Thermodynamic properties and optical absorption of polaron in monolayer graphene under laser eld

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Abstract

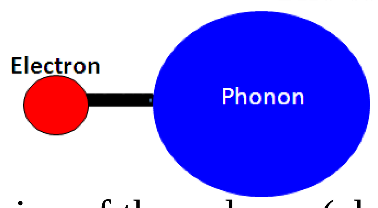
In this work, we use the variational method to investigate thermal properties and optical absorption of polaron in monolayer graphene under laser field. We have shown that the energies and the optical absorption of the system strongly depend on laser parameters and graphene characteristics. We found that the simple model adopted to calculate the optical absorption was enough accurate to investigate the optical absorption coecient of the polarons in graphene. We observe that the laser assists the polaron in the optical absoprtion phenomenon. We observe that temperature, the phonon and electron interaction, laser and wave number aect the disorder in the system.

Introduction

With intensive research in eld of nanotechnology recently, much attention has been given on graphene studies from the many aspects in experiments and theories. Graphene gets comprehensively applications as a thin structure due to its only physical valuable characteristics and many electronical applications. Graphene gets several interesting properties like a very high thermal conductivity and extraordinary high room temperature which makes it especially interesting to examine other thermal properties of graphene Polaron is a quasiparticle discover by Lev Landau in 1933, it is characterized by energy, effective mass, mobility, etc. These properties are dependent of the strength of the electron and crystal lattice interaction, the frequency of the movement of the electron and even of the quality of the vibration of the lattice. The properties of polaron are very interesting nowadays. Understanding the role of phonon interaction scattering and polaron scattering is of primary interest and important. The important characteristics enhance here is particularly for new nanostructures like graphene. it is important to note that, laser eect have neither been investigated in conventional 2D materials nor in graphene. What will the laser's effect on the decoherence of polaron in graphene. This is an important matter that need to be investigate.

Model and method

The total Hamiltonian of the system is described by



$$H_P = H_e + H_{ph} + H_{e-Ph} \qquad (1)$$

The Hamiltonian of the polaron (electron-phonon interaction) in the presence of the laser field in the system can be written as:

$$H = \begin{bmatrix} 0 & V_F\left(P_x + \frac{e}{c}By - i\left(P_y - \frac{e}{c}Bx\right)\right) \\ V_F\left(P_x + \frac{e}{c}By + i\left(P_y - \frac{e}{c}Bx\right)\right) & 0 \end{bmatrix} + \sum_k \hbar\omega a_k^+ a_k + \sum_k V_k \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix} \left(a_{-k}^+ + a_k\right) e^{i\vec{k}\vec{r}} \qquad (2)$$

Let us insert the linear combination of annihilation and creation operators,

$$\begin{cases} P_x = \lambda\left(b_x^+ + b_x\right) \\ r_I = \frac{i}{\lambda}\left(b_I^+ - b_I\right), \quad I = x, y \end{cases} \qquad (4)$$

Where, $$\lambda = \sqrt{\frac{|e|cE}{\hbar\Omega}\cos(\Omega t)} \qquad (3)$$

The second LLP transformation used is given by

$$U = \exp\left[\sum_k\left(\phi_k a_k^+ - \phi_k^* a_k\right)\right] \qquad (5)$$

The system's expectation energy is given by the relation

$$E_n = \left\langle \Psi_n \middle| H' \middle| \Psi_n \right\rangle \qquad (6)$$

Analytical Parameters

I. Optical absorption of polaron

On the base of the Fermis golden principle, the optical absorption coefficient for an incident photon with energy from the fundamental state of a free polaron is

$$\Gamma(\hbar\Omega) = -\frac{e^2D^2(\Omega-\omega_0)^2}{\rho\pi Cn\varepsilon_0\lambda^4\hbar^5\Omega^2\upsilon^3\left|(\Omega-\omega_0)\right|}\exp\left(-\frac{8m^2(\Omega-\omega_0)^2}{\hbar^2\lambda^2}\right)\left|-\lambda^2-\frac{4m^2}{\hbar^2}(\Omega-\omega_0)^2\right|^2 \qquad (7)$$

II. Thermodynamic properties of polaron

$$S_q = k_B\frac{1-\sum_{i=1}^{w}P_i^q}{1-q}, \quad (q\in\mathbb{R}) \qquad (8)$$

$$P(E_i) = \begin{cases} \frac{\left[1-\beta(1-q)E_i\right]^{\frac{1}{1-q}}}{Z_q}, & \left[1-\beta(1-q)E_i\right]^{\frac{1}{1-q}} > 0 \\ 0 & \text{Ohterwise} \end{cases}$$

$$Z_q = \sum_{levels}\left[1-\beta(1-q)E_i\right]^{\frac{1}{1-q}}$$

$$U_q = -\frac{\partial}{\partial\beta}\ln_q Z_q \qquad (9)$$

$$C_q = T\frac{\partial S_q}{\partial T} = \frac{\partial U_q}{\partial T} = -T\frac{\partial^2 F_q}{\partial T^2} \qquad (10)$$

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Simulation Results

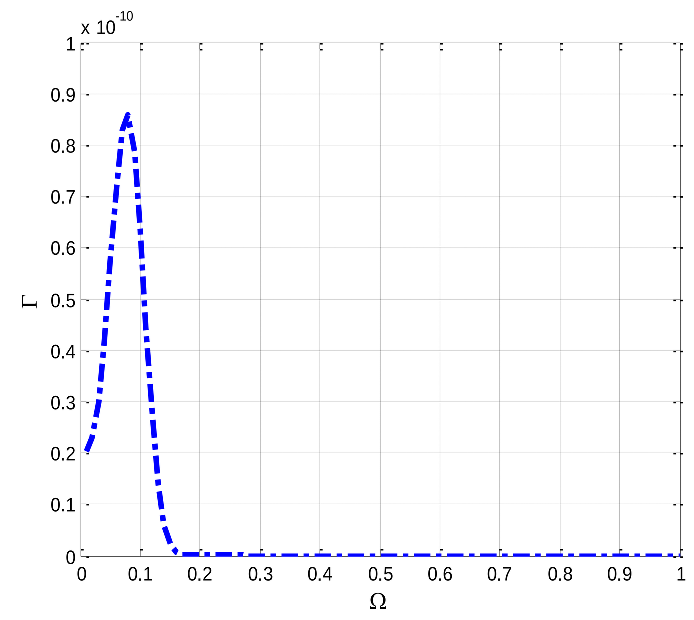

Fig 1: Optical absorption of polaron as function of laser energy

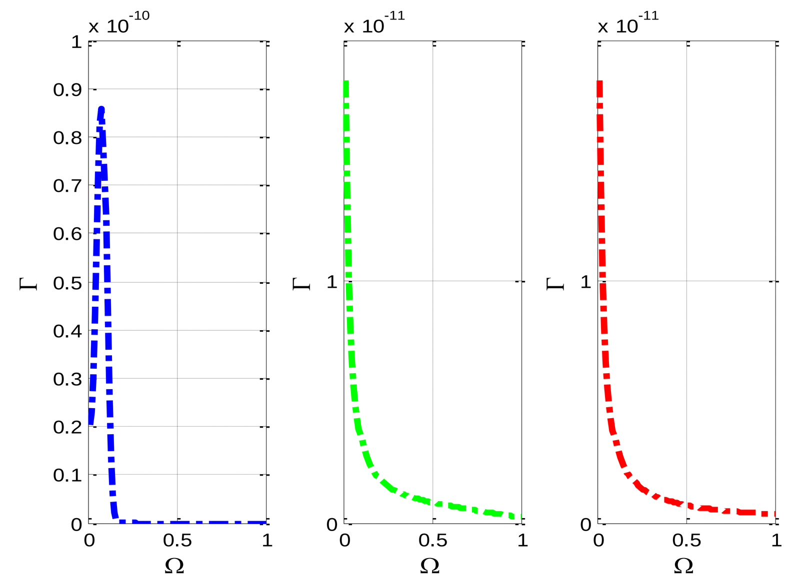

Fig 2: Optical absorption as function of laser energy for different values of laser amplitude.
E=0.008 (blue curve); E=10 (green curve); E=100 (red curve)

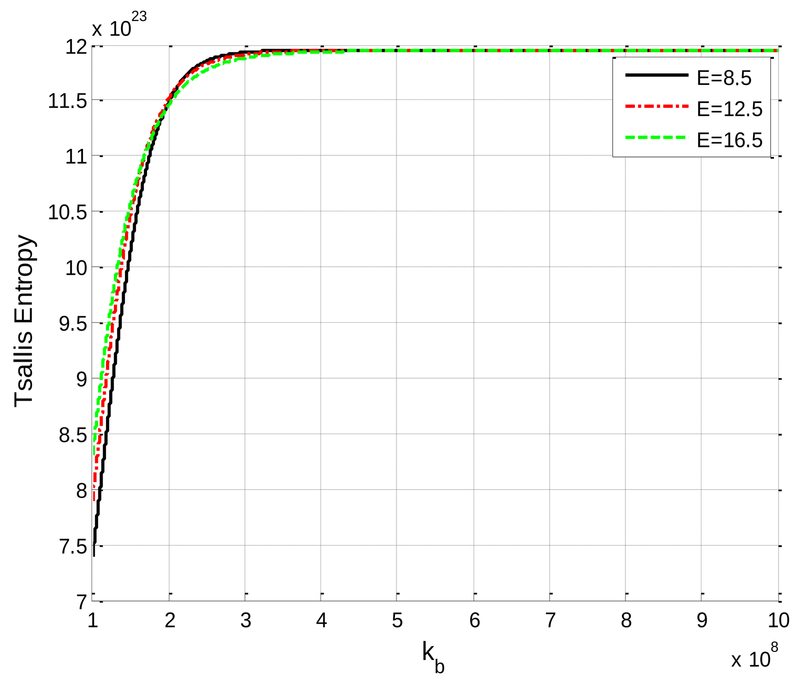

Fig 3: Tsallis entropy as function of wave number for different values of laser amplitude.

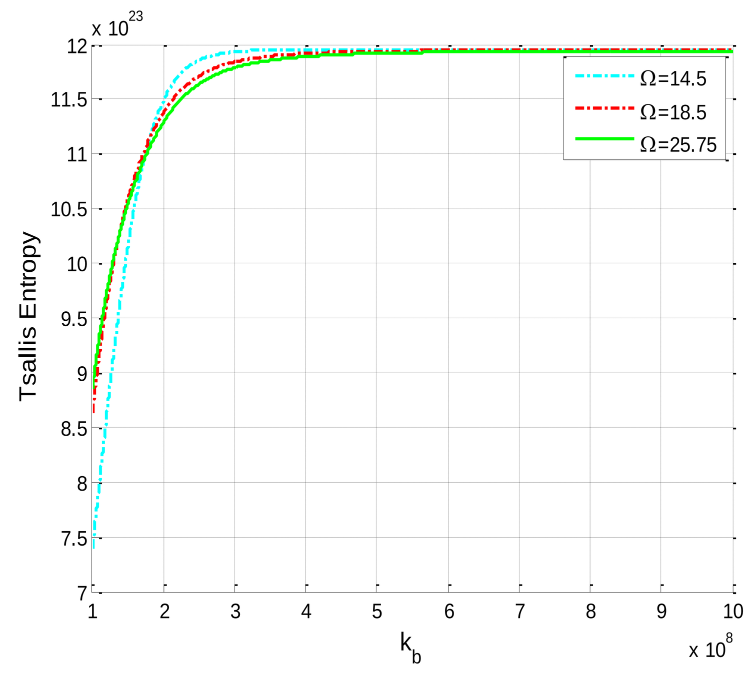

Fig 4: Tsallis entropy as function of wave number for different values of laser frequency.

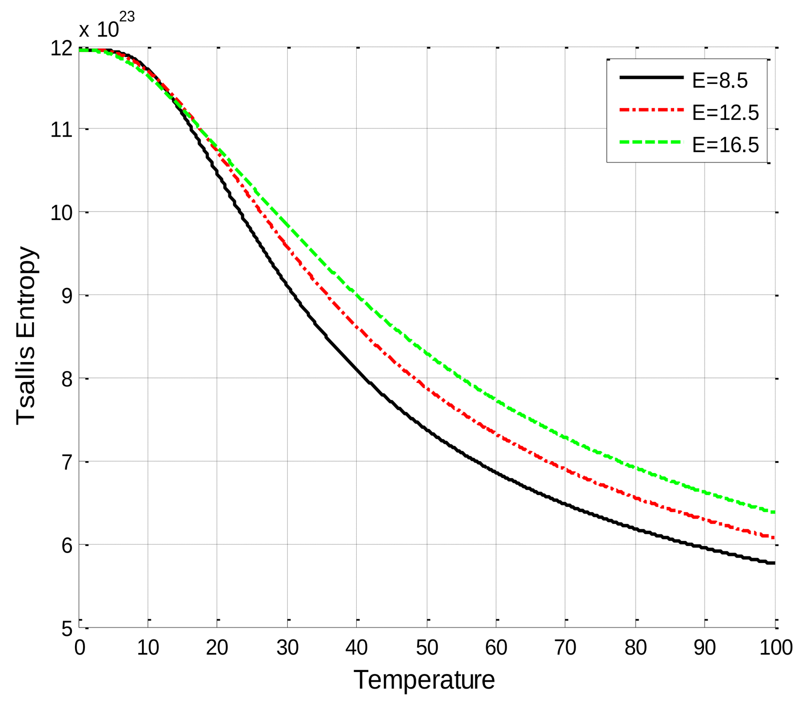

Fig 5: Tsallis entropy as function of temperature for different values of laser amplitude

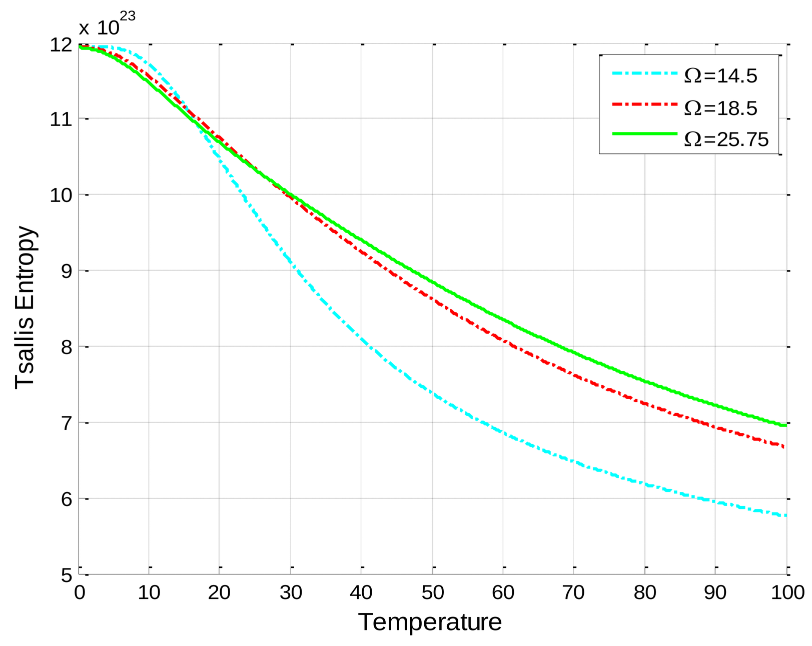

Fig 6: Tsallis entropy as function of temperature for different values of laser frequency

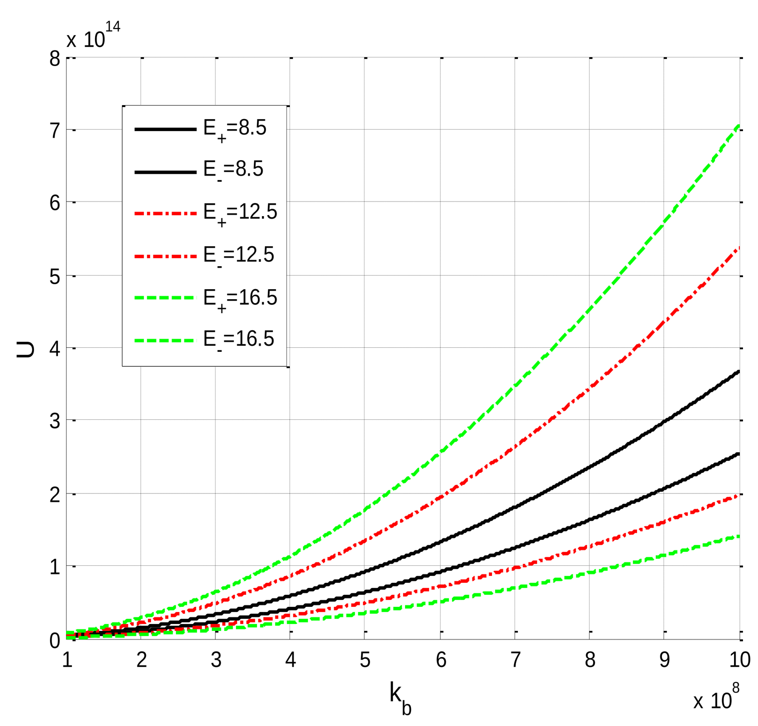

Fig 7: Internal energy variation as function of wave number for different values of laser amplitude

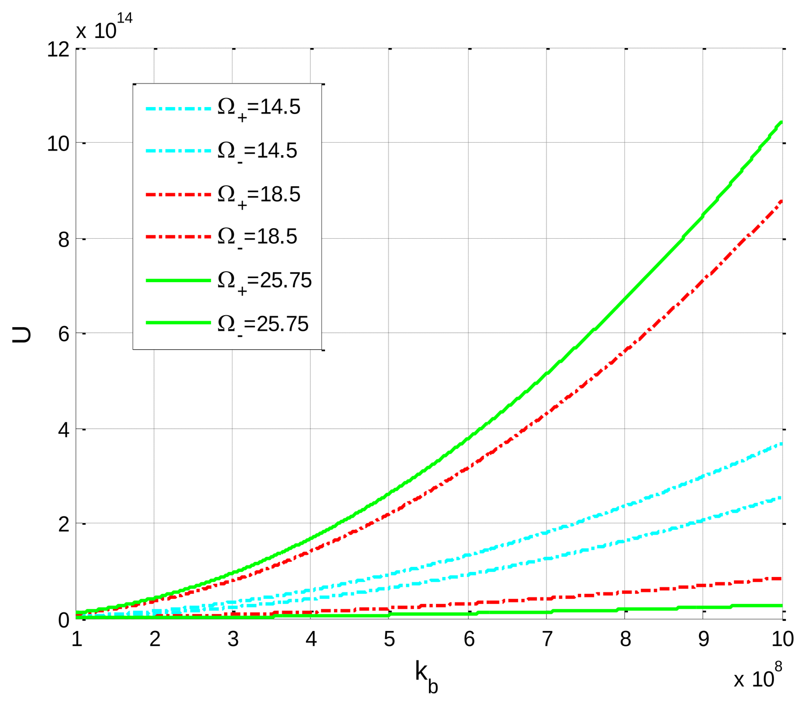

Fig 8: Internal energy variation as function of wave number for different values of laser frequency

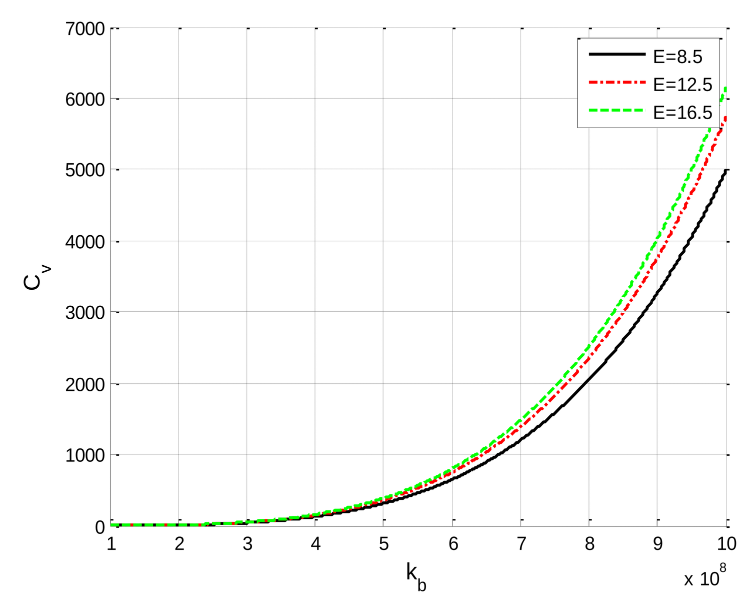

Fig 9: Heat capacity as function of wave number for different values of laser amplitude

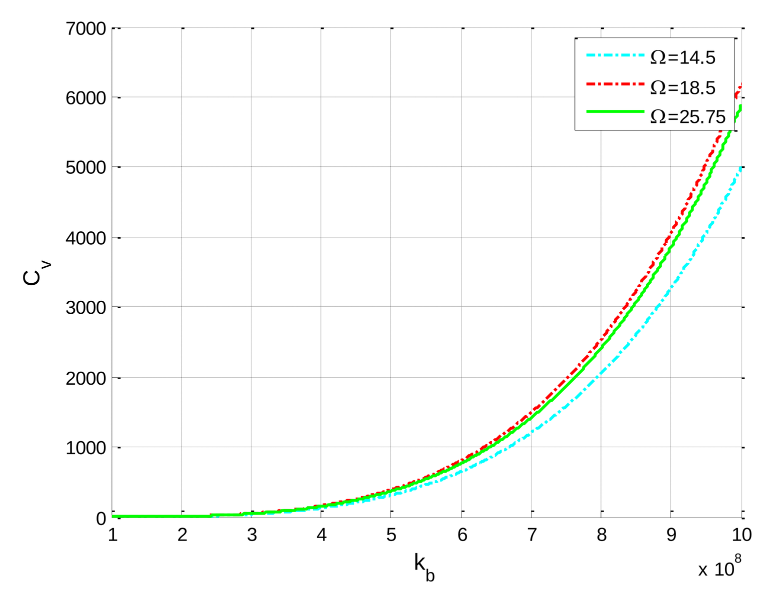

Fig 10: Specific heat as function of wave number for different values of laser frequency

Conclusion

The optical absorption have been evaluated and strongly depends on the laser parameter. We found that the energies of absorbed photons (laser) in these materials are in the infrared region, which enhance the understanding of infrared absorption in monolayer materials. We also remark that the entropy increases with enhancing laser amplitude and laser frequency because the system disorder increases. With increasing wave number, laser amplitude and laser frequency, we strongly enhance the capacity of system to store energy. These parameters of laser act as confinement for the system when the Landau-type levels are formed. The effect of laser starts to overcome the wave number and the specific heat starts to rise. From the curves, we see an interplay between electron phonon interaction and laser in graphene. The laser field acts as a scaling parameter to recalibrate the magnitude of the specific heat. We hope that these theoretical results can stimulate the progress of the related experiments.