, $\hat{\mathbf{S}}_x$, $\hat{\mathbf{S}}_y$, and $\hat{\mathbf{S}}_z$, only act on the electron spin part of the state ket;

therefore, the diagonal elements of the matrix $\langle f | \hat{\mathbf{S}}_j | i \rangle$ are evaluated as

$$\langle f | \hat{\mathbf{S}}_z | i \rangle = \langle F = 2, m_F = 1 | \hat{\mathbf{S}}_z | F = 2, m_F = 2 \rangle, \quad (7.39)$$

$$= \left(\frac{1}{2} \left\langle \frac{3}{2}, \frac{1}{2}; \frac{3}{2}, -\frac{1}{2} \right| + \frac{\sqrt{3}}{2} \left\langle \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2} \right| \right) \frac{\hbar}{2} \left| \frac{3}{2}, \frac{1}{2}; \frac{3}{2}, \frac{1}{2} \right\rangle, \quad (7.40)$$

$$= 0 = \langle i | \hat{\mathbf{S}}_z | f \rangle, \quad (7.41)$$

$$\langle f | \hat{\mathbf{S}}_x | i \rangle = \langle F = 2, m_F = 1 | \left(\frac{\hbar}{2} [(|+\rangle \langle -|) + (|- \rangle \langle +|)] \right) | F = 2, m_F = 2 \rangle, \quad (7.42)$$

$$= \left(\frac{1}{2} \left\langle \frac{3}{2}, \frac{1}{2}; \frac{3}{2}, -\frac{1}{2} \right| + \frac{\sqrt{3}}{2} \left\langle \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2} \right| \right) \frac{\hbar}{2} \left| \frac{3}{2}, \frac{1}{2}; \frac{3}{2}, -\frac{1}{2} \right\rangle, \quad (7.43)$$

$$= \frac{\hbar}{4} = \langle i | \hat{\mathbf{S}}_x | f \rangle, \quad (7.44)$$

$$\langle f | \hat{\mathbf{S}}_y | i \rangle = \langle F = 2, m_F = 1 | \left(\frac{\hbar}{2} [-i(|+\rangle \langle -|) + i(|- \rangle \langle +|)] \right) | F = 2, m_F = 2 \rangle, \quad (7.45)$$

$$= \left(\frac{1}{2} \left\langle \frac{3}{2}, \frac{1}{2}; \frac{3}{2}, -\frac{1}{2} \right| + \frac{\sqrt{3}}{2} \left\langle \frac{3}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2} \right| \right) i \frac{\hbar}{2} \left| \frac{3}{2}, \frac{1}{2}; \frac{3}{2}, -\frac{1}{2} \right\rangle, \quad (7.46)$$

$$= \frac{i\hbar}{4} = -\langle i | \hat{\mathbf{S}}_y | f \rangle. \quad (7.47)$$

As for the imaginary part of the double curl of the Green's function, recalling (7.5) and taking the imaginary parts of both sides, we get

$$\text{Im} \left[\nabla \times \nabla \times \overleftrightarrow{\mathbf{G}}(\mathbf{r}, \mathbf{r}', \omega) \right] = \frac{\omega^2}{c^2} \text{Im} \left[\overleftrightarrow{\mathbf{G}}(\mathbf{r}, \mathbf{r}', \omega) \right]. \quad (7.48)$$

For magnetic traps, the offset field for preparing the initial state of the atoms is usually oriented parallel to the current carrying wire [50, 53, 54, 56, 95]. If we want to calculate the spin flip rate in this case, we need to modify the Green's tensor accordingly by transforming the coordinate system so that the z -axis is aligned with the direction of the offset magnetic field, i.e. the G_{yy} and G_{zz} elements are switched (see Figure 7.4).

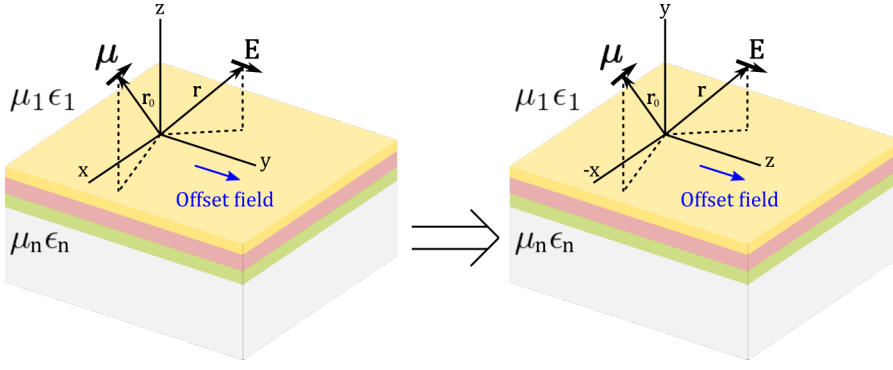


Figure 7.4: The transformation from the old coordinate system in which the z -direction is perpendicular to the surface to the new coordinate system in which the z -axis is parallel to the direction of the offset field (blue arrow). In the new coordinates, the dipole is located at distance y_0 above the interfaces.

Now that all the terms in the expression for the spin flip rate (7.21) can be evaluated, we can start exploring the Johnson noise lifetimes in various planar structures, be they pure metal slabs or graphene-based structures.

7.2.3 Results and discussion

It is stressed in [13,14] that $\text{Im}[\epsilon], \text{Im}[\mu] > 0$; however, here we take $\mu = 1$ as an approximation to the full complex permeability. This enables good estimates of the lifetimes to be made and, crucially, compared for different materials and structures.

Lifetimes of trapped atoms near metal slabs

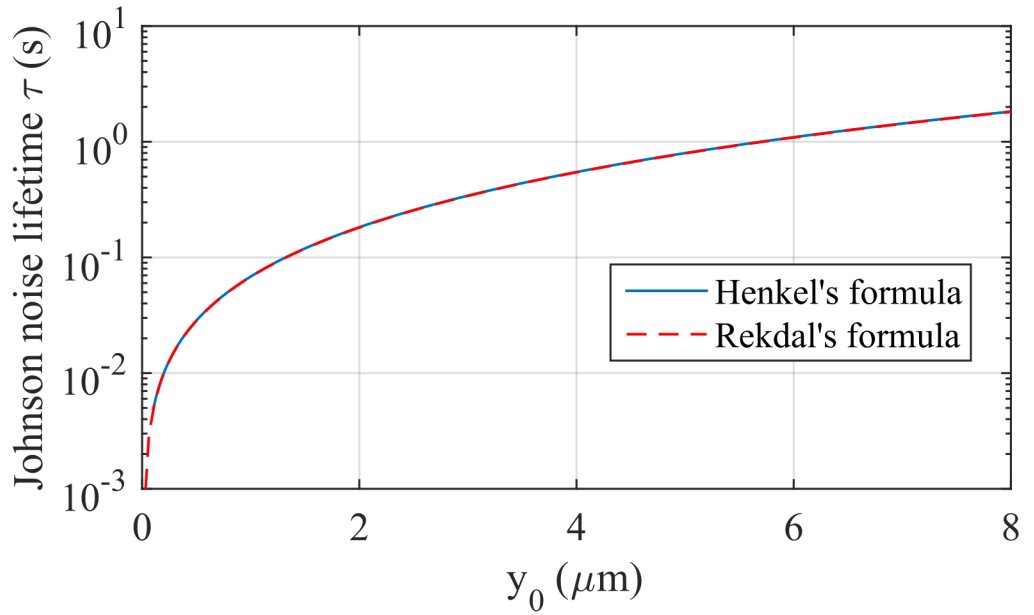


Figure 7.5: Johnson noise lifetimes, τ , calculated versus trapping distance, y_0 , of an ensemble of ultra-cold ^{87}Rb atoms above a copper slab, characterised by skin depth $\delta = 88 \mu\text{m}$, with thickness of $2 \mu\text{m}$ (see text). Blue curve is obtained from evaluating (7.21) and red dashed curve is calculated based on the formula taken from Lin *et al.* (2004). Our lifetime predicted by the formula derived by Rekdal *et al.* (2004) is similar to the lifetime calculated from the interpolation of Henkel's formula. Parameters: $T = 300 \text{ K}$, $\omega = 2\pi \times 560 \text{ kHz}$.

Let us first compare our calculated lifetime associated with spin flips from state $|F = 2, m_F = 2\rangle$ to state $|F = 2, m_F = 1\rangle$, defined in the new coordinates (right diagram of Figure 7.4), with the lifetime previously reported in [68]. We will choose the parameters of the trap to coincide with theirs. The temperature is 300 K. The copper slab for the simulation has infinite length and width, while its thickness is $2 \mu\text{m}$. Its permittivity is given by [24] $\epsilon_r = 2ic^2/\omega^2\delta^2$,

where $\delta = 88 \mu\text{m}$ is the skip depth at transition frequency of 560 kHz [95]. The offset field points in the $+z$ -direction. Note that trapped ^{87}Rb atoms do not have the same temperature as the trap; they have been cooled down to μK temperatures and become quasi Bose-Einstein condensates. We can see from Figure 7.5 that our calculated lifetime based on the approach outlined previously quantitatively agree with the lifetime calculated using the formula that interpolated the spin flip rates derived by Henkel *et al.* using the fluctuation-dissipation theorem [54].

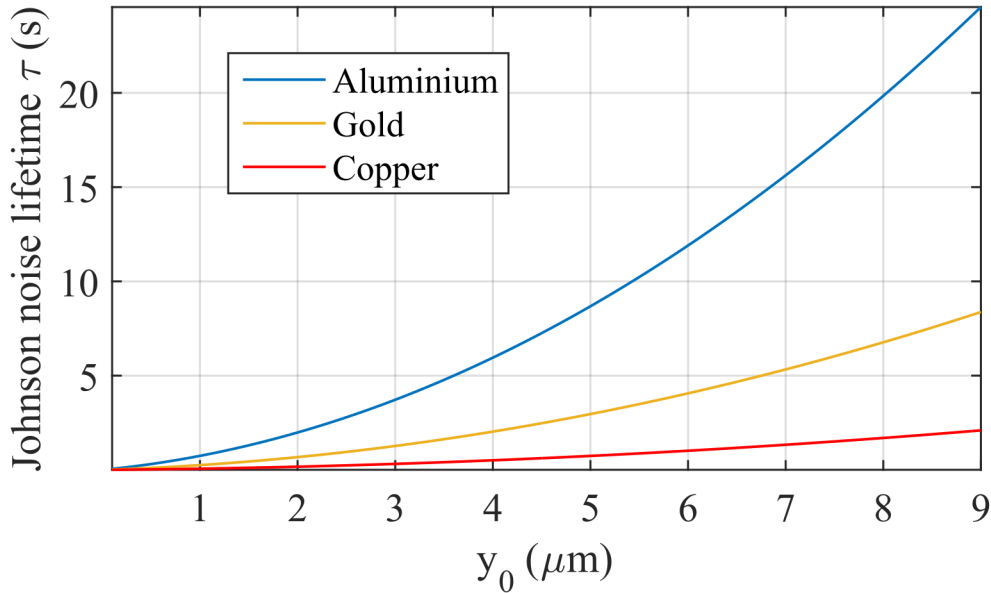


Figure 7.6: Johnson noise lifetimes, τ , calculated versus trapping distance, y_0 , for an ensemble of ultra-cold ^{87}Rb atoms trapped above three different surfaces of thickness $2 \mu\text{m}$: copper (red curve), gold (yellow curve), aluminium (blue curve). Each metal has different permittivity which is calculated using Eq. (6.11): $-6.54 \times 10^2 + 1.72 \times 10^{11}i$ for aluminium, $2.01 \times 10^{12}i$ for copper, and $-1.64 \times 10^4 + 5.03 \times 10^{11}i$ for gold. The permittivity of copper is the largest and aluminium the smallest, resulting in different spin-flip lifetimes, which decrease with increasing permittivity. The lifetimes increase with trapping distance as expected. Parameters: $T = 300 \text{ K}$, $\omega = 2\pi \times 560 \text{ kHz}$.

With the success of Rekdal's formula in comparison with Henkel's, we will move on and investigate the Johnson noise lifetimes for ^{87}Rb atoms near thin metal slabs such as gold, copper, and aluminium. The permittivity of copper is cal-

culated using the skin depth $\delta = 85 \mu\text{m}$. The dielectric constant of aluminium can be described by the Drude model given in (6.11) with $\hbar\omega_p = 15.565 \text{ eV}$ and $\hbar\Gamma = 0.608 \text{ eV}$ [88]. Here, we have taken a spin-flip frequency of $2\pi \times 560 \text{ kHz}$, corresponding to the offset field of 0.8 T , and a temperature of 300 K . Figure 7.6 shows the Johnson noise lifetimes, τ , calculated versus trapping distance, y_0 , for three different metal slabs of thickness $2 \mu\text{m}$: copper (red curve), gold (yellow curve), aluminium (blue curve). The lengths of the lifetimes, in descending order, are aluminium, gold then copper. Since copper has the highest imaginary part of the permittivity, while aluminium the lowest, this reveals that Johnson noise lifetimes vary inversely with the imaginary part of the permittivity, which is associated with the absorptive properties of materials and their conductivity. Lower conductivity metals yield longer lifetimes.

Lifetimes of trapped atoms near graphene-based structures

We now investigate the lifetimes of ^{87}Rb atoms trapped above graphene-based planar structures. Let us start with a single layer of graphene suspended in vacuum. Since the Johnson noise depends on the material's reflectance, we expect the lifetimes of the trapped atoms near graphene, which has far lower reflectance than metals, to be far longer than the lifetimes near metals. Figure 7.7 shows the comparison of the Johnson noise lifetimes, τ , calculated for an ensemble of ultra-cold ^{87}Rb atoms near a single layer of graphene suspended in vacuum and near a $2 \mu\text{m}$ -thick copper slab. The Johnson noise lifetime obtained in the case of the single layer of graphene is far longer than that in the case of the $2 \mu\text{m}$ -thick copper slab. Also, undoped graphene yields a longer lifetime than doped graphene. This makes sense because undoped graphene has a fewer electrons. Since the thickness of the copper slab coincides with the thickness of the main guide wire in the atom chip described in [68], we can see that novel atom chips which use graphene wires are promising and have a potential to replace the present generation of atom chips which use metal wires.

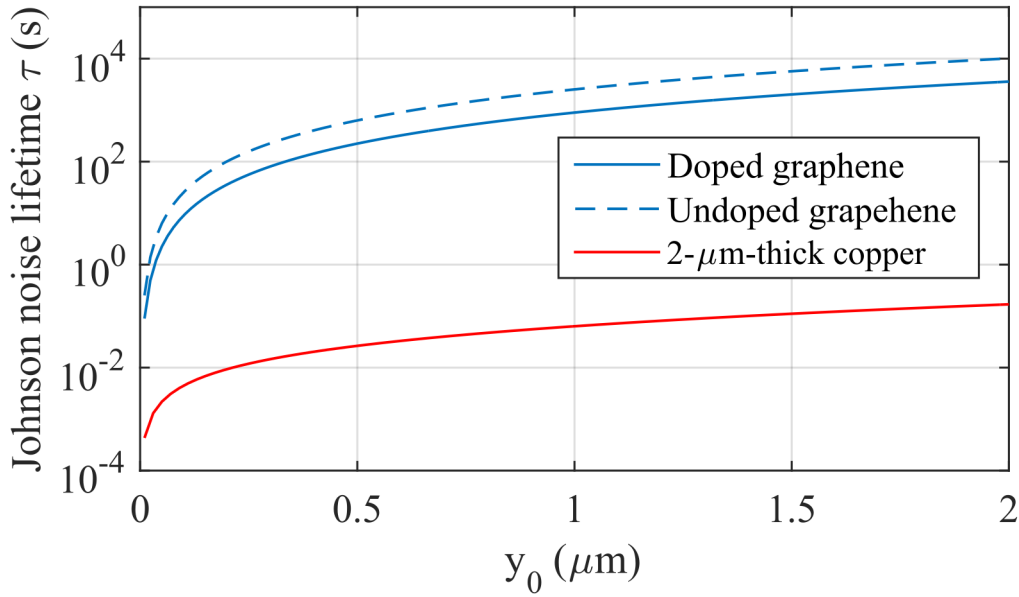


Figure 7.7: Johnson noise lifetimes, τ , calculated versus trapping distance, y_0 , of an ensemble of ultra-cold ^{87}Rb atoms trapped above a single layer of undoped graphene (dashed blue curve), doped graphene with $E_F = 0.1\text{ eV}$ (solid blue curve) and a $2\text{ }\mu\text{m}$ -thick copper slab (solid red curve). The graphene monolayer yields a far longer lifetime than the $2\text{ }\mu\text{m}$ -thick copper slab as a result of having far lower reflectance. Undoped graphene produces a longer lifetime than doped graphene as expected. Parameters: $T = 300\text{ K}$, $\omega = 2\pi \times 560\text{ kHz}$, and $\gamma = 4\text{ THz}$, for graphene.

Now that we have seen the comparison between metals and graphene regarding their associated Johnson noise lifetimes, we will divert our interest back to investigating the Johnson noise in graphene-based structures. Let us look at the validity of our model by first considering the variation of the lifetime with the atom-surface distance.

Figure 7.8 shows the Johnson noise lifetimes, τ , calculated versus trapping distance, y_0 , of an ensemble of ultra-cold ^{87}Rb atoms trapped above a single layer of graphene suspended in vacuum. It can be seen that the lifetimes increase with increasing trapping distance, approaching the free-space lifetime, determined by the free-space Green's function, of about $2 \times 10^{18}\text{ s}$ in the very long distance regime. This confirms that our model is valid in the limit $y_0 \rightarrow \infty$.

The oscillation of the lifetime in the kilometre regime in (b) emerges from the exponential term in Eq. (7.17) as the wavelength of the electromagnetic wave due to spin-flip transitions is comparable with the separation distance between the atom and the graphene surface.

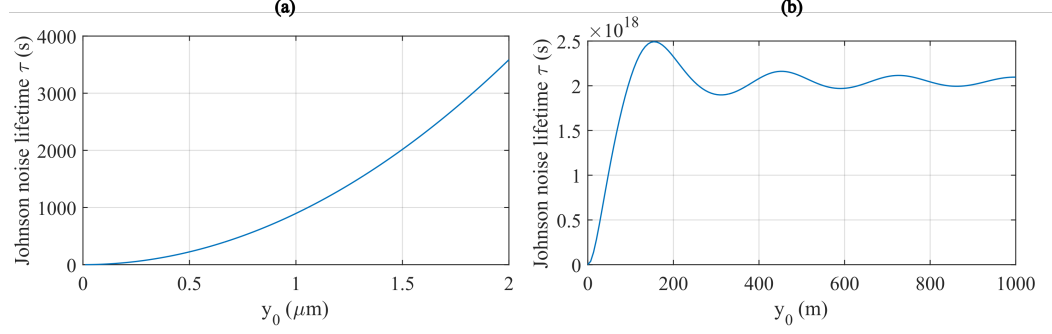


Figure 7.8: Johnson noise lifetimes, τ , calculated versus trapping distance, y_0 , of an ensemble of ultra-cold ^{87}Rb atoms trapped above a single layer of graphene suspended in vacuum: (a) trapping distance up to 0–2 μm , (b) trapping distance up to 1000 m. Johnson noise lifetimes increase with increasing trapping distance to a certain point before reaching the limit of the free-space lifetime of $\sim 2 \times 10^{18}$ s. The oscillating characteristic in (b) comes from the exponential term in Eq. (7.17). Parameters: $T = 300$ K, $\omega = 2\pi \times 560$ kHz, and $E_F = 0.1$ eV, $\gamma = 4$ THz, for graphene.

Next, we investigate the dependence of Johnson noise lifetimes on temperature. In our model, the temperature appears in two places: graphene’s optical conductivity and via Bose-Einstein function describing the mean number of thermal photons per mode at the frequency ω of the spin flip. Referring back to Figure 5.2, we can see that, in sub-THz regime, temperature hardly affects the conductivity. Therefore, Johnson noise lifetimes only depend on the thermal fluctuations of photons. Figure 7.9 shows Johnson noise lifetimes, τ , calculated versus trapping distance, y_0 , for ^{87}Rb atoms trapped near a single layer of graphene suspended in vacuum for $T = 200$ K, 300 K, and 400 K. It is not so surprising that the Johnson noise lifetimes increase when the temperature decreases and vice versa because increasing temperature increases both the thermal motion of electrons in graphene and the population of virtual and real photons.

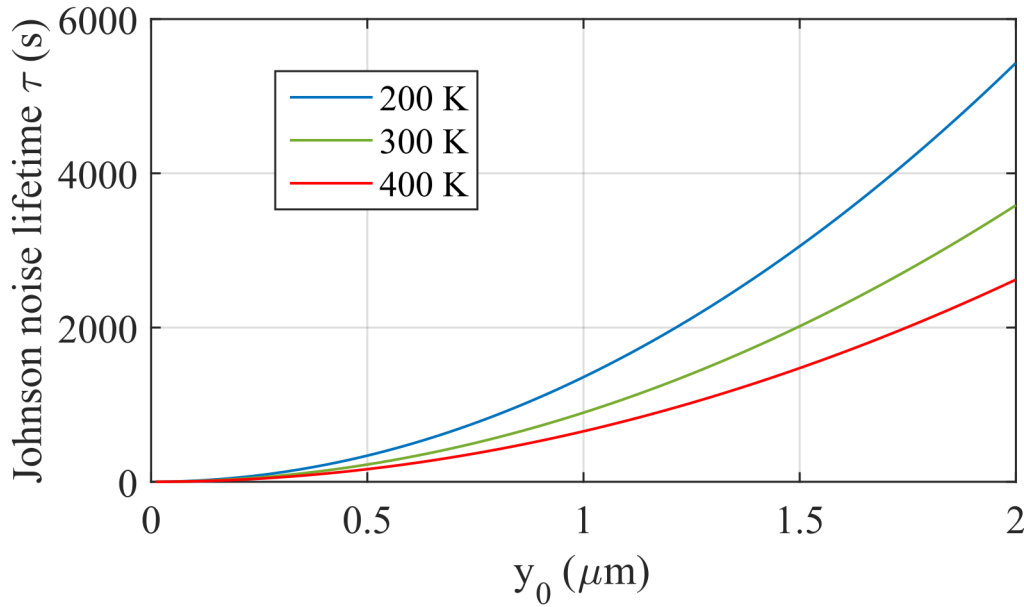


Figure 7.9: Johnson noise lifetimes, τ , calculated versus trapping distance, y_0 , of an ensemble of ultra-cold ^{87}Rb atoms trapped above a single layer of graphene suspended in vacuum for three different graphene temperatures: $T = 200\text{ K}$, 300 K , and 400 K (blue, green, red curves, respectively). For non-zero temperature, other than spontaneous decay, the decay of the atoms is also induced by thermal excitations resulting in shorter lifetimes as temperature increases. Parameters: $\omega = 2\pi \times 560\text{ kHz}$, and $E_F = 0.1\text{ eV}$, $\gamma = 4\text{ THz}$, for graphene.

Another parameter we have yet to explore is the relaxation rate of electrons in graphene. As we have mentioned before, this relaxation rate can be interpreted exactly as in the Drude model for metals. Higher relaxation rates imply shorter times between each collision of an electron with ion cores or defects. On the other hand, very clean and high quality graphene will have very low relaxation rates, i.e. the electrons are less restricted spatially.

Fig. 7.10 shows the lifetimes, calculated for four different values of electron relaxation rates: $\gamma = 1\text{ THz}$, 2 THz , 3 THz , and 4 THz (blue, red, yellow and green curves, respectively). The lifetimes increase as the relaxation rates increase. The explanation for this is that electrons in graphene with high relaxation rates can move more freely and will behave more like free electrons.

Compared to metals whose electron relaxation rates are ~ 100 THz, the average graphene electron's relaxation rate is two orders of magnitude lower. That graphene gives far longer Johnson noise lifetimes must therefore be from its other properties such as very low density of states.

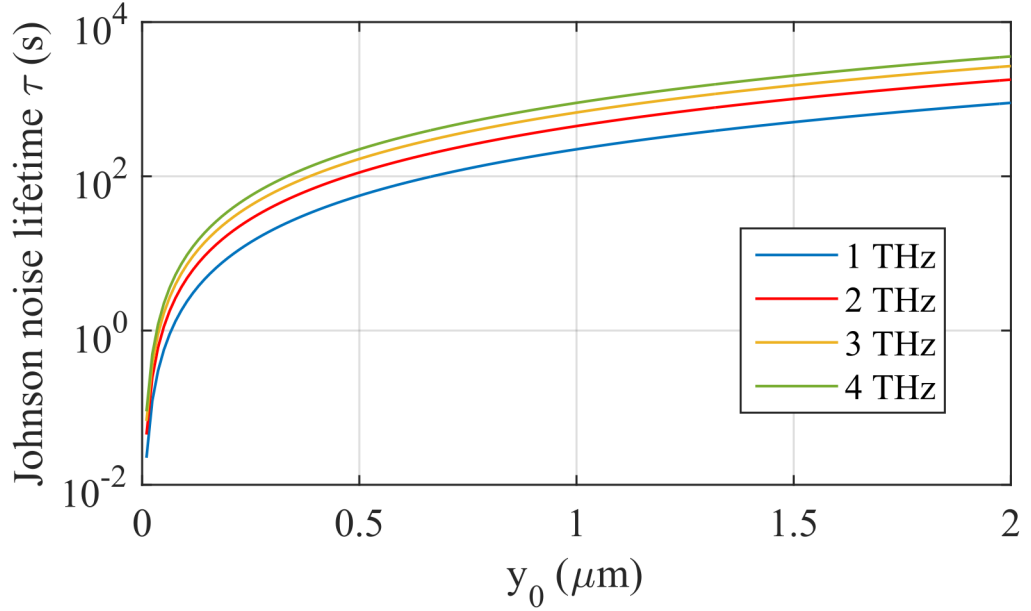


Figure 7.10: Johnson noise lifetimes, τ , calculated versus trapping distance, y_0 , of an ensemble of ultra-cold ^{87}Rb atoms trapped above a single layer of graphene with different electron relaxation rates: $\gamma = 1$ THz, 2 THz, 3 THz, and 4 THz (blue, red, yellow and green curves, respectively). The Johnson noise lifetime increases as the relaxation rate increases. Parameters: $\omega = 2\pi \times 560$ kHz, and $E_F = 0.1$ eV.

For the sake of satisfying our own curiosity, it is interesting to see how the Johnson noise lifetime changes when the magnetic moment quantisation axis of the atom is vertically oriented to the surface of the interfaces. The difference between these two states is that, for the quantisation axis oriented parallel to the surface, the G_{xx} and G_{yy} elements of the Green's function are associated with the horizontal and vertical directions, respectively, whereas, for the quantisation axis oriented perpendicular to the surface, both the G_{xx} and G_{yy} elements are associated with only the horizontal direction. Considering the matrix elements $\langle f | \hat{\mathbf{S}}_j | i \rangle$ in (7.21), we can see that only the components of the noise fields that are parallel to the quantisation axis induce spin flips. This

tells us that only the xx - and yy -diagonal elements of the Green's function play the role in determining the Johnson noise lifetime. To prepare an atom in a vertical magnetic moment state, an offset field in the vertical direction to the surface is applied.

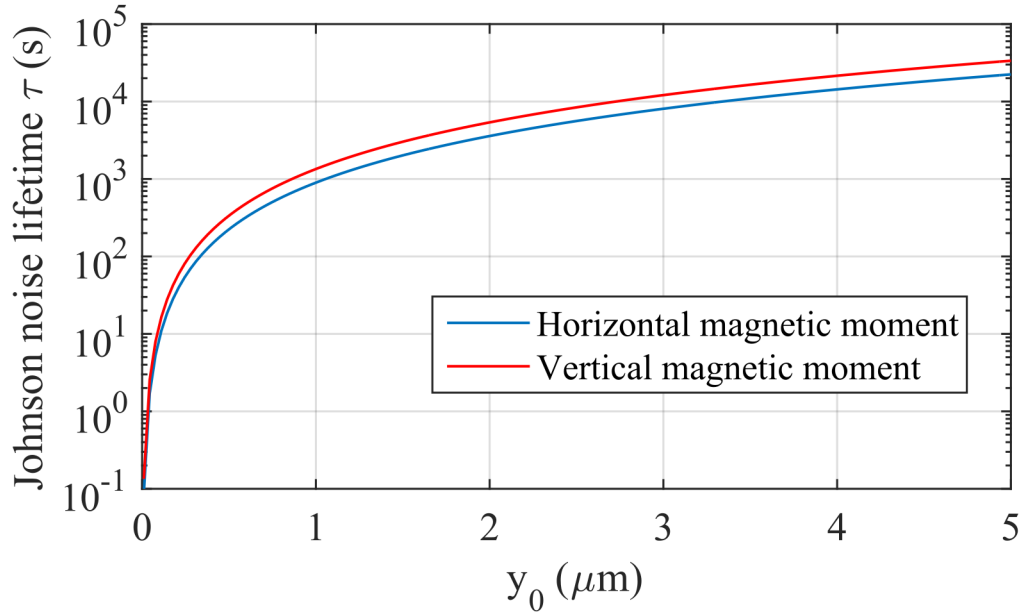


Figure 7.11: Johnson noise lifetimes, τ , calculated versus trapping distance, y_0 , of an ultra-cold ^{87}Rb atom near a single layer of graphene suspended in vacuum for two different configurations of the magnetic moment of the atom: (red curve) vertical magnetic moment, (blue curve) horizontal magnetic moment. Different configurations of the magnetic moment are prepared by changing the direction of the offset field. The spin-flip rate for the atom in the vertical magnetic moment state is lower than that in the horizontal magnetic moment state; therefore, the lifetime for the atom in the vertical magnetic moment state is longer than that in the horizontal magnetic moment state. Parameters: $T = 300\text{ K}$, $\omega = 2\pi \times 560\text{ kHz}$, and $E_F = 0.1\text{ eV}$, $\gamma = 4\text{ THz}$, for graphene.

Figure 7.11 shows the Johnson noise lifetimes, τ , calculated versus trapping distance, y_0 , of an ultra-cold ^{87}Rb atom near a single layer of graphene suspended in vacuum for two different configurations of the magnetic moment of the atom. The atom in the vertical magnetic moment state has a lower spin-flip rate than the atom in the horizontal magnetic moment state, hence a longer lifetime for the atom in the vertical magnetic moment state. Considering the Green's function, we can know that the s-polarisation of evanescent waves dominates. Since s-polarised waves (transverse-electric waves), in contrast with

p-polarised waves, tend to have their magnetic fields pointing in the vertical direction, they interact more strongly with the magnetic moment aligned in the vertical direction. Therefore, the contribution from the G_{yy} element of the Green's tensor for the case in which the magnetic moment quantisation axis is parallel to the surface is bigger than that for the vertical quantisation axis case, resulting in higher spin-flip rates, hence shorter lifetimes.

Let us move on to considering more complicated graphene-based structures. The type of structure under consideration is illustrated in Figure 6.2 in chapter 6, where, here, $d = 1.4$ nm, and adjacent graphene layers are separated only by vacuum. There is no special reason, regarding the optics of the structure, why we take $d = 1.4$ nm; it is only that we have considered this similar d value before. The temperature and ω remain the same as the previous calculation (i.e. $T = 300$ K, $\omega = 2\pi \times 560$ kHz) and the atom-surface distance is $1\text{ }\mu\text{m}$. In Figure 7.12, we can see the calculated results: the Johnson noise lifetime decreases as the number of graphene layers increases. The explanation for this is that increasing the number of graphene layers increases the number of free electrons in the surface and, hence, their overall thermal noise. It is noteworthy that a Johnson noise lifetime of 31 s can be achieved even when there are 30 layers of graphene. Since, in the modelling of the current graphene-based atom chips, the graphene wires are only one-layer thick [25], this indicates a promising potential of novel graphene-based atom chips.

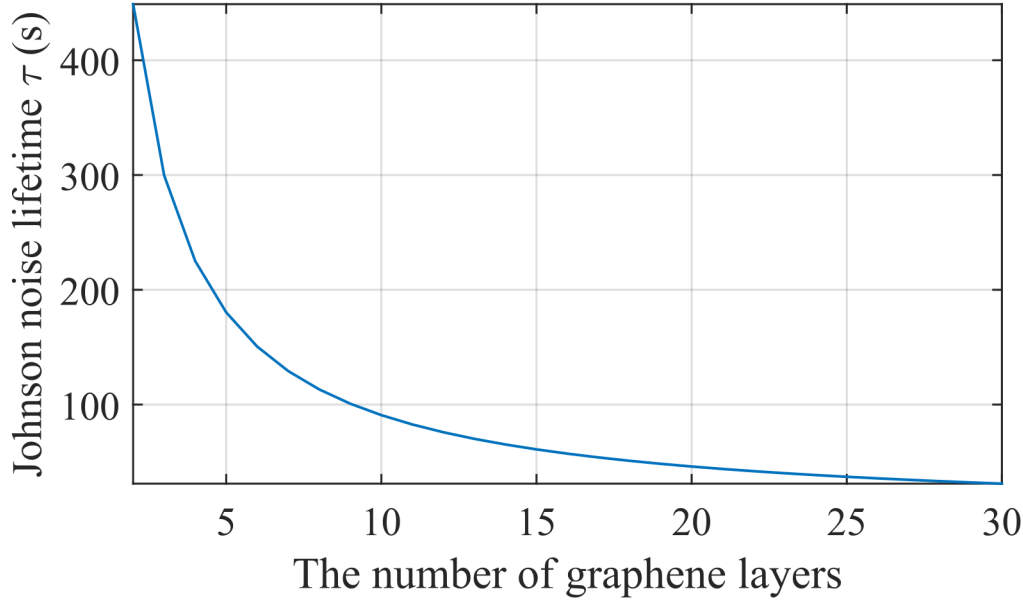


Figure 7.12: Johnson noise lifetimes, τ , calculated versus the number of graphene layers, of an ensemble of ultra-cold ^{87}Rb atoms trapped at the distance $y_0 = 1\text{ }\mu\text{m}$, for the structure illustrated in Figure 6.2 with vacuum between graphene layers. As expected, Johnson noise lifetime decreases as the number of graphene layers increases. However, it is still comparatively longer than the lifetime calculated above metal slabs even at $N = 30$, highlighting the promising potential of graphene-based atom chips in which only a few graphene layers are needed. Parameters: $T = 300\text{ K}$, $\omega = 2\pi \times 560\text{ kHz}$, $d = 1.4\text{ nm}$, and $E_F = 0.1\text{ eV}$, $\gamma = 4\text{ THz}$, for graphene.

We will now consider three-layer structures consisting of combinations of graphene and hBN layers. The trap parameters are the same except now we have $N = 3$. We start with the structure that we are familiar with, which is the graphene/hBN/graphene heterostructure, labelled Gr/hBN/Gr in Figure 7.13. The conductivity of each hBN monolayer is obtained from the four-parameter semi-quantum model in the same manner as described in the previous chapter. In the calculation of the reflection coefficients by the transfer-matrix method, the hBN monolayer is assumed to have no thickness, so is the graphene monolayer. The second structure is composed of three layers of graphene (Gr/Gr/Gr) and the last one is two layers of hBN enclosing a single layer of graphene (hBN/Gr/hBN).

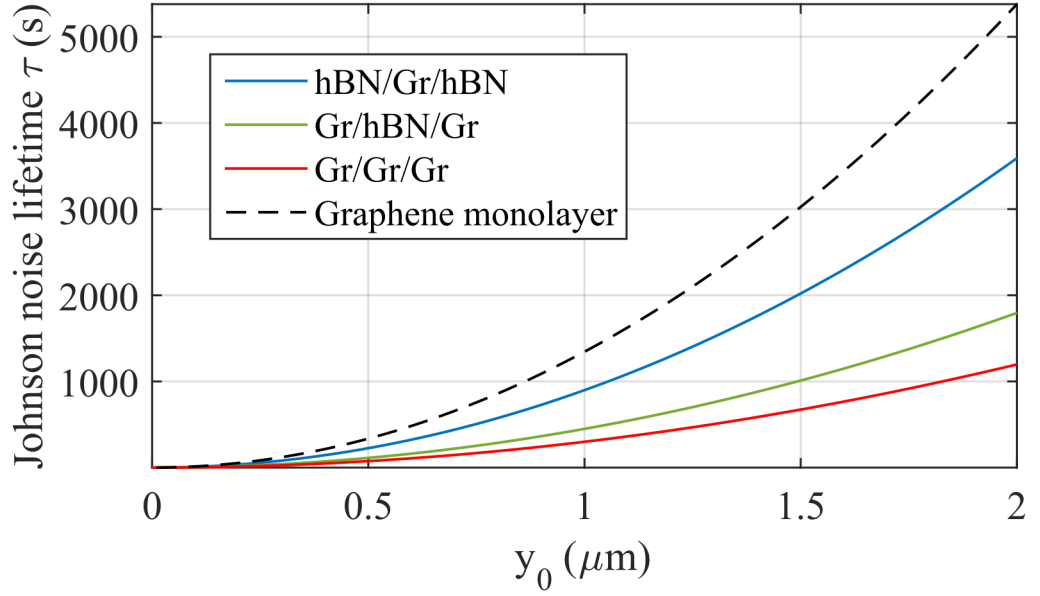


Figure 7.13: Johnson noise lifetimes, τ , calculated versus trapping distance, y_0 , of an ensemble of ultra-cold ^{87}Rb atoms trapped above three different 3-layer structures. The first configuration is two graphene layers enclosing an hBN monolayer, denoted by Gr/hBN/Gr; the second is a stack of three graphene layers (Gr/Gr/Gr); the last structure is a graphene monolayer encased by two hBN layers, denoted by hBN/Gr/hBN, and their corresponding lifetimes are plotted in green, red, and blue curve, respectively. The Johnson noise lifetime for a graphene monolayer is also added for comparison. The conductivity of hBN is obtained from the four-parameter semi-quantum model introduced in chapter 6. We can see that the Gr/Gr/Gr structure gives the strongest Johnson noise due to higher optical conductivity. With hBN enclosing graphene, the lifetime increases. This shows the potential of graphene-based atom chips that use hBN coating on the graphene layers to prevent contamination due to adsorption and polarisation of Rb atoms directly on the graphene [72]. Parameters: $T = 300$ K, $\omega = 2\pi \times 560$ kHz, $d = 1.4$ nm, $N = 3$, and $E_F = 0.1$ eV, $\gamma = 4$ THz, for graphene.

In Figure 7.13, it can be seen that the Gr/Gr/Gr structure gives the shortest lifetime, the Gr/hBN/Gr structure has a moderate lifetime, and the atoms trapped near the hBN/Gr/hBN structure have the longest Johnson noise lifetime. If we recall the weak Casimir-Polder potential of hBN (see Figure 6.4), it is reasonable that the structures with hBN layers will give longer Johnson noise lifetimes than the structure without hBN. This could be useful in developing graphene-based atom chips as we can coat the graphene wires with hBN to prevent contamination and, at the same time, reduce the thermal spin flip

rate of the trapped atom cloud [72].

7.3 Chapter Summary

We have given an introduction to the present generation of atom chips and laid out the theoretical foundations for atom-cloud lifetime calculations, including the dyadic Green's function and the quantum physics of spin angular momenta and Johnson noise. We have encountered an issue of not knowing the exact expression for the complex magnetic permeability of diamagnetic metals; however, we have made progress by taking a simple value of the permeability. We started calculating the Johnson noise lifetimes by considering pure metal slabs and compared the results obtained from Henkel's formula [53, 54] and Rekdal's formula [95]. The rest of the chapter considered more complex graphene-based structures. We have found that, in general, graphene-based structures give lower Johnson noise than metal structures, showing the performance advantage of graphene-based atom chips. In future work, we will try to find analytical expressions derived from Rekdal's formula in asymptotic limits and compare them with Henkel's. We will also try to find analytical expressions for the complex permeability, allowing us to explore more metal-based structures and get more accurate results. Furthermore, we will try to figure out possible implementations of graphene-based atom chips.

Chapter 8

Conclusion and Outlook

In this thesis, we have studied the electronic and optical properties of graphene monolayers and the quantum dynamics of atoms near graphene-based interfaces in the context of field-effect transistors and atom chips. At the start of this PhD research, miniaturisation of transistors by employing the peculiar properties of graphene was one of the hot research topics in the Universities of Manchester and Nottingham. We carried on the work on graphene-based transistors [40] by following the graphene-based device models to show that we can fine-tune the device tunnel-current characteristics by altering the device parameters such as the misalignment angle and the bias gate voltages. We also discussed the tunnelling process and found that the like-band tunnelling dominates in a low bias voltage regime up to the value at which the tunnel current reaches its peak, while the unlike-band tunnelling was dominant after that point. We then extended our research scope to investigate the variation of tunnel current with barrier thickness and temperature. We investigated the resonant tunnelling condition and showed the viability of graphene-based transistors that can withstand a high working temperature. Future work could include investigating electrodes made of different novel 2-dimensional materials.

The rest of the thesis, commencing from Chapter 5, is devoted to the study

of graphene-based atom chips. However, within the scope of this thesis, we have inclined more towards understanding the physics of atom-field interactions of atoms near-graphene multilayers rather than considering the trapping currents and fields, which are now well understood. We started by looking into the optical properties of graphene and laying out a computational method (transfer-matrix method) for calculating the Fresnel reflection coefficients for planar structures. This method proved to be very versatile as it can be used to calculate the reflection coefficients of structures comprising one to thousands of graphene layers with ease. We used this method to explore the optical properties of various graphene-based structures such as Fabry-Pérot resonators and photonic crystals. In Chapter 6, we studied quantum fluctuations of charge and fields and derived an expression for the Casimir-Polder potential within the Born-Oppenheimer approximation, rather than the Lifshitz formula [60]. We then calculated the Casimir-Polder potential experienced by a ^{87}Rb atom near a graphene monolayer using both the transfer-matrix method and analytical reflection coefficients in Dirac model. We compared the Casimir-Polder potentials calculated for a graphene monolayer, an hBN monolayer and a thin slab of gold: we found that the graphene and hBN layers yielded far weaker Casimir-Polder attractions than the gold slab. We then investigated the Casimir-Polder potential as a function of the atom-surface distance in the graphene/hBN/graphene heterostructures. We have found that, in general, a structure with a thicker hBN slab produces a higher Casimir-Polder attraction in the sub-micron atom-surface separation regime. We also investigated the effect of Bragg's condition on the variation of the Casimir-Polder potential with the hBN thickness. We chose three different models to describe the optical properties of the hBN slab. We have found a common feature which occurs in all the models: the Casimir-Polder potential becomes more attractive as the hBN thickness increases. This result agrees with the conclusion made in [25] that the Casimir-Polder potential monotonically approaches the values

for bulk materials as the hBN thickness increases.

The last section in Chapter 6 integrated the work on the gated graphene-based transistor studied in Chapters 3 and 4 with an attempt to vary the Casimir-Polder potential near the structure. We showed that the Casimir-Polder attraction becomes slightly weaker when the Fermi energy of the graphene layer deviates from 0, i.e. from the Dirac point. In the context of graphene-based atom chips, this study showed significant performance advantages of the graphene-based atom chips over the present generation of atom chips which use metal wires. In Chapter 7, we considered the Johnson noise lifetimes of ^{87}Rb Bose-Einstein condensates trapped near metal slabs and graphene-based structures. We showed that the imaginary part of the permittivity of a metal plays a crucial role in determining the lifetimes: a metal with a larger imaginary part of the permittivity produces a stronger Johnson noise. We compared the Johnson noise lifetimes associated with a single layer of graphene and a thin copper slab and found that a single layer of graphene yields a far longer lifetime than a thin copper slab. We also examined the validity of our spin-flip rate model by investigating the variation of the Johnson noise lifetime with the atom-surface distance and found that the lifetime approaches the value of the lifetime in free space in the limit that the atom-surface distance approaches infinity. We showed that the Johnson noise lifetime decreases with increasing environment temperature and as the number of graphene layers increases. Lastly, we showed that the Johnson noise lifetime increases when we add layers of hBN, hinting that the use of hBN coating could be advantageous in the development of graphene-based atom chips.

Possible future work would include, in regards to exploring metal-based structures, trying to find better models of the optical properties of metals, which provide analytical expressions for the complex permeability. This could include

trying to investigate the Casimir-Polder potential and Johnson noise lifetime for a range of novel multilayered systems. This can be done easily since we have now developed a solid theoretical formalism. Searching for the materials that yield repulsive Casimir-Polder forces would also be very interesting. Regarding the Johnson noise lifetime calculations, considering other possible spin-flip processes such as a spin flip from $|F = 2, m_F = 1\rangle$ to $|F = 2, m_F = 0\rangle$ would also give more accurate lifetimes. Another possible future direction includes considering the effect of quantum tunnelling in gated graphene-based heterostructures on the Johnson noise lifetime and thereby predicting the total lifetime of the trapped atoms more accurately. Last but not least, figuring out possible implementations of graphene-based atom chips is crucial for future experimental work with cold atoms.

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