Nanoelectronic Modeling (NEMO) for High Fidelity Simulation of Solid-State Quantum Computing Gates

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Extending the world's most comprehensive semiconductor quantum device simulation tool to model quantum computing gates

Project Started in April 2002

This research was carried out by at the Jet Propulsion Laboratory, California Institute of Technology under a contract with the National Aeronautics and Space Administration.

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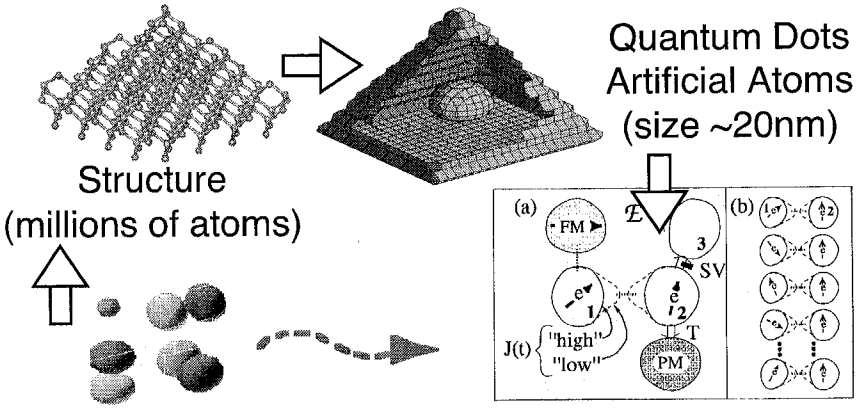
Objective

- Narrow experimental qubit parameter space
- Development of a comprehensive suite of modeling tools for solid state qubit devices
- Atomic level material description.
- Charge and spin coherent devices.
- Charge and spin transport in NEMO 1-D.
- Electronic structure in NEMO 3-D.
- Compute interactions and decoherence.



Approach

- Leverage about 50,000 hours NEMO 1-D and 12,000 hours NEMO 3-D development.
- Incorporate capabilities to model SiGe (close tie to Wisconsin group, v. d. Weide)
- Incorporate atomistic treatment of magnetic fields and impurities in semiconductors.
- Incorporate many-body effects through Hartree & configuration interaction (3-D).
- Provide data to circuit simulation (Williams)

Status

- Project started in April 2002
- Collaboration with Wisconsin on Si QDots.
- Completed atomistic SiGe parameterization.
- Atomistic magnetic field and charge interaction
- Theory of spin transport using NEGF
- Begun study of decoherence times in single and coupled quantum dots.
- 9 papers (submitted, in preparation, in print)

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Progress on last year's objectives

- Incorporated external magnetic fields and charge interactions into NEMO 3-D.
- Studied the magnetic field induced spin effects and many body effects in coupled QDs.
- Completed the SiGe tight binding parameterization (VCA) and begin study QDs.
- Developed theory to spin transport across heterojunctions using NEGF.
- Begun study of decoherence times in single and coupled quantum dots.

+Collaborated with Wisconsin group: confinement-based splitting of degenerate valleys.
+Computed phonon spectr of quantum dot arrays in atomistic model including strain.
+Hired new full time person: Dr. Seungwon Lee, Ohio State U, NCSA, UC Berkeley.

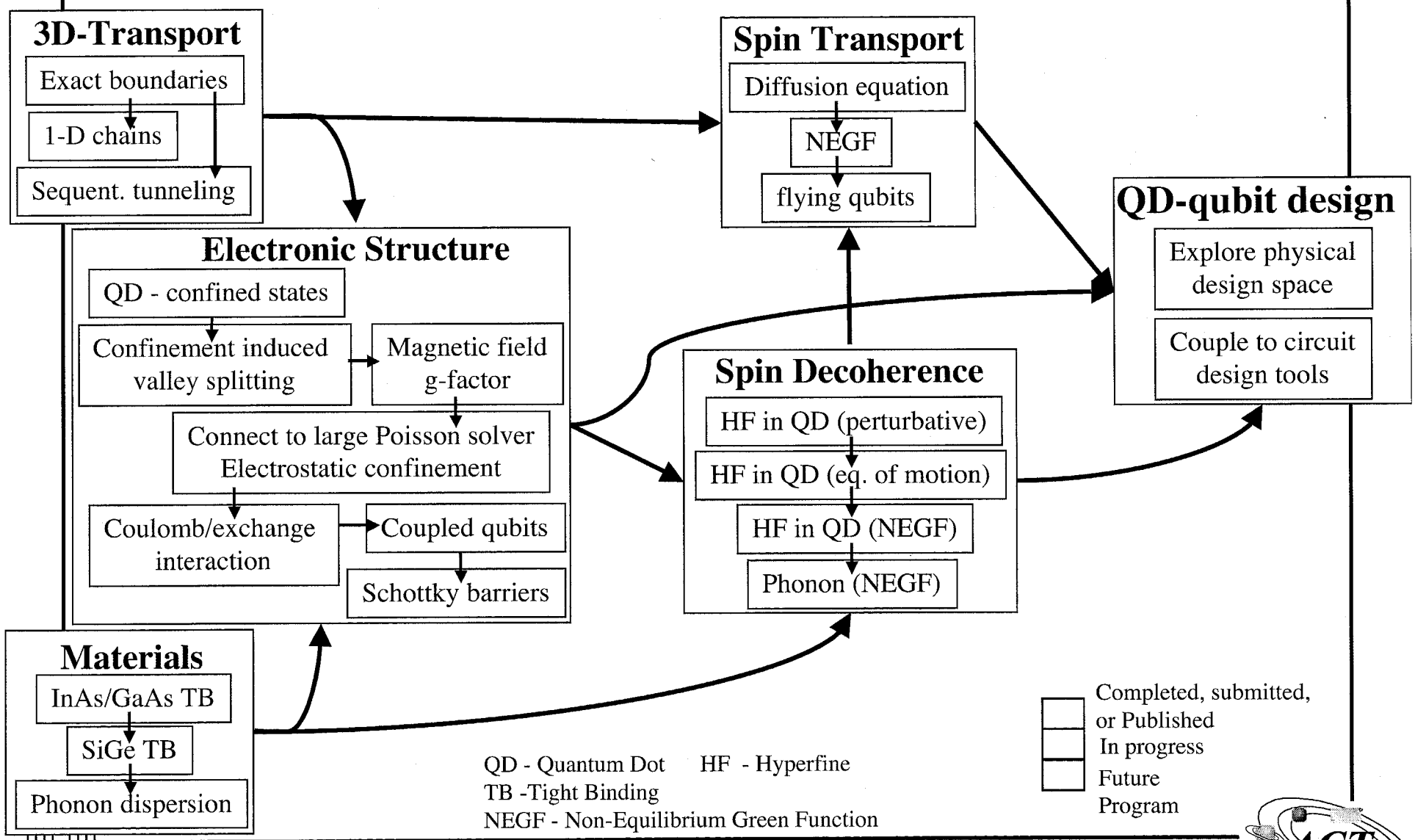
Research plan for the next 12 months

- Continue to collaborate with Wisconsin group on Si/SiGe quantum dot designs
- Continue NEGF development for spin transport.
- Estimate spin de-coherence times in systems of individual and coupled quantum dots. Compare different material systems.
- Develop and implement open boundary conditions of various approximations in NEMO 3D

Long term objectives (demonstrations)

- Demonstrate exploration of the design space of semiconductor QD-based qubit gates using realistic physics-based models.
- Aid experimentalists (like Wisconsin group) with design tool to narrow parameter space.
- Aid circuit theorists (like Colin Williams, JPL) with input to circuit design tools.

Roadmap to High Fidelity Simulation of Solid-State QC Gates 2003



QD - Quantum Dot HF - Hyperfine
TB -Tight Binding
NEGF - Non-Equilibrium Green Function

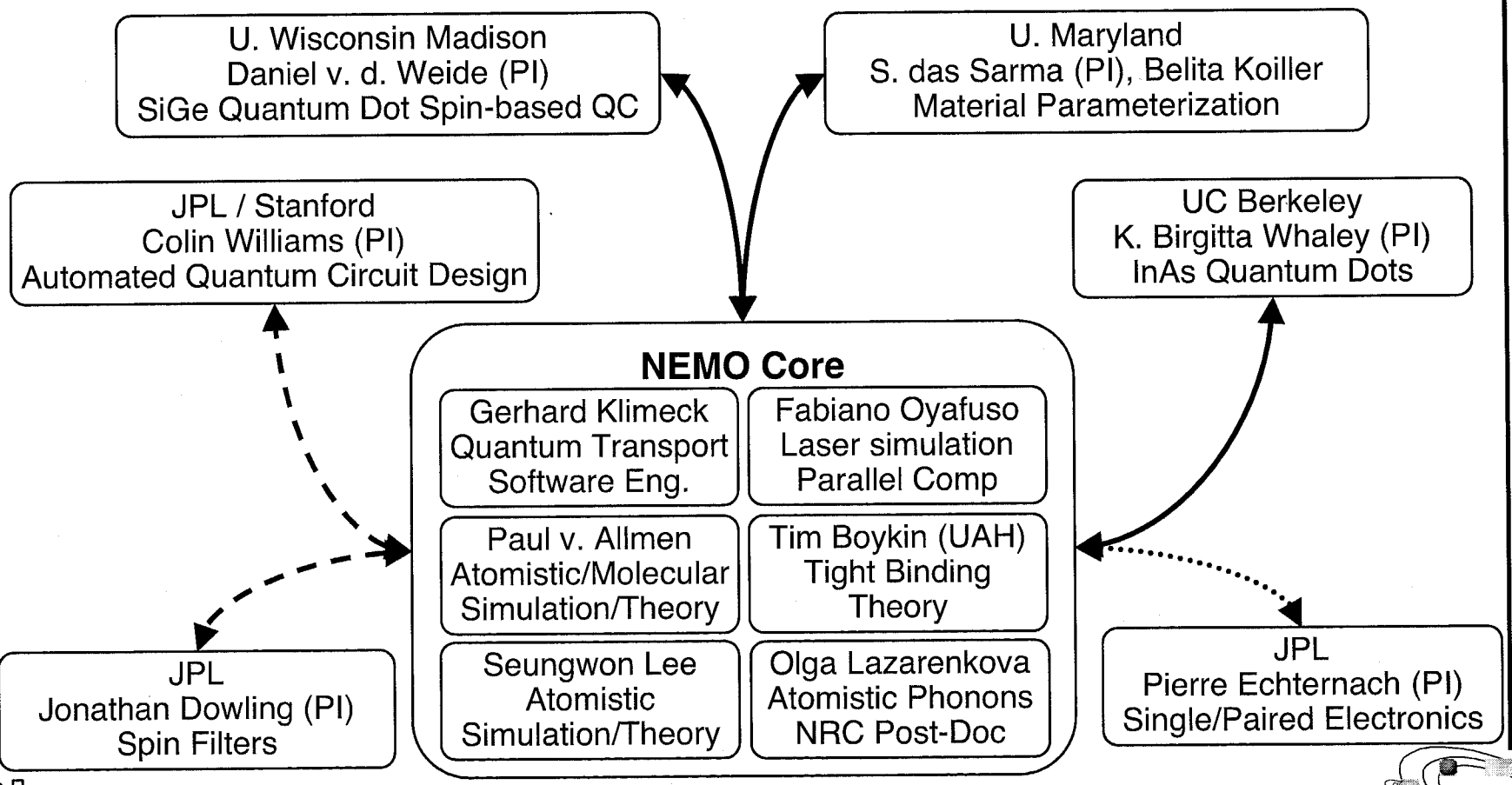
Year 1 & 2 Milestone Chart

(after 16 months of work)

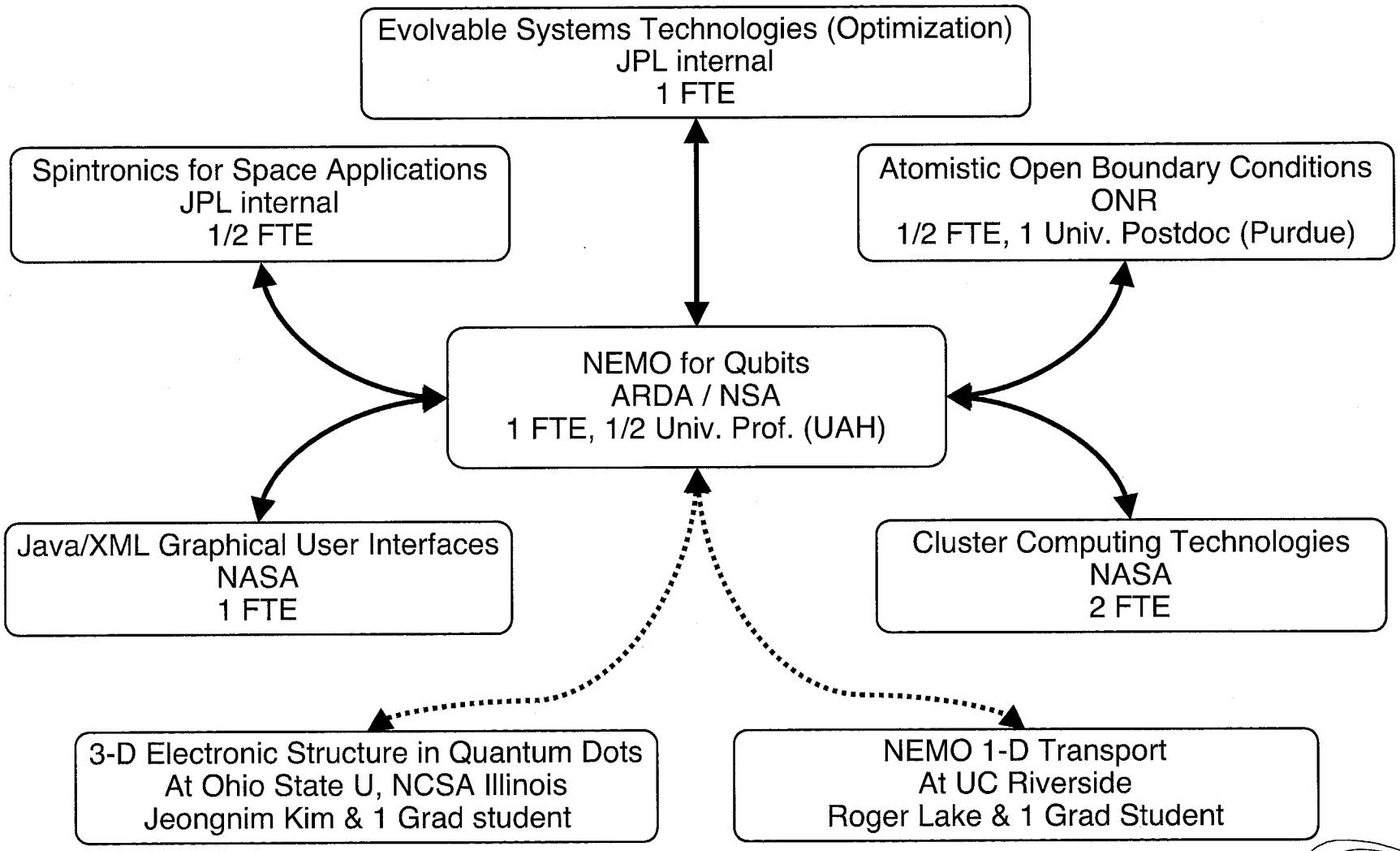
- ***Milestone 1:*** **Establish at least one collaboration with an experimental group currently funded by ARDA to model issues on their experimental device structures.**
  - Developed theory of confinement induced state splitting (to be published)
  - Simulation support for 3-D lateral quantum dot designs. Imported Wisconsin simulation data into NEMO 3-D.
- ***Milestone 2 (year 1):*** **External magnetic fields into 3-D.** (Completed)
  - Software completed, incorporated new eigenvalue solvers.
  - Study coupled quantum dots..
- ***Milestone 3 (year 1):*** **Parameterize the Si/Ge material system.**
  - 3-D alloy treatment of SiGe implemented.
  - Study of large scale quantum dots.
- ***Milestone 4 (year 1):*** **Hartree and Exchange into 3-D.**
  - Software completed.
  - Study of coupled dots.
- ***Milestone X (year 2):*** **Model spin transport in heterostructures.**
  - Simulated time dependent spin precession across semiconductor interfaces (with drift diffusion).
  - Developed non-equlibrium Green function based theory.
- ***Milestone 5 (year 2):*** **Study spin de-coherence times.**
  - Begun work on hyperfine interaction.
  - Compute phonon spectra in realistically sized atomistic system.
- ***Milestone 6 (year 2):*** **Compare different material systems.**
  - Developed GaAs/InAs and Si/Ge parameterization.
  - Study different device configurations.
- ***Milestone 7 (year 2):*** **Develop and implement open boundary conditions.**
  - Begun prototype development.
- ***Milestone 8 (year 2):*** **Magnetic impurities and spontaneous spin polarization.**
  - No work begun. After discussion with program mangement: will drop this milestone for increased support of experimental Wisconsin group.

✓ Completed
✓ In progress
✓ Eliminated with program mgmt. approval

NEMO Team and Teaming
within NSA/ARDA/ARO Quantum Computing Funding



Existing Synergistic Projects / Funding



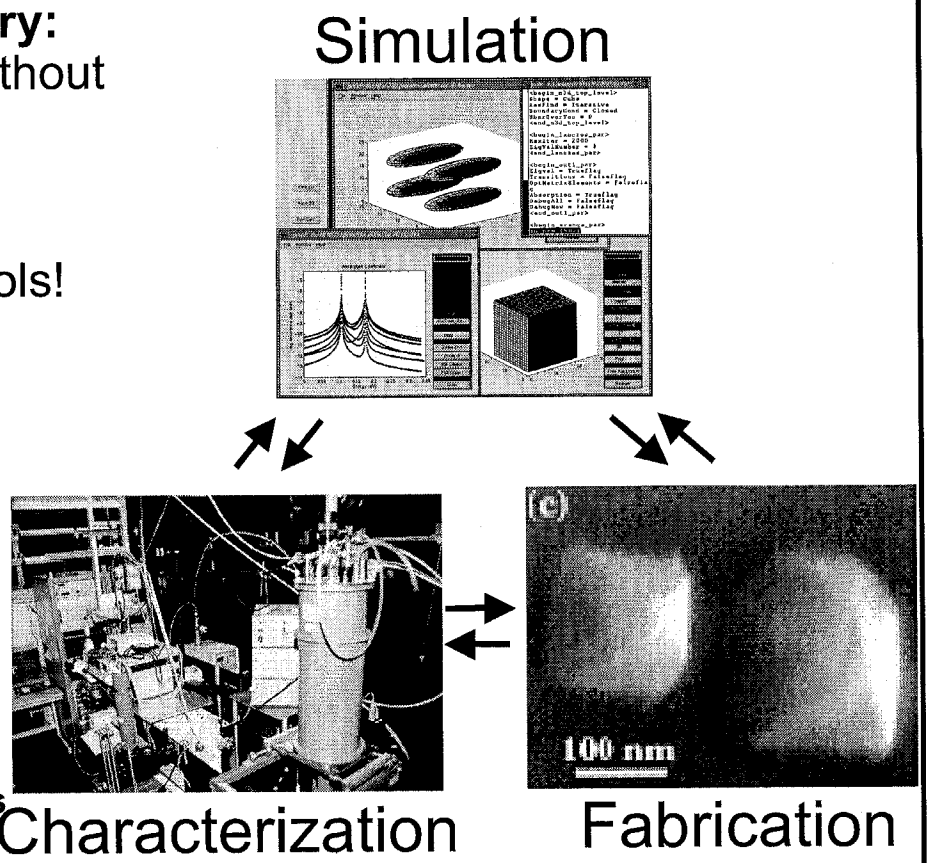
Simulation is essential for Quantum Devices

Premise:
- A scalable quantum computer will be implemented in solid state devices.

Hint from the Semiconductor Industry:
- No new devices / circuits designed without software!

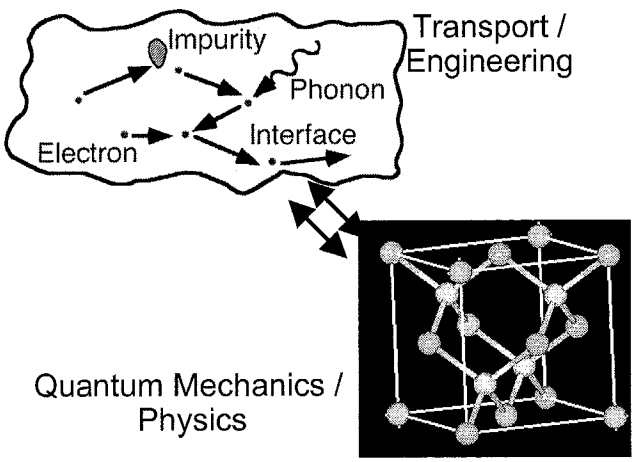
Problems:
- There are no physical qubit design tools!
- Design space is huge
  - Choice of materials, shapes, orientations, dopings, heat anneals
- Characterizations are incomplete and invasive / destructive

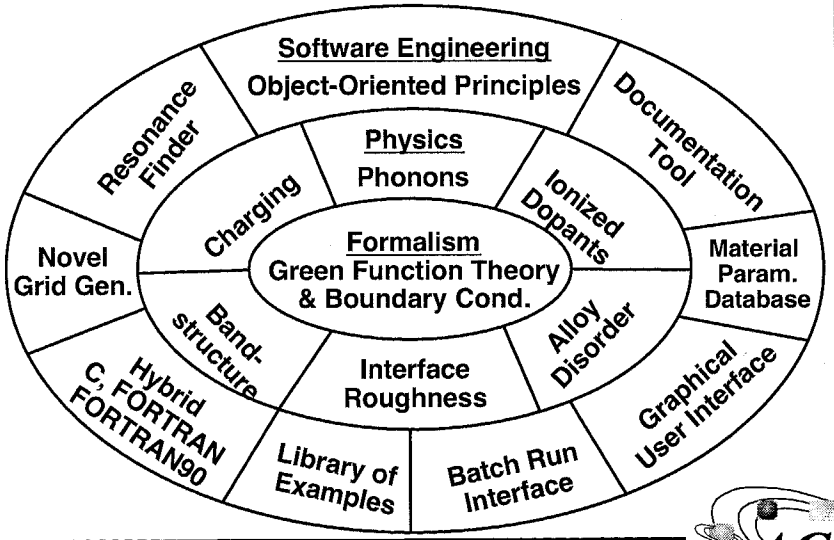
Simulation Impact:
- Aid Design. Fast, cost effective.
  -> Device performance
  already successful for 1-D quantum devices
- Aid Characterization
  - Non-invasive, More accurate
  -> Structure and doping analysis
  already successful for 1-D quantum devices



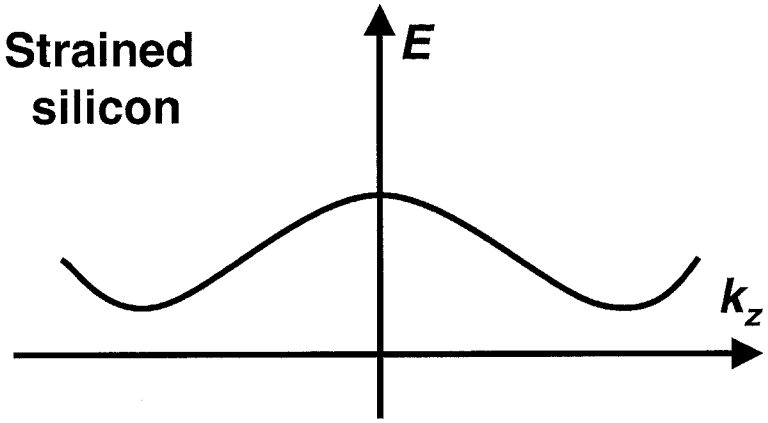
NEMO:
A User-friendly Quantum Device Design Tool

- NEMO 1-D was developed under a NSA/NRO contract to Texas Instruments and Raytheon from '93-'98 (>50,000 person hours, 250,000 lines of code).
- NEMO 1-D maintained and NEMO 3-D developed at JPL '98-'02 (>12000 person hours) under NASA funding. Since '02 NSA and ONR funding.
- NEMO is THE state-of-the-art quantum device design tool.
  - First target: transport through resonant tunneling diodes (high speed electronics).
  - Second target: electronic structure in realistically large nano devices (detectors).
  - Newly set target: qubit device simulation.
- Bridges the gap between device engineering and quantum physics.
- Based on Non-Equilibrium Green function formalism NEGF - Datta, Lake, and Klimeck.
- Used at Intel, Motorola, HP, Texas Instruments, and >10 Universities.



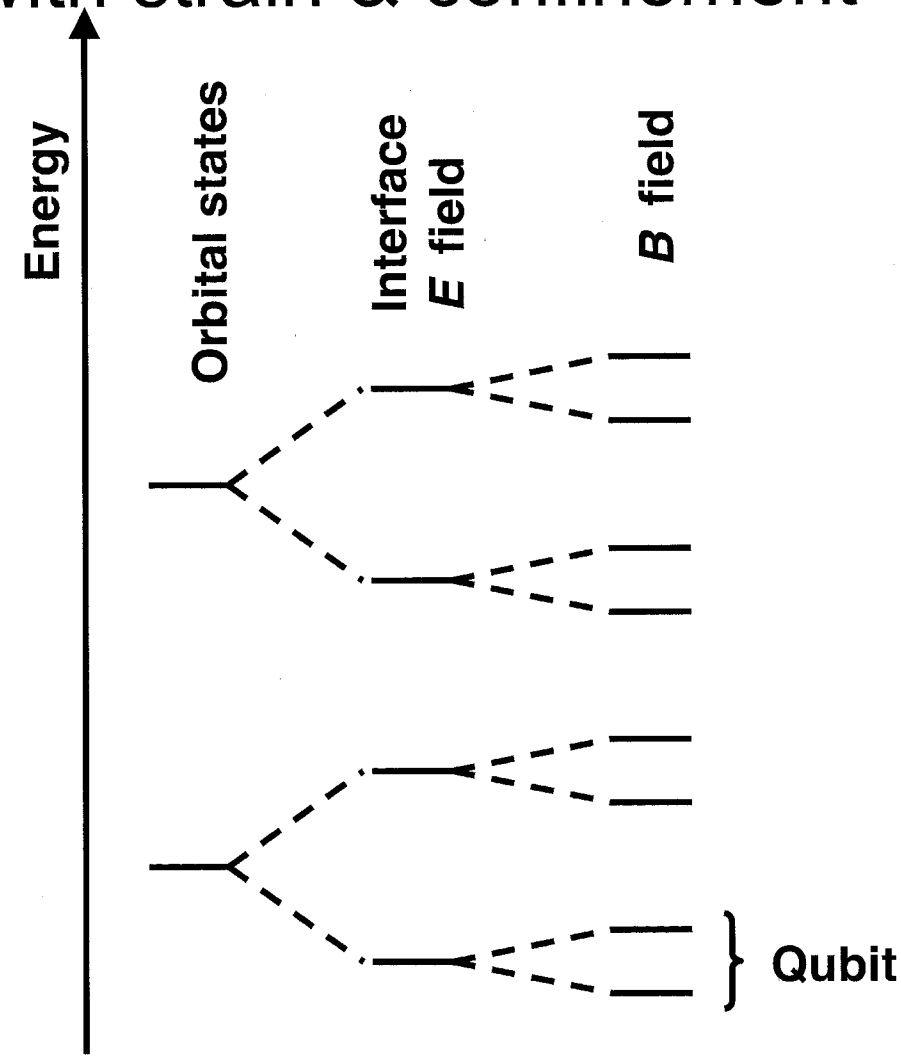


Quantum Dot Quantum Computing in Si:
Lifting Degeneracies with strain & confinement



Valley degeneracy in X direction is broken by interface and electric field

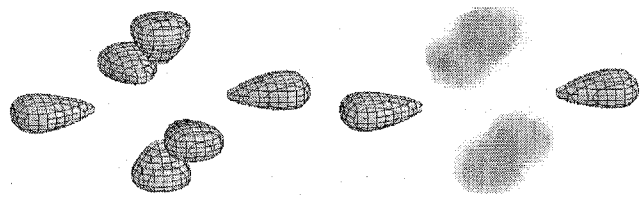
Are the qubit states separated enough from higher energy states?



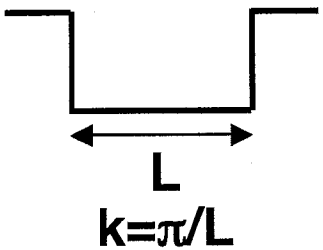
Quantum Dot Quantum Computing in Si:

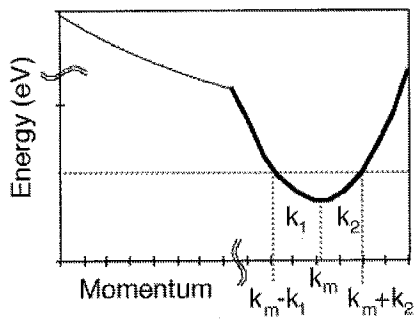
Lifting Degeneracies - strain & confinement

- **Bi-axial strain on Si.** **Lifting 4 of the 6 degenerate valleys ΔE>100meV**



- **Confinement in 1D:** **Valley Splitting ΔE~1meV**





4 propagating states

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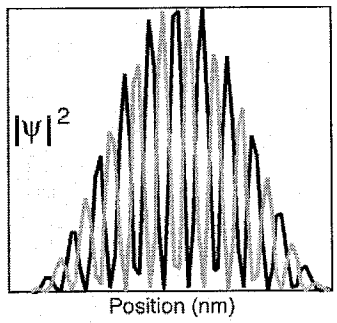
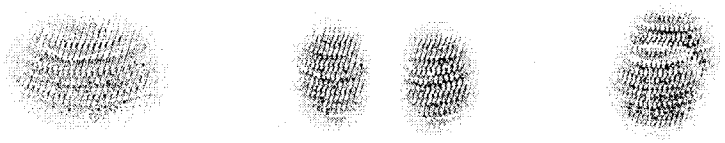
2 bound states
$k_{1/2}$ envelope
k_m fast oscillations



- **Confinement in 3D:** **(1D heterostr. & 2D lat gates & mag. field) ΔE~0.1meV**



Magnetic-Field Effects on Confined States

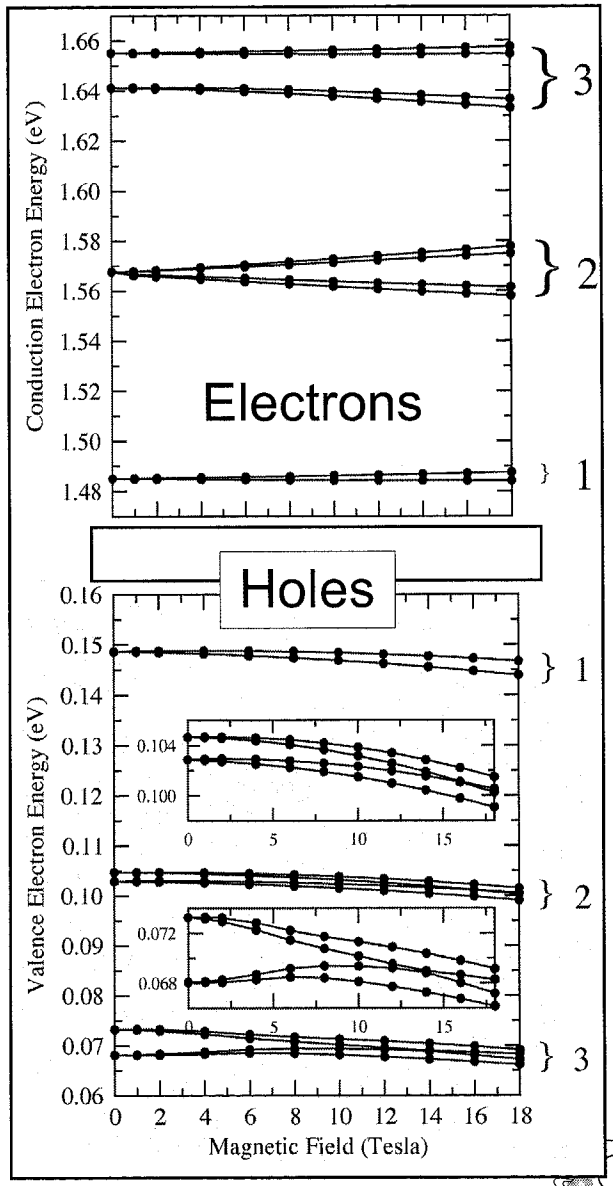
- Study InAs/GaAs QDs
- Zeeman Interaction splits the levels into spin-up and -down levels.
- Effective g-factor ($g^* = (E_\uparrow - E_\downarrow)/\mu_B B$)

Electrons:

- g* ranges from 2 to 3.5.
- InAs dot g* is very different from g* of InAs bulk (-15).
- Experimental measurements report g*=0.5-1.6 for InAs dots. [Thornton et al., Appl. Phys. Lett. **73**, 354 (1999)]

Holes:

- Zeeman interaction splits hole levels into Jz = 3/2 and - 3/2 levels.
- Zeeman interaction couples closely-spaced hole levels.
- g* varies from 0.65 to 2.66



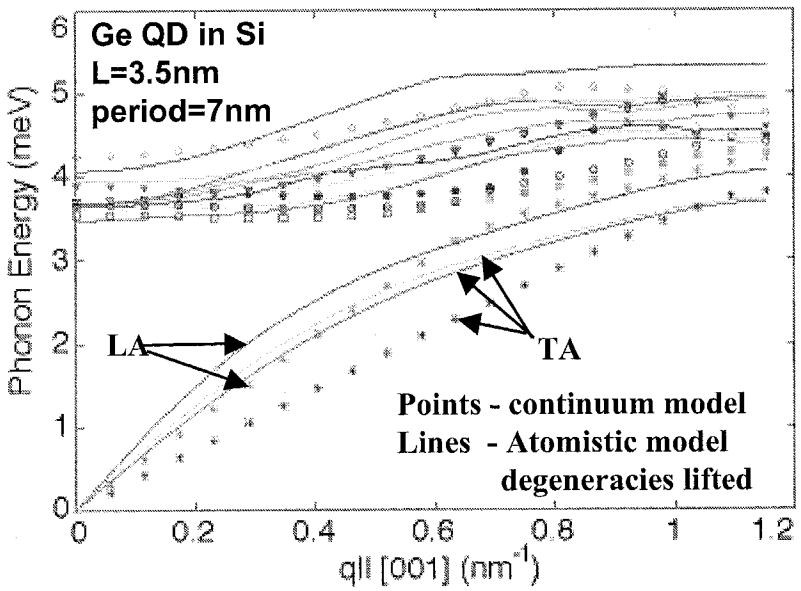
Phonon Spectra based on Atomistic Simulations

Objective:

- Calculate atomic vibration (phonon) spectrum of nanostructures

Problem / Motivation:

- Decoherence mechanism.
- Effects on thermal and electronic conductivity.
- Creation of nano-coolers and high efficient thermoelectric generators



Approach:

- Compute phonon spectrum within atomistic Keating model in NEMO 3-D
- Realistically extended structure.
- Including strain.

Status:

- The serial version implemented in NEMO 3-D
- Tests on bulk Si and Ge phonon dispersions
- Comparison of atomistic and continuum approaches for phonon spectra of QDs arrays
- Studied effect of strain
- Continuum theory breakdown for even number of monolayers (T_d symmetry), atomic model handles O_d and T_d symmetry)

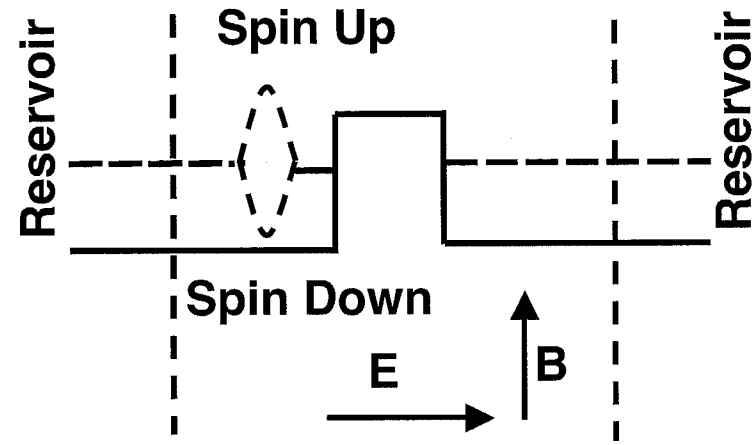
Spin Dynamics and Spin Transport with Non Equilibrium Green Functions

Objective

- Simulate spin transport across interfaces
- Simulate spin transport between qubits

Challenge

- Simulate spin transport on equal footing with spin relaxation, decoherence and precession



Approach

- Non equilibrium Green function formalism
- Extend NEMO to fully time dependent problems including magnetic field and spin relaxation and decoherence

Status

Established formalism for non-equilibrium transport with spin precession in magnetic field

$$G_{00}^{<0}(t,t') = g_{00}^{<0}(t-t')M^{<}(t,t')$$

$g_{00}^{<0}(t-t')$ Spinless Surface Green Function

$$M^{<}(t,t') = \begin{pmatrix} \cos\frac{\omega_L t}{2}\cos\frac{\omega_L t'}{2} & -i\cos\frac{\omega_L t}{2}\sin\frac{\omega_L t'}{2} \\ i\sin\frac{\omega_L t}{2}\cos\frac{\omega_L t'}{2} & \sin\frac{\omega_L t}{2}\sin\frac{\omega_L t'}{2} \end{pmatrix}$$

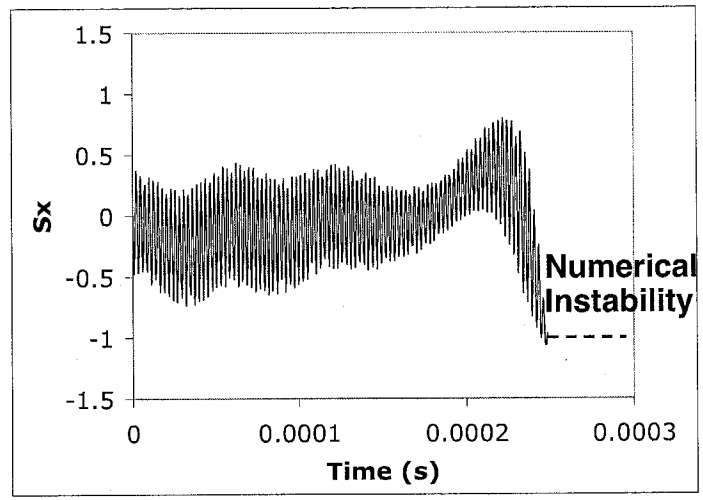
Hyperfine Interaction Induced Electron Spin Decoherence

Objective

Simulate electron spin decoherence due to hyperfine interaction with nuclei.

Challenge

1. Overcome divergence in second order perturbation term *(A. Khaetskii, D. Loss and L. Glazman, PRB 67, 195329, 2003).*
2. Include external magnetic field.



Approach

Explicit solution of the equations of motion for the average electronic and nuclear spins and for the correlation functions.

Hyperfine Hamiltonian

$$H_{HF} = \sum_j A_j S \cdot I_j$$

$$A_j = \frac{2}{3}\mu_0 \gamma_e \gamma_N \left|\psi(R_j)\right|^2$$

$$\partial_t \langle S_\alpha \rangle = -\sum_{j=1}^{N} A_j \varepsilon_{\alpha\beta\gamma} \langle S_\beta I_{j\gamma} \rangle$$

$$\partial_t \langle I_{j\alpha} \rangle = -A_j \varepsilon_{\alpha\beta\gamma} \langle I_{j\beta} S_\gamma \rangle$$

$$\partial_t \langle S_\alpha I_{n\alpha'} \rangle = -\sum_{j=1}^{N} A_j \varepsilon_{\alpha\beta\gamma} \langle S_\beta I_{j\gamma} I_{n\alpha'} \rangle - A_j \varepsilon_{\alpha'\beta\gamma} \langle S_\alpha I_{j\beta} S_\gamma \rangle$$

Collaborations -> Impact on Quantum Computing

We are here to learn!

U. Wisconsin Madison
Daniel v. d. Weide (PI)
SiGe Quantum Dot Spin-based QC

U. Maryland
S. das Sarma (PI), Belita Koiller
Material Parameterization

JPL / Stanford
Colin Williams (PI)
Automated Quantum Circuit Design

UC Berkeley
K. Birgitta Whaley (PI)
InAs Quantum Dots

NEMO Core

Gerhard Klimeck
Quantum Transport
Software Eng.

Fabiano Oyafuso
Laser simulation
Parallel Comp

Paul v. Allmen
Atomistic/Molecular
Simulation/Theory

Tim Boykin (UAH)
Tight Binding
Theory

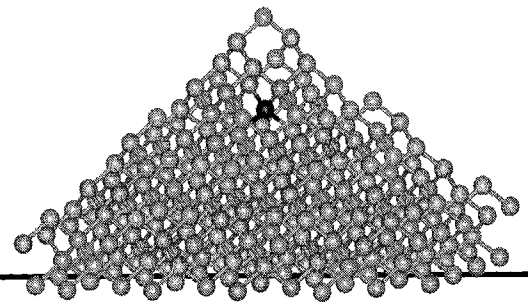
Seungwon Lee
Atomistic
Simulation/Theory

Olga Lazarenkova
Atomistic Phonons
NRC Post-Doc

JPL
Jonathan Dowling (PI)
Spin Filters

JPL
Pierre Echternach (PI)
Single/Paired Electronics

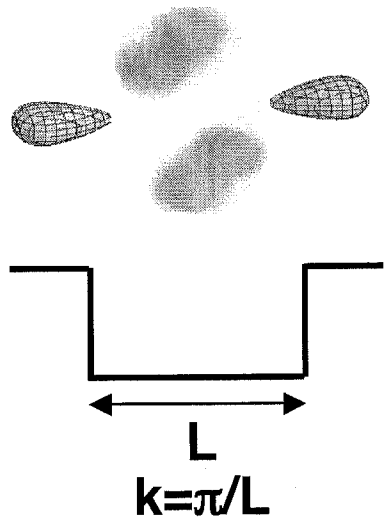
Single Electron
Spintronics

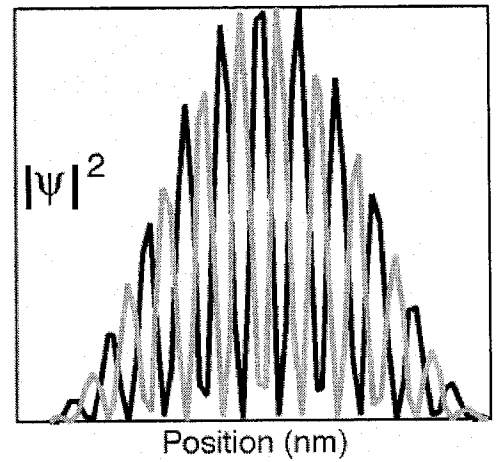


Single Nucleus
Spintronics

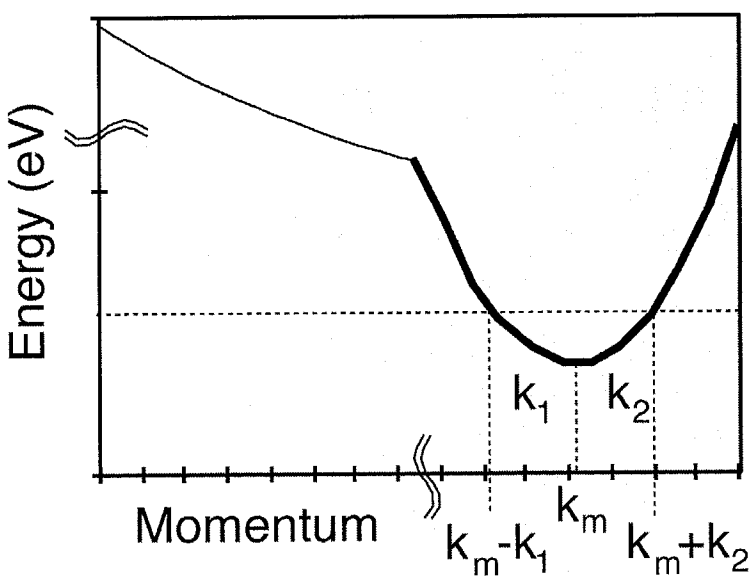
Backup

1D Confinement Creates Valley Splitting:





Valley Splitting ΔE~1meV



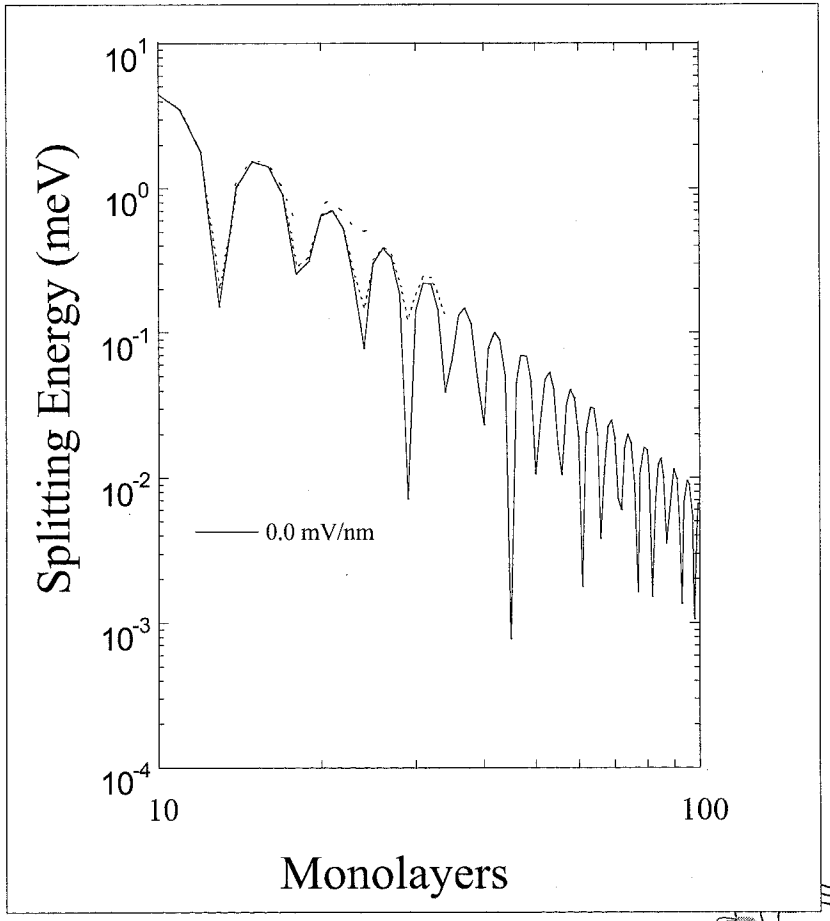
4 propagating states

↓

2 bound states
$k_{1,2}$ envelope
k_m fast oscillations

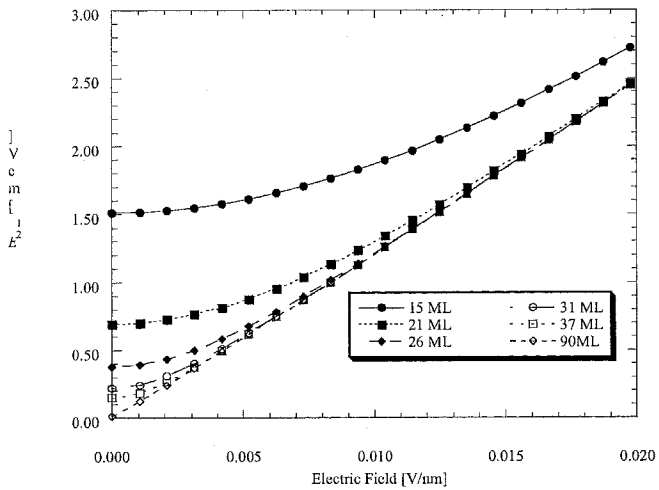
Splitting Behavior With Quantum Well Width

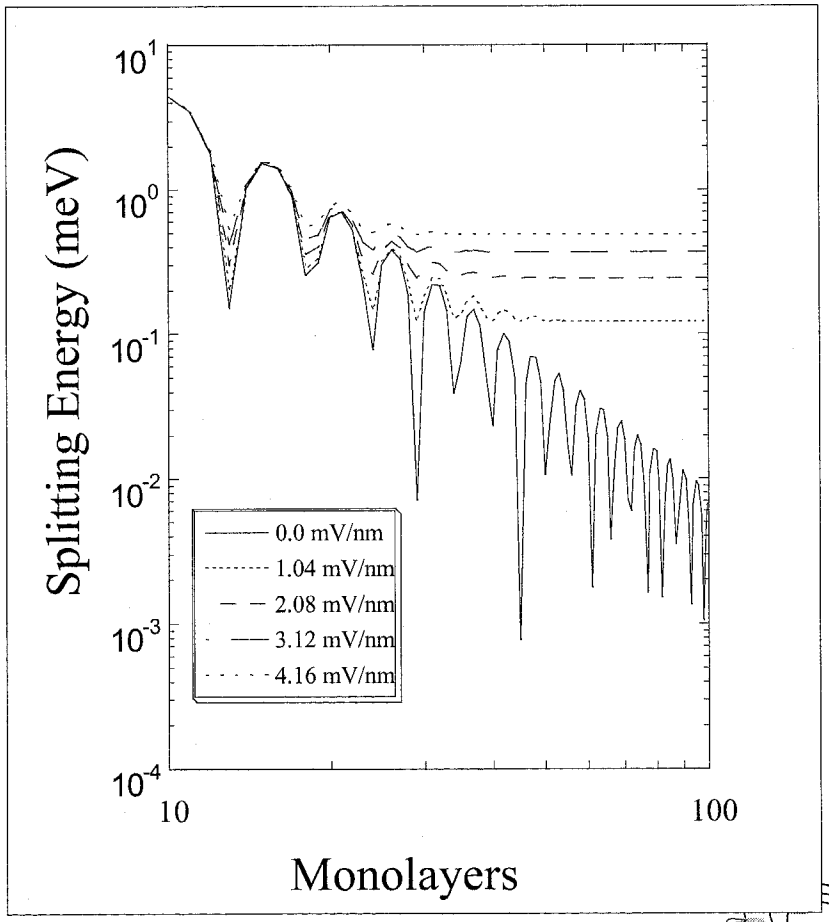
- Strained Si QW, Hardwall BCs
- Oscillations with Monolayers (decay as ML^{-3})



Splitting Behavior With Quantum Well Width and Electric Field

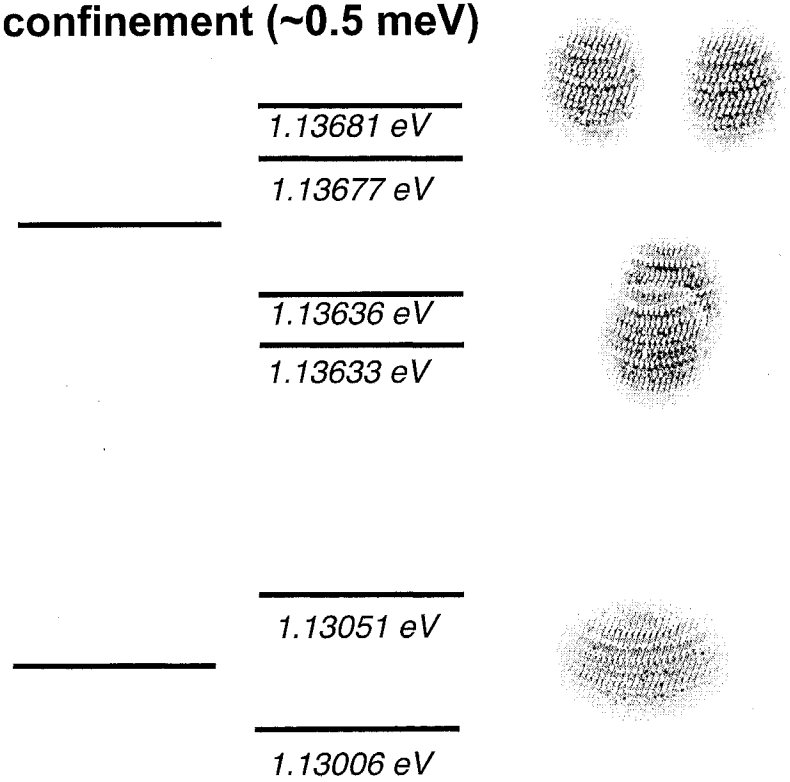
- Strained Si QW, Hardwall BCs
- Oscillations with Monolayers
- Oscillations decay with increasing Field
- Decay significant once drop/ML is of order zero-field splitting
- For fixed *L*, splitting linear at high field, nonlinear at low field



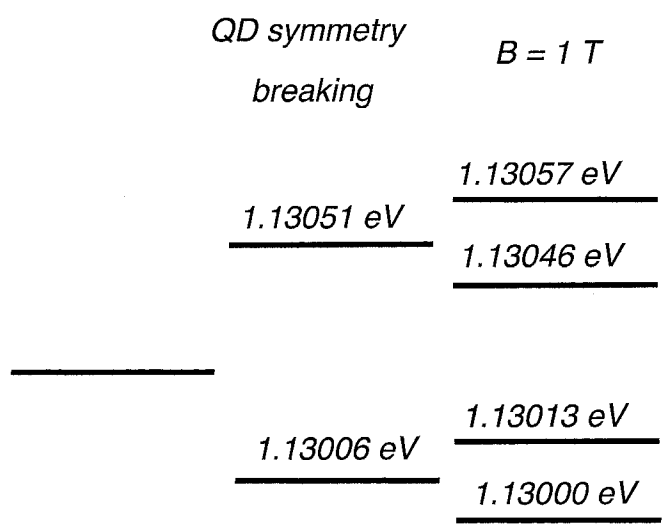


Relative Size of State Splitting
3-D Electronic structure of low-lying states

- Valley splitting due to breaking of translational invariance is typically smaller than splitting due to confinement (~0.5 meV)

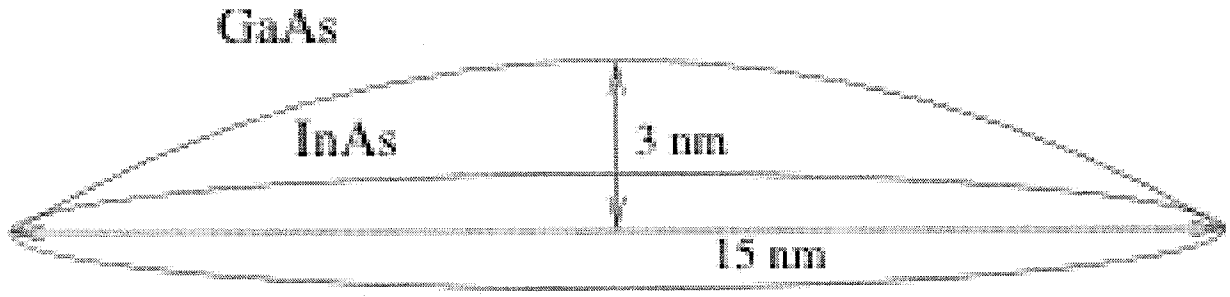


- Even with a large B=1.0T, Zeeman splitting is much smaller than valley splitting (~0.12 meV).



Model for InAs self-assembled dot

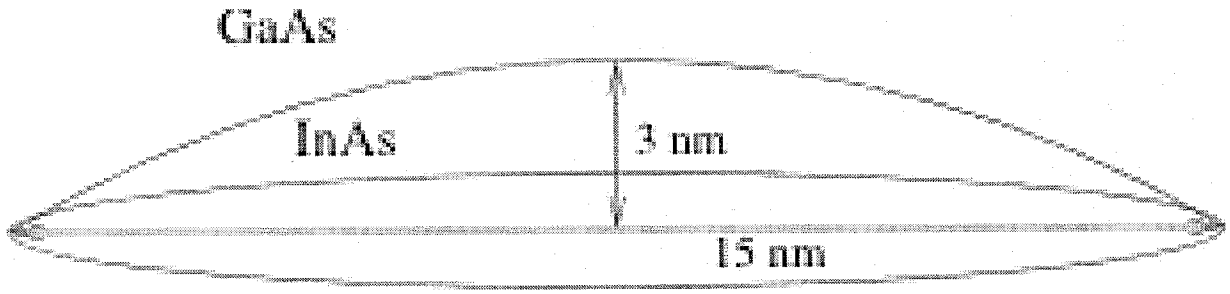
- **System geometry**



- **Strain profile model:** Atomic elasticity model
  [P. N. Keating, Phys. Rev. B **145**, 637 (1966)]
  Strain energy as a function of bond length and bond angle.
  GaAs strained buffer is 15nm in all directions (total of 2,764,600 atoms).
- **Electronic structure model:** Tight-binding Hamiltonian
  Basis orbitals: sp^3d^5 s*, parameters generated by a genetic algorithm.
  Matrix Size : 2,090,880 = 104,544 atoms X 10 basis orbitals X 2 spins
- **Eigenvalue solver:** Arnoldi method with PARPACK
  Computation on a Beowulf cluster with 30 nodes.
  Currently memory limited, in process of system upgrade right now.

Model for InAs self-assembled dot

- **System geometry**



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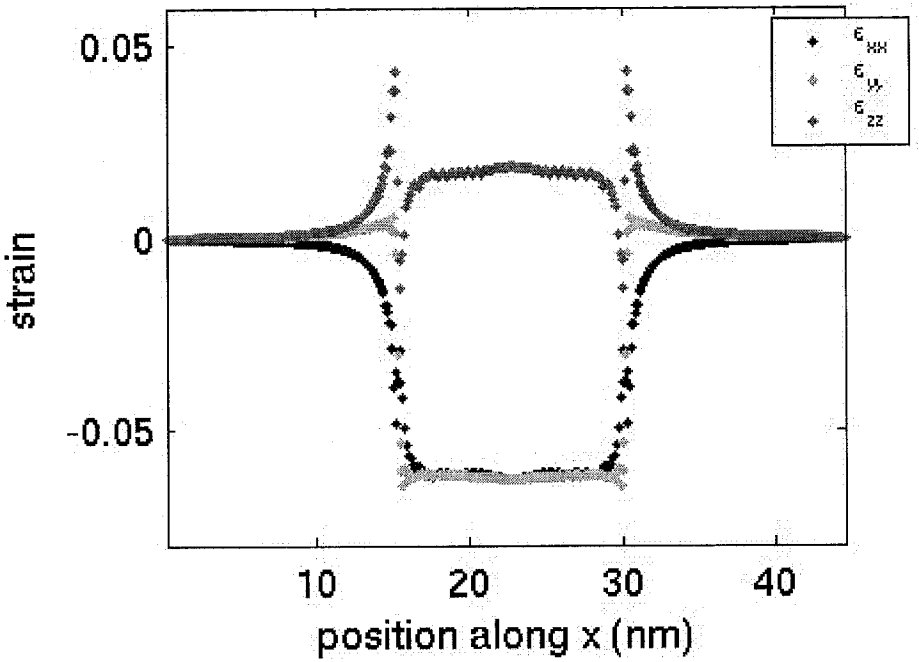


Strain Profile

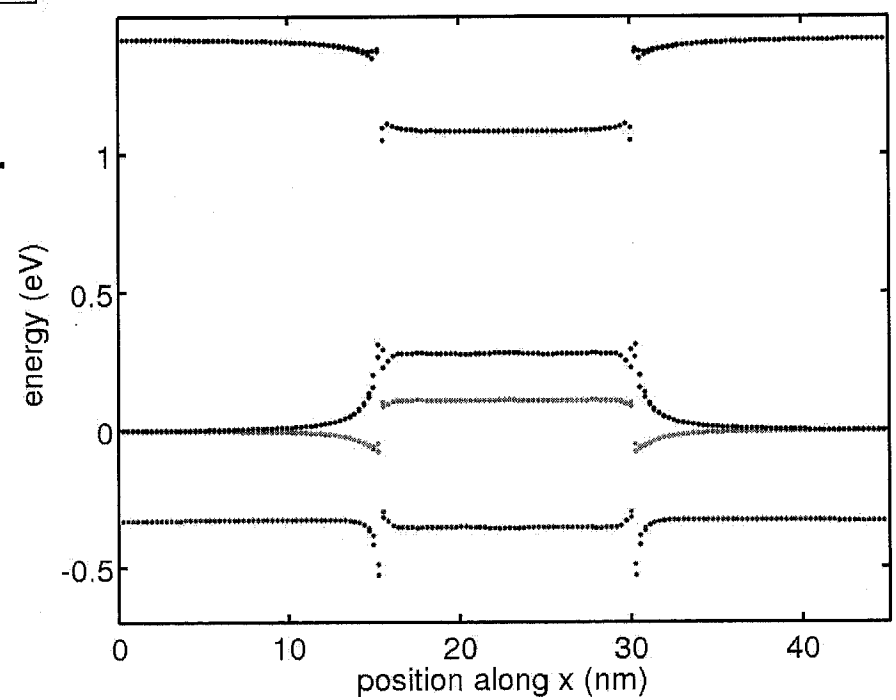
Inside InAs dot,

- Compressive strain in x-y plane.
- Stretching strain in growth direction.

Band Profile

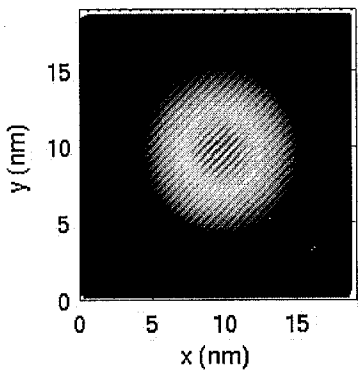
Inside InAs dot,

- Conduction-band edge shifts up from 0.6 eV to 1.1 eV.
- Valence-band edge shifts up from 0.22 eV to 0.28 eV.
- Strain splits heavy-hole and light-hole bands by 0.17 eV.

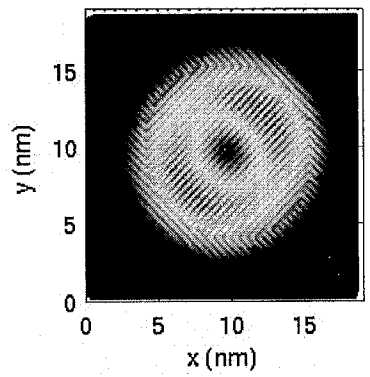


Charge Distribution of Electron and Hole States

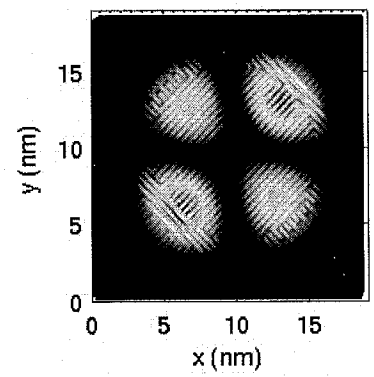
1st Electron (L=0)



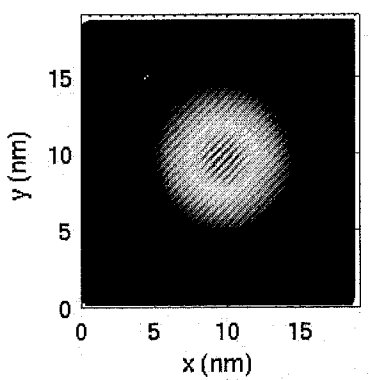
2nd Electron (L=1)



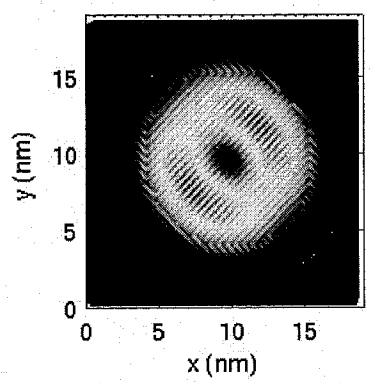
3rd Electron (L=2)



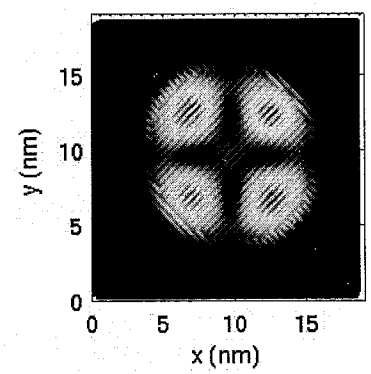
1st Hole (L=0)



2nd Hole (L=1)

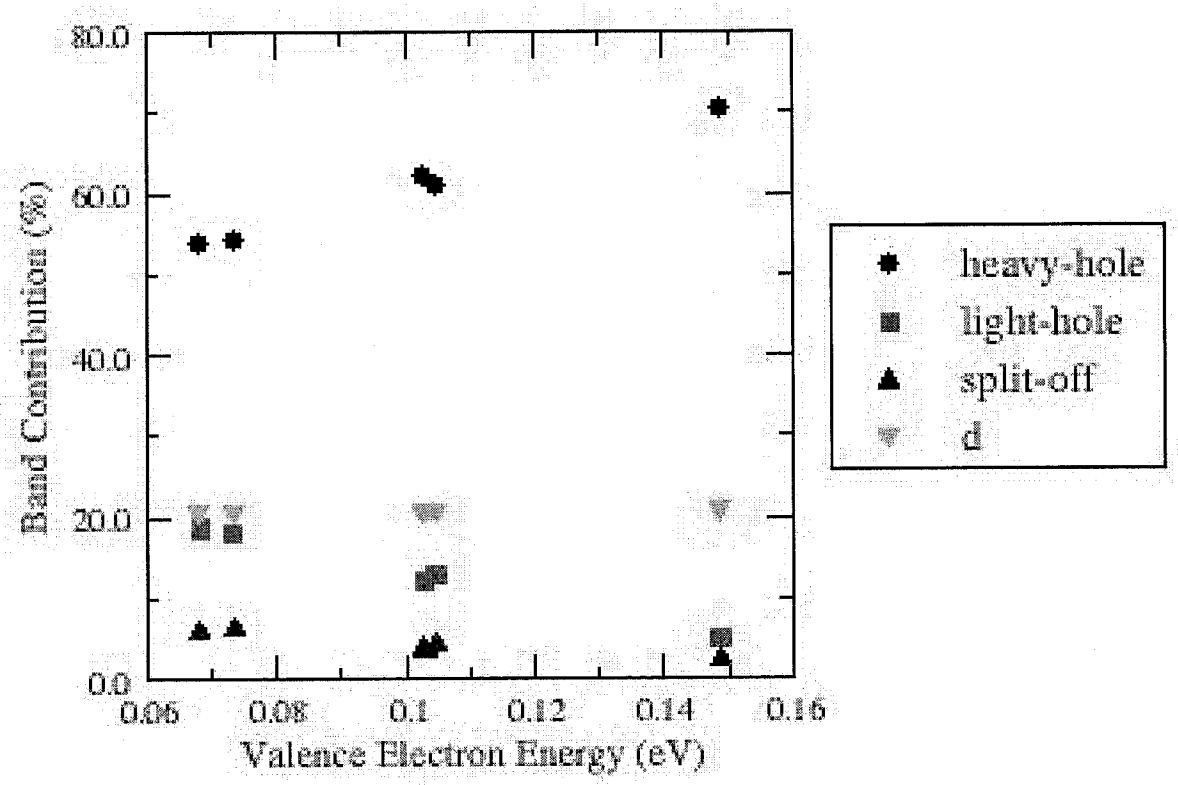


3rd Hole (L=2)



Band Origin of Hole Levels

- The lowest hole level is mainly from heavy-hole and d bands.
- Light-hole band contribution increases as the hole energy increases.
- d-band contribution is constant ~20%.



Tight-binding model for magneto-optical response

- **Gauge-invariant modification of tight-binding Hamiltonian**
  [M. Graf and P. Vogl , Phys. Rev. B **51**, 4940 (1995)]

$$\varepsilon_i = \varepsilon_i^0 + \mu_B B \cdot \sigma$$ **Onsite interaction**

$$t_{ij} = t_{ij}^0 \exp\left(-\frac{ie}{\hbar c}\int_{R_j}^{R_i} A \cdot dr\right)$$ **Nearest-neighbor interaction**

- **Absorption rate between conduction and valence levels**
  [S. Lee et al., Phys. Rev. B **66**, 235307 (2002)]

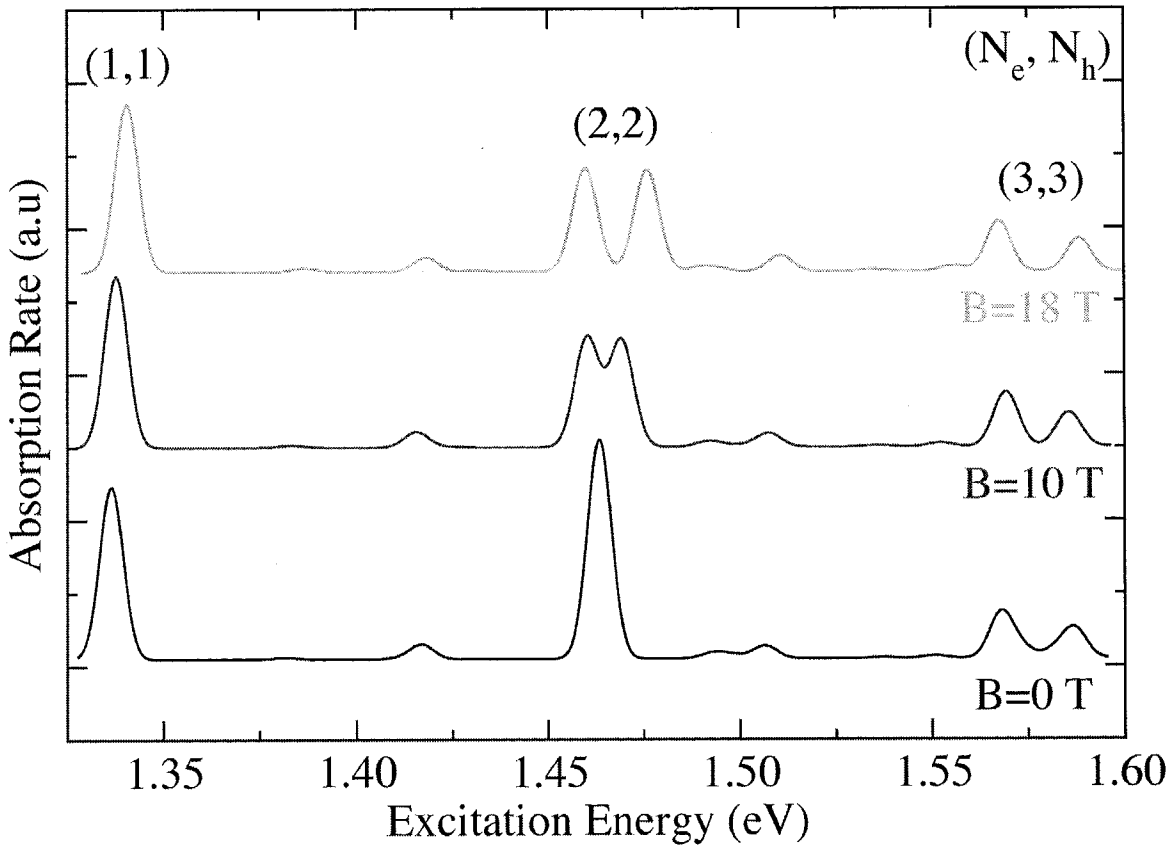
$$\Gamma(E) = \frac{2\pi}{\hbar}\left|\langle c \mid \hat{r} \mid v\rangle\right|^2 \delta(E_c - E_v - E)$$

$$\langle c|\hat{r}|v\rangle = \sum_{ij} c_j^* v_i \left[\hat{r}_i \delta_{ij} + \langle j|\delta\hat{r}_i|i\rangle\right]$$

Magneto-Optical Response

- Selective dipole coupling between electron and hole levels.
- The selectivity remains intact even at a high magnetic field.

$$\Delta L = 0 \;\&\; \Delta j = 1$$



Hyperfine Interaction

Hyperfine Hamiltonian

$$H_{HF} = \frac{16\pi}{3}\sum_j \mu_B \mu_j \delta(r - R_j)(I_j \cdot S)$$

$$= \frac{16\pi}{3}\sum_j \mu_B \mu_j \left|\Psi(R_j)\right|^2 (I_j \cdot S)$$

$$= \sum_j A_j I_j \cdot S \equiv g_e \mu_B B_N \cdot S$$

Hyperfine coupling constant

$$A_j = \frac{16\pi}{3}\mu_B \mu_j \left|\Psi(R_j)\right|^2$$

Effective nuclear magnetic field

$$B_N = \frac{1}{g_e \mu_B}\sum_j A_j I_j$$

Electron precession frequency

$$\omega_e = g_e \mu_B B_N / \hbar$$

$$= \sum_j A_j I_j / \hbar$$

Nuclear precession frequency

$$\omega_j = A_j S / \hbar$$

Spin Dephasing in an Ensemble of Dots

- Effective nuclear magnetic field (B_N) is randomly distributed.
- Electron spin of each dot precesses with different ω_e.
- This leads to ensemble average spin dephasing.

$$T_2^* \sim 1/\sqrt{\langle \omega_e^2 \rangle}$$

Spin Decoherence in a Single Dot

- Hyperfine coupling constant (A_j) is non-uniform.
- Each nuclear spin precesses with different frequency ω_j.
- This leads to electron spin decoherence.

$$T_2 \sim 1/\sqrt{\langle \omega_j^2 \rangle}$$

Electron Spin Correlator

Hamiltonian with external magnetic field and nuclear hyperfine field

$$H = g_e \mu_B B \cdot S + \sum_j A_j I_j \cdot S = g_e \mu_B (B + B_N) \cdot S$$

$$= g_e \mu_B (B_z + B_{Nz}) S + \frac{1}{2} \sum_j A_j (I_j^+ S^- + I_j^- S^+)$$

$$= \hbar \omega_e S + \sum_j \hbar \omega_j (I_j^+ S^- + I_j^- S^+)$$

Electron and nuclear state

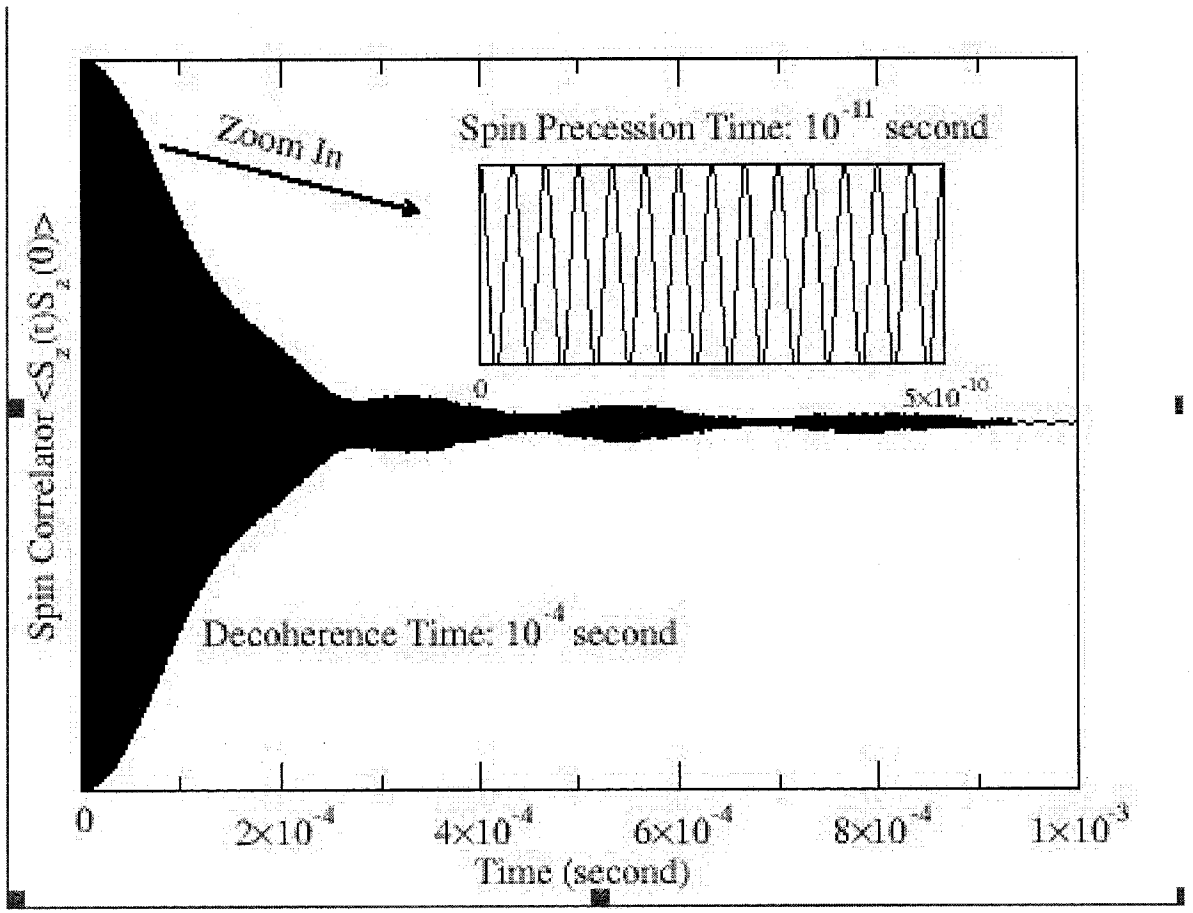
$$\left|\Psi(t)\right\rangle \approx \left|\Uparrow_e, \{I_{jz}\}\right\rangle - \sum_j \frac{\omega_j}{\omega_e + \omega_j} \left(1 - e^{-i(\omega_e t + \omega_j t)}\right) I_j^+ \left|\Downarrow_e, \{I_{jz}\}\right\rangle$$

Electron spin correlator

$$\left\langle \Psi(t) \middle| S_z(t) S_z(0) \middle| \Psi(t) \right\rangle = \frac{1}{4} \left[1 - \sum_j \frac{2\omega_j^{\,2}}{(\omega_e + \omega_j)^2} (1 - \cos(\omega_e t + \omega_j t)) \left\langle \{I_{jz}\} \middle| I_j^- I_j^+ \middle| \{I_{jz}\} \right\rangle \right]$$

Electron Spin Decoherence and Dephasing

- Electron precession time $T_p \sim 10^{-11}$ s with B=1 T.
- Electron spin decoherence time $T_2 \sim 10^{-4}$ s.
- Electron spin dephasing time $T_2^* \sim 10^{-8}$ s.



Summary

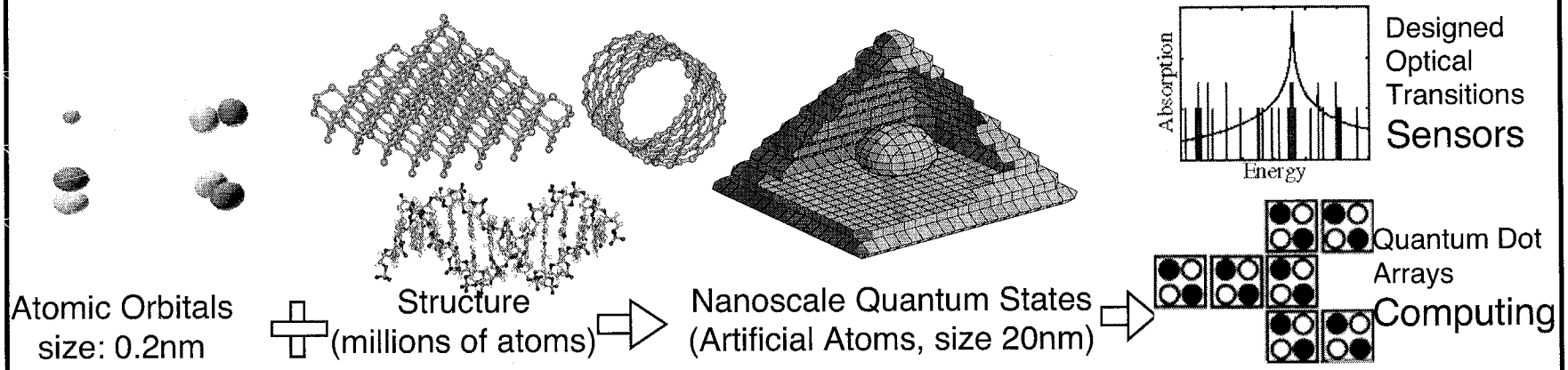
Theoretical Approach

- ✓ Nearest-neighbor $sp^3d^5s^*$ tight-binding model for electronic structure.
- ✓ Atomic elasticity model (Keating Model) for strain.
- ✓ Spin correlator for electron spin decoherence.

Main Results

- ✓ Inside the dot, strain shifts up conduction-band edge and splits heavy- and light-hole bands.
- ✓ Effective electron g-factors are between 2 and 3.5.
- ✓ Magnetic field couples closely-spaced hole levels.
- ✓ Dipole interaction selectively couples electron and hole levels, and the selective coupling remains intact even at high magnetic fields.
- ✓ Nuclear hyperfine interaction leads to $T_2 = 10^{-4}$ s and $T_2^* = 10^{-8}$ s.

NEMO: Nanoelectronic Modeling Agenda



Problem:

Nanoscale device simulation requirements:

- Cannot use bulk / jellium descriptions, need description of the material atom by atom => use pseudo-potential or local orbitals
- Consider finite extent, not infinitely periodic => local orbital approach
- Need at minimum one million atoms. => need massively parallel computers
- The design space is huge: choice of materials, compositions, doping, size, shape.
  => **need a design tool**

Approach:

- Leverage NEMO 1-D:
  - 25 person years at TI / Raytheon
  - 250,000 lines of code.
- Use local orbital description for individual atoms in arbitrary crystal / bonding conf.
  - Use s, p, and d orbitals
  - Use genetic algorithm for fitting
- Compute mechanical strain in the system.
- Develop parallel algorithms to generate eigenvalues/vectors of very large matrices ($N=3.2\times10^8$ for a 16 million atom system).
- Develop prototype GUI for (NEMO-3D)

Tight Binding Material Parameterization

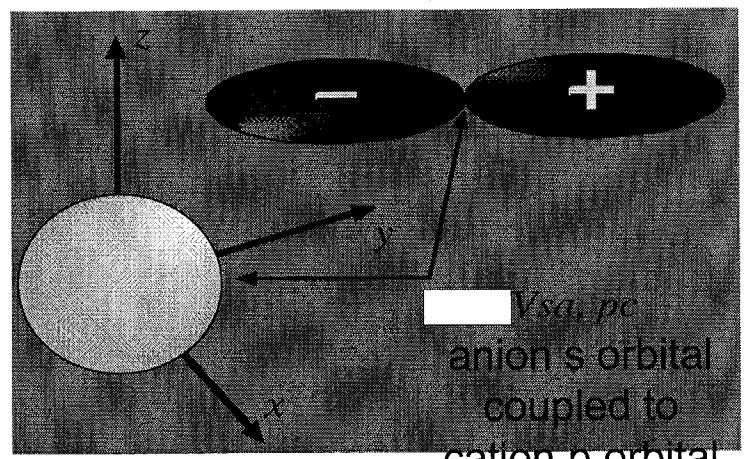
Bulk Semiconductors are described by:
- Conduction and valence bands, bandgaps (direct, indirect), effective masses
- 10-30 physically measurable quantities

Tight Binding Models are described by:
- Orbital interaction energies.
- 15-30 theoretical parameters

Analytical approach:
- Exact diagonalization at Γ for $sp^3d^5s^*$
- Formulas developed by Tim Boykin at UAH for effective masses and bandgaps from interaction energies

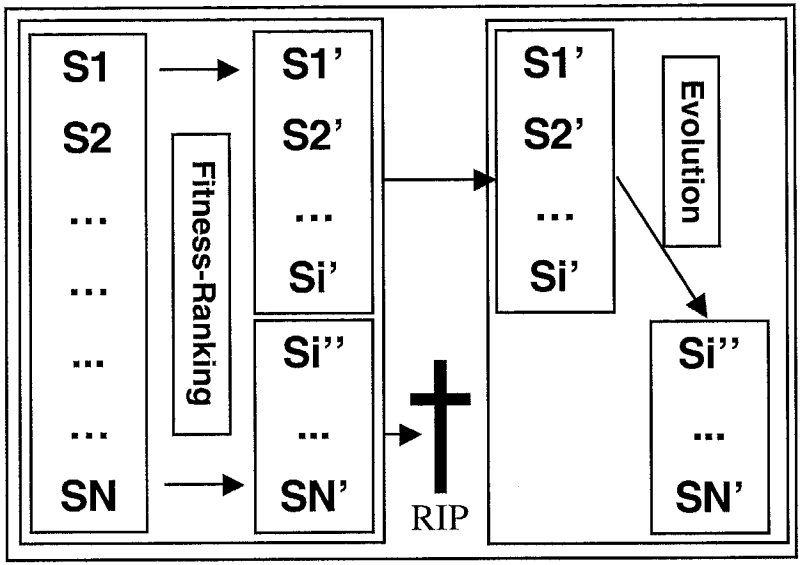
Numerical approach:
- Use a genetic algorithm to do fitting.

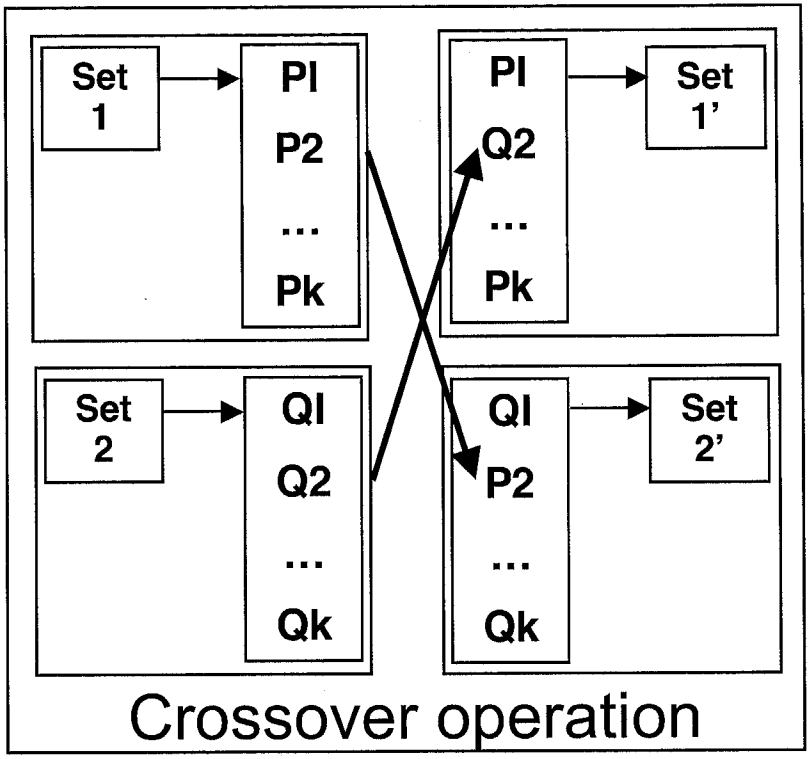
- Match experimental data in various electron transport areas of the Brillouin zone:
  - Effective masses of electrons at Γ, X and L
  - Effective masses of holes at Γ
  - Band edges at Γ, X and L

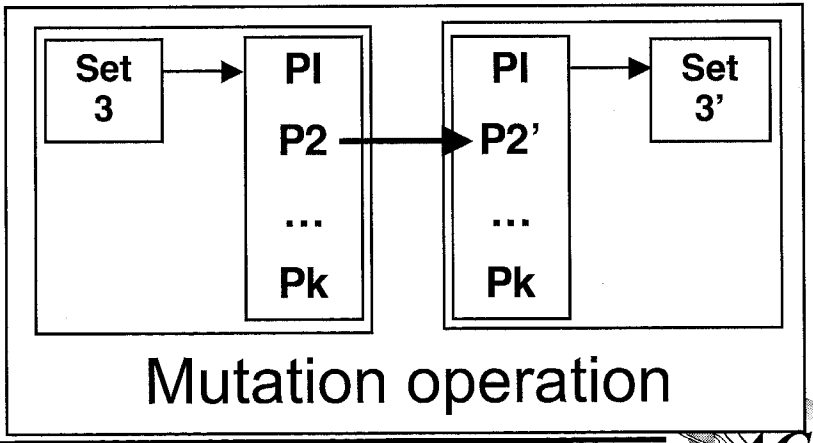


15-30 theoretical interaction energies

Genetic Algorithm





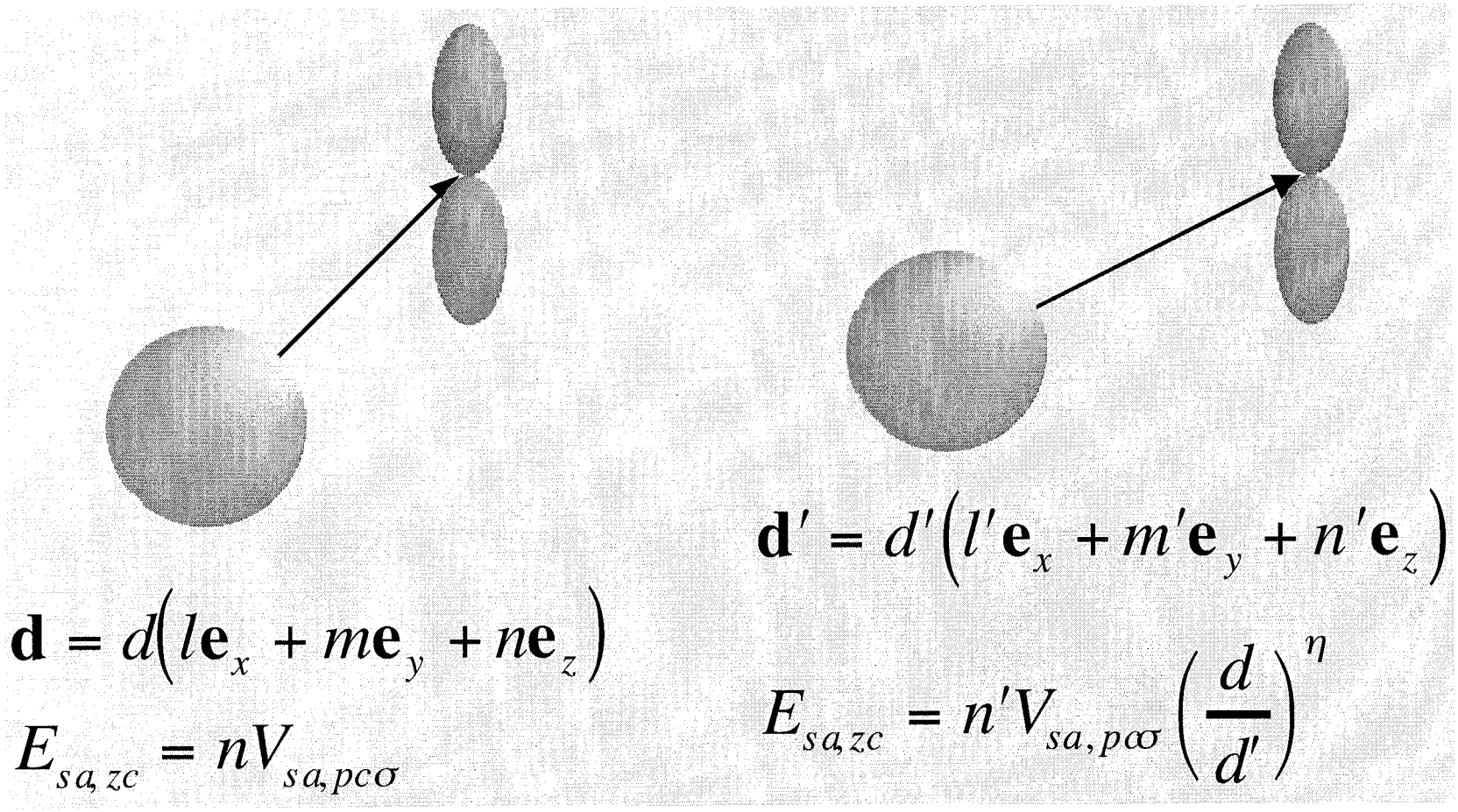


- Genetic algorithm parameter optimization is based on:
  - Survival of good parameter sets
  - Evolution of new parameter sets
  - Persistence of diversity (ensures global exploration)

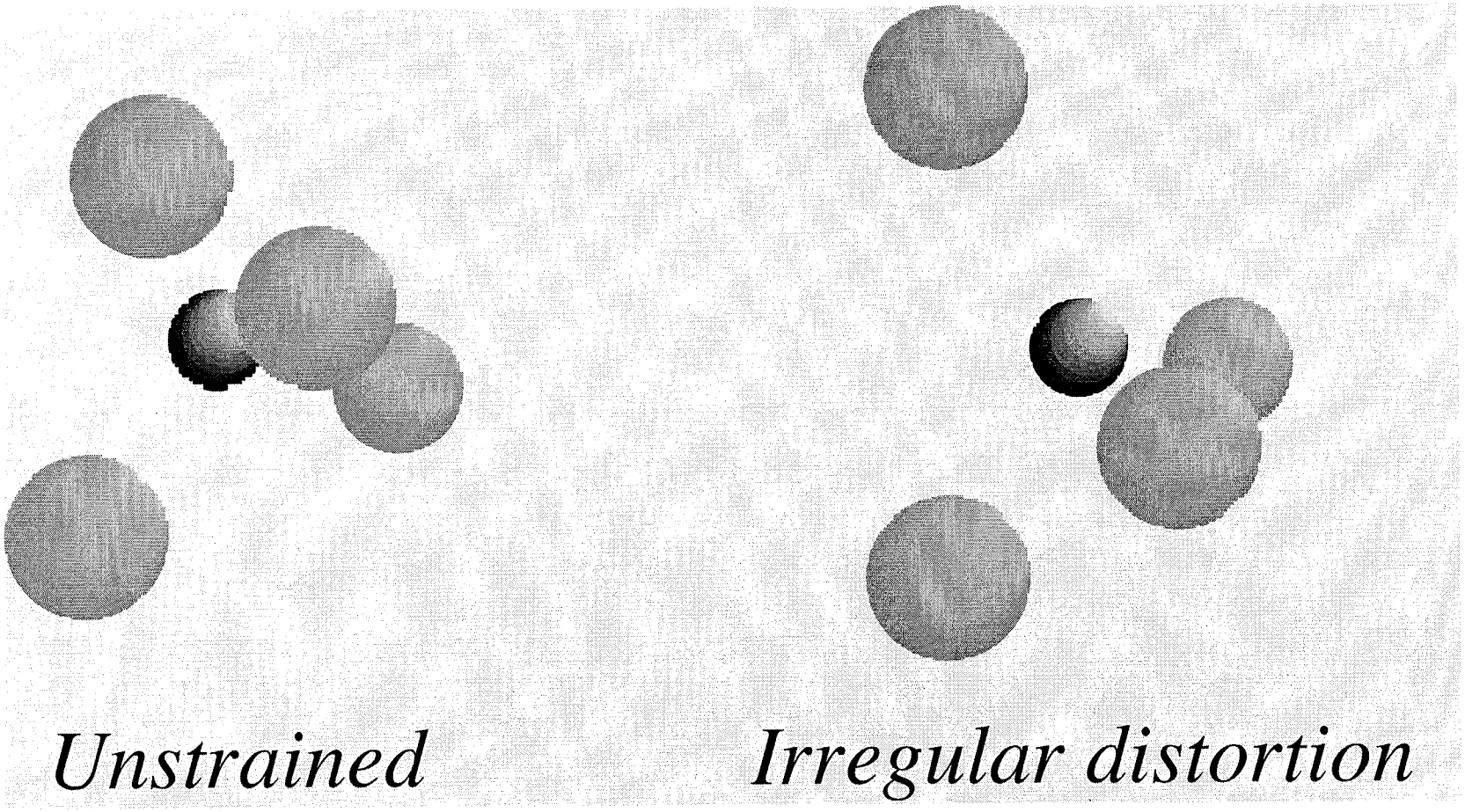
- Basic Operations:
  - Crossover – gross exploration
  - Mutation – fine tuning

Modeling Strain

Bond Lengths and Angles Change



Distortions: Regular and Irregular



On-site Parameters Change

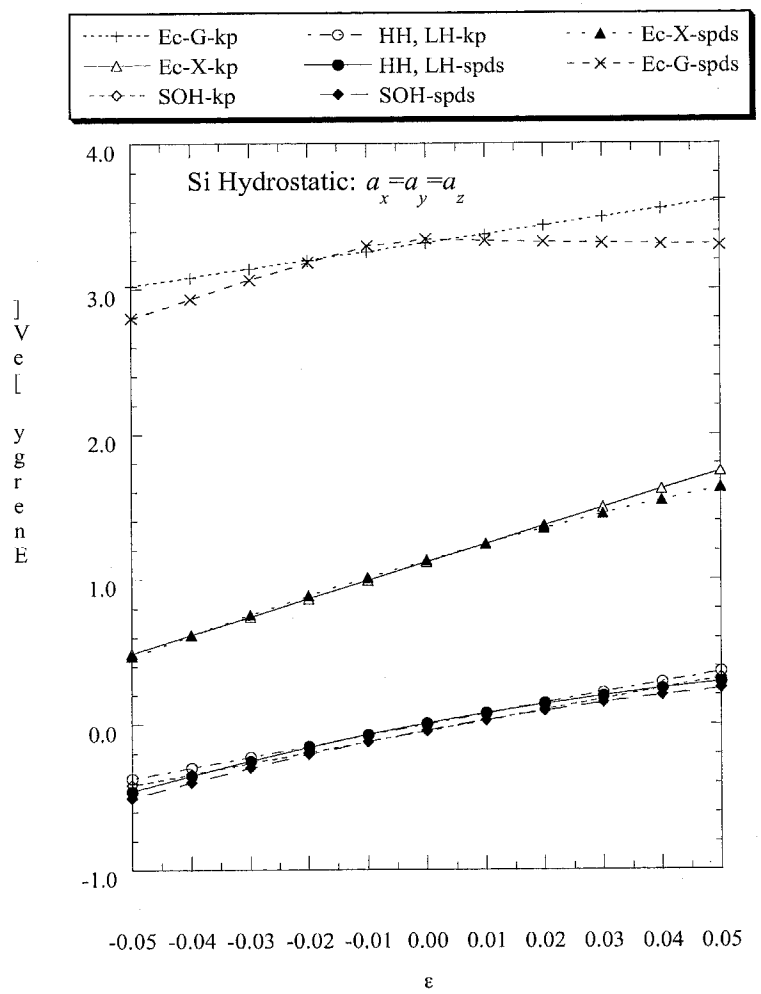
- Overlaps of true atomic orbitals change due to altered bond angles, lengths
- Must compute new orthonormal basis – use Lowdin procedure
- Need new overlaps – use Harrison's form

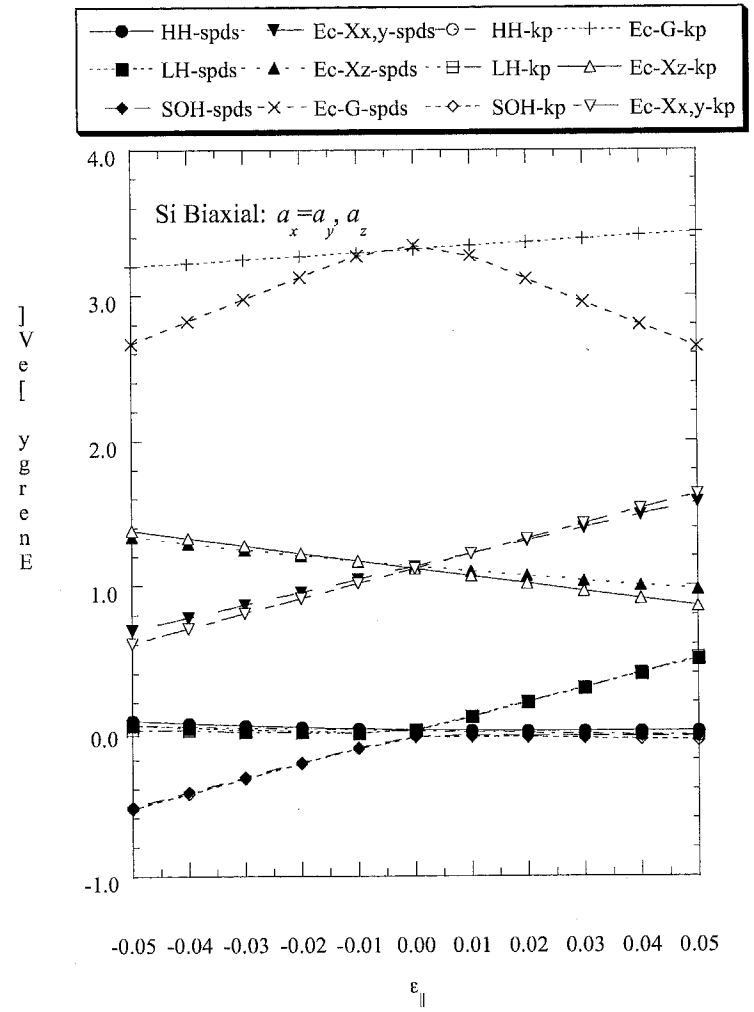
$$S_{(n',\mu'),(n,\mu)} = K_{(n',\mu'),(n,\mu)} \frac{v_{(n',\mu'),(n,\mu)}}{\varepsilon^{(0)}_{(n',\mu')} + \varepsilon^{(0)}_{(n,\mu)}}$$

- Gives new nearest-neighbor parameters
- ALSO give new On-Site parameters
- New fitting parameters, *C*, which characterize changed overlaps
- Procedure valid for arbitrary displacements
- End result is…

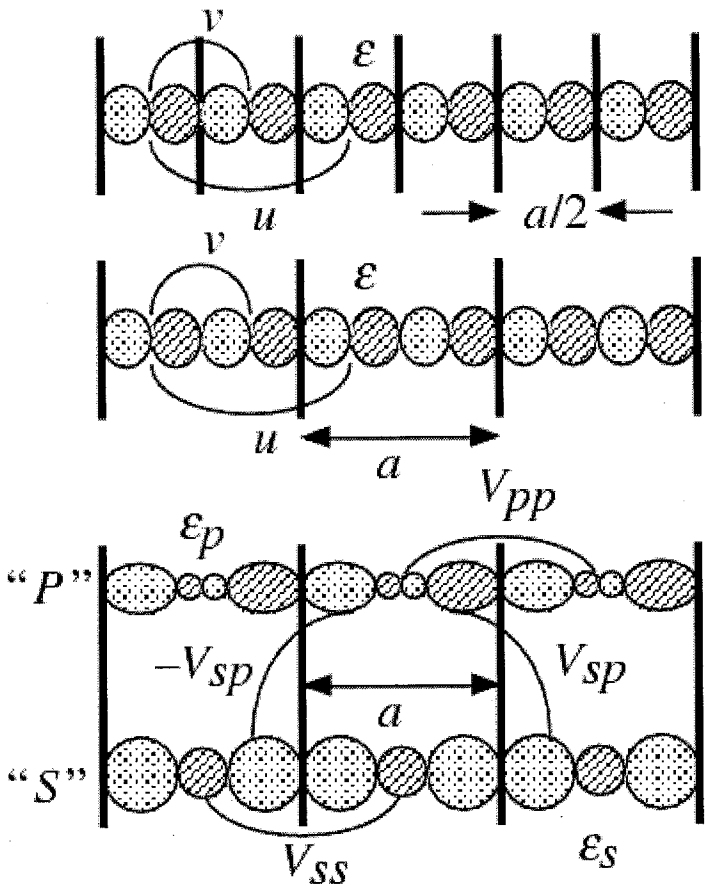
$$\varepsilon'_{i,\alpha} = \varepsilon_{i,\alpha} + \sum_{\substack{j,\beta \\ j \in NN-i}} C_{(j,\beta),(i,\alpha)} \frac{v^2_{(j,\beta),(i,\alpha)} - v'^2_{(j,\beta),(i,\alpha)}}{\varepsilon_{j,\beta} + \varepsilon_{i,\alpha}}$$

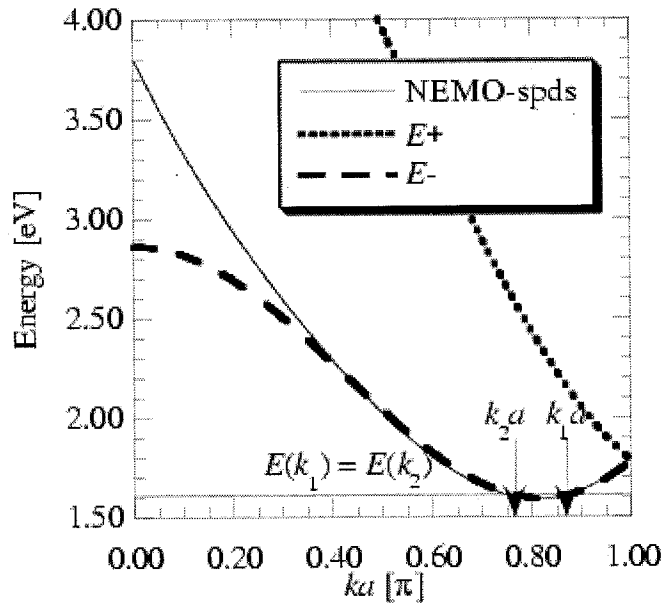
Si: Strain Behavior





Analytical Model: 1-band and 2-band tight binding

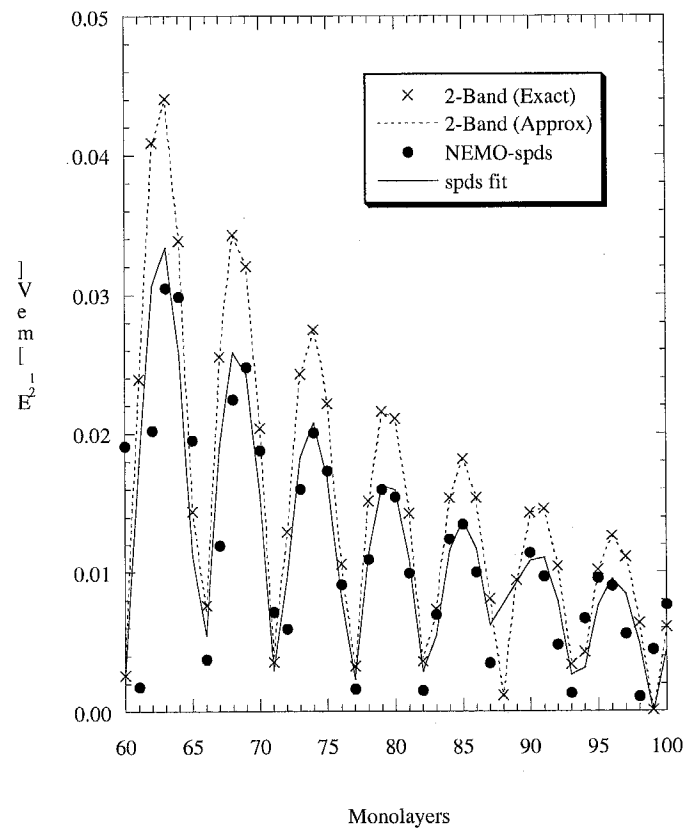




Splitting: 2-Band and spds

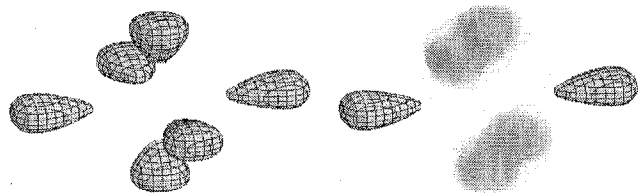
- Zero field splitting oscillates with *L*
- Strained Si QW, hardwall BCs
- Calculated with NEMO and 2-Band
- Minima occur when phase-matching of the 2 states are nearly the same at interfaces
- Splitting follows same functional form for both (*S* = no. atoms):

$$E_{21} \approx \frac{16\pi^2 u}{(S+2)^3}\left|\sin\left[(S+2)\phi_0\right]\right|\sin(\phi_0), \quad \sin(\phi_0) = \sqrt{1-\left(\frac{v}{4u}\right)^2}$$

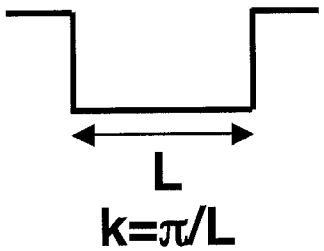


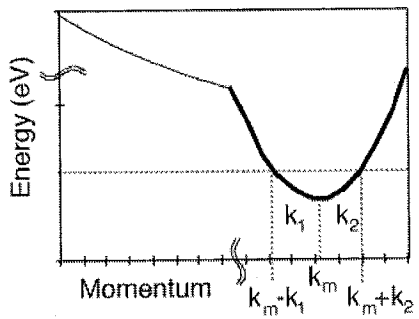
Outline

- **Bi-axial strain on Si.** Lifting 4 of the 6 degenerate valleys $\Delta E > 100$meV



- **Confinement in 1D:** Valley Splitting $\Delta E \sim 1$meV

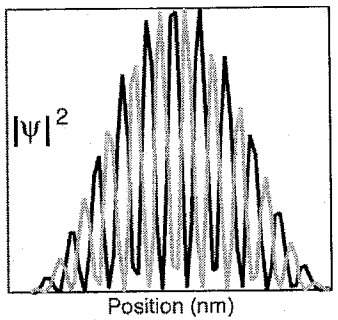




4 propagating states

↓

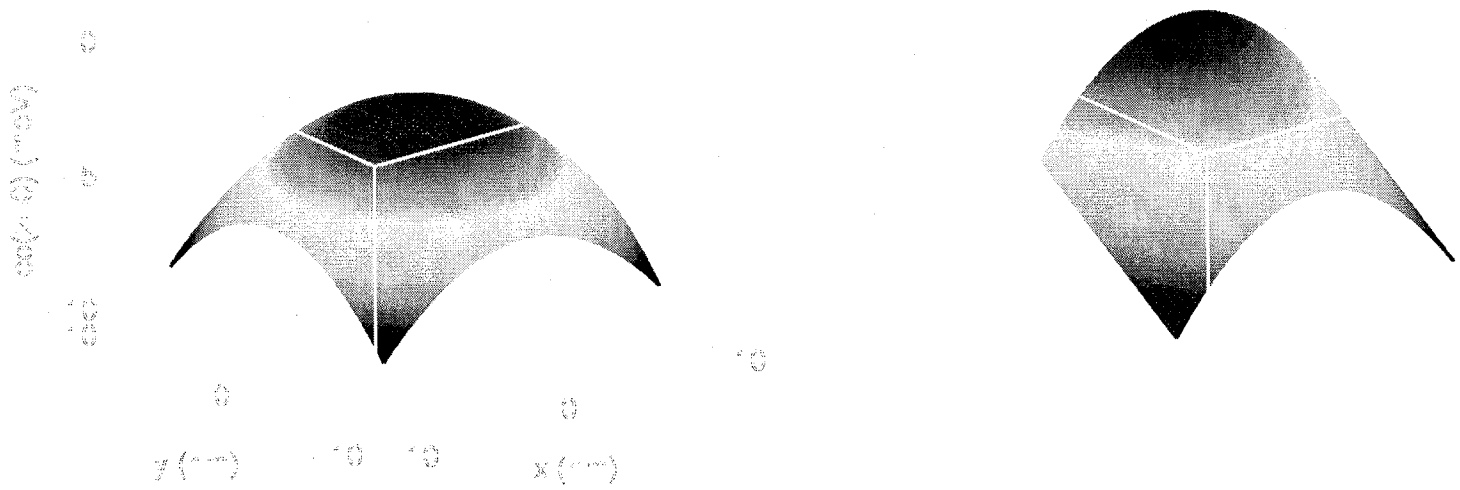
2 bound states
$k_{1/2}$ envelope
k_m fast oscillations



- **Confinement in 3D:** (1D heterostr. & 2D lat gates & mag. field)

- **Conclusions**

1D Heterostructure Confinement
2D Electrostatic confinement in Si QW



- **Geometry:**
  - 5nm quantum well lattice-matched to $Si_{0.2}Ge_{0.8}$ (0.8% tensile strain)
  - non-zero field along z and lateral electrostatic confinement.
  - Rescaled problem size from (5×10^4 atoms) WI group

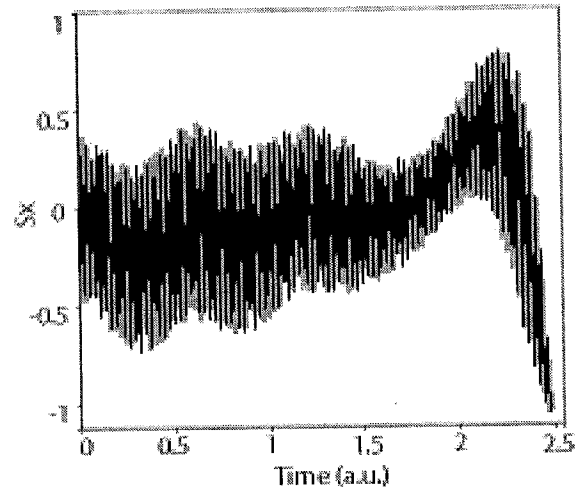
Hyperfine Interaction Induced Electron Spin Decoherence

Objective

Simulate electron spin decoherence due to hyperfine interaction with nuclei

Challenge

Develop alternative method to perturbational approach previously used: avoid divergence in second order perturbation term.



Approach

Explicit solution of the equations of motion for the average electronic and nuclear spins and for the correlation functions.

$$H_{HF} = -\frac{2}{3}\mu_0\gamma_e\gamma_N \sum_j \left|\psi(R_j)\right|^2 S\cdot I_j$$

$$= -\gamma_e S\cdot B_N$$

$$= -\gamma_N \sum_j I_j \cdot B_j$$

$$\partial_t \langle S\rangle = \gamma\langle S\times B_N\rangle$$

$$\partial_t \langle I_j\rangle = \gamma\langle I_j\times B_j\rangle$$

$$\partial_t \langle S_x I_{jx}\rangle = \gamma\left(B_{Nz}\langle S_y I_{jx}\rangle - B_{Ny}\langle S_z I_{jx}\rangle\right) + \gamma_N\left(B_{jz}\langle S_x I_{jy}\rangle - B_{jy}\langle S_x I_{jz}\rangle\right)$$

Details to be discussed at the poster with Paul von Allmen