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Electron-phonon dynamics in transition metal dichalcogenides quantum dot after short pulse radiation

Presented by:

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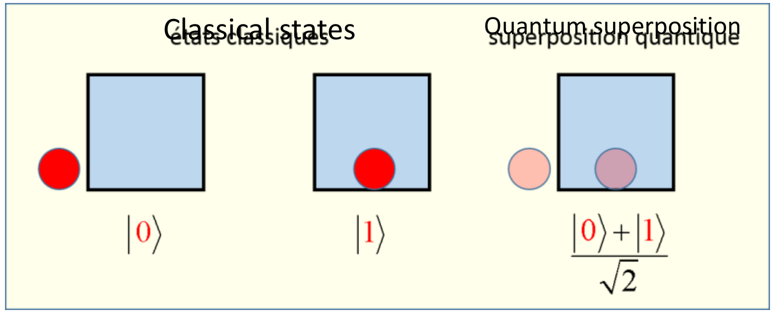
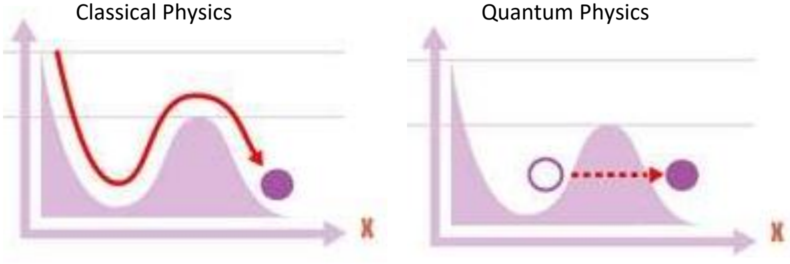
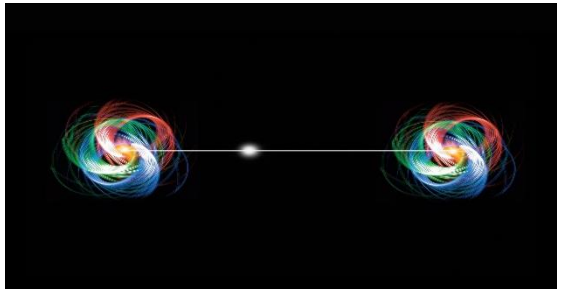
CONTEXT

1900 Birth of quantum physics

Some atypical properties and behaviour





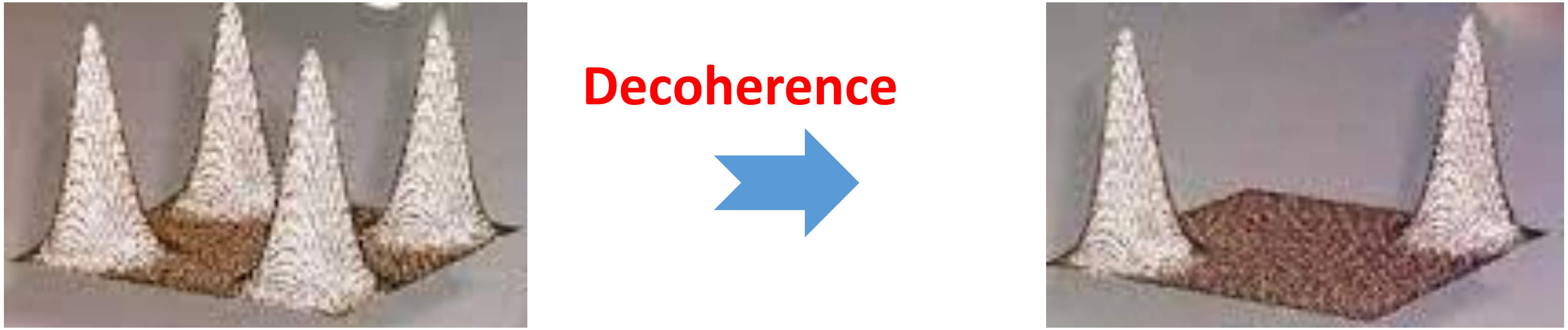


Superposition states

Tunelling effect

Entanglement

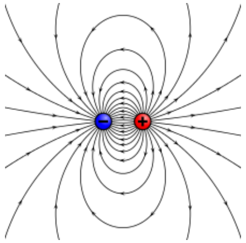
CONTEXT


Decoherence

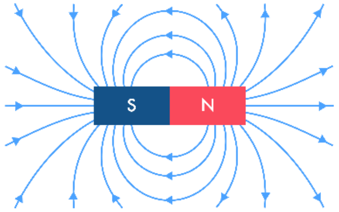
Loss of quantum properties when the system is immersed in an environment

CONTEXT

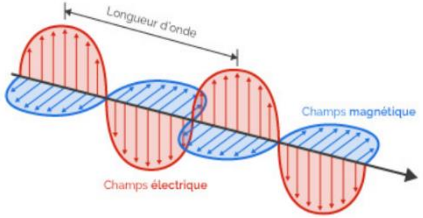
The environment can be:



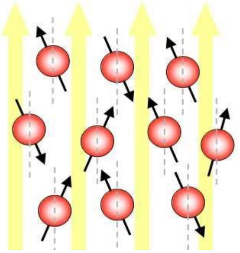
Magnetic



Electrical



Electromagnetic



Spin

Several methods have been developed to study this type of system:

- **Lee Low Pines Method or modified Lee Low Pines Method**
- **Pekar type method**
- **Feynmann Path Integral approach**

Different from graphene, 2D DMTs have a wide bandgap range from the visible to the infrared spectrum and above all the possibility to control the bandgap.

This ability to control the band gap has led to several research projects in this area.

Related work

1933

Work on quasiparticle called Polaron

LANDAU
Phys. Z. Sowjetunion3, 664

2010

The direct bandgap of TMD has been produced, with prospective solicitations for high electron mobility transistors and light-emitting diodes

Mak et al
Phys. Rev. Lett. 105, 136805

2016

Experimental work demonstrates that polar substrates are necessary in the derivation of some physical properties of TMD

Liu et al
Adv. Mater. 28, 6457

2021

The polaron in radiofrequency spectrum study have been done in others quasiparticles in TMD monolayers with external field

Kenfack-Sadem et al
J.electr. Mater. 50, 2911

2021

Study of thermodynamic properties of polaron in TMDs

Diffo et al
Phys. Lett. A 385,126958

2021

Transition frequency and dynamic of polaron in Transition Metal Dichalcogenides under radiowaves and microwaves

Nguepnang et al

PROBLEM

What is the effect of microwave and radiowave on dynamic of polaron in two-dimensionals materials particularly the TMDs

⬇

Which **parameter** should we study to **analyse the influence of the environnement** on the studied system?

OBJECTIF

we consider a polaron in TMD under the radiation of both microwave and radiowave and present their effect on enegies and lifetime of polaron supported by a polar substrate. We take into considerations both the surface optical (SO) phonon mode brought by polar substrates and intrinsic longitudinal optical (LO) phonon mode.

Specific Objectives

- Construct the Hamiltonian of the problem
- Derive the energies of the system
- Determine the lifetime of polaron in TMDs

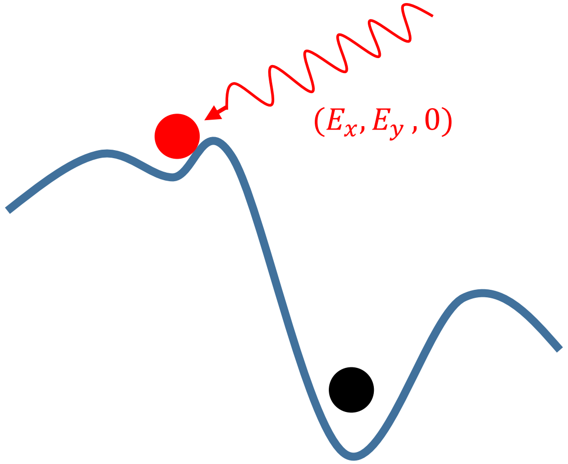
PLAN OF THE PRESENTATION

1. Method
2. Results
3. Conclusion and perspectives

01.

METHOD

Hamiltonian of the model



Potential energy in x-y plane

Phonon energy

$$H = V_F \tau \left[\frac{P_x^2}{2m}\sigma_x + \frac{P_y^2}{2m}\sigma_y + \frac{m\vartheta^2 x^2}{2}\sigma_x + \frac{m\vartheta^2 x^2}{2}\sigma_x + \sigma_z G \right] + \tau \frac{P_z^2}{2m} + A_2 \cos(\beta t + \phi)\sigma_y + A_1 \cos\theta t \sigma_x + \sum_{k,\upsilon} \hbar\omega_\upsilon a_k^+ a_k + \sum_{k,\upsilon} \left(T_{k,\upsilon} a_k e^{i\vec{k}\vec{r}} + T_{k,\upsilon}^* a_k^+ e^{-i\vec{k}\vec{r}} \right) \quad (1)$$

Kinetic energy of electron in x-y direction

Energy of the radiation of a microwave and a radiofrequency

Energy of interaction between phonons and electron

Calculations

$$\left(E_{0\pm}\right)_{SO}=\pm\begin{bmatrix}2\left(\frac{e^2\eta\hbar\vartheta Q_{0,SO}\left(k,\chi,z_0\right)}{4\pi\varepsilon_0}\right)^2\left(\sum_{\upsilon=1}^{2}\frac{\hbar\omega_{SO,\upsilon}}{\left(\hbar\omega_{SO,\upsilon}+\sqrt{2}\hbar\vartheta V_F\right)^2}\right)^2+\frac{1}{2}\left(V_F\hbar\vartheta\right)^2\\+V_F\hbar\vartheta\left(A_1\cos\theta t+A_2\cos\left(\beta t+\phi\right)\right)+A_1^2\cos^2\theta t+A_2^2\cos^2\left(\beta t+\phi\right)+G^2\\+\left(V_F\hbar\vartheta+A_1\cos\theta t+A_2\cos\left(\beta t+\phi\right)\right)\times\left(\frac{e^2\eta\hbar\vartheta Q_{0,SO}\left(k,\chi,z_0\right)}{2\pi\varepsilon_0}\right)\left(\sum_{\upsilon=1}^{2}\frac{\hbar\omega_{SO,\upsilon}}{\left(\hbar\omega_{SO,\upsilon}+\sqrt{2}\hbar\vartheta V_F\right)^2}\right)\end{bmatrix}^{\frac{1}{2}}$$

$$\pm\hbar\vartheta l_z\pm\frac{e^2\eta Q_{0,SO}\left(k,\chi,z_0\right)}{4\pi\varepsilon_0}\sum_{\upsilon=1}^{2}\left(\frac{\hbar\omega_{SO,\upsilon}}{\hbar\omega_{SO,\upsilon}+\sqrt{2}\hbar\vartheta V_F}\right)^2\mp\frac{e^2\eta Q_{0,SO}\left(k,\chi,z_0\right)}{2\pi\varepsilon_0}\sum_{\upsilon=1}^{2}\left(\frac{\hbar\omega_{SO,,\upsilon}}{\hbar\omega_{SO,\upsilon}+\sqrt{2}\hbar\vartheta V_F}\right) \tag{2}$$

$$\left(E_{0\pm}\right)_{LO}=\pm\begin{bmatrix}2\left(\frac{e^2\eta_0L_m\hbar\vartheta\hbar\omega_{LO}}{4\pi\varepsilon_0\left(\hbar\omega_{L0}+\sqrt{2}\hbar\vartheta V_F\right)^2}Q_{0,LO}\left(k,\chi,\nu\right)\right)^2+\frac{1}{2}\left(V_F\hbar\vartheta\right)^2\\+V_F\hbar\vartheta\left(A_1\cos\theta t+A_2\cos\left(\beta t+\phi\right)\right)+A_1^2\cos^2\theta t+A_2^2\cos^2\left(\beta t+\phi\right)+G^2\\+\left(V_F\hbar\vartheta+A_1\cos\theta t+A_2\cos\left(\beta t+\phi\right)\right)\left(\frac{e^2\eta_0L_m\hbar\vartheta\hbar\omega_{LO}}{2\pi\varepsilon_0\left(\hbar\omega_{L0}+\sqrt{2}\hbar\vartheta V_F\right)^2}Q_{0,LO}\left(k,\chi,\nu\right)\right)\end{bmatrix}^{\frac{1}{2}}$$

$$\pm\hbar\vartheta l_z\pm\frac{e^2\eta_0L_m\left(\hbar\omega_{LO}\right)^2}{4\pi\varepsilon_0\left(\hbar\omega_{L0}+\sqrt{2}\hbar\vartheta V_F\right)^2}Q_{0,LO}\left(k,\chi,\nu\right)\mp\frac{e^2\eta_0L_m\hbar\omega_{LO}}{2\pi\varepsilon_0\left(\hbar\omega_{L0}+\sqrt{2}\hbar\vartheta V_F\right)}Q_{0,LO}\left(k,\chi,\nu\right) \tag{3}$$

According to the Fermi golden rule, the rate of transition from ground to first excited state is evaluated. Thus The lifetime of polaron using the golden principle is given by:

FOR SO phonons

$$\frac{\hbar}{\tau}=\frac{e^2\eta}{2\varepsilon_0}\left(-\frac{1}{\left(\frac{\chi^2}{\zeta}+\frac{\chi^2}{2\xi}\right)k_c+2z_0}\exp\left(-\left(\frac{1}{\zeta}+\frac{1}{2\xi}\right)k_c^2\chi^2-2k_cz_0\right)+\frac{1}{2z_0}\right)\sum_{\upsilon=1}^{2}n_k\hbar\omega_{SO;\upsilon}$$

FOR LO phonons

$$\frac{\hbar}{\tau}=\frac{e^2\eta_0L_m\hbar\omega_{LO}n_k}{2\varepsilon_0}\int_0^{k_c}\exp\left(-\frac{k^2\chi^2}{\zeta}-\frac{k^2\chi^2}{2\xi}\right)\left[erfc\left(\frac{k\nu}{2}\right)\right]^2dk \tag{4}$$

02.

RESULTS

Energy polaron in TMDs

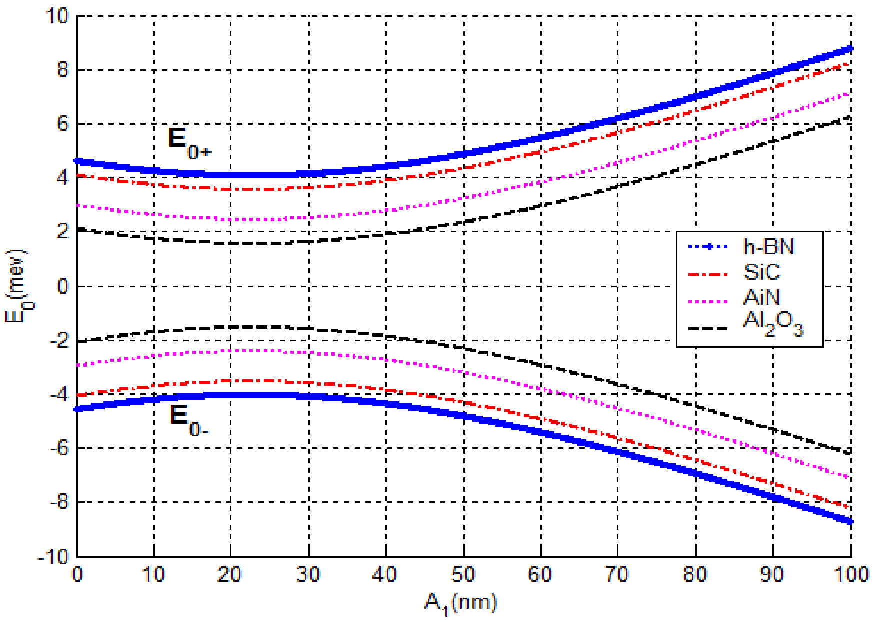


Fig. 1: Ground-state energy of exciton polaron with SO phonon mode as function of amplitude of RW for different polar substrate and for $\beta = 2Ghz\,; \alpha = 4000\,khz; A_2 = 30\,nm$

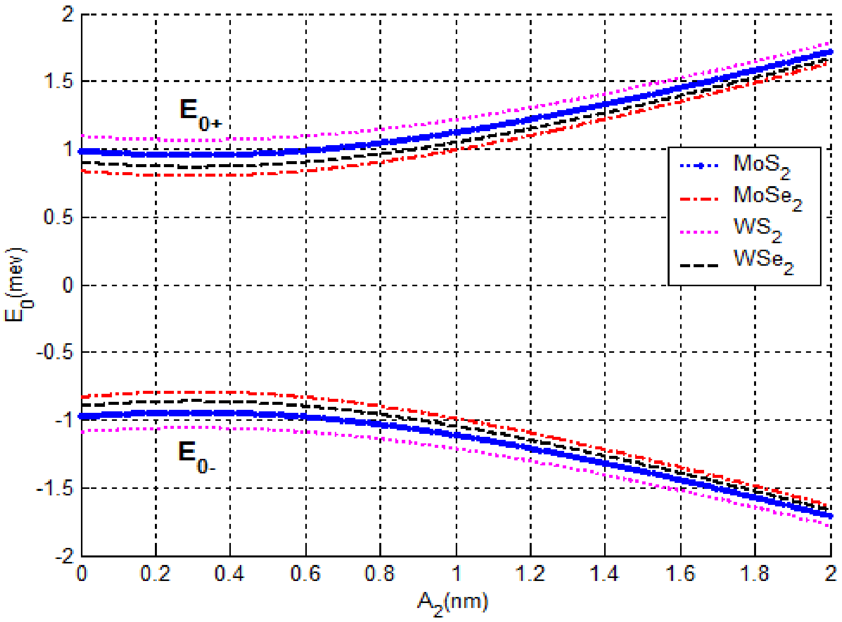


Fig. 2: Ground-state energy of exciton polaron with SO phonon mode as function of amplitude of MW for different polar substrate and for $\beta = 2Ghz\,; \alpha = 4000\,khz; A_1 = 75nm$

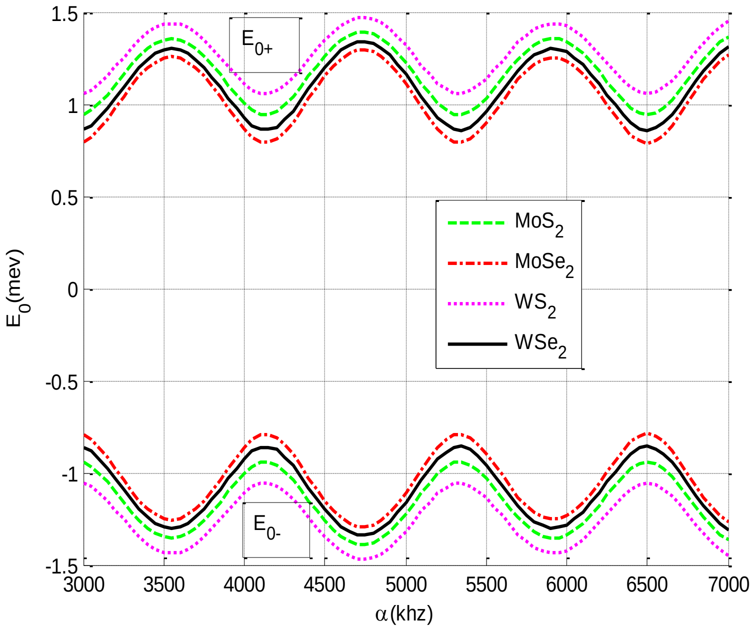


Fig. 3: Ground-state energy of exciton polaron with LO phonon mode as function of frequency of RW for different TMD monolayer and for $\beta = 2Ghz\,; A_1 = 10nm\,; A_2 = 2nm$

The fundamental energy increases sharply with the increasing of the amplitude the RW and linearly with the amplitude of the MW. Thus as the RW and the MW can be considering as a potential of confinement, they increase the ground state energy of polaron in MoS_2 monolayer by increasing their amplitude, thus increasing the modulated bandgap. Comparing the modulated bandgap of the MoS_2 monolayer

Lifetime polaron in TMDs

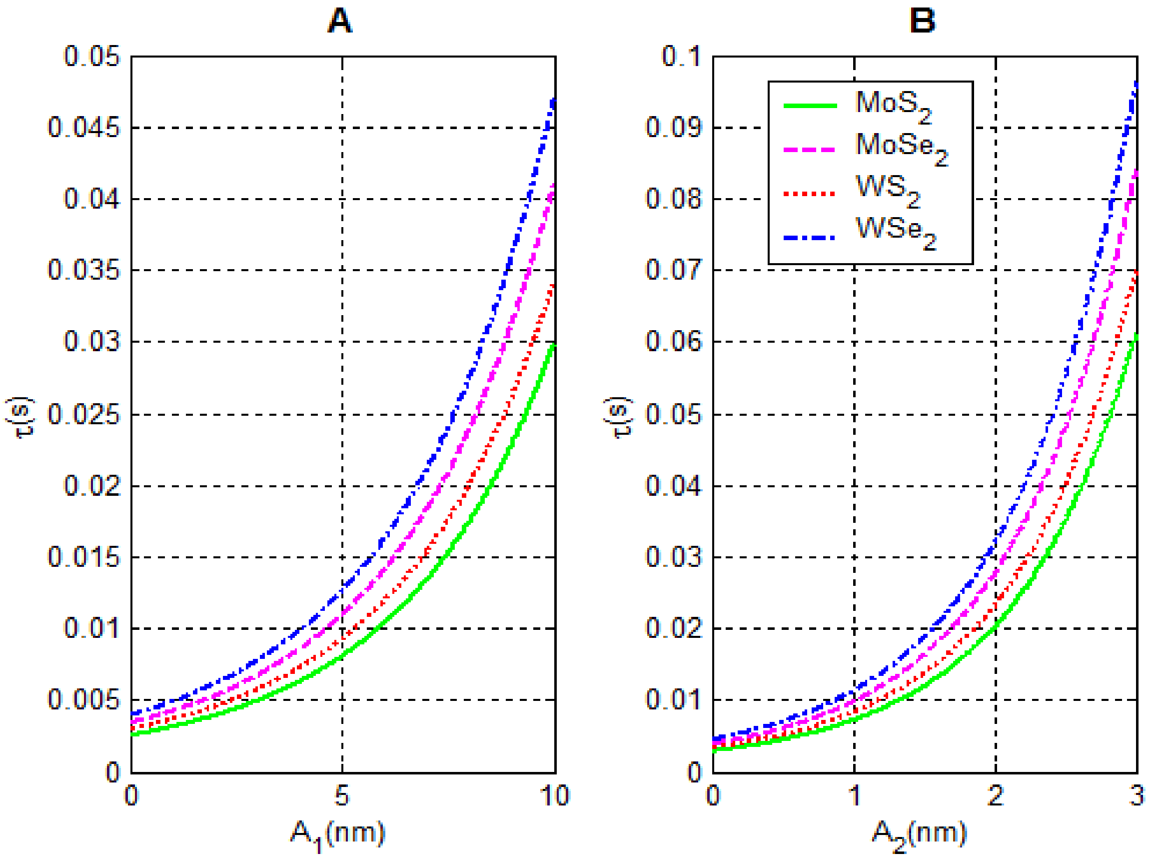


Fig. 4 : Life time of polaron with LO phonon mode as function of amplitide of RW (fig. 14A) for $\beta = 2Ghz;\alpha = 4000khz;A_2 = 2nm$ and amplitude of MW (fig. 14B) for $\beta = 2Ghz;\alpha = 4000khz;A_1 = 5nm$ and for differents TMDs monolayers

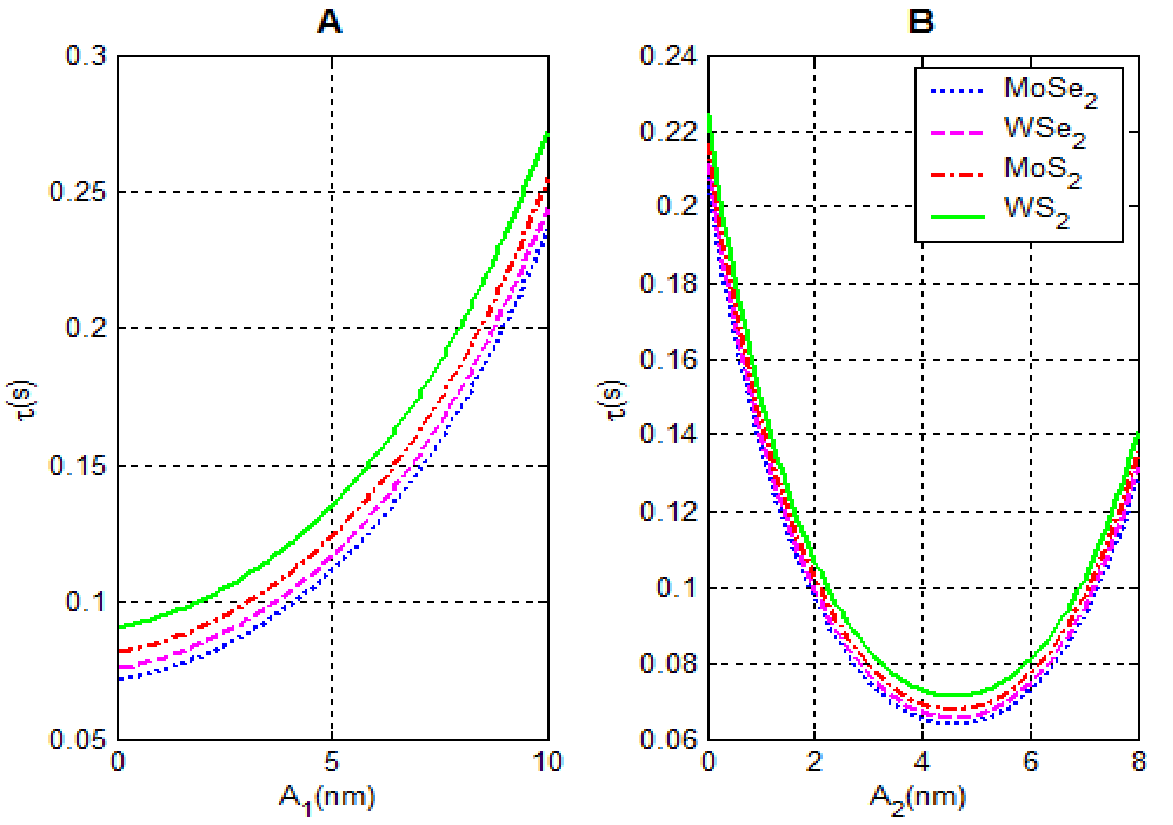


Fig. 5: Life time of polaron with SO phonon mode as function of amplitide of RW (fig. 15A) for $\beta = 2Ghz;\alpha = 4000khz;A_2 = 2nm$ and amplitude of MW (fig. 15B) for $\beta = 2Ghz;\alpha = 4000khz;A_1 = 5nm$ and for differents TMDs monolayers

For SO phonon mode, polaron lives longer in TMD with disulphide than with diselenides whereas for LO phonon mode polaron lives longer in TMD with diselinides than with disulphide, which means that the type of electron-phonon coupling also affects polaron lifetime in TMD monolayers.

03.

CONCLUSION AND PERSPECTIVES

CONCLUSION

1

In this work, we have evaluated the dynamics of polaron in transition metal dichacogenide in the presence of both radiowaves and microwaves. The ground and first excited state energies have been derived using Pekar variational method,

2

When both surface optical and intrinsic longitudinal optical phonon modes are taken into consideration

- the radiowaves, microwaves and polar substrates can been used to switch the polaron energies and the lifetime of polaron
- the microwaves and the radiowaves create fluctuations in the energies levels of polaron,

APPLICATIONS

1

- Improvement of information transmission in optical fibres
- Securing information

2

- Information storage
- Improving semiconductor performance

PERSPECTIVES

1

Dynamics of spontaneous exciton-polaron emission with multiple transitions

2

Compare the results on Transition Metal dichalcogenides with the one obtained in graphene

3

Apply the results using Density Functional Theory

SCIENTIFIC PRODUCTIONS

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