Simulating Light Absorption and Emission in Materials

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Abstract. In this paper, the author builds a simple model for light absorption and emission in materials, with a special focus on graphene. This is mainly due to its extraordinary optical properties near the Dirac points, as well as the band gap opening due to external electric field perturbations. A fully quantum mechanical treatment of light as well as the matter electrons is used. The theoretical model is based upon quantum optics, quantum dynamics, as well as electronic band theory, capturing the essence of the light-matter interaction happening among materials, while simplifying the mathematical description. The author uses Python simulation to test the efficacy of this model and observes the steady state absorption rate. Meanwhile, this work also studies the dynamical properties of the system including excited state probability and the expectation value of photon number in the beam. The numerical result is in good accordance with experimental evidence, where similar trends are observed, paving the way for relevant theoretical and experimental researches on the optical properties of graphene and other materials.

Keywords: Band structure, Light-matter interaction, Graphene, Absorption rate.

1. Introduction

Since its discovery, graphene has captured the interest of a broad community of researchers due to its unique optical and electronic properties, connecting the field of optics, electronics, quantum information and quantum sensing [1,2,3]. Graphene owns many fascinating properties due to its two dimensional nature as well as its hexagonal atomic arrangements. As a result, it could be used to build optical modulators [4] and photon detectors [5] due to its interesting light matter interaction properties. However, the existing models for graphene light absorption and emission, and more generally, the light-matter interaction properties of an arbitrary material with a given band structure, are always too complicated, smearing out the physical essence of such process. Therefore, it is needed that a simple model that captures the essence of light-matter interaction of materials be built.

In this paper, the author concentrates on the topic of simulating the light absorption and emission properties of materials, with a particular focus on graphene. This endeavor integrates the principles of band theory and the quantum description of light, aiming to unravel the complex interplay between electronic structures and light-matter interactions. The objective is to provide a simplified model of how materials like graphene interact with electromagnetic radiation, paving the way for innovative applications in various technological domains.

Graphene, a single layer of carbon atoms arranged in a hexagonal lattice, has emerged as a material of immense interest due to its extraordinary electronic, optical, and mechanical properties. Its unique band structure, featuring Dirac cones at the K and K' points, leads to electrons behaving as massless Dirac fermions [6]. This results in exceptional electrical conductivity and allows for a wide range of light absorption frequencies. This paper aims to delve into the optical properties near Dirac points by leveraging band theory, a fundamental framework in solid-state physics that describes the energy levels of electrons in a material. Through simulations and theoretical analysis, the author aims at offering a clear and simple physical perspective on how materials like graphene absorb and emit light. These insights have far-reaching implications, from the development of highly efficient photo-detectors and solar cells to the creation of innovative optoelectronic devices. By bridging the gap between fundamental physics and practical applications, This work stands at the forefront of advancing materials science and technology, opening doors to cutting-edge innovations and solutions.

2. Theory

2.1. Band Structure of Graphene

To begin with, the author presents the lattice geometry of graphene. As shown in Fig. 1, in an infinitely extending graphene-like structure, for any lattice site i, the vectors δ_{ij} connecting its nearest neighbors can be defined as one of the followings: $\delta_1 = a(-1,0)$; $\delta_2 = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$; $\delta_3 = a\left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right)$. As each unit cell of graphene hosts two different types of atoms, denoted A and B, respectively. It is a common approach to define a respective set of creation and annihilation operators $\hat{a}_i^\dagger, \hat{a}_i, \hat{b}_j^\dagger, \hat{b}_j$ for each atom. In this manner, the graphene electronic Hamiltonian can be described as follows, using tight bonding approach where only the nearest neighbor hopping terms are included

$$\hat{H}_{gr} = -t \sum_{\langle ij \rangle} \left(\hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i \right). \tag{1}$$

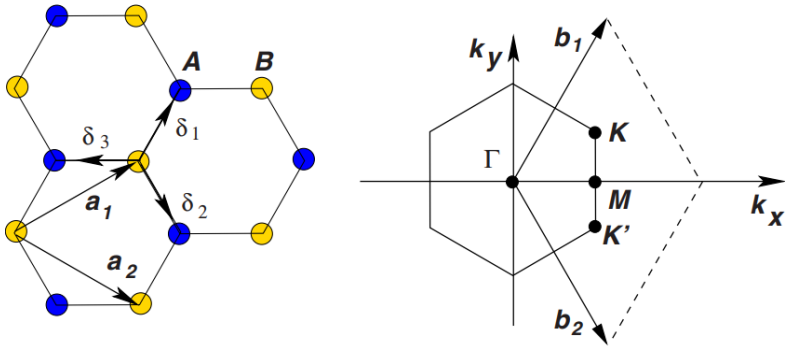


Fig. 1 Left Panel: Real space representation of graphene. Right Panel: K space representation of graphene [6].

The creation and annihilation operators can be transformed onto the momentum basis

$$\begin{cases} \hat{a}_i^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{ikR_i} \hat{a}_k^\dagger \\ \hat{b}_j^\dagger = \frac{1}{\sqrt{N}} \sum_{k'} e^{ik'R_j} \hat{a}_{k'}^\dagger \end{cases} \tag{2}$$

Using the identity $\sum_i e^{iR_i(k-k')} = N\delta(k-k')$, the graphene electronic Hamiltonian could be formulated as the tensor product of the sub-lattice Hamiltonian $H(k)$ and the projector onto the momentum basis of the electrons $\hat{c}_k^\dagger \hat{c}_k = |k\rangle\langle k|$, similar to the approach used when dealing with the Hamiltonian of Su-Schrieffer-Heeger chain [7]

$$\hat{H}_{gr} = -t \sum_k H(k) \otimes \hat{c}_k^\dagger \hat{c}_k . \tag{3}$$

The sub-lattice Hamiltonian has the form

$$\mathrm{H(k)} = \begin{pmatrix} 0 & \mathrm{f^*(k)} \\ \mathrm{f(k)} & 0 \end{pmatrix} \tag{4}$$

where f(k) is highly dependent upon the geometric properties of the lattice structure. By using $R_j = R_i + \delta_{ij}$, it is obtained that

$$\mathrm{f(k)} = \sum_{\mathrm{j}} \mathrm{e}^{\mathrm{ik}\delta_{\mathrm{ij}}} = \mathrm{e}^{-\mathrm{ik_x a}} + 2\mathrm{e}^{\mathrm{ik_x}\frac{\mathrm{a}}{2}} \cos\left(\mathrm{k_y}\frac{\sqrt{3}}{2}\mathrm{a}\right). \tag{5}$$

After diagonalizing the sub-lattice Hamiltonian, the energy-momentum dispersion relationship of graphene $\mathrm{E(k)}$ can be obtained. The $\pm$ showcases the energy distinction between the valence and the conduction band, respectively [8]

$$\mathrm{E(k)} = \pm \mathrm{t}\sqrt{1 + 4\cos^2\left(\mathrm{k_y}\frac{\sqrt{3}}{2}\mathrm{a}\right) + 4\cos\left(\mathrm{k_y}\frac{\sqrt{3}}{2}\mathrm{a}\right)\cos\left(\mathrm{k_x}\frac{3}{2}\mathrm{a}\right)}. \quad (6)$$

Notice that, the valence and conduction bands meet at special points in the k space. People usually denote these points K as Dirac points, as the behavior of electrons near these points resembles the massless Dirac fermions emergent in the Dirac equation for relativistic particles. The Dirac points can be located at (K_x, K_y), with their coordinates being $\left(0, \pm\frac{4\pi}{3\sqrt{3}a}\right)$; $\left(\pm\frac{2\pi}{3a}, \pm\frac{2\pi}{3\sqrt{3}a}\right)$. The energy dispersion relationship could be expanded in the neighborhood of these Dirac points

$$\mathrm{E(k')} = \mathrm{E}\left(\mathrm{K_x}, \mathrm{K_y}\right) + \frac{\partial \mathrm{E}}{\partial \mathrm{k_x}}\left(\mathrm{K_x}, \mathrm{K_y}\right)\delta\mathrm{k_x} + \frac{\partial \mathrm{E}}{\partial \mathrm{k_y}}\left(\mathrm{K_x}, \mathrm{K_y}\right)\delta\mathrm{k_y} + \cdots. \quad (7)$$

The dispersion relationship becomes linear with k near Dirac points $E(\mathrm{k}) = \hbar \mathrm{v_F}|\mathrm{k}|$ where $v_F = \frac{3ta}{2\hbar}$.

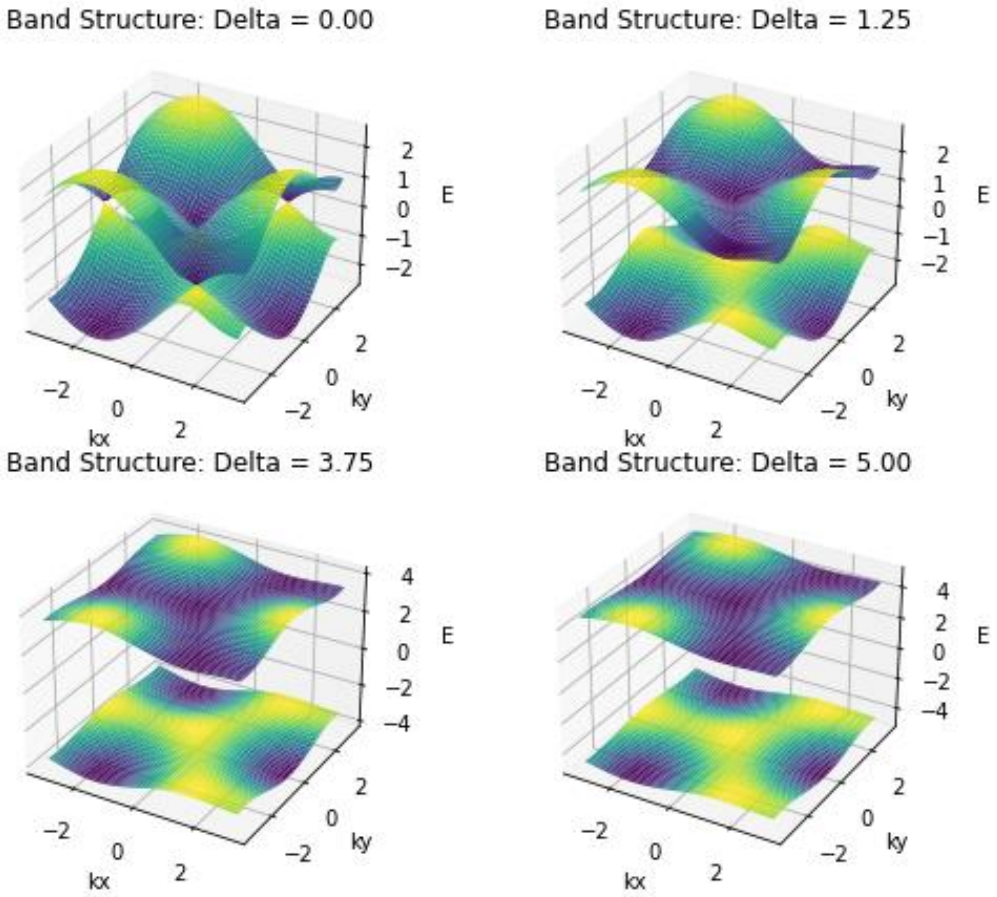


Fig. 2 The energy dispersion relationship of graphene $\mathrm{E(k)}$ in the entier first Brillouin zone, satisfying Eq. (6). Parameters k_x, k_y range from $-\pi$ to π. In this simulation, $\mathrm{a} = \frac{4}{3\sqrt{3}}$, $\hbar = \mathrm{v_F} = 1$, $\mathrm{t} = \frac{2\hbar \mathrm{v_F}}{3\mathrm{a}} = \frac{\sqrt{3}}{2}$. Δ takes the values 0, 1.25, 3.75 and 5.00, respectively.

Equivalently, the sub-lattice Hamiltonian could be expressed in terms of Pauli operators near Dirac points $\widehat{H}(k) = \hbar \mathrm{v_F}\left(\mathrm{k_x}\hat{\sigma}_\mathrm{x} + \mathrm{k_y}\hat{\sigma}_\mathrm{y}\right)$. In many cases, people are interested in the behavior of graphene

under the external tuning of electric field [9]. In this case, one slightly modifies the form of the sublattice Hamiltonian $H(k)$ near Dirac points

$$H(k) = \hbar v_F\left(k_x\hat{\sigma}_x + k_y\hat{\sigma}_y\right) + \hbar\Delta\hat{\sigma}_z. \tag{8}$$

Fig. 2 illustrates the band structure of graphene under external electric field tuning in the first Brillouin zone. As Δ increases, the opening of band gap is observed. This indicates that the band gap at Dirac points increases to a finite value, indicating the transition from semi-metal to semi-conductor, and finally to insulator.

Given an arbitrary dispersion relationship $E(k)$, it is always possible to calculate the density of states (DOS) with respect to the electron energy E by integrating over the momentum space:

$$D(E) = \frac{g_s}{2\pi^n}\int d^n k\,\delta\left(E - E(k)\right) \tag{9}$$

where $\delta\left(E - E(k)\right)$ stands for Dirac delta function, while g_s stands for the electron spin degeneracy, usually taking the value 2, and n stands for the dimensionality of the system. Using Eq.(9), a linear density of states near Dirac points with respect to the energy E can be obtained, as well as the lattice wave vector k:

$$\rho(E) = \frac{2}{\pi\hbar^2 v_F^2}|E| = \frac{2}{\pi\hbar v_F}|k| \tag{10}$$

Unlike the DOS for a free electron in 2d, which is a step-like function with respect to electron energy, the linear DOS with energy near Dirac points gives rise to special optical and electronic properties of graphene. Fig. 3 demonstrates this fascinating linear trend.

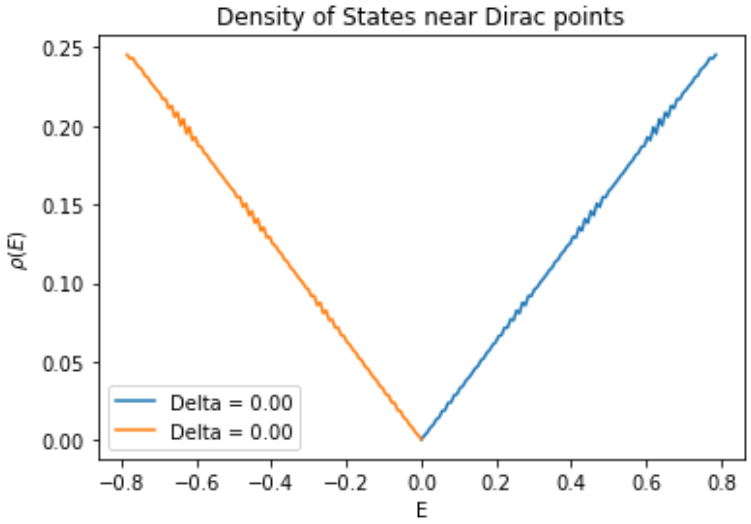


Fig. 3 The density of states (DOS) of graphene near Dirac points with respect to electron energy E. The blue line illustrates the conduction band DOS, while the orange line indicates the valence band DOS. The Fermi energy is set to 0.

In the following section, a generalized model for light absorption and emission of an arbitrary material with a given dispersion relationship $E(k)$ will be introduced. As will be shown, this simple model can capture the essential dynamics of light-matter interaction in graphene.

2.2. Model for Photon Absorption and Emission

In this section, the author will build a simple model describing photonic absorption and emission processes based on the electronic band structure theory, and a fully quantized theory of light. Quantum mechanically, the entire procedure could be understood as the unitary evolution of state vectors defined on the Hilbert space $\mathcal{H}_{ph}\otimes\mathcal{H}_e$, where $\mathcal{H}_{ph}$ denotes the photonic subspace, with the

corresponding eigenstates being the photonic Fock states $\{\otimes_k|n_k\rangle\}$, and $\mathcal{H}_e$ denotes the electronic subspace, its eigenstates being expressed as the eigenvectors on the momentum basis $\{|\mathrm{k}\rangle\}$, when the spin degrees of freedom σ is omitted for simplicity. Therefore, the eigenvectors of the combined Hilbert space could be defined as $\{(\otimes_{\mathrm{q}}|\mathrm{n_q}\rangle)\otimes|\mathrm{k}\rangle\}$, and any state vector will be the linear combination of these basis states.

Usually, the unitary time evolution operator $\mathrm{U(t)} = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}\mathrm{t}}$ could be expressed as the evolution of the Hamiltonian $\hat{H}$ describing the entire system for a time period t, when the effects of external decoherence could be neglected. The total Hamiltonian could be expressed as:

$$\hat{H} = \hat{H}_{ph} + \hat{H}_e + \hat{H}_{int}. \tag{11}$$

The photonic Hamiltonian $\hat{H}_{ph}$ is as follows:

$$\hat{H}_{ph} = \sum_{q,\lambda} \hbar\omega_q \left(\hat{a}^\dagger_{q,\lambda}\hat{a}_{q,\lambda} + \frac{1}{2}\right) \tag{12}$$

where the summation over different photonic modes q is performed. λ is the polarization index. For single mode laser with fixed polarization, the entire Hamiltonian will be reduced to $\hbar\omega\left(\hat{\mathrm{a}}^\dagger\hat{\mathrm{a}} + \frac{1}{2}\right)$.

The electronic Hamiltonian $\hat{H}_e$, in real space, could be expressed as the infinite summation of the terms corresponding to the onsite interaction, the nearest neighbor hopping, the next nearest neighbor hopping and so on:

$$\hat{H}_e = \triangle \sum_i \hat{c}_i^\dagger \hat{c}_i - t\sum_{\langle ij\rangle}\left(\hat{c}_i^\dagger\hat{c}_j + \hat{c}_j^\dagger\hat{c}_i\right) + t'\sum_{\langle\langle ij\rangle\rangle}\left(\hat{c}_i^\dagger\hat{c}_j + \hat{c}_j^\dagger\hat{c}_i\right) + \cdots \tag{13}$$

If a Fourier transformation onto the momentum basis is performed, it is possible to arrive at a description of the electronic Hamiltonian in the full Hilbert space using tensor product, similar to what is obtained in Eq. (4) for the graphene example:

$$\hat{H}_e = \sum_k H(k)\otimes\hat{c}_k^\dagger\hat{c}_k \tag{14}$$

where $H(k)$ signifies the Hamiltonian for the degrees of freedom within a unit cell, $c_k^\dagger, c_k$ are the creation and annihilation operators for the mutually non-interacting electrons with a given momentum k.

The interaction Hamiltonian $\hat{H}_{int}$ is vital for the construction of the theory, as it formulates the interactions of the photons and the electrons inside the material:

$$\hat{H}_{int} = \sum_{k,k,q,\lambda} \hbar g_{kk',q\lambda}\left(\hat{a}_{q,\lambda}\hat{c}^\dagger_{k',c}\hat{c}_{k,v} + \hat{a}^\dagger_{q,\lambda}\hat{c}^\dagger_{k,v}\hat{c}_{k',c}\right). \tag{15}$$

Note that $\hat{H}_{int}$ comprises of the summation over the photonic modes q, the polarization λ, as well as the electronic modes k, k', where k and k' represent the electron momentum before and after the interaction with the photon, respectively. The label v denotes the valence band electrons, while the label c denotes the conduction band electrons. In most cases, the photonic momentum is orders of magnitude smaller than the electronic momentum. In this regard, one approximately models the electronic transition from the valence band to the conduction band when a photon is absorbed by a direct transition, where the differences in electronic momentum k, k' can be neglected, due to the conservation of momentum, unless in some TMDCs where indirect transitions with the aid of electron-phonon interactions become dominant [10]. In the graphene case, Eq. (15) reduces to:

$$\hat{H}_{int} = \hbar g(\hat{a} + \hat{a}^\dagger)(\hat{\sigma}\cdot\vec{\varepsilon}) \tag{16}$$

where $\vec{\varepsilon}$ is the polarization vector of light in the xoy plane.

An important rule governing the photonic absorption and emission process associated with the electronic transition is the Fermi Golden Rule

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar}\left|\langle f|\hat{H}_{int}|i\rangle\right|^2 \delta\left(E_f - E_i - \hbar\omega\right) \tag{17}$$

where $\Gamma_{i\to f}$ means the transition rate from the initial state i to the final state f. This quantity is proportional to the square of the norm of the interaction Hamiltonian matrix value $\left|\langle f|\hat{H}_{int}|i\rangle\right|^2$, and a specific Dirac function term $\delta\left(E_f - E_i - \hbar\omega\right)$ showcasing that the transition is allowed only if the incident photon energy $\hbar\omega$ matches the energy difference between the initial and the final state $E_f - E_i$. These resonant transitions are the major contributions to photonic absorption and emission properties of a given material, while the off-resonant transitions are not taken into consideration in the scope of this paper.

The optical absorption rate, for example, can be formulated as:

$$W_{i\to f} = \frac{2\pi}{\hbar}\iint dk_{i,v}dk_{f,c}\left|\langle f,c|\hat{H}_{int}|i,v\rangle\right|^2 \delta\left(E_{f,c} - E_{i,v} - \hbar\omega\right)\rho\left(E_{f,c}\right)\rho\left(E_{i,v}\right) \tag{18}$$

where the integration over all possible initial states $|\mathrm{i,v}\rangle$ at the valence band, as well as all possible final states $|\mathrm{f,c}\rangle$ at the conduction band is performed, $\rho\left(E_{f,c}\right), \rho\left(E_{i,v}\right)$ accounts for their respective density of states, which could in principle be derived by the energy band structure of a given material if $\mathrm{E(k)}$ is known, as demonstrated in Eq. (11).

Usually, the optical absorption rate $W_{i\to f}$ is a function of the frequency ω of the incident photon beam. However, it is often considered as a static, time-independent quantity, featuring the transitions from one energy eigenstate of the time-independent Hamiltonian $\hat{H}$ to another. Meanwhile, the quantum dynamics of the system is also worth discussing, and thus it is necessary to define the excited state probability P_e to quantify the behavior of the electrons under the influence of the incident photon beam:

$$P_e = \sum_n |\langle n,c|\psi\rangle|^2 \tag{19}$$

where $|\psi\rangle = \sum_{\mathrm{n'}} \psi_{\mathrm{n'c}}|\mathrm{n',c}\rangle + \psi_{\mathrm{n',v}}|\mathrm{n',v}\rangle$ is an arbitrary time-dependent quantum state, and the excited state probability is calculated by summing over all the possible Fock basis states $|\mathrm{n}\rangle$. In the case of graphene, the sublattice Hamiltonian $\mathrm{H(k)}$ is represented by a 2 by 2 matrix, and thus could be modeled using a quasi two level system. Note that equivalently, the excited state could be represented by $|\mathrm{c}\rangle$, the quantum state vector representing the electron inside the conduction band, while the state $|\mathrm{v}\rangle$ signifies the electron inside the valence band, resembling the ground state.

Besides, the expectation value of the photonic number operator $\langle\hat{N}\rangle$ is another quantity that will be used in this paper. It is defined as $\langle\hat{N}\rangle = \langle\psi|\hat{N}|\psi\rangle$. Although this theoretical model captures the essence of the light - matter interaction of a given material, employing a full, quantum mechanical description of the light and the matter. However, the limitations are obvious. The electronic Hamiltonian $\hat{H}_e$ is simplified such that the many body interactions between electrons are neglected. However, this effect may lead to many interesting dynamics like exciton formation and nonlinear optical absorption and emission. What's more, the spin effect of the electrons are also neglected. Last but not least, to simplify the numerical simulation, only a single mode photon beam is considered in this work. But it is natural to generalize this theoretical model to multi-mode photon beams. Developing a more detailed and nuanced approach might be the focus of future works.

3. Simulations

In this section, the author performs Python simulation using the model established in Sec.2.2, taking the monolayer graphene as a specific example for illustration. In the simulation, only a small range of k values near Dirac points is considered, as the maximum deviation of lattice momentum away from the Dirac point K is set to $\frac{\pi}{4}$, where in this simulation, the center of the first Brillouin zone to the edge of the hexagon is π. In this regime, the linear approximation of the dispersion relation remains effective.

As this model uses the photonic description of light, it is required to set a maximum number of photons N in a beam in the simulation. The initial state is defined as $|N\rangle\otimes|v\rangle$, where there are N photons in the beam, while the graphene electrons are in the valence band, unexcited. As the quantum photon beam gradually couples to the material with a coupling constant g, the probability of the electrons being in the excited state, equivalently, the conduction band, changes with time.

As observed in Fig. 4, the excited state probability increases with time to approximately 0.5, and then starts oscillating around this value. This behavior could somehow be interpreted as the excited state probability - time curve being attracted towards the 'equilibrium'. When the light-matter coupling constant $g = 0$, the time evolution of the excited state probability resembles a sinusoidal pattern, but the trajectory quickly becomes irregular when the coupling is turned on. In the meantime, it is surprising that when the frequency ω of the external light is increased, the time evolution of excited probability becomes attracted to the 'equilibrium' value 0.5, featuring fewer and fewer wild oscillations. What's more, the polarization vector, defined as $\vec{\varepsilon} = \begin{pmatrix}\cos\theta \\ \sin\theta\end{pmatrix}$, parameterized by the angle θ, modifies the excited state probability with time by introducing some specific peaks at certain time points. This effect becomes increasingly noticeable when the evolution time gets longer. In order to shift the 'equilibrium', the external electric field, parameterized by Δ is required. As Δ increases, it becomes less likely for the electrons to occupy the excited state, assuming that Δ is positive. This means that the entire curve is shifted towards the direction of smaller P_e values. This could somehow explain the change of optical properties of graphene under doping effects [9]. The $P_e - t$ relationships using different k_x, k_y samples are also simulated. And the time evolution plots showcase a similar trend for different lattice momentum values. Hence, only $k_x = 0.13$, $k_y = 0.20$ is shown.

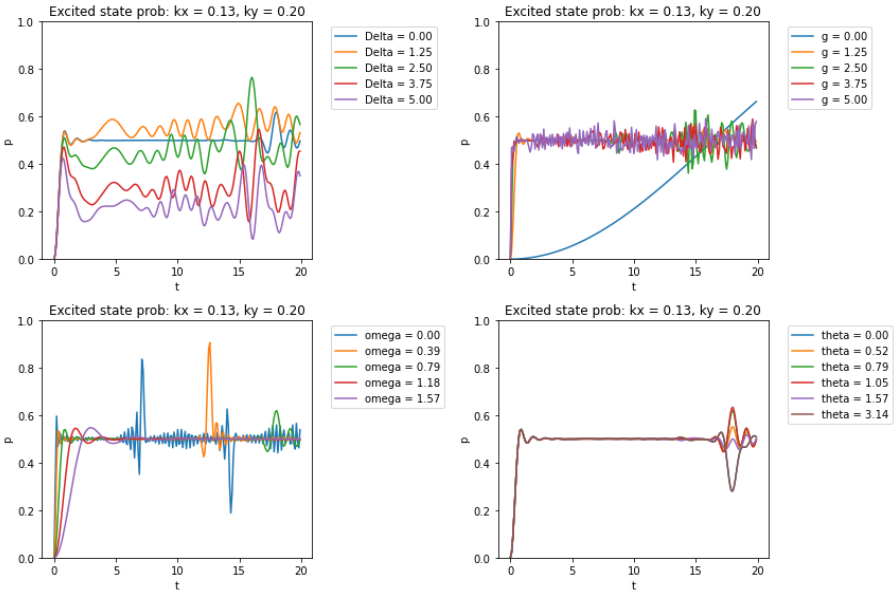


Fig. 4 The time evolution of excited state probability (the state representing electrons inside the conductance band) when $k_x = 0.13$, $k_y = 0.20$. The subplots show the different curves when the control parameters of the quantum system are varied. The maximum number of photons $N = 50$.

Besides the excited state probability, it is also worth examining the expectation value of photon numbers $\langle N \rangle$ evolving with respect to time. A special case to consider is when the coupling constant $g = 0$, indicating no couping. Therefore, the expectation value of photon number in the beam remains constant. When the coupling is gradually turned on, the decreasing rate of $\langle N \rangle$ becomes larger. Observing the $T = 50$ evolution curve shown in Fig. 5, when the coupling is turned on, the expectation value of photon number becomes oscillating with time, similar to the excited state probability. Based upon what has been understood from Fig. 4, the external electric field strength Δ and the photon frequency ω, when increased, suppress the light absorption at this particular k point due to the decrease of resonance terms. The trend is clearly observed in Fig. 5 as well, because the changing rate of $\langle N \rangle$ decreases. Surprisingly, the polarization angle θ does not significantly affect the absorption of photon, at least in terms of $\langle N \rangle$.

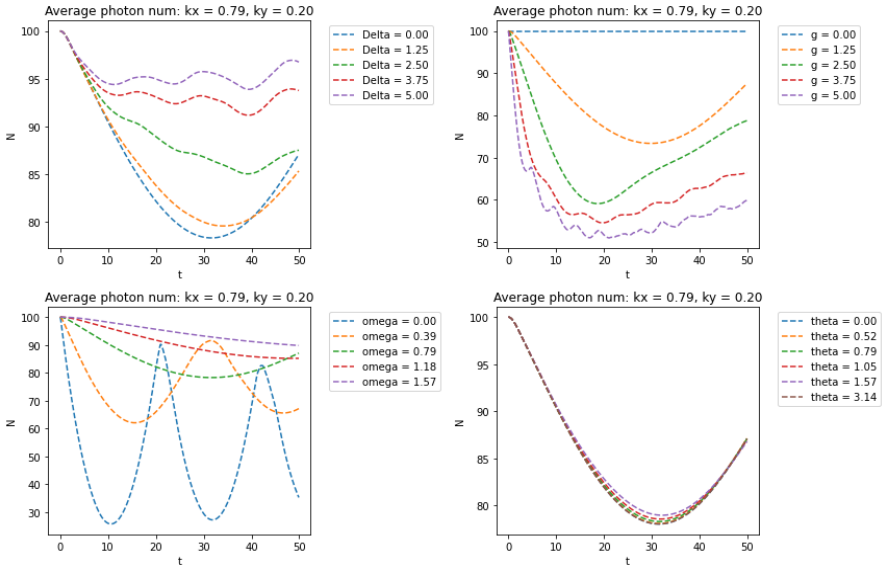


Fig. 5 Average photon number with respect to time. The total evolution time $T = 50$. The momentum values are $k_x = 0.79$, $k_y = 0.20$. The subplots show the different curves when the control parameters of the quantum system are varied with maximum photon number $N = 50$.

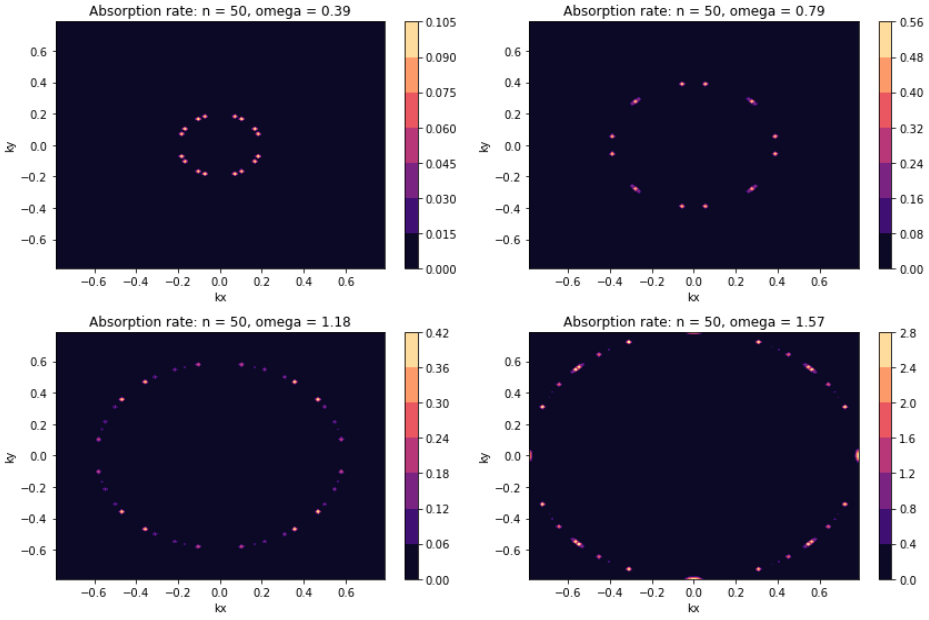


Fig. 6 Absorption rate integrating over the entire selected momentum space. The photon number $n = 50$. The incident photon frequency ω takes the value $[0.39, 0.79, 1.18, 1.57]$ respectively. k_x, k_y range from $-\frac{\pi}{4}$ to $\frac{\pi}{4}$. Other parameters are fixed to be $\Delta = 0$, $g = 1$, $\theta = \frac{\pi}{4}$.

Apart from the dynamical properties, the steady state absorption rate induced by Fermi Golden Rule is also plotted in Fig. 6. For different values of ω, the bright region gradually moves towards higher k_x and k_y. These bright regions correspond to the resonance region, while for most k values, the resonance condition is not satisfied, thus the steady state absorption rate is not significant. In this simulation, the Dirac delta function is approximated by using lorentzian distribution with $\sigma = 0.001$.

The author also simulated the case where the photon number considered increases, there a significant increase in the absorption rate. However, it is too early to conclude that whether the absorption rate will continue to increase with larger values of n. It is believed that similar to saturated absorption (SA), the absorption rate would finally settle at a fixed value [11]. In this paper, the case where $n = 50$ is displayed.

4. Experimental Evidence

Groundbreaking experimental work has established the remarkable optical properties of graphene. A seminal study revealed graphene's universal broadband absorption of approximately 2.3% of incident light over a wide spectral range [12]. Furthermore, ultrafast optical spectroscopy techniques have elucidated the dynamics of excited carriers in graphene. Measurements using differential transmission spectroscopy demonstrate extremely rapid relaxation times of photoexcited Dirac fermions on the order of hundreds of femtoseconds [13].

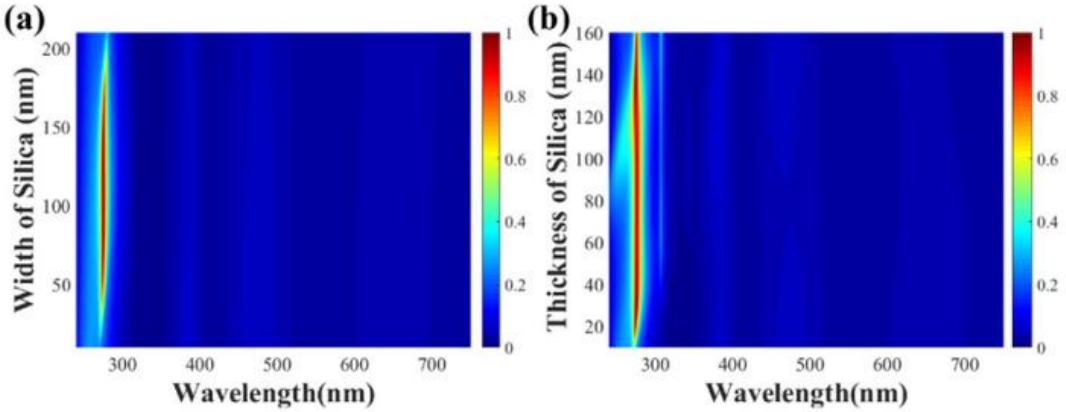


Fig. 7 Measured absorbance of graphene with varying wavelength and the thickness, width of silica substrate [13].

Fig. 7 demonstrates the measured absorbance of graphene with varying wavelength. This result indicates that the integrated absorbance is highly dependent upon the wavelength (frequency) of the incoming photons, selecting only the resonant case. This is in accordance with the results obtained in Fig. 6. There is also subsequent research on how modifying graphene through doping, patterning, or integration with other materials can tailor its light interaction for various applications. And to understand the essence of these new, emergent properties may require a more sophiscated theoretical model, with the simple model in this paper as a starting point.

5. Conclusion

In this paper, the author developed a simple theoretical model for light absorption and emission of materials with a given band structure $E(k)$, based on the theory of electronic band structure, quantum optics and quantum dynamics. Starting from these basics, the author can recover the essence of light matter interaction process. The author then tested this model using graphene as an example. As one of the most famous two-dimensional materials, graphene hosts many interesting properties, especially near the Dirac points, where both the energy-momentum dispersion relationship and the DOS-energy relationship becomes linear. Based upon this, the author simulated the integrated absorption rate from one steady eigenstate of the time independent Hamiltonian to another. The results obtained fit the

experimental data, where a large area of low absorbance due to off resonance is observed, while only in some specific regions of the momentum space where high absorbance becomes noticeable. Besides the static properties, the author also performed a simulation of the full quantum dynamics of this system, by calculating the excited state probability and the expectation value of photons in the beam, the author found that the optical properties of such system could be tuned by parameters including the external field strength Δ, input photon beam frequency ω, light - matter coupling strength g and the polarization angle θ. As the evolution time of the quantum system T increases, the oscillatory behavior of these quantities could be observed. The irregularity of these patterns signifies the complex nature of the light matter interaction procedure. This model paves the way for future research on relevant optical properties of graphene, as well as different methods to tune these properties. From chemical doping, external electric and magnetic field, to adding layers of graphene and twisting them to some specific 'magic angles. To better understand these properties beyond the simple, single layer graphene, a more detailed theoretical model based on what has been discussed in this paper could be developed. This could be the focus of future works.

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