Coupled electromechanical effects in the electronic properties of nanostructures

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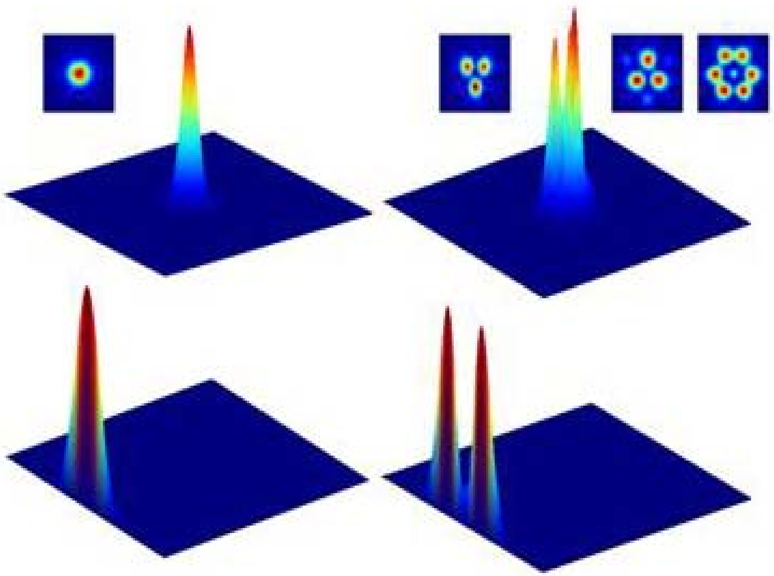

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Gregorio Millan Institute, Spain

Outline

- ***Coupled effects in nanostructures of different materials***

- ***g-factor and spin relaxation in III-V semiconductor QDs***

- ***Berry phase in Quantum Dots***

- ***Conclusions***

Theoretical model:

Prabhakar, Melnik, Bonilla
JAP (2013)

The total electromechanical energy density for nanostructures (nanowires,QDs,supperlattices)

$$U_s = \frac{1}{2} C_{iklm} \; \varepsilon_{ik} \; \varepsilon_{lm}$$

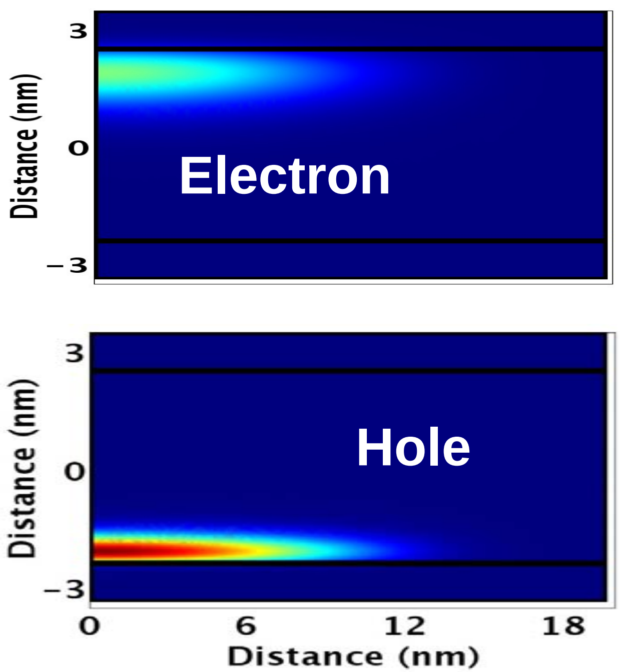
$$\sigma_{ik} = C_{iklm}\varepsilon_{lm} + e_{nik}\partial_n V$$

$$D_i = e_{ilm}\varepsilon_{lm} - \hat{\varepsilon}_{in}\partial_n V + P_{sp}$$

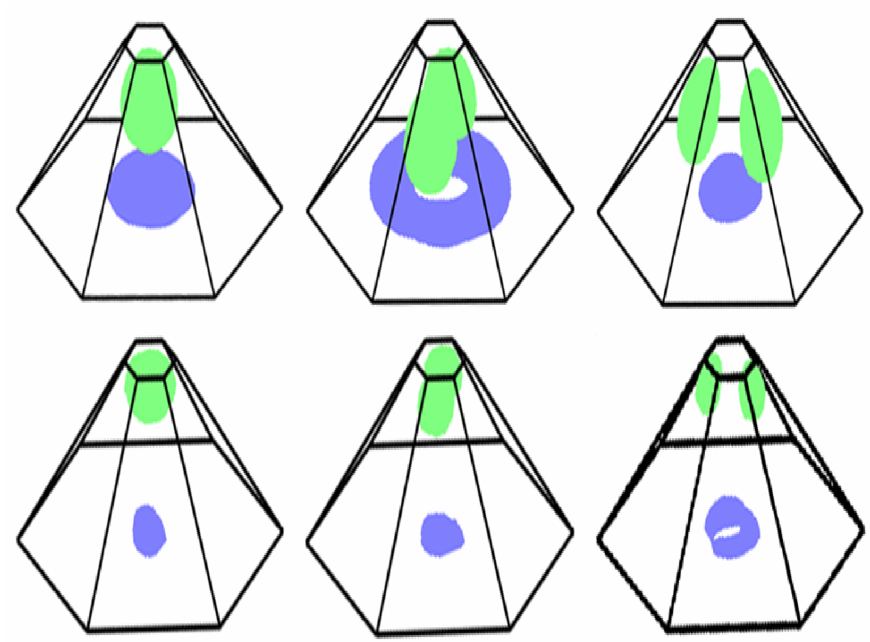
We solve Navier and Maxwell equations

$$\partial_j \sigma_{ij} = 0$$

$$\partial_i D_i = 0$$



AlN/GaN QDs



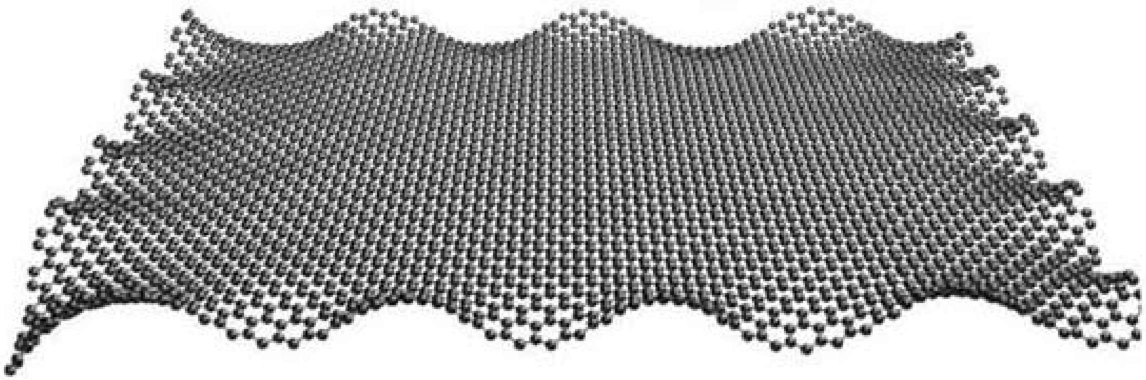
Motivation: Experimental observation of ripples seen in graphene sheet

Thompson-Flagg et al., EPL (2009)

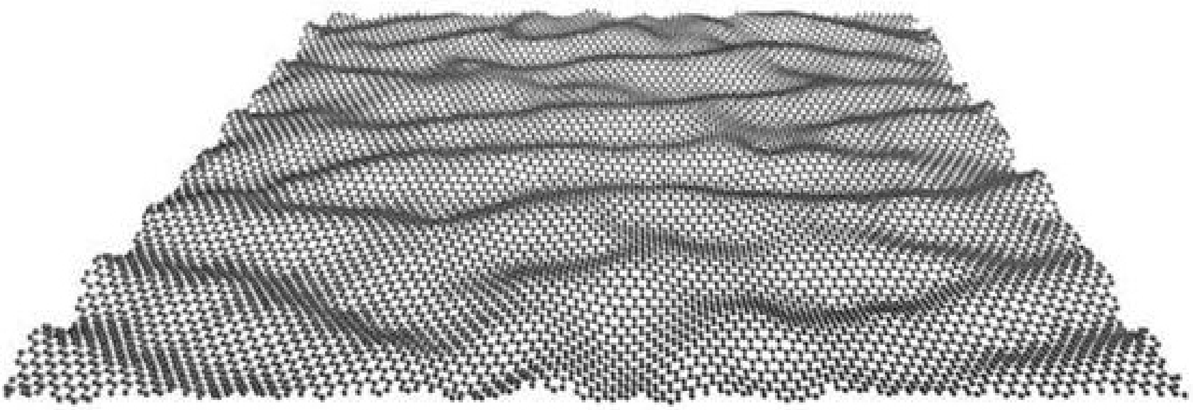
- **Thermal fluctuation should induce smaller ripple waves which does not match with the experimental observation Nature Nanotechnology (2009)**

- **Ripples can be induced as a consequence of adsorbed OH molecules in random sites.**

- **Theoretical model has been developed by Bonilla and Carpio PRB (2012)**



Ripples produced by edge effects alone in graphene sheet, 10nmx10nm.



Ripples produced by 20% coverage of OH in graphene sheet, 10nmx10nm.

Theoretical model:

The total elastic energy density for the two dimensional graphene sheet

$$U_s = \frac{1}{2} C_{iklm} \ \varepsilon_{ik} \ \varepsilon_{lm}$$

$$\partial_k \sigma_{ik} = F^k_{ext} / t$$

$$F^k_{ext} = \tau_e q \cos(q x_k)$$

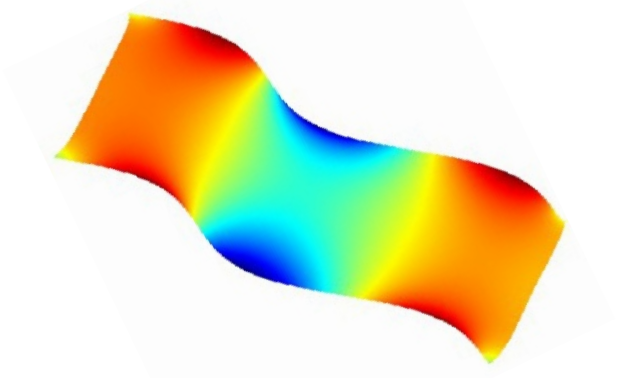
This provides two coupled Navier equations as:

$$\left(C_{11}\partial_x^2 + C_{66}\partial_y^2\right) u_x + \left(C_{12} + C_{66}\right) u_y = F^x_{ext} / t$$

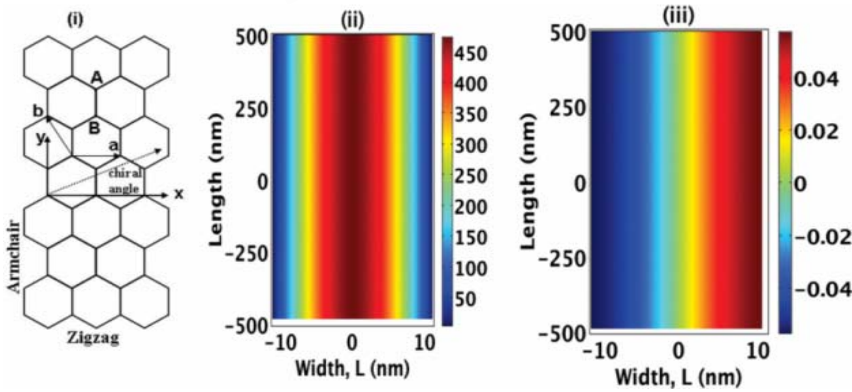
$$\left(C_{66}\partial_x^2 + C_{11}\partial_y^2\right) u_y + \left(C_{12} + C_{66}\right) u_x = F^y_{ext} / t$$

We solve these two coupled equations to investigate the ripple waves in graphene.

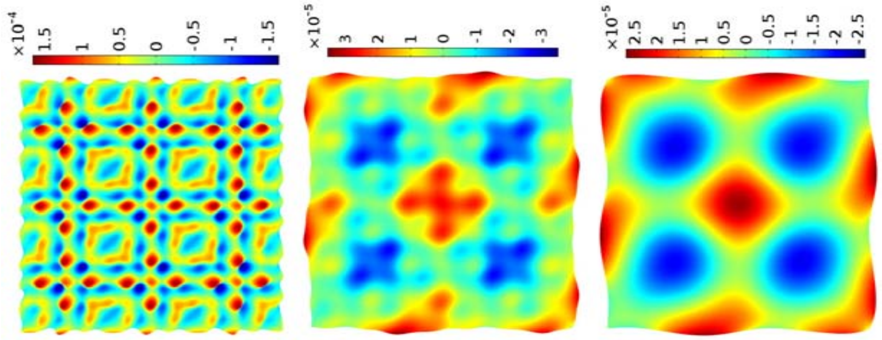
Prabhakar, Melnik, Bonilla
PRB (2014)



Prabhakar, Melnik, Bonilla
PRB (2016)



Future work



Influence of ripple waves in the Band diagram of graphene:

Hamiltonian for single and bilayer graphene can be written as

$$H = v_F \left(\sigma_x P_x + \sigma_y P_y\right)$$

$$H = \begin{pmatrix} U(x,y) & AP_+ & 0 & 0 \\ AP_- & U(x,y) & 0 & 0 \\ 0 & 0 & -U(x,y) & -AP_- \\ 0 & 0 & -AP_+ & -U(x,y) \end{pmatrix}$$

$$P_\pm = P_x \pm P_y, \; and \;\; P = p + eA$$

$$A = \left(2\varepsilon_{xy}, \varepsilon_{yy} - \varepsilon_{xx}, 0\right)\beta / a$$

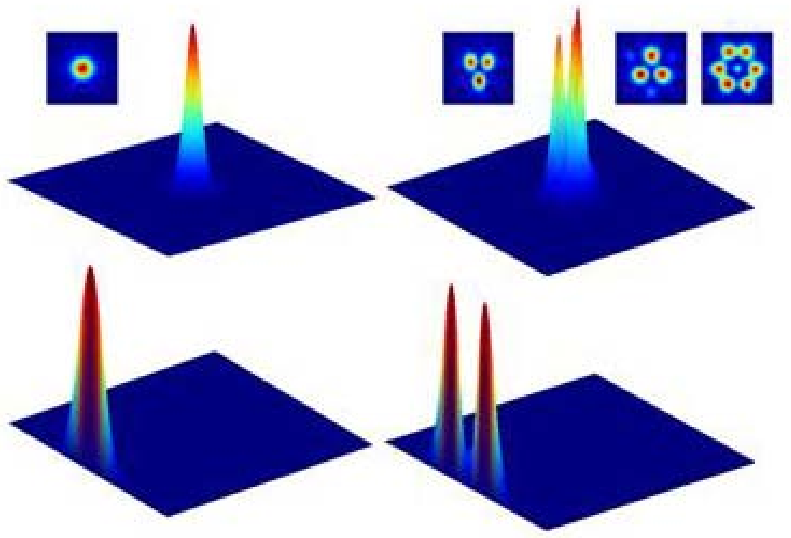
- ***Our goal is to treat strain tensor components as a pseudomorphic vector potential.***

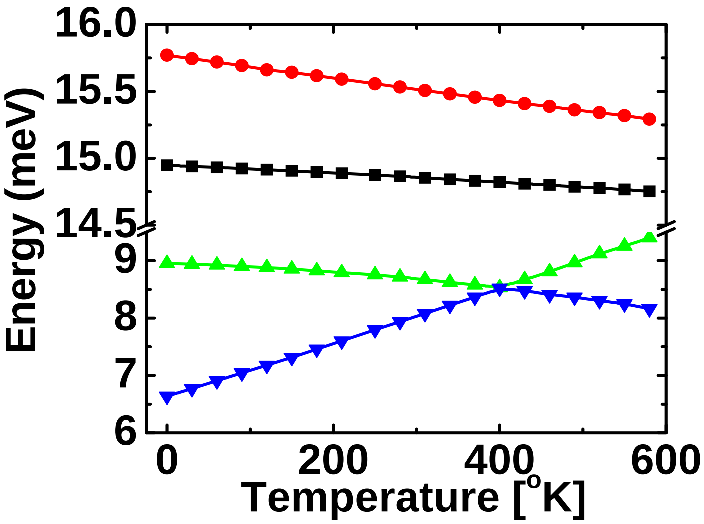
- ***Then, we investigate the influence of electromechanical effects on the band structure of single and bilayer graphene.***

Band diagram of graphene at Dirac point

Graphene Quantum Dots:

Prabhakar, Melnik, Bonilla PRB (2014)





•Level crossing points for zigzag states can be observed.

•Such level crossings are absent in the states formed at the center of the graphene sheet due to the presence of three-fold symmetry.

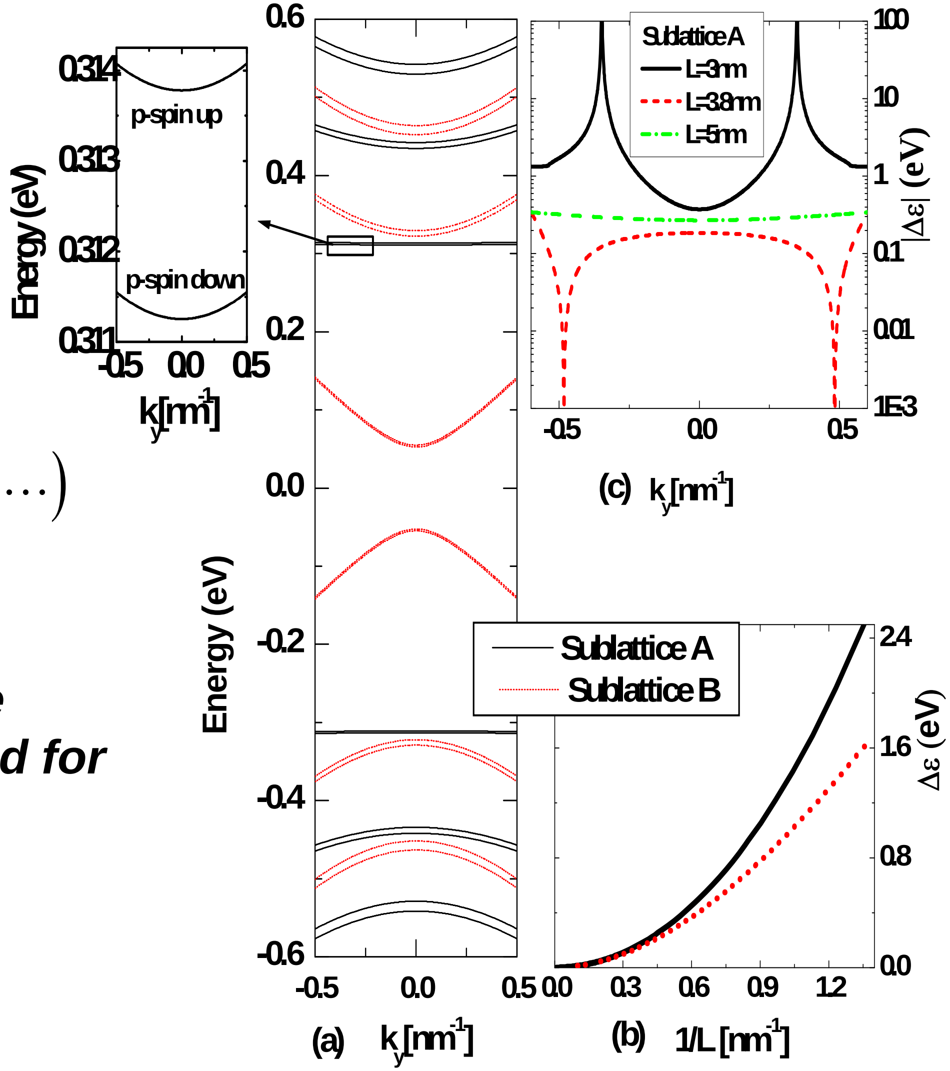
Influence of ripple waves in the band diagram of graphene nanoribbons

Prabhakar, Melnik, Bonilla
PRB (2016)

$$H = v_F\left(\sigma_x\left(p_x - eA_x\right) + \sigma_y\left(p_y - eA_y\right)\right) + \frac{1}{2} g_0 \mu_B B_s \sigma_z$$

$$A = \left(2\varepsilon_{xy}, \varepsilon_{yy} - \varepsilon_{xx}, 0\right)\beta / a$$

$$B_s = \nabla \times A = B_0 \cos(qx),\ B_0 \propto \frac{\tau_e}{L}$$



Note that

$$B_s = -B_0 \cos(q\hat{x}) \approx -B_0\left(1 - q^2/2 + q^4/24 - \cdots\right)$$

•Pseudo-spin splitting energy is in the range of meV and can not be neglected for smaller ribbon width.

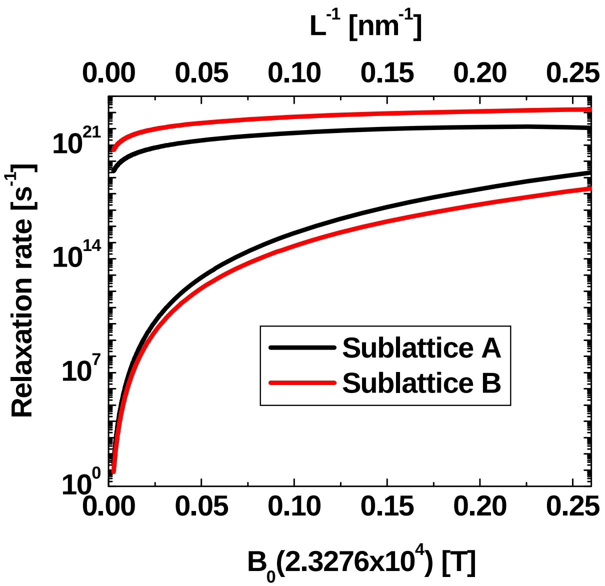
•Sublattices A and B have different energy spectra.

Pseudo-spin life time caused by in-plane phonon modes

Prabhakar, Melnik, Bonilla
PRB (2016)

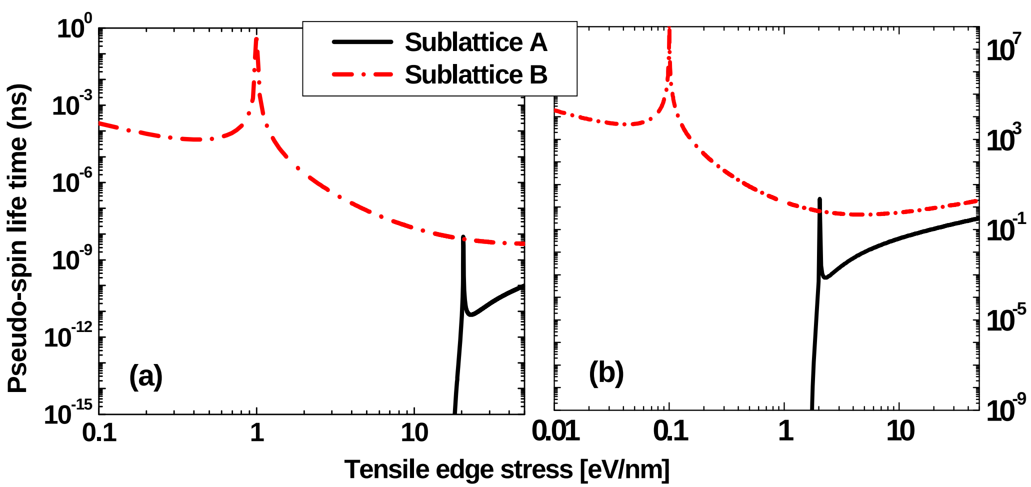
The interaction of electron and in-plane phonon modes is written as

$$u_{ph}^{k\alpha}(r) = i\sum_{\alpha=l,t}\sqrt{\frac{\hbar}{2\rho A_r \omega_{k\alpha}}}\,|k|\,\Xi_{kj} e^{ik.r} b_{q\alpha} + h.c.$$



We apply the Fermi-Golden Rule to find the transition rate

$$\frac{1}{T_1} = \frac{V}{(2\pi)^2\hbar}\sum_{\alpha}\int d^3k\,|<1|u_{ph}^{k\alpha}|2>|^2\,\delta(\hbar\omega_{k\alpha} - E_2 + E_1)$$



- ***Relaxation rate vanishes like*** B_0^5 ***and*** L^{-9} ***and*** τ_e^{-1}
- ***Cusp-like structures can be seen due to pseudo-spin up and down band crossing***

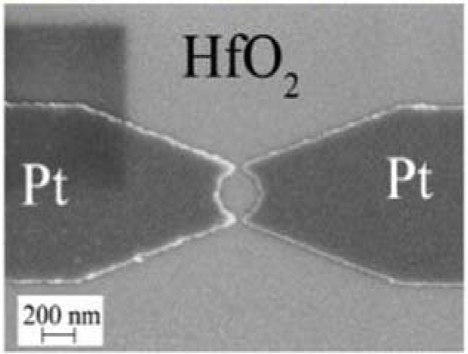
QDs for spintronics

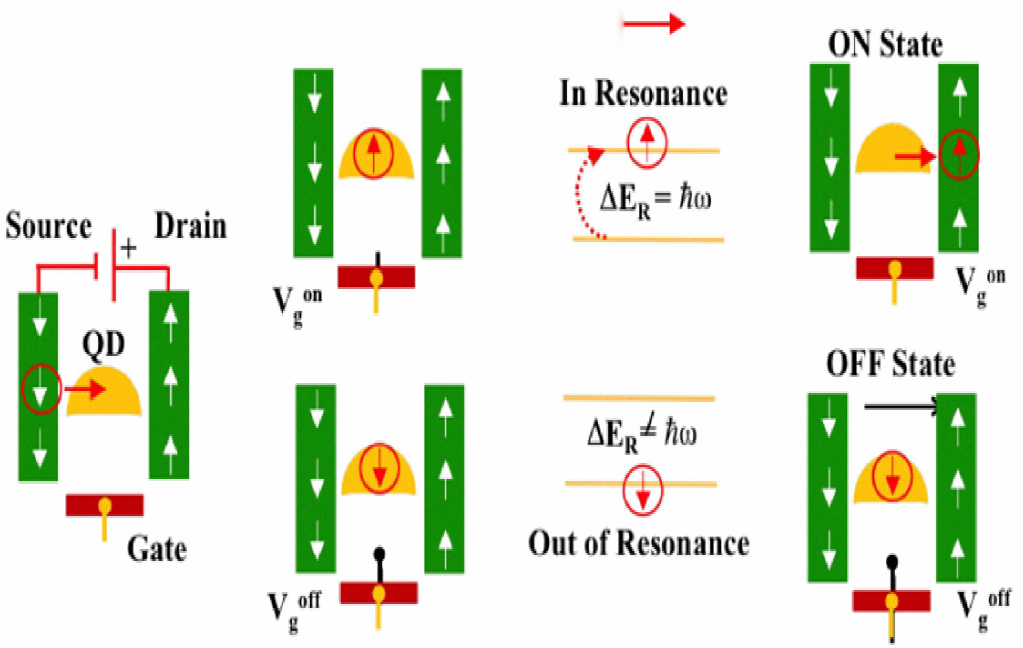
Schematics of spin single electron transistors (SET): QDs

Bandyopadhyay et al., PRB (2000)

Prabhakar, Raynolds PRB (2009)

SEM of a 2D-0D heterodimensional prototype





Tunnel injection of one spin-polarized electron per QD

Splitting of QD ground state is controlled by gate voltage V_g

Spins in resonance with RF field will flip (ON State), non-resonant spins will not (OFF State)

Hamiltonian of quantum dots in III-V semiconductors

$$H = H_0 + H_z + H_R + H_D$$

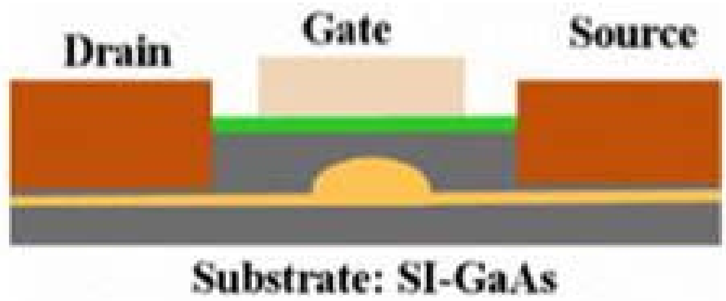
$$H_0 = \frac{\vec{P}^2}{2m} + \frac{1}{2} m \omega_0^2 \left(ax^2 + by^2\right) + \frac{1}{2} g_0 \mu_B \sigma_z B$$

•The lack of structural inversion asymmetry leads to Rashba spin-orbit coupling

$$H_R = \frac{\gamma_R e E}{\hbar}\left(\sigma_x P_y - \sigma_y P_x\right)$$

•Bulk inversion asymmetry leads to Dresselhaus spin-orbit coupling

$$H_D = \frac{\gamma_D}{\hbar}\left(\frac{2meE}{\hbar^2}\right)^{2/3}\left(-\sigma_x P_x + \sigma_y P_y\right)$$



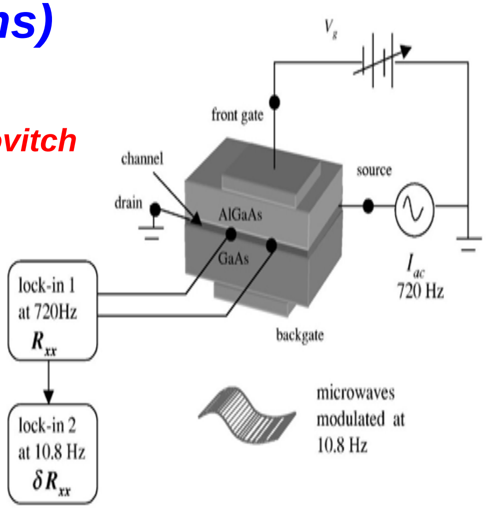
$$g = \frac{\left(\varepsilon_{0,0,-1/2} - \varepsilon_{0,0,+1/2}\right)}{\mu_B B}$$

•Better understanding of g-factor is the key parameter for the design of QD devices

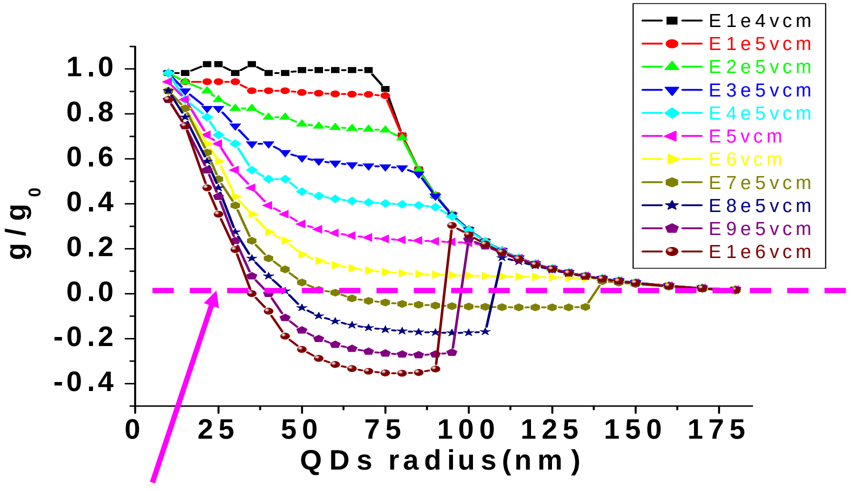
•Electrical control of “g” (physical mechanisms)

Theory: Prabhakar and Raynolds
PRB 79, 195307 (2009)

Experiment: Jiang and Yablonovitch
PRB 64, 041307 (2001)

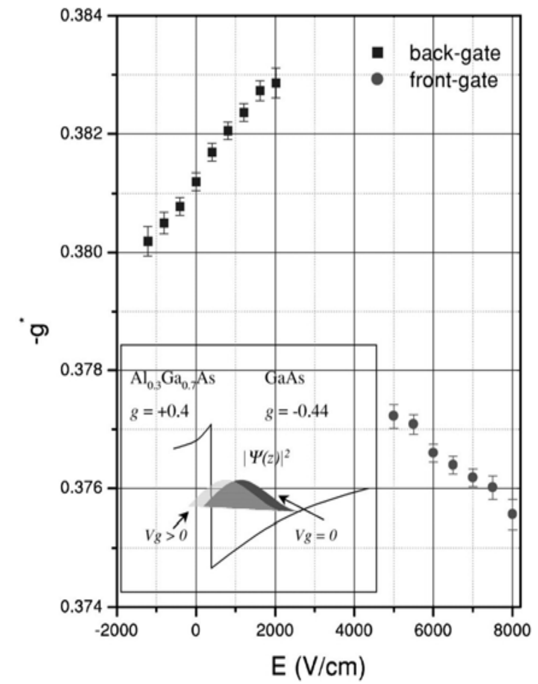


•Wave function overlap: ***electric fields can “move” the wave function to sample different materials (e.g. GaAs has g = -0.44; AlGaAs has g = +0.4)***



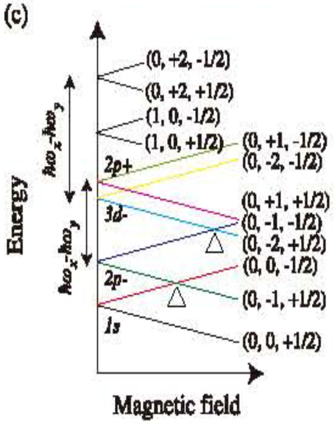
g-factor changes its sign

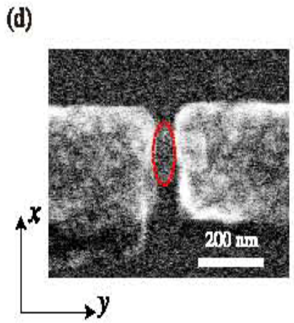
$$g = \frac{\left(\varepsilon_{0,0,-1/2} - \varepsilon_{0,0,+1/2}\right)}{\mu_B \mathrm{B}}$$

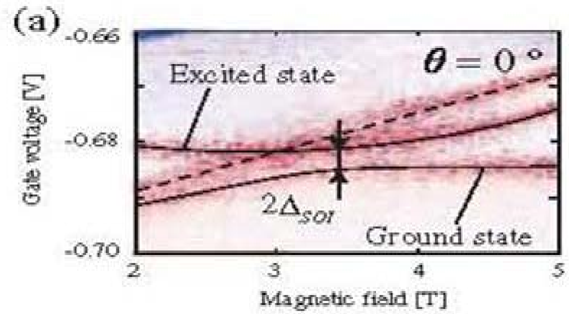


Spin states in InAs QDs: Experiment vs Theory

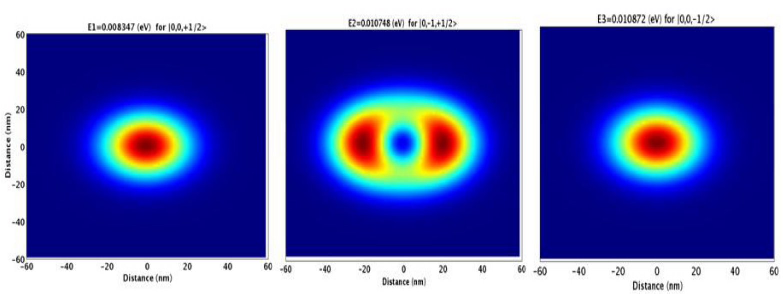
Experiment: Takahashi et. al
PRL 104, 246801 (2010)

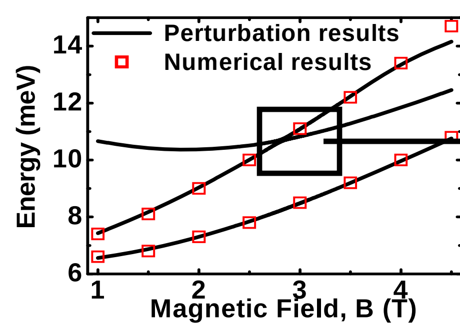


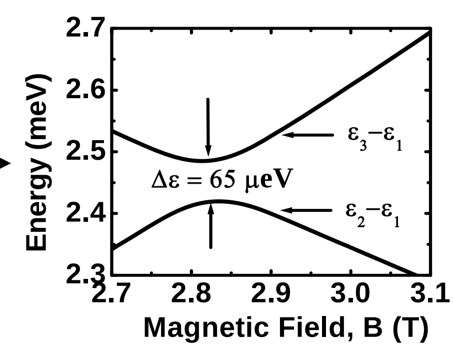




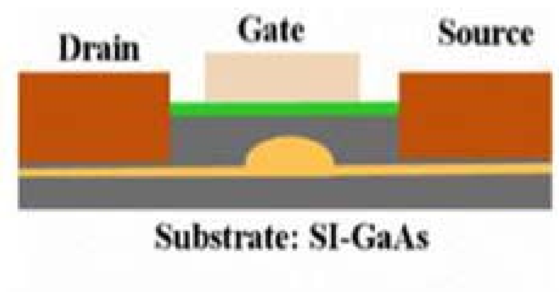
Prabhakar, Melnik, Raynolds
PRB 84, 155208 (2011)







Phonon mediated spin transition rates

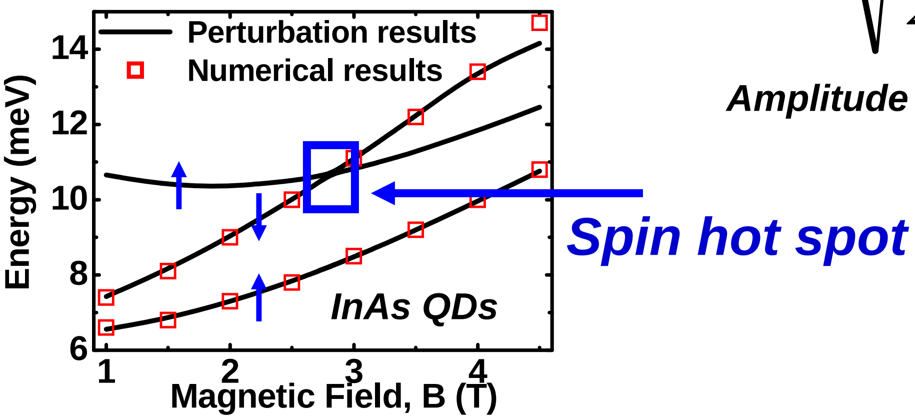


$$H = H_0 + H_z + H_R + H_D$$ ***Total Hamiltonian of a QD***

The interaction of electron and piezo-phonon is written as

$$u_{e-ph}^{q\alpha} = \sqrt{\frac{\hbar}{2\rho V \omega_{q\alpha}}} e^{-i(\hat{q}.\hat{r} - \omega_{q\alpha} t)} e A_{q\alpha} b_{q\alpha} + h.c.$$

Amplitude of the electric field created by piezo-phonon strain



Consider one longitudinal and two transverse phonon modes. Polarizations directions are

$$\hat{e}_l = (\sin\theta\cos\varphi,\ \sin\theta\sin\varphi, \cos\theta)$$

$$\hat{e}_{t1} = (\cos\theta\cos\varphi,\ \cos\theta\sin\varphi, -\sin\theta)$$

$$\hat{e}_{t2} = (-\sin\varphi,\ \cos\varphi, 0)$$

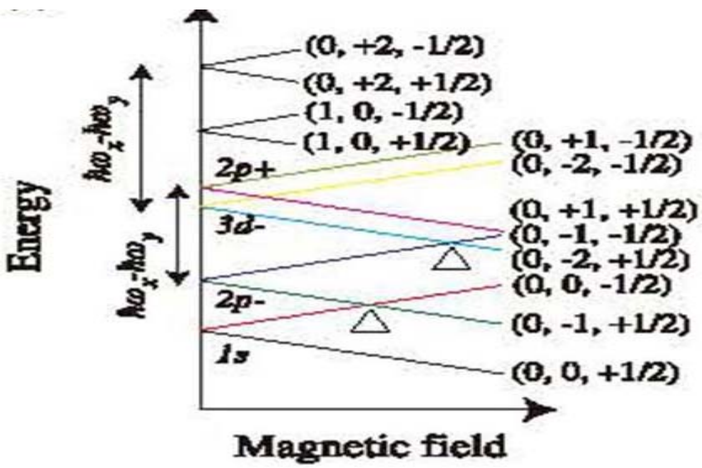
Prabhakar, Melnik, Raynolds PRB (2011)

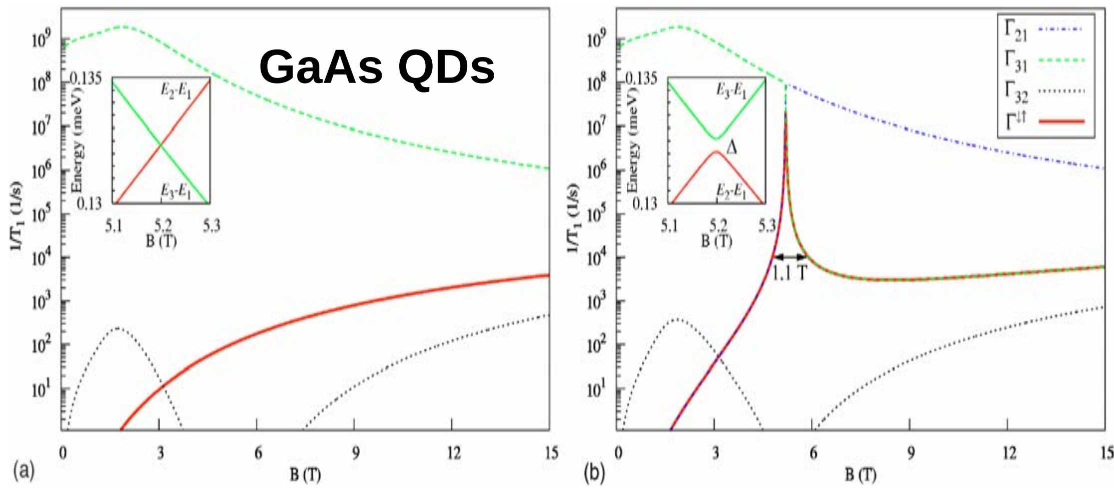
We apply Fermi-Golden Rule to find the transition rate

$$\frac{1}{T_1} = \frac{V}{(2\pi)^2 \hbar} \sum_\alpha \int d^3q \, |\langle 1 | u_{e-ph}^{q\alpha} | 2 \rangle|^2 \underbrace{\delta(\hbar\omega_{q\alpha} - E_2 + E_1)}_{\text{Conservation of energy}}$$

Conservation of energy

Phonon mediated spin transition rates





Dresselhaus case

Rashba case

D. Loss group PRB 71 (2005)

•Cusp-like structure can be seen for the pure Rashba case in the phonon mediated spin-flip rate

• However, spin-flip rate is a monotonous function of the magentic fields for the pure Dresselhaus case

Why? Need some Math

Why only Rashba spin-orbit coupling gives cusp-like structures?

Prabhakar, Melnik, Bonilla
PRB 87, 235202 (2013)

$$\frac{1}{T_1}=\frac{V}{(2\pi)^2\hbar}\sum_\alpha \int d^3q\,|<1|u^{q\alpha}_{e-ph}|2>|^2\,\delta(\hbar\omega_{q\alpha}-E_2+E_1)$$

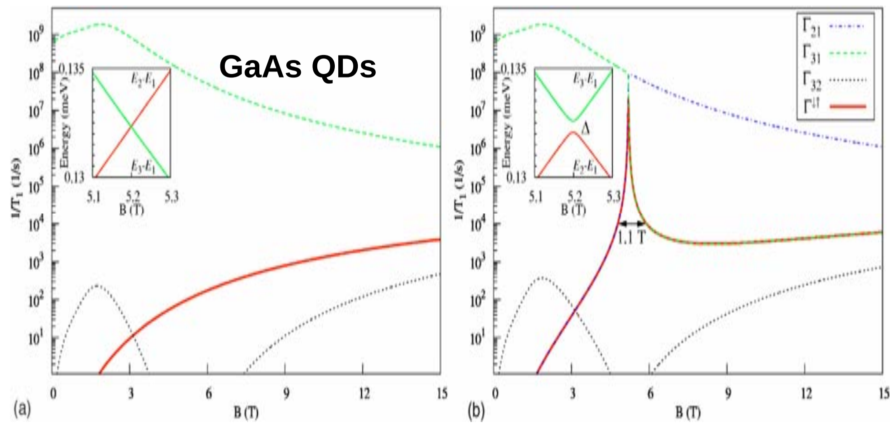
$$\frac{1}{T_1}=\frac{(eh_{14})^2(g\mu_B B)^3}{35\pi\hbar^4\rho}\left(\frac{1}{s_l^5}+\frac{4}{3}\frac{1}{s_t^5}\right)\left(|M_R|^2+|M_D|^2\right)$$

$$M_R=\frac{\alpha_R}{\sqrt{2}\hbar\Omega}\left[\frac{1}{1-\frac{\Delta}{\hbar(\Omega+\frac{\omega_c}{2})}}-\frac{1}{1+\frac{\Delta}{\hbar(\Omega-\frac{\omega_c}{2})}}\right]$$

$$M_D=\frac{\alpha_D}{\sqrt{2}\hbar\Omega}\left[\frac{1}{1+\frac{\Delta}{\hbar(\Omega+\frac{\omega_c}{2})}}-\frac{1}{1-\frac{\Delta}{\hbar(\Omega-\frac{\omega_c}{2})}}\right]$$

$$\Delta = g_0\mu_B B$$

Never find the accidental degeneracy point



Dresselhaus case **Rashba case**

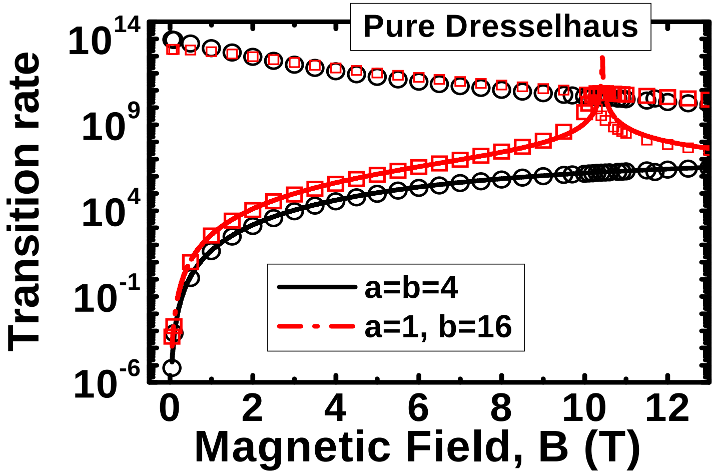
Also see D. Loss group
PRB 71, 205324 (2005)

•Accidental degeneracy point is also called the spin hot spot.

•Since the spin-flip rate at or nearby the level crossing point is enhanced by several order of magnitudes, it provides the most favorable condition for the design of spin based logic gates

•Bulk g-factor is –ve. Only Rashba coupling has accidental degeneracy which provides the cusp-like structure in the spin-flip rate.

Phonon mediated spin transition rates: anisotropic effects



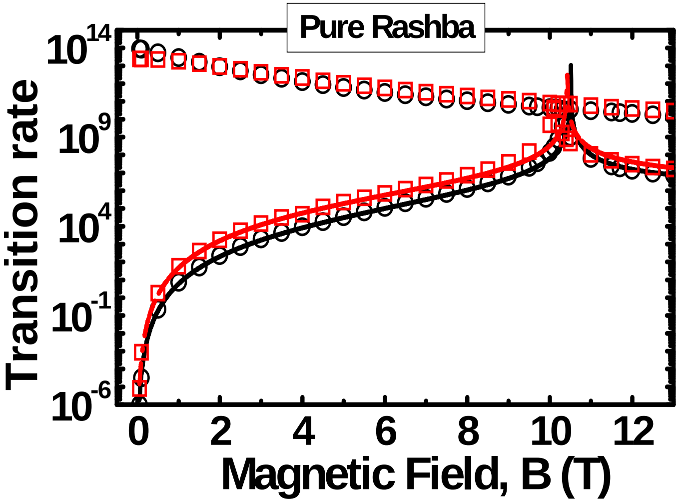
Bulaev and Loss PRB (2005)

For circular QDs

- **Cusp-like structure can be seen for pure Rashba case.**
- **Spin-flip rate is a monotonous function for pure Dresselhaus case**

Our proposal: anisotropic effects

Prabhakar, Melnik and Bonilla; PRB (2013)



Spin transition rate is obtained from the Fermi-Golden Rule

$$\frac{1}{T_1} = \frac{V}{(2\pi)^2 \hbar} \sum_{\alpha} \int d^3 q \, |<1| u_{e-ph}^{q\alpha} |2>|^2 \, \delta\left(\hbar\omega_{q\alpha} - E_2 + E_1\right)$$

Summary:

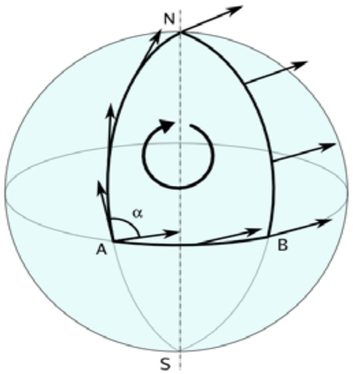
- **The spin hot spot (i.e., the cusp like structure) due to accidental degeneracy point in the phonon mediated spin-flip rates has been observed for the pure Dresselhaus spin-orbit coupling case**

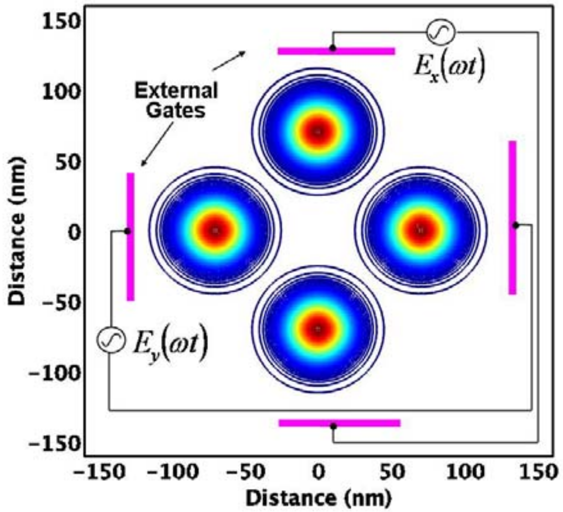
Berry phase in QDs

Geometric phase factors accompanying adiabatic changes (Berry Phase)

According to Schrödinger Equation, the state $|\Psi(t)\rangle$ of the system evolves

$$\hat{H}(R(t))|\Psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle$$





At any instant,

$$\hat{H}(R)|n(R)\rangle = E_n(R)|n(R)\rangle$$

$$|\Psi(t)\rangle = \exp\left\{\frac{-i}{\hbar}\int_0^t dt'\, E_n(R(t'))\right\}\exp(i\gamma_n(t))|n(R(t))\rangle$$

Dynamical Phase Factor ***Berry phase***

Prabhakar, Melnik, Bonilla PRB (2014)

M. Berry Proc. R. Soc. Lond. A 392,45-57(1984)

$$\gamma_n = -Im\iint_C dS \bullet \sum_{m\neq n}\frac{\langle n(R)|\nabla_R\hat{H}(R)|m(R)\rangle\times\langle m(R)|\nabla_R\hat{H}(R)|n(R)\rangle}{(E_m(R)-E_n(R))^2}$$

Manipulation of spin through Berry phase in III-V semiconductor QDs

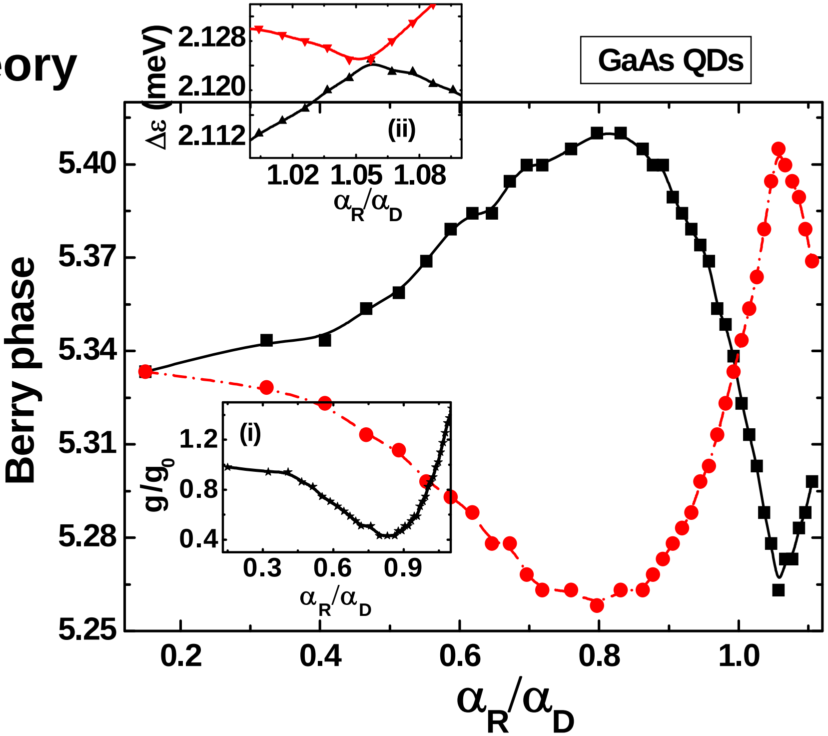
Prabhakar, Melnik, Bonilla PRB (2014)

- We apply non-degenerate perturbation theory
- We find the Berry phase in QDs as

$$\gamma_{0,0,\pm 1/2} = \mp \frac{\pi}{2} \frac{\left(\hbar\omega_+ \xi_- r_0\right)^2}{\left[\hbar\Omega_- \pm \xi_-^2 \left(\frac{\alpha_R^2}{\rho_+} - \frac{\alpha_D^2}{\rho_-}\right)^2\right]^2}$$

$$\rho_\pm = \hbar\Omega_- \pm \Delta;\ \Delta = g_0 \mu_B B$$

$$\omega_\pm = \Omega \pm \frac{\omega_c}{2};\ \Omega = \sqrt{\omega_0^2 + \frac{1}{4}\omega_c^2}$$



- Interplay between Rashba and Dresselhaus spin-orbit couplings in the Berry phase has been explored
- Sign change in the g-factor has been observed
- Level crossing in the Berry phase can be obtained
- Berry phase is higly sensitive to the magnetic fields, QDs radii and the electric fields along z-direction

Extension of Berry Phase for degenerate case: disentangling operator method

For non degenerate state,

$$\left|\Psi(t)\right\rangle = exp\underbrace{\left\{\frac{-i}{\hbar}\int_0^t dt'\; E_n\left(R\left(t'\right)\right)\right\}}_{\text{Dynamical Phase Factor}} \underbrace{exp\left(i\gamma_n(t)\right)}_{\text{Berry phase}}\left|n\left(R(t)\right)\right\rangle$$

For a degenerate state, geometric phase factor is replaced by a non-Abelian unitary operator acting on the initial states within the subspace of a degeneracy

$$\left|\Psi_a(T)\right\rangle = \exp\left\{\frac{-i}{\hbar}\int^T E(t)\,dt\right\}\hat{U}_{ab}\left|\Psi_b(0)\right\rangle$$

$\hat{U}_{ab} =$ *Non-Abelian Unitary transformation*

F. Wilczek and A. Zee; PRL 52, 2111, (1984)

- ***We seek to apply the Feynman disentangling operators to find the exact evolution operators for the Hamiltonian associated to QDs***

Quantum dot orbiting in a closed path in the plane of 2DEG

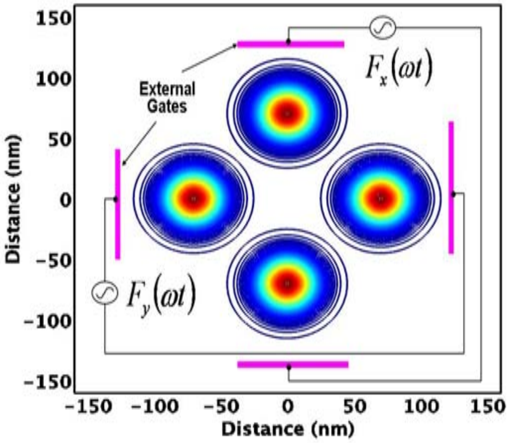
$$P_x = -R_0 m\omega \sin \omega t \qquad P_y = R_0 m\omega \cos \omega t$$

For the pure Dresselhaus case;

$$U_{ad} = T \exp\left[-i\int_0^{2\pi} d\phi \frac{R_0}{l_{so}}\left(\sigma_x \sin\phi + \sigma_y \cos\phi\right)\right]$$

Prabhakar, Raynolds, Inomata, Melnik
PRB 82, 195306 (2010)

Consider both Rashba and Dresselhaus spin-orbit couplings



$$H_{\pm} = \left(\alpha P_y - \beta P_x\right) \mp i\left(\beta P_y - \alpha P_x\right)$$

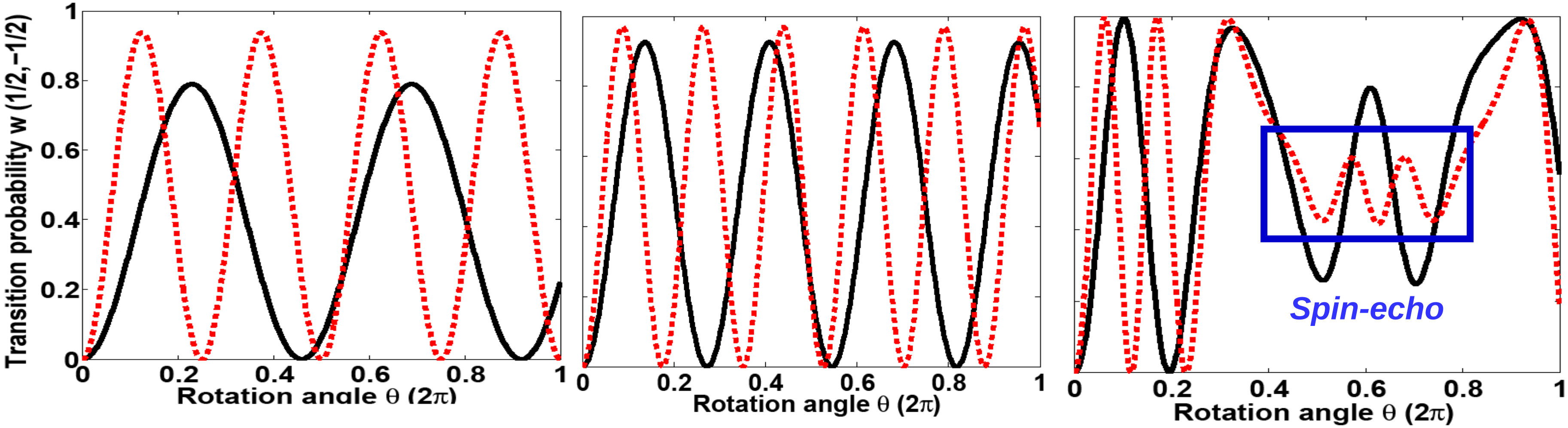
- ***We find the evolution operator and investigate the interplay between the Rashba and the Dresselhaus spin-orbit couplings***
- ***We apply the Feynman disentangling operators scheme to find the exact evolution operator.***

Results: Evolution of spin dynamics during the adiabatic movement of the QDs in the plane of 2DEG

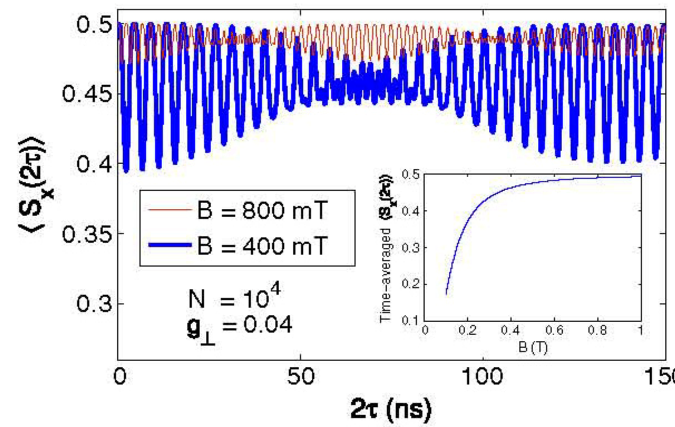
Prabhakar, Raynolds, Inomata, Melnik.
PRB 82, 195306 (2010)

$E=5x10^5$ V/cm (black)
$E=10^6$ V/cm (red)
R_0=500nm

Rashba case **Dresselhaus case** **Mixed case**

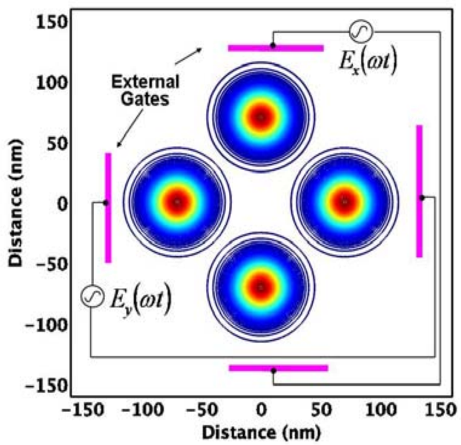


- *Spin-flip transition probability is enhanced with the gate controlled electric fields.*
- *Periodicity of the propagating waves is reduced with increasing electric fields which provides a shortcut to flip the spin rapidly.*
- *Periodicities of the propagating waves are different for the pure Rashba and pure Dresselhaus cases. As a result, we find the spin echo due to a superposition of Rashba and Dresselhaus spin waves.*

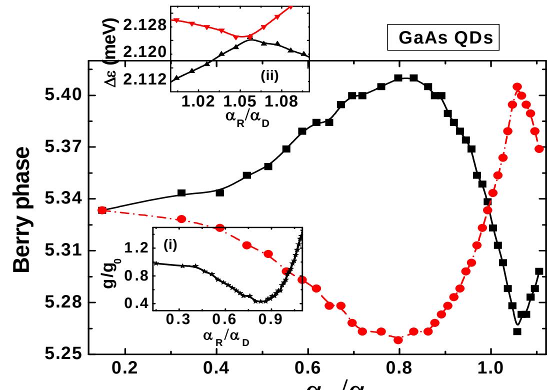


Coish et. al (PRL 2012); Spin-echo found in heavy holes Interacting with nuclear spins

Summary:

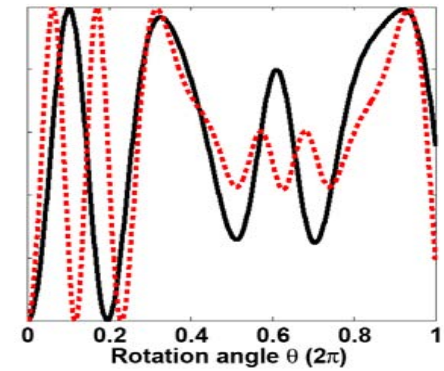


Prabhakar, Melnik, Bonilla PRB (2014), EPJB (2015)



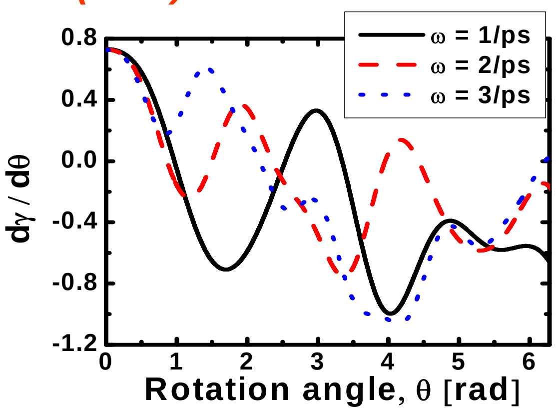
Sign change in the g-factor is reflected in the manipulation of spin via Scalar Berry phase.

Prabhakar, Raynolds, Inomata, Melnik, PRB (2010)



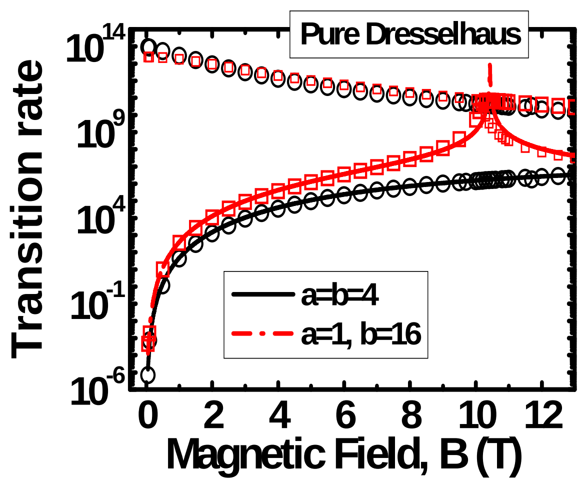
Exact evolution operator is found via Feynman disentangling operators scheme. Spin echo dynamics is observed.

Prabhakar, Melnik, Inomata APL (2014).



We propose a method to flip the spin completely by an adiabatic transport of quantum dots.

Prabhakar, Melnik and Bonilla; PRB (2013)



Spin hot spot due to anisotropy effect in Dresselhaus spin-orbit coupling

Prabhakar, Melnik, Bonilla PRB (2016)