Modern Challenges in Coupled Quantum-Continuum Modeling and Control of Closed and Dissipative Systems

Roderick Melnik

Wilfrid Laurier University & University of Waterloo, Canada
Guelph-Waterloo Institute of Physics
The MS2Discovery Interdisciplinary Research Institute

http://www.m2netlab.wlu.ca
http://www.ms2discovery.wlu.ca

Predictive Multiscale Materials Modeling Workshop,
Research Team:

Sanjay Prabhakar
Bin Wen
Rakesh Dhote
Max Paliy
Shyam Badu

Collaborators:

James Raynolds, USA
Luis Bonilla, Spain
Hector Gomez, Spain
Morten Willatzen, Denmark
Bruce Shapiro, USA

SHARCNET / COMPUTE CANADA
Outline of This Talk

- Introduction: multiple scales and their coupling.
- Going all the way down. Nanoscale: what is next?
- A hierarchy of physics-based mathematical models and coupling.
  - Geometric and materials nonlinearities.
  - Variational formulations and coupling procedures.
- Higher order nonlinear effects: phase transformations.
- Controlling nanoscale objects and future applications.
- Going to the cell level and below: multiscale approaches for biological nanostructures.
Since the undoubted attractiveness of ab initio atomistic approaches and first principles calculation is necessarily accompanied by severe computational limitations, the question is how far can we proceed with these approaches?

2. Atomic forces entering Hamiltonians in such calculations are already approximate. Add to this coupled multiscale effects, including those from larger scales.

P. Krajewski et al, E. Karpov et al
Biological Nanostructures and the Design of Life

1 nanometer = $10^{-9}$ meter
It is roughly 100,000 times smaller than the thickness of human hair.
Importance and Universality of Interacting Spatio-Temporal Scales

γνῶθι σεαυτόν → Nosce te ipsum → Know thyself

Diagram showing different scales and models, from atomic to organismal, with corresponding time scales and processes.
Quantum-Continuum Approaches

- The information from the atomistic scale can be passed and built into continuum models (VAC models, hierarchical multiscale)
- Concurrent multiscale (QCM, BSM, e.g. Quantum-to-Stochastic-Multiresolution-Continuum), in iterative manner with complete coupling (convergence depends on a degree of coupling)
- A combination of the above (e.g., embedding the HM into the CS)
- Via entropy maximization (quantum models at the mesoscale)
Nanoscale, Low Dimensional Nanostructures & The Kingdom of Electrons

- Low dimensional nanostructure (LDN) - a tiny structure made of a solid material.
- It is so tiny (typically consisting of 1,000 - 10,000 atoms) that an electron (a fundamental constituent of matter that has no known components or substructure) inside it is severely restricted in its movement.
- Now, when an electron’s motion is so severely constrained, its kinetic energy can assume only certain allowed values that are determined by the size and shape of the LDN, as well as the material making up these low dimensional nanostructures.

Quantum wires\(^1\)  
Quantum dots\(^2\)  
Nanowire superlattices\(^3\)

\(^1\)Karlsson et al Appl. Phys. Lett. 90, 101108 (2007)  
\(^3\)Caroff et al Nature Nanotechnology 4, 50 - 55 (2009)
The top-down approach in mathematical modelling of LDSNs

The Liouville equation for the evolution of the position-velocity probability density $f(x, v, t)$:

$$\partial_t f + v \cdot \text{grad}_x f + \frac{1}{m} F \cdot \text{grad}_v f = 0,$$

$$F = -qE, \quad t > 0, \quad x \in \mathbb{R}^3, \quad v \in \mathbb{R}^3,$$

Under the assumption $E_{eff} = -\text{grad}_x V_{eff}$ the effective field equation is reducible to the Poisson equation

$$-\epsilon_s \Delta V_{eff} = \rho.$$

Simplify and the integration of the Vlasov equation leads to a macroscopic conservation law:

$$q \partial_t n - \text{div} J = 0, \quad J = -q \int vFdv.$$
The scattering rate, $s$, is a highly non-regular function allowing us to define the collision frequency (and the corresponding collision operator) and the relaxation time (average time between two consecutive collisions at $(x, k)$)

$$\lambda = \int s(x, k, k') dk', \quad \tau(x, k) = 1/\lambda(x, k), \quad k \in B,$$

where the integral is taken over the Brillouin zone $B$ of the lattice.

- Relaxation time hierarchy of mathematical models (QHM,...)
- We move here from continuum (fluid dynamics like) model to account for discretness of the problem.

A fundamental (bottom-up) approach to modelling LDSNs is based on the mixed-state Schrodinger equation coupled to Poisson’s equation for the electrostatic potential.
The formation of LDSNs (in particular quantum dots) is a competition between the surface energy in the structure and strain energy.

Technologically, all effective methodologies are based on self-assembly where the final result is often many (dozens and even hundreds) self-assembled dots sitting on the wetting layer and randomly distributed over it, having

- different size,
- shape, and, ultimately,
- properties.
• Inside of your computer are tiny switches that are only 100 nanometers wide. About 1,000 of these switches can fit across the width of a single hair.

• One important property of quantum dots is their exceptionally large surface-to-volume ratios -- sensing, targeted drug delivery, catalysis, etc (all applications where S/V large values are needed).

• Lasers, Optical Amplifiers; Sensors (as an alternative to CCD and CMOS technology, Si – only 50% light-absorbing efficiency)

• QDs for high-resolution, low-energy televisions.

[M. Simmons et al, M. Fuchsle]
Nanoscale and Multiscale: Biology, Bioengineering, and Biomedical

- QD-based DNA nanosensors where rapid and highly sensitive detection of DNA is critical in diagnosing genetic diseases and cancer (they are capable to detect and count the DNA strands linked to cancer);

- Quantum dots and novel techniques for drug delivery and therapy
  1. Microscopy and multiplexed histology
  2. Flow-cytometry
  3. Drug delivery
  4. Photodynamic therapy
  5. *In vivo* whole animal and clinical imaging (e.g., angiography)
  6. Tissue mapping and demarcation (e.g., sentinel lymph node)
  7. Real time detection of intracellular events, signalling, and bio-sensing
  8. Tracking cell migration (e.g., stem cells)
  9. Low cost but sensitive point-of-care detection (e.g., lateral flow)
  10. Environment and bio-defence

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10 - 20 nm
Quantum Dots, Nanorods, and Forests

Thorsten Dziomba: GeSi QDs, 15 nm high, 70nm in diameter, Vvedenski, Wang et al
Recall a classical example:
Newton’s prediction of the speed of sound before the development of thermodynamics.

**Coupled Problems:**

- Drift and diffusion/reaction are intrinsically coupled (such models span from the dynamics of cell cycles: R.M., Wei, Moreno-Hagelsieb, to risk modeling, Zhang, R.M.).

- Coupled electro-elasticity equations (see R.M., on well-posedness and regularity, R.M. et al, including piezoelectricity)

- Coupled nonlinear thermo-elasticity equations: (Matus, R.M., Wang, Dhote, Zu)

- Coupled problems in quantum mechanics, e.g. for low dimensional nanostructures such as quantum dots (Lassen, R.M., Willatzen), as well as nanowire superlattices (Bonilla, Alvaro, Carretero, R.M., Prabhakar).
Coupling: Universality and Numerical Approaches

• Due to universality of coupling and multiscale interactions, *coupled dynamic problems* are the rule rather than an exception in mathematical modeling and its applications.

• Coupled problems: the general variational principles, from where we derive numerical approximations which conserve the most important properties of the original system, e.g., energy.
The importance of coupling at the nanoscale

- Low dimensional nanostructures (such as quantum wells, quantum wires, quantum dots) have been modeled predominantly with simplistic quantum mechanical approximations, e.g. linear Schrödinger models in the steady-state approximation.

- New technological advances in applications of low-dimensional semiconductor nanostructures clearly demonstrate that such approximations become inadequate.

- Experiments (e.g., A. Zaslavsky et al): effects at different scales that may influence substantially optoelectromechanical properties of the nanostructures - strain relaxation, piezo-, thermal, magnetic, and other effects coming from different physical fields coupling.
We need some **averaging over atomic scales**:
- empirical tight-binding,
- pseudopotential, and
- $k \cdot p$ approximations.

The $k \cdot p$ (envelope function) theory represents the electronic structure in a continuum-like manner and is well suited for incorporating additional effects into the model such as strain and piezoelectric and other coupled effects, including higher order nonlinear effects.
Physics-based models and the choice of basis functions

The accuracy of the $k \cdot p$ approximation depends on the choice of the functional space where the envelope function is considered.

From the physical point of view:

The basis functions that span such a space correspond to subbands within conduction and valence bands of the semiconductor material.

The number of basis functions: 1-8. The choice is a balance between the accuracy of the model and computational feasibility of its solution.

Physical effects for the WZ (hexagonal crystalline lattice) materials that are important to include into the model:

- spin-orbit and crystal-field splitting,
- valence and conduction band mixing (due to a large band gap typical for these materials).
The model for the WZ materials

The model, in its general setting, is based on 6 valence subbands and 2 conduction subbands (accounting for spin up and down situations) and we need to solve the following PDE eigenvalue problem with respect to eigenpair \((\Psi, E)\):

\[
H \Psi = E \Psi, \quad \Psi = (\psi_S^\uparrow, \psi_X^\uparrow, \psi_Y^\uparrow, \psi_Z^\uparrow, \psi_S^\downarrow, \psi_X^\downarrow, \psi_Y^\downarrow, \psi_Z^\downarrow)^T
\]  

(1)

where

- \(\psi_X^\uparrow \equiv (|X > | \uparrow)\) denotes the wave function component that corresponds to the X Bloch function of the valence band with the spin function of the missing electron “up”,

- the subindex “S” denotes the wave function component of the conduction band, etc,

- \(E\) is the electron/hole energy.
All current models for bandstructure calculations we are aware of are based on the original representation of [Bir1974] where strain is treated on the basis of infinitesimal theory with Cauchy relationships between strain and displacements.

Geometric irregularities make this approximation inadequate.

Material nonlinearities (stress-strain relationships): strain remains of orders of magnitudes smaller of the elastic limits.

- Semiconductors are piezoelectrics and higher order effects may become important (e.g., at the level of device simulation).
- Elastic and dielectric coefficients, being functions of the structure geometry, are nonlinear, but the elasticity is treated by the valence-force-field approaches.
HeQuad Structure: A GaAs/InAs/InSb Quantum Dot

(a) GaAs
(b) GaSb

Diagram showing dimensions:
- Y-axis: 80nm
- X-axis: 180nm, 200nm
- Z-axis: 35nm, 14nm, 40nm
- Scale: 10 nm
Both deformational energy and piezoelectric field functionals should be included consistently (RM2000 – WLVM2006).

However, most results obtained so far in the context of bandstructure calculations are pertinent to minimization of elastic energy only ([O’Reily2000], [Fonoberov2003],...)

Could be Ok for ZB materials (where the piezoelectric effect is relatively small), but not for the WZ.

We need to solve simultaneously equations the elasticity equations and Maxwell equation.

Even for the linear constitutive model, the coupling between the field of deformation and the piezoelectric field is of fundamental importance (Pan, Jogai2003, WLVM2006).
While on the atomic scale we are attempting to move directly to new atomic positions of all particles after deformations, in our approach we move from the variation in displacements to the variation of deformation (as in the Hamilton principle):

$$\delta \int_{t_1}^{t_2} (L + W) dt = 0,$$

where

$$L = \int_V \left[ \frac{1}{2} (\sigma^T \epsilon + E^T D) - \rho \dot{u}^T \delta u \right] dV + \int_{S_\sigma} F_1^T u ds + \int_{S_\varphi} F_2^T \varphi ds,$$

where $F_1$ and $F_2$ are surface force and surface charge (with surface areas, $S_\sigma$ and $S_\varphi$), respectively.
In our case, we couple this model to the weak form of the Schrodinger equation equivalent to finding stationarity conditions for the following functional:

\[
\Phi(\Psi) = -\frac{\hbar^2}{2m_0} \int_{\tilde{V}} (\nabla \Psi)^T \mathcal{H}^{(\alpha,\beta)} \nabla \Psi \, dv - E \int_{\tilde{V}} \Psi^T \Psi \, dv \tag{8}
\]

with respect to the wave function vector field \( \Psi \) defined in (1).
Excited states accounting for piezoeffect
Widening of the band-gap due to lattice misfit and piezo effects.
Influence of finite size in NWSLs

Electron

Hole

Electron

Hole

M^2NeT Laboratory
www.m2netlab.wlu.ca
With coupling: piezo-electromechanical effects in wurtzite NWSLs
Critical radius and barrier localization
Symmetry breaking in low dimensional nanostructures

Cylindrical symmetry is broken
Effect of thermal stresses in quantum dots and wires\textsuperscript{1,2,3,4}

– Increase in the magnitude of the mechanical stress/strain; Decrease in the electric potential and the electric field

– Significantly higher influence on electro-mechanical properties in wurtzite nanostructures as compared to zinc blend

– Influences of the phase transformations and phase stability in nanostructures

– A significant reduction in electronic state energies due to thermal loadings has been observed.

\textsuperscript{4}Wen B and Melnik R V N \textit{Appl. Phys. Lett.} Vol. 92, 261911, 2008
Modeling of the nanowire superlattices

We assume that the NWSL consists of alternate layers of AlN/GaN and is embedded in AlN matrix. The dimensions and geometrical details of the NWSL are given in above Figures.
The potential difference creates a deeper potential well, for holes at the negative end and at the positive end for electrons. Thus, the decrease in potential difference with temperature leads to a shallower potential well, which will result in relatively less confinement. In the present case we observe the highest value of electric potential in the second layer of GaN.
Magneto-thermo-electromechanical effects

Magneto-thermo-electromechanical effects

**AlN/GaN QDs**

- $E_1 = 4.91$ eV
- $E_2 = 4.95$ eV
- $E_1 = 4.33$ eV
- $E_2 = 4.43$ eV

**GaN/BaTiO$_3$ QDs**

- $E_1 = 3.85$ eV
- $E_2 = 3.86$ eV
- $E_1 = 1.96$ eV
- $E_2 = 1.97$ eV
Shape Memory Properties (Lagoudas)
SMA Applications at Submicron Scale

Okamura et al. (2007)

Johnson et al.

Luskin et al. (2004)

Zakharov et al. (2012)

Rozman et al. (2012)
Microstructures - Nanograin

† Dhote, R.M., Zu et al. 2012 (CMS)
Microstructure Evolution – $e_2$

t = 0

t = 500

t = 600

t = 800

t = 1100

t = 1400
Microstructure Evolution – e2

Evolution

Evolved microstructure

† Dhote, Gomez, R.M., Zu 2013 (Proc. Sci.)
Open and Coupled/Interconnected Systems, Probabilistic Dissipation & Control

• **Open System** interacts with its environment, e.g. by exchanging matter, energy, or information.

• **Coupled System** consists of interacting subsystems/fields

• *A major source of uncertainty* is coming from the fact that the classical systems theory treats input, output, and signal flow graphs *ab initio*.

• **Dissipation theory** is formulated in terms of generalized energy inequalities in probabilistic sense via vacuum expectations of stored and supplied energies. Examples are developed for *open quantum systems* + *exosystem*.

• Non-smooth control, LD for Hamiltonian vector fields
Spin & geometry

Applications:

Schematics of spin single electron transistors (SET): QDs

Bandyopadhyay et al. PRB 61, 13813 (2000)

Manipulation of spin through Berry phase

R.M. with Prabhakar and Bonilla, arxiv: 1211:2936;

QDs for laser and light emitting diodes applications
Hamiltonian of quantum dots in III-V semiconductors: isotropic vs anisotropic

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

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

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

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

where

$$\omega_0 = \sqrt{\frac{\hbar}{m\ell_0}}, \quad E$$

are control variables
**Possible spin SET prototype QDs: g-factor**

*g-factor tuning by several different mechanisms*

- Gate controlled electric fields along z-direction
- Lateral size of the QDs in the plane of 2DEG
- Notice that the g-factor changes its sign

![Wavefunctions of GaAs QDs in the plane of 2DEG](image)

\[ g = \frac{\varepsilon_{0,0,1/2} - \varepsilon_{0,0,-1/2}}{\mu_B B} \]
Spin states in InAs QDs: Experiment vs Theory

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

Numerical results

Energy (meV)

Magnetic Field, B (T)

2.7  2.8  2.9  3.0  3.1

2.3

2.4

2.5

2.6

2.7

\( \Delta \varepsilon = 65 \mu \text{eV} \)

\( \varepsilon_2 - \varepsilon_1 \)

\( \varepsilon_3 - \varepsilon_1 \)

Energy (meV)

Magnetic Field, B (T)

2.7  2.8  2.9  3.0  3.1

2.3

2.4

2.5

2.6

2.7

R.M. with S.P. et al  
PRB 84, 155208 (2011)

\[ U(x, y) = \frac{1}{2} m \omega_0^2 (ax^2 + by^2) \]

\[ [H_{xy}, p_z] = 0 \]

\[ \langle p_z \rangle = (\hbar k)^2 = \hbar^2 \left( \frac{2meE}{\hbar^2} \right)^{2/3} \]

\( E=1.6 \times 10^4 \text{ V/cm} , \)

\( l_0=28 \text{ nm}, \)

\( a=1.5, b=4 \)

SEM of a 2D-0D heterodimensional prototype

R.M. with S.P. et al  
PRB 84, 155208 (2011)
Summary:

- Anisotropy effects push the g-factor towards bulk crystal.
- Electric and magnetic field tunability of the g-factor in InAs QDs is shown to cover a wide range of g-factors through a strong Rashba spin-orbit coupling.
- Rashba and Dresselhaus spin-orbit couplings themselves induce the anisotropy in the g-factor in QDs.
- Level crossing point can be achieved with the accessible values of the QD radii and magnetic fields.
- Next, we look at the phonon mediated spin transition rate in such quantum dots.
Phonon mediated spin transition rates in III-V semiconductor QDs: Anisotropy effects

\[ H = H_0 + H_z + H_R + H_D \]

Total Hamiltonian of a QD

The interaction of electron and piezo-phonon is written as

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

Amplitude of the electric field created by piezo-phonon strain

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

- \[ \hat{e}_l = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta) \]
- \[ \hat{e}_{t1} = (\cos \theta \cos \varphi, \cos \theta \sin \varphi, -\sin \theta) \]
- \[ \hat{e}_{t2} = (-\sin \varphi, \cos \varphi, 0) \]

Apply Fermi-Golden Rule to find the transition rate

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

Conservation of energy

Perturbation results

Numerical results

InAs QDs

Spin hot spot

Energy (meV)

Magnetic Field, B (T)

PRB 84, 155208 (2011)

PRB 68, 155330 (2003)

APL 100, 023108 (2012)

D. Loss et. al.
PRL 95, 076805 (2005)

R.M. with Prabhakar and Bonilla

Das Sarma et. al.
Phonon mediated spin transition rate

Confining potential for circular QDs

\[ U(x, y) = \frac{1}{2} m \omega_0^2 \left( x^2 + y^2 \right) \]

Spin transition rate is obtained from Fermi-Golden Rule

\[ \frac{1}{T} = \frac{V}{(2\pi)^2 \hbar} \sum_\alpha \int d^3 q |<1| u_{e-ph}^{q\alpha} |2>|^2 \delta(\hbar \omega_{q\alpha} - E_2 + E_1) \]

Results: D. Loss group
PRB 71, 205324 (2005)

- Cusp-like structure can be seen for the pure Rashba case in the phonon mediated spin-flip rate
- Spin-flip rate is a monotonous function of the magnetic fields for the pure Dresselhaus case

Why?
Why only the Rashba spin-orbit coupling gives a cusp-like structure?


Bulk g-factor is –ve. Only the Rashba coupling has accidental degeneracy which provides a cusplike structure in spin-flip rates.

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

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

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

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

\[
\Delta = g_0 \mu_B B
\]

Accidental degeneracy point is also called the spin hot spot.

The spin-flip rate at or nearby the level crossing point is enhanced by several orders of magnitude which provides the most favorable condition for the design of spin based logic gates.
Controlling nanostructures

Spin, g-factor of QDs, anisotropy, and geometry

• Spins in a QDs can be manipulated by several different mechanisms such as gate controlled electric fields along z-direction, magnetic fields and spin-orbit couplings.
• Spin-orbit coupling itself induces anisotropy in QDs
• Anisotropy induces the suppression of g-factor towards bulk crystal
• Anisotropy either extends the g-factor to larger QDs radii as well as to larger magnetic fields or vice versa.

Phonon mediated spin transition rates:

• Anisotropy enhances the phonon induced spin-flip rates
• Only Rashba coupling induces the spin hot spot in symmetric QDs
• However, anisotropy breaks the in-plane rotational symmetry. As a result, we discovered the spin-hot spot for the pure Dresselhaus spin-orbit coupling case.
**Spin & geometry**

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

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

\[
\nu_{0,0,1/2} = \frac{-e^2 \ell^2}{\hbar \omega_+ - \omega_+^2 \left(\frac{\alpha_R^2}{\rho_+} - \frac{\alpha_D^2}{\rho_-}\right)^2} \int_C ds
\]

- \( \rho_{\pm} = \hbar \omega_{\pm} \pm \Delta; \Delta = g_0 \mu_B B \)

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

- Interplay between Rashba and Dresselhaus spin-orbit couplings in the Berry phase has been explored

- Sign change in the g-factor can be seen for GaAs QDs

- Level crossing in the Berry phase can be obtained

- Berry phase is highly sensitive to the magnetic field, QDs radius and the electric fields along z-direction

**Graphs and charts**

- GaAs QDs
- InAs QDs

**Arxiv:** 1211:2936
Extension of Berry Phase for degenerate case: Disentangling operator method

For a non degenerate state, we have:

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

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

$$\Psi_a (T) = \exp \left\{ \frac{-i}{\hbar} \int_0^T E(t) dt \right\} \hat{U}_{ab} |\Psi_b (0)\rangle$$

$\hat{U}_{ab} = \text{non Abelian unitary transformation}$

We seek to apply the Feynman disentangling technique to find the exact evolution operators for the Hamiltonians associated with QDs.

Finding exact evolution operators has important implications for quantum computing
Quantum dot orbiting in a closed path in the plane of 2DEG

San-Jose et al
PRB 77, 045305 (2008)

\[ P_x = -R_0 m \omega \sin \omega t \quad P_y = R_0 m \omega \cos \omega t \]

For pure Dresselhaus case:

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

\[
\approx 1 - i \sigma_z \frac{2\pi R_0^2}{l_{so}}
\]

Our proposal:
PRB 82, 195306 (2010)

Consider both Rashba and Dresselhaus spin-orbit couplings

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

• Find the evolution operator and investigate the interplay between the Rashba and the Dresselhaus spin-orbit couplings
• We apply the Feynman disentangling operator scheme to find the exact evolution operator.
Evolution of spin dynamics during the adiabatic movement of the QDs in the plane of 2DEG

PRB 82, 195306 (2010)

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.

Periodicity of the propagating waves are different for pure Rashba and pure Dresselhaus cases. As a result, we find the spin echo due to superposition of Rashba and Dresselhaus spin waves.

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

- Adiabatic control of spin states in QDs through geometric phase has been proposed and analyzed in detail.
- Non-zero scalar Berry phase in the lowest Landau levels of QDs can be achieved from higher orbital states that are only differed by one quantum number.
- Berry phase is highly sensitive to the gate controlled electric fields, QDs radius and magnetic fields.
- Exact analytical solution of spin propagator of QDs has been found.
- Electron spin transition probability in QDs is enhanced with the gate controlled electric fields.
- Complete spin-flip takes place only for the case of equal strength of Rashba and Dresselhaus spin-orbit couplings which provides the presence of persistent spin-helix in QDs.
Modelling biological systems: RNA nanostructures

- Understanding of RNA led to the emergence of the "RNA architectonics" (a set of recipes for (self-)assembly of the RNA nanostructures of arbitrary size and shape.

- Although better suited for nanoengineering applications and medicine, compared to the DNA, the RNA bring a number of additional challenges (one is much larger structural modularity and diversity of the tertiary structural building blocks, e.g. 200 vs 20 for DNA)

- To be successful in developing coarse-grained (mesoscopic) models, it is essential to have input data from full molecular dynamics simulations.
Figure 1: A sample initial configuration from our MD simulations: (RNA hexaring + 165 Mg$^{2+}$ ions + 88664 H$_2$O). Top and side views of one simulation box (water is not shown).
Figure 2: Number of ions within 5 Å of RNA versus time for two selected temperatures and for a number of concentrations of Na and Mg ions. The colour coding is explained in the body of figures. The scale of the $y$-axis for Mg$^{2+}$ ions is set up twice smaller than that for the Na$^+$ ions to allow some better visual comparison. The sets of the curves in the lower parts of the plots belong to the Cl ions, whose adsorption onto the nanoring is much lower.
Stability conditions under quenching

**Figure 3:** Side and top views of the RNA nanoring in the "physiological solution" of Na (580 Na) after 4 ns equilibration at $T = 510$ K. Bottom snapshot: same for "barely neutralized" system (330 Na), it depicts the break of the nanoring in the kissing loop area. Na atoms situated within 5Å of the RNA ring only are shown in green, together with the bound water molecules (red and white). Cl atoms are not shown.
Evolution of the RNA nanoring
Figure 4: Top views of the RNA nanoring in the barely "neutralized" systems (165 Mg or 330 Na) after 1 ns "quenched" equilibration at $T = 310$ K starting from high temperature configurations. Only those Mg and Na atoms that have been located within 5 Å of RNA nanoring in the beginning of the runs are shown (such representations allow to visualise the process of the evaporation of the ions from the nanoring). Mg atoms are shown in green, Na atoms are shown in yellow. Waters that have been located in the first solvation spheres for Mg and Na in the beginning of the runs are shown in red and white. The phosphorus and two nonbridging oxygens atoms in each phosphate group are shown as brown and red spheres.
A hierarchy of coarse-graining methodologies

Here we analyze a range of possible coarse-graining methodologies with the three bead approximation leading to the best results.

Phosphate, sugar group and the nucleobase are used as the first, second and the third bead respectively.
The Boltzmann Inversion Method (multistate iterative)

RNA nanotube modeled from the eight and ten nanorings using VMD tool
THANK YOU

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