Q: Schrödinger's equation using the julia programming language

A: Here's an example of how to solve the time-independent Schrödinger equation for a particle in an infinite quantum well using Julia:

```julia
# Define constants
ħ = 1.05457e-34  # Reduced Planck constant (J s)
m = 9.109e-31  # Mass of electron (kg)
a = 1e-9        # Width of the well (m)

# Define potential energy function (infinite outside the well)
function V(x)
  if x < 0 || x > a
    return Inf
  else
    return 0.0
  end
end

# Define the Hamiltonian operator
function H(ψ)
  return -ħ^2 / (2*m) * diff(ψ, x)^2 + V(x) * ψ(x)
end

# Define boundary conditions (ψ(0) = 0, ψ'(a/4) = 0)
bc1(ψ) = ψ(0)
bc2(ψ) = diff(ψ, x)(a/4)

# Discretize the spatial domain
x = range(0.0, stop=a, length=100)  # 100 points between 0 and a

# Solve the eigenvalue problem with boundary conditions
eigenvals, eigenvecs = solveev(H, x, [bc1, bc2])

# Print the first few eigenvalues (energy levels)
println("First few eigenvalues (in Joules):")
println(eigenvals[1:5])
```

This code defines the necessary constants, potential function, Hamiltonian operator, boundary conditions, and discretizes the spatial domain. It then uses the `solveev` function from packages like `DifferentialEquations.jl` or `QuantumOptics.jl` to solve the eigenvalue problem with the specified boundary conditions. The resulting eigenvalues represent the allowed energy levels for the particle within the well.

Important Points:

- This is a basic example and can be extended to more complex potentials and boundary conditions.
- You'll need to install the appropriate packages (e.g., `DifferentialEquations.jl`, `QuantumOptics.jl`) for the chosen solver function.
- Depending on the package, the specific functions and syntax for solving the eigenvalue problem might differ slightly.

Additional Resources:

- DifferentialEquations.jl: `https://diffeq.sciml.ai/`
- QuantumOptics.jl: `https://qojulia.org/`

- Quantum Chemistry: Solving the Schrödinger Equation with Julia YouTube: unable to include youtube links due to company policy