QM Formalism for a COMSOL Quantum-Dot Solar-Cell Project

0. What we are doing in the project (simple, but correct)

Project goal (in one line). We use COMSOL to compute how adding quantum dots (QDs) and applying bias modifies the electronic states and carrier transport, and we translate that into device-level performance indicators (e.g., absorption edges, current, recombination trends, or qualitative improvements relative to a baseline).

Why we do it. QDs create *confined* states inside a host semiconductor. Those states can:

- shift effective absorption/transition energies (useful for harvesting sub-bandgap photons in intermediate-band ideas),
- change carrier localization (affecting recombination and collection),
- alter band profiles (especially under applied voltage).

How COMSOL connects to quantum mechanics. We split the work into two coupled views:

1. **Quantum view (Wavefunction/eigenstates):** solve an eigenvalue problem for confined states in the QD potential.
2. **Device view (Electrostatics + carriers):** solve Poisson + continuity equations (often stationary or time-dependent) with band offsets, doping, generation, and recombination.

The formalism topics below are the *mathematical justification* for these two views.

1 Hilbert Space → what COMSOL is storing

A quantum state is a vector $|\psi\rangle$ in a Hilbert space. In position space, this is a wavefunction $\psi(\mathbf{r})$ that must be square-integrable and normalizable:

$$\int_{\Omega} |\psi(\mathbf{r})|^2 \, d\mathbf{r} = 1.$$

COMSOL meaning: When you run an *Eigenvalue* study, COMSOL approximates ψ on a mesh. The mesh + basis functions are the "discretized Hilbert space."

Exercise 1 (Normalization and probability; solved)

Problem. Suppose in 1D a trial confined state is

$$\psi(x) = A\sin\Big(\frac{\pi x}{L}\Big), \quad 0 < x < L.$$

Find A such that $\int_0^L |\psi(x)|^2 dx = 1$, and interpret $|\psi|^2$.

Solution.

$$1 = \int_0^L A^2 \sin^2\Big(\frac{\pi x}{L}\Big)\, dx = A^2 \cdot \frac{L}{2} \;\Rightarrow\; A = \sqrt{\frac{2}{L}}.$$

Interpretation. $|\psi(x)|^2$ is the probability density of finding the carrier at position x. In COMSOL plots, higher $|\psi|^2$ inside the dot means stronger localization in the QD.

2 Observables and Hermitian Operators → why eigenvalues are real

An observable is represented by an operator $\hat{A}$. Physically meaningful observables must be **Hermitian** so measured values are real.

The key operator for confined states is the Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m^*}\nabla^2 + V(\mathbf{r}),$$

where m^* is the effective mass and $V(\mathbf{r})$ is the potential energy (constructed from band offsets, electrostatics, and geometry).

COMSOL meaning:

- m^*: material parameter per domain (QD vs barrier).
- $V(\mathbf{r})$: band edge profile + offsets (and optionally electrostatic potential).
- The *Eigenvalue* study is solving $\hat{H}\psi_n = E_n\psi_n$.

Exercise 2 (Why energy levels shift when QD size changes; solved)

Problem. Using a simple 1D infinite-well approximation, the energy levels are

$$E_n \approx \frac{n^2\pi^2\hbar^2}{2m^*L^2}.$$

If you reduce the dot confinement length from L to $L/2$, by what factor does E_1 change?

Solution.

$$E_1(L/2) = \frac{\pi^2\hbar^2}{2m^*(L/2)^2} = \frac{\pi^2\hbar^2}{2m^*} \cdot \frac{4}{L^2} = 4E_1(L).$$

Project insight. This is the cleanest explanation for a common COMSOL result: smaller dots ⇒ higher confined energies ⇒ shifted transition energies. Even if your real QD is truncated-conical and barriers are finite, the trend remains.

3 Eigenfunctions of a Hermitian Operator → mode shapes you plot

For a Hermitian $\hat{H}$,

$$\hat{H}\psi_n = E_n\psi_n, \quad E_n \in \mathbb{R},$$

and eigenfunctions are orthonormal:

$$\int_\Omega \psi_n^*(\mathbf{r})\psi_m(\mathbf{r})\, d\mathbf{r} = \delta_{nm}.$$

Exercise 3 (Orthogonality and why it matters; solved)

Problem. Explain in one sentence why orthogonality is useful when computing transitions (e.g., absorption between states).

Solution. Orthogonality ensures each state contributes independently; transition strengths are computed from overlaps like $\langle\psi_f|\hat{O}|\psi_i\rangle$, and orthogonality prevents "double counting" of the same physical mode.

Project insight. When you compare QD vs no-QD, you are effectively comparing two different eigen-bases and their transition energies.

4 Generalized Statistical Interpretation → how QM feeds device physics

The expectation value of $\hat{A}$ is

$$\langle A\rangle = \int_\Omega \psi^*(\mathbf{r})\, \hat{A}\, \psi(\mathbf{r})\, d\mathbf{r}.$$

COMSOL meaning: If you compute $|\psi|^2$ and see localization in the dot, you can anticipate:

- stronger confinement (good for creating discrete levels),
- but possibly increased recombination if carriers remain trapped.

Exercise 4 (A direct link to "where carriers are"; solved)

Problem. Let $\Omega_{\mathrm{QD}} \subset \Omega$ be the QD region. Define the probability that an electron is inside the dot and state the practical interpretation.

Solution.

$$P_{\mathrm{QD}} = \int_{\Omega_{\mathrm{QD}}} |\psi(\mathbf{r})|^2\, d\mathbf{r}.$$

If P_{QD} is high, the state is QD-localized; if low, it is more delocalized into barriers/wetting layer. This directly supports your claims about "QD-confined states" in the paper-style discussion.

5 Uncertainty Principle → why confinement forces energy quantization

$$\Delta x\,\Delta p \geq \frac{\hbar}{2}.$$

Simple meaning. If the dot confines carriers to small Δx, momentum uncertainty Δp increases, which increases kinetic energy and thus raises eigenvalues.

Exercise 5 (Quick estimate; solved)

Problem. If a dot confines an electron to $\Delta x \sim L$, estimate Δp and the kinetic energy scale.

Solution.

$$\Delta p \sim \frac{\hbar}{2L}, \qquad E_{\text{kin}} \sim \frac{(\Delta p)^2}{2m^*} \sim \frac{\hbar^2}{8m^*L^2}.$$

Project insight. This scaling is the same message as Exercise 2: confinement controls energy levels. It is the clean physical story behind your parameter sweeps (QD size, barrier thickness, etc.).

6 Dirac Notation → what your simulation is "really" doing

Dirac notation compresses the same ideas:

$$|\psi\rangle \leftrightarrow \psi(\mathbf{r}), \quad \langle H\rangle = \langle\psi|\,\hat{H}\,|\psi\rangle\,.$$

COMSOL meaning: Discretization turns $\hat{H}$ into a matrix H and $|\psi\rangle$ into a vector; COMSOL solves $H\mathbf{u} = E\mathbf{u}$.

7 Schrödinger Equation in 3D → your QD geometry (the core)

For a 3D QD in a heterostructure:

$$-\frac{\hbar^2}{2m^*}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}).$$

Why this matters for the project. This equation is the reason QDs produce discrete subbands. Once you have E_n and ψ_n, you can argue (with evidence) that your QD design introduces new states compared with the control device.

Exercise 6 (Finite barrier insight; solved)

Problem. In a finite barrier V_0, do eigenfunctions vanish exactly outside the dot?

Solution. No. They decay exponentially into the barrier (wavefunction "leakage"). Practically, this means barrier thickness and height control coupling between dots/layers, which can change transport and recombination in device simulations.

8 Hydrogen Atom Analogy → how to explain QDs professionally

Hydrogen has quantized energy levels due to Coulomb confinement. A QD has quantized levels due to *geometric + band offset* confinement. That is why QDs are called **artificial atoms**.

Exercise 7 (One-sentence paper-style statement; solved)

Problem. Write a single professional sentence connecting this analogy to your simulation results.

Solution. "The computed discrete eigenenergies and localized eigenmodes confirm that the embedded quantum dots behave as artificial atoms, introducing quantized subband states relative to the bulk reference structure."

9 Angular Momentum and Spin → what you can (and can't) claim

For highly symmetric dots, angular momentum quantizes and can create degeneracies. Spin introduces (at least) a two-fold degeneracy.

Practical project rule. If your COMSOL model does not explicitly include spin-orbit or Zeeman terms, you should:

- mention spin only as a conceptual note,
- avoid claiming spin-resolved splitting unless you simulated it.

1. How this becomes a COMSOL workflow (the "how" in plain language)

A defensible workflow for a report/paper is:

1. **Build geometry and materials:** QD + barrier + surrounding layers.
2. **Define potential profile $V(\mathbf{r})$:** via band offsets and electrostatics assumptions.
3. **Eigenvalue study:** extract E_n and ψ_n, plot $|\psi_n|^2$ and interpret confinement/leakage.
4. **Device study:** run Poisson + carrier transport with and without QDs to show trends.
5. **Parameter sweeps:** QD size, barrier thickness, doping, applied bias V_{app} to produce "new" results.

2. A final exercise that aligns with your current COMSOL issue (bias sweeps; solved conceptually)

Problem. You observe convergence at $V_{\text{app}} = 0$ but failures at 0.05 or 0.1. Give one physically meaningful explanation and one numerical explanation.

Solution (simple and correct).

- **Physical:** bias changes band bending strongly; if QDs introduce localized charge and strong gradients, the nonlinear system becomes harder to satisfy.
- **Numerical:** stationary solvers are sensitive to initial guesses; a bias jump can be too large. Continuation (ramping) and tighter damping are typically required to track the solution branch.

Project insight. This is not a "random COMSOL problem"; it is a normal consequence of nonlinear coupled PDEs under bias.

Conclusion (what you should say in the presentation)

We use Hilbert-space formalism and Hermitian eigenproblems to justify the extraction of QD-confined states in COMSOL. Those states explain why QD geometry and band offsets change transition energies and localization. Then we connect these quantum outputs to device-level transport under applied bias to argue improvement (or controlled change) versus a baseline structure, supported by parameter sweeps and physically interpretable trends.