

Study of Linear and Nonlinear Optical Properties of Graphene Based on the Dirac Equation

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Outline

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- Introduction of Klein-Gordon and Dirac equation

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- Introduction of graphene

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- Method

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- Result



Relativistic wave equation or Klein-Gordon equation

$$\checkmark \quad i\hbar \frac{\partial \psi}{\partial t} = \left[-\frac{\hbar^2}{2m_0} \nabla^2 + V(x) \right] \psi(x, t)$$

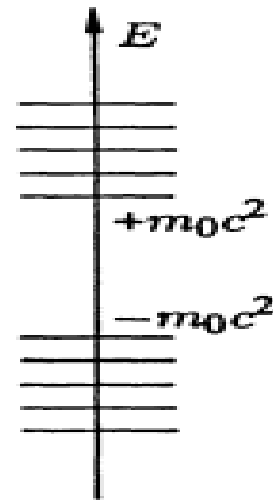
$$\checkmark \quad \hat{E} = \frac{\hat{p}^2}{2m_0} + V(x)$$

$$\checkmark \quad p^\mu p_\mu = \frac{E^2}{c^2} - p \cdot p = m_0^2 c^2$$

$$\checkmark \quad \hat{p}^\mu \hat{p}_\mu \psi = m_0^2 c^2 \psi$$

$$\checkmark \quad \rho = \frac{i\hbar}{2m_0 c^2} \left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right)$$

Probability density





Dirac equation

- Dirac Equation an Overview:

- ✓ $\hat{p}^\mu \hat{p}_\mu = m_0^2 c^2$

- ✓ $\hat{p}^\mu \hat{p}_\mu - m^2 c^2 = (\beta^k p_k + mc)(\gamma^\lambda p_\lambda - mc)$

- ✓ $(p^0)^2 - (p^1)^2 - (p^2)^2 - (p^3)^2 = (\gamma^0)^2 (p^0)^2 + (\gamma^1)^2 (p^1)^2 + (\gamma^2)^2 (p^2)^2 + (\gamma^3)^2 (p^3)^2 + (\gamma^0 \gamma^1 + \gamma^1 \gamma^0) p_0 p_1 + (\gamma^0 \gamma^2 + \gamma^2 \gamma^0) p_0 p_2 + (\gamma^0 \gamma^3 + \gamma^3 \gamma^0) p_0 p_3 + (\gamma^1 \gamma^2 + \gamma^2 \gamma^1) p_1 p_2 + (\gamma^1 \gamma^3 + \gamma^3 \gamma^1) p_1 p_3 + (\gamma^2 \gamma^3 + \gamma^3 \gamma^2) p_2 p_3$



Dirac equation

✓ Puli matrix

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}$$

✓ the energy and momentum factor

$$(\hat{p}^\mu \hat{p}_\mu - m^2 c^2) = (\beta^k p_k + mc)(\gamma^\lambda p_\lambda - mc) = 0$$

✓ The dirac final equation

$$i\hbar\gamma^\mu \partial_\mu \psi - mc\psi = 0$$



Visual Comparison: Dirac vs. Klein-Gordon Equation

Dirac Equation

$$H_D \psi = E \psi$$

Relativistic equation for spin- $\frac{1}{2}$ particles

Applies to fermions (e.g., electrons in graphene)

Linear energy-momentum relationship



Klein-Gordon Equation

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 + \frac{m^2 c^2}{\hbar^2} \right) \phi = 0$$

Relativistic equation for scalar particles

Applies to bosons (e.g., scalar fields in quantum field theory)

Quadratic energy-momentum relationship



Graphene

What is Graphene?

A single layer of carbon atoms in a hexagonal lattice.

Extraordinary properties: High electrical conductivity, strength, and optical transparency.

Relationship Between Graphene and the Dirac Equation

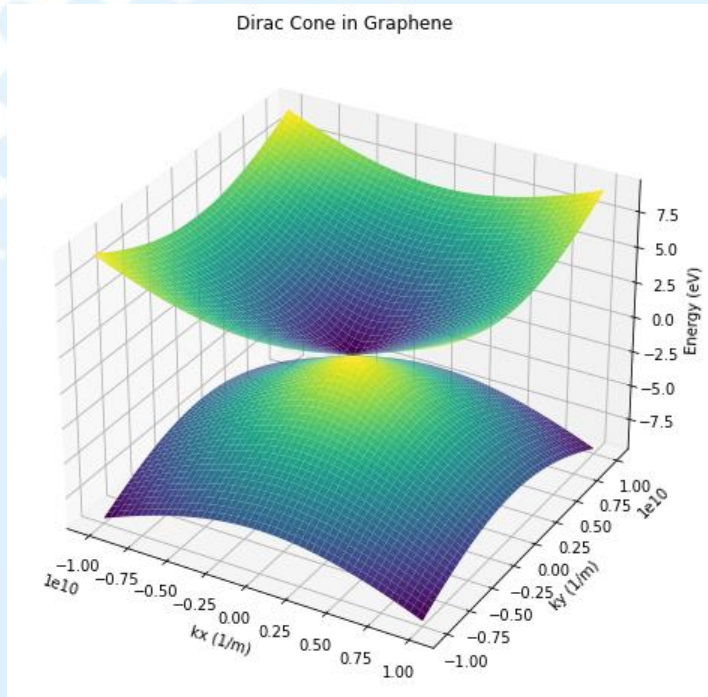
In graphene, electrons behave like massless Dirac fermions.

The electronic structure near the Dirac points in graphene is described by the Dirac equation.

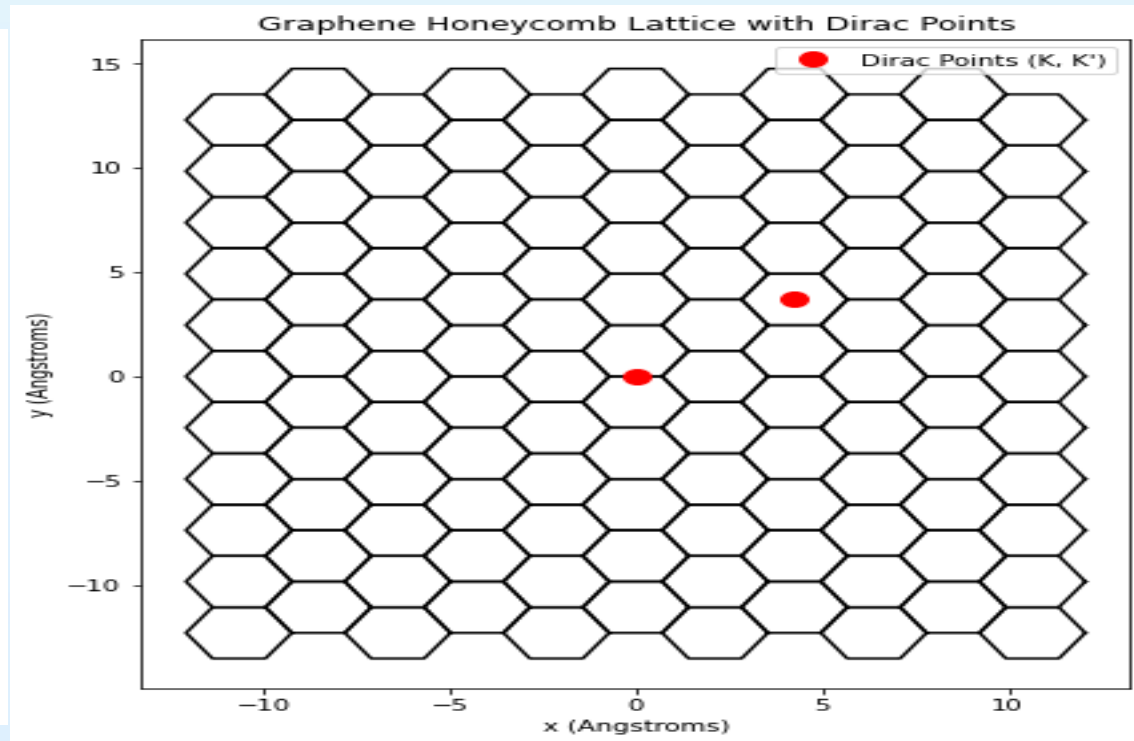


Dirac cones Graphene

Dirac Cone in Graphene

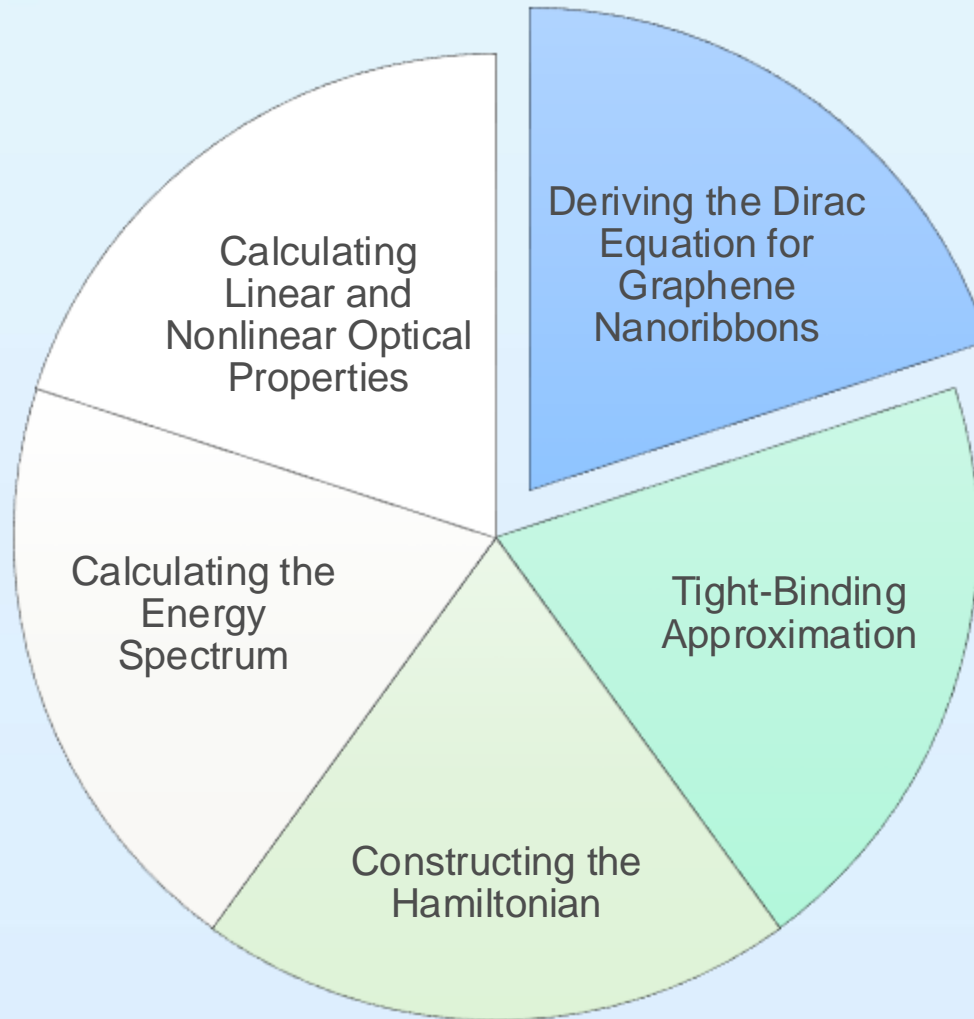


Graphene Honeycomb Lattice with Dirac Points





Methodology





Equations

- ✓ Dirac equation for 2D

$$v_F = (\sigma_x k_x + \sigma_y k_y) \psi = E \psi$$

- ✓ Boundary Conditions and Hamiltonian for Zigzag and Armchair Nanoribbons

$$\psi(x=0) = \psi(x=L) = 0$$

$$\psi_A(x=0) = \psi_A(x=L) = 0$$

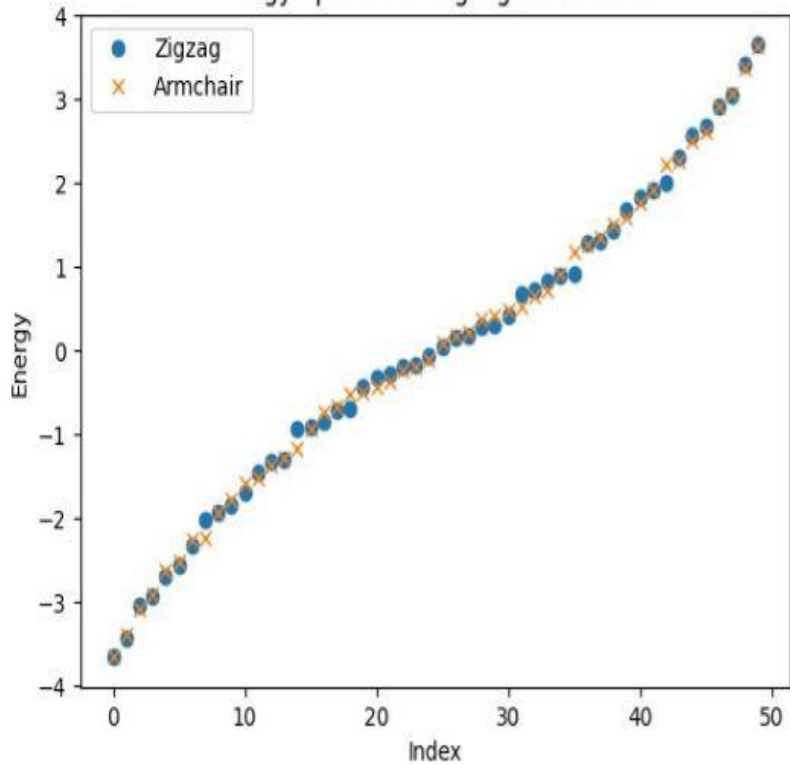
$$\psi_B(x=0) = \psi_B(x=L) = 0$$

$$H = -t \sum_{\langle i,j \rangle} (c_i^\dagger c_j + hc)$$

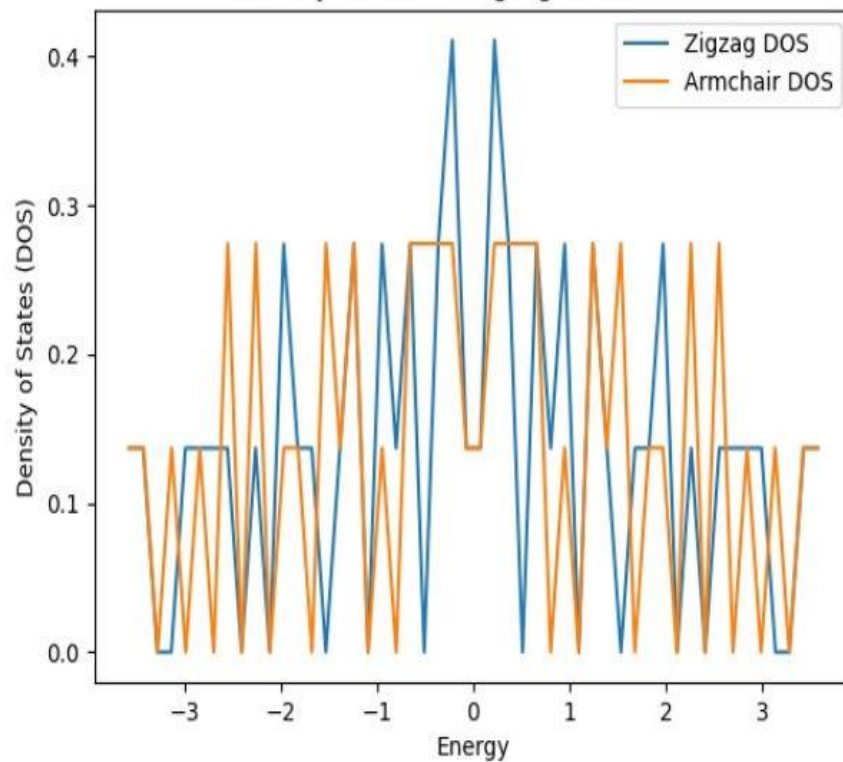


Density of state, energy spectrum

Energy Spectrum: Zigzag vs Armchair



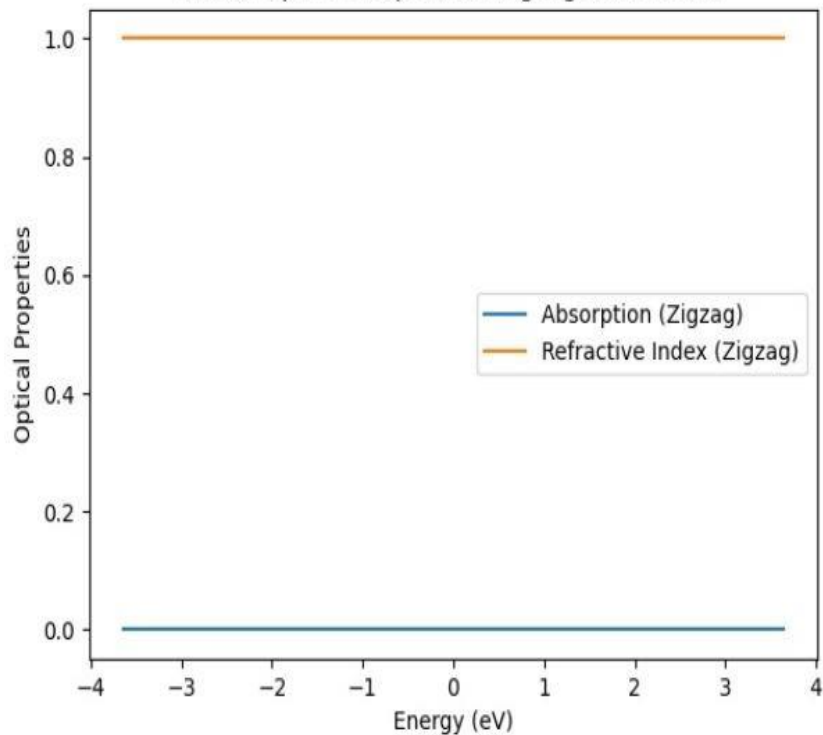
Density of States: Zigzag vs Armchair



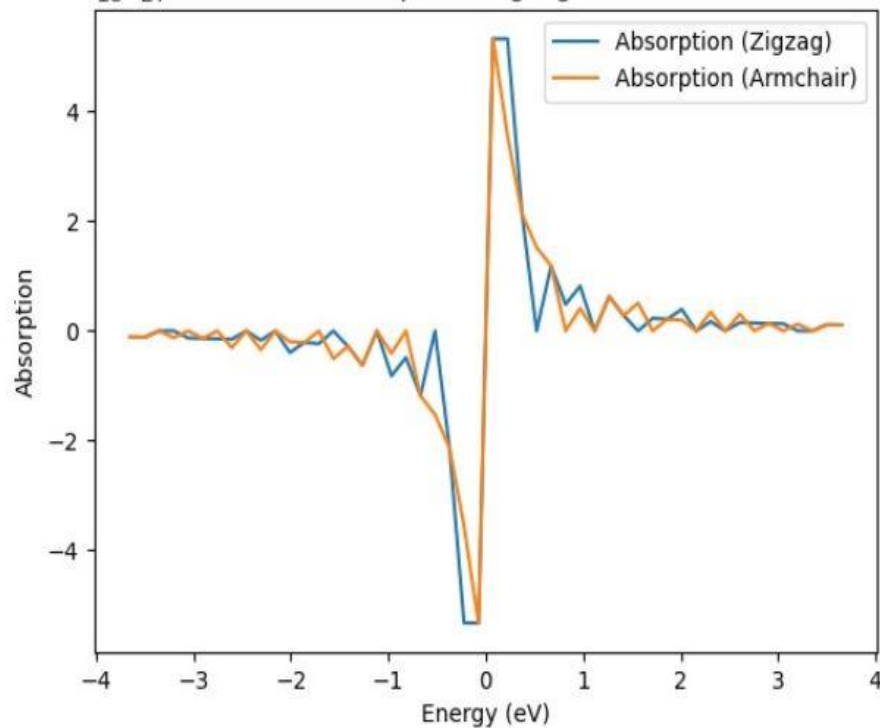


Linear Optical Properties

Linear Optical Properties: Zigzag Nanoribbon

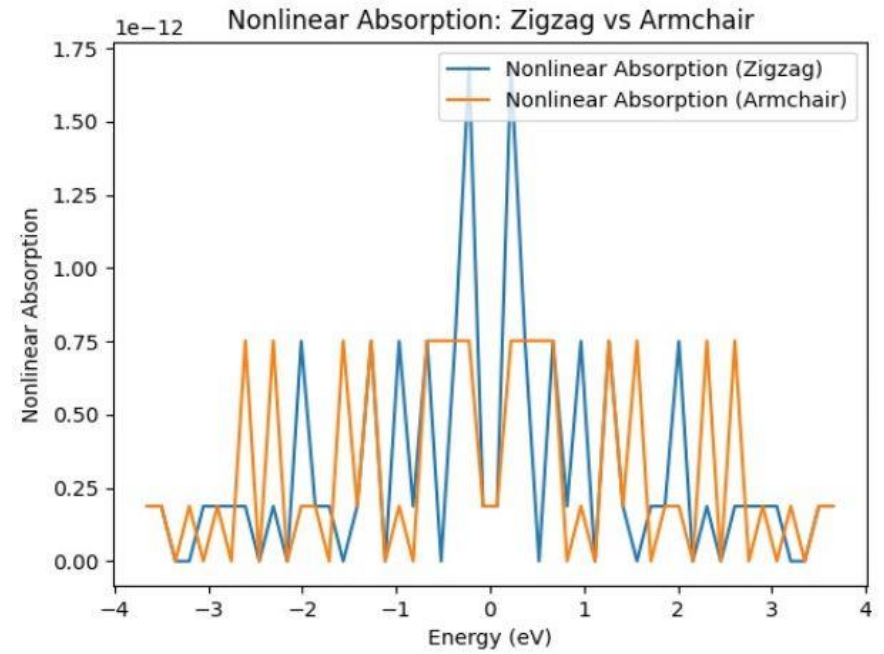
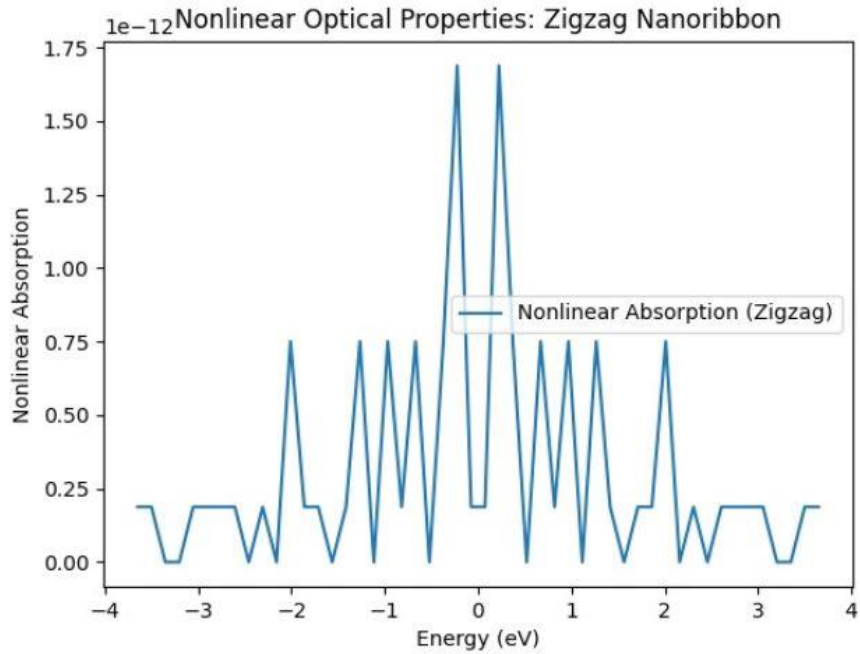


1e-27 Linear Absorption: Zigzag vs Armchair





Non Linear Optical Properties





Thank you for your attention