Quantum Mechanics Applications Using the Time Dependent Schrödinger Equation in COMSOL Multiphysics® Software

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Abstract

INTRODUCTION:
COMSOL is used for obtaining the quantum mechanics wave function Ψ(x,y,z,t) as a solution to the time dependent Schrödinger equation [1]. Probability determination of a particle being at a spacial point is treated by the "Schrödinger wave function formulation". This involves solving field pde's, thus is adaptable to COMSOL. The solutions provide quantum mechanics students , a supplementary understanding of how the Ψ(x,y,z,t) behaves in simple examples.

USE OF COMSOL MULTIPHYSICS®:
Time independent Schrödinger's equation was solved using COMSOL [3-7]. Here, the "transient study type" is employed using the General Form PDE interface. An incident plane wave of the form Ψ= ΨoExp(ikx-iωt), with Ψo=1.0 , is implemented by driving the model end face with Ψ= ΨoExp(-iωt)., The Ψo amplitude is gradually increased from ε to 1.0 over two time cycles in order to avoid the suddenly applied driver's real part @ t=0. Further, an absorbing boundary condition is developed.

RESULTS:
Bar Model
A 2-D bar is solved for testing FEM accuracy of the time-dependent Ψ propagation vs. a Laplace transform exact solution using [8]. Non-dimensional time (τ=t/T) and length (χ=x/λ) quantities are scaled w.r.t. the incident wave period T= 2π/ω and wave length λ= 2π/k . Figure 1 shows agreement between the exact and FEM solution for Ψ vs x/λ at τ=t/T=1.5 as the solution builds, heading towards the desired ΨoExp(ikx-iωt). The Figure 2 plot shows the solution at time τ=t/T=4.0, where the Ψo unit amplitude is reached and illustrates the absorbing boundary is working.

Slit Model
Similar to above except here a two slit barrier is at the end of the bar, with width λ/4 slit opening. Figure 3 displays three snapshots in 3a) τ=t/T=3.0, 3b) τ=4.0 and 3c) τ=6.0. The real part Ψ illustrates the diffraction progressing vs. time. Figure 3d) is at τ=6.0, with | Ψ|^2 plotted, where a banded interference pattern evolves like ones observed experimentally [2]. In Figure 4 a plot of | Ψ|^2 vs. coordinate y/λ shows the bands, where the slice location is the dashed line in Figure 3c.

The value of Ψ|^2 is lower directly opposite the slit as say compared to values either directly above or below the slit, thus illustrating the wavelike diffraction of Ψ.

The probability of a particle being in a ΔA=λ/4 x λ/4 probability zone is addressed by evaluating ∬ Ψ|^2 dA over each zone in Figure 3d . Upon taking the ratio of an integrated zone (e.g. upper) divided by the integration over the mid zone (in-line with slit) , it is 1.74 times more probable that a particle is found in the upper zone then in mid zone and 1.57 times more probable if it is found in the lower zone then in mid zone.

CONCLUSION:
The agreement between the exact vs FEM solution for a 2-D bar example with absorbing boundary conditions, was good. Solutions to the incident harmonic wave upon a two slit barrier, produced diffraction patterns showing bands of null zones due to wave destructive interference. This illustrates the wave like diffraction behavior of particles at the atomic scale.

Reference

[1] Leonard. Susskind,et al., Quantum Mechanics, Basic Books New York, 2014.

[2] Kenneth W. Ford, 101 Quantum Questions, Harvard University Press, Cambridge Ma, 2012.

[3] COMSOL Multiphysics PhysicsBuilderManual Version 5.1, Pages 242-259.

[4] COMSOL Multiphysics "Equations Based" Example, Version 5.1, "Conical Quantum Dot".

[5] Mikhail V. Kisin, "Modeling of the Quantum Well and Cascade Semiconductor Lasers using 8-Band Schrödinger and Poisson Equation System", Proceedings of COMSOL Conference, Oct. 4-6, 2007, Newton, MA, USA. pp. 489-493.

[6] Mikhail V. Kisin, et al., "Modeling of III-Nitride Quantum Wells with Arbitrary Crystallograph Orientation for Nitride-Based Photonics", COMSOL Technical Papers and Presentations Archives.

[7] Y. Yao, et al., "Numerical Study of Exciton States of Core?shell CdTe/CdS Nanotetrapods by using COMSOL Multiphysics", COMSOL Technical Papers and Presentations Archives.

[8] Peter P. Valkó, P et al., Comparison of Sequence Accelerators for the Gaver Method of Numerical Laplace Transform Inversion, Computers & Mathematics with Applications, (2002),implemented in Mathematica®.

Figures used in the abstract

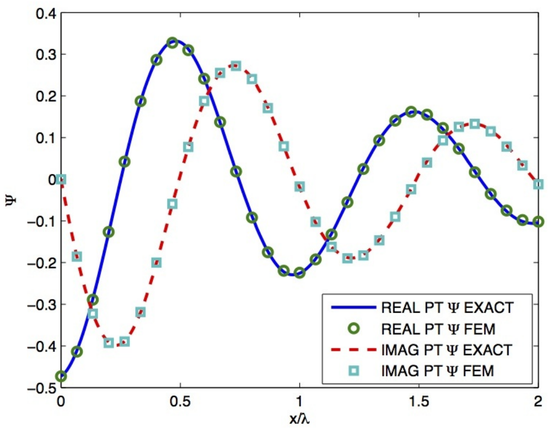

Figure 1: Wave Function Ψ vs x/λ at τ=t/T =1.5 for Exact vs. COMSOL FEM 2D Plane Wave Bar Solution

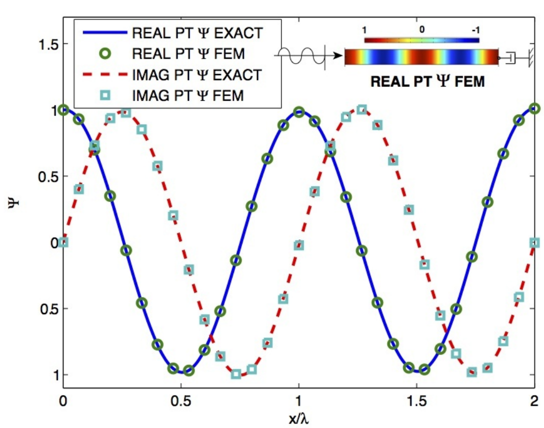

Figure 2: Wave Function Ψ vs x/λ at τ=t/T =4.0 for Exact vs. COMSOL FEM 2D Plane Wave Bar Solution

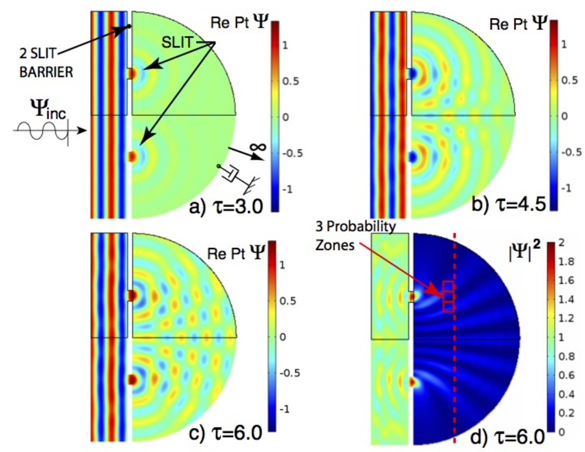

Figure 3: Real Part Ψ of Wave Function over the spatial field, at times : a) τ=t/T =3.0, b) τ=t/T 4.5, c) τ=t/T 6.0 and d) magnitude squared |Ψ|^2 at time : τ=t/T =6.0

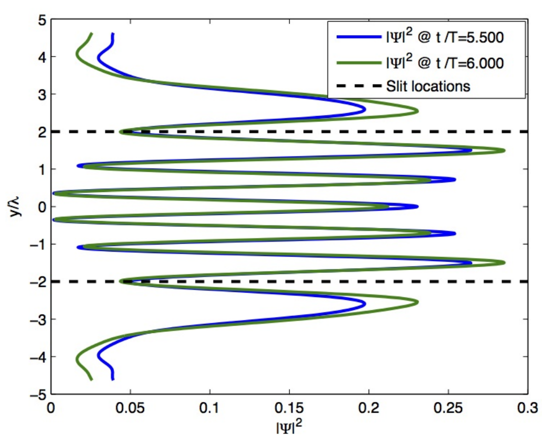

Figure 4: Wave Function Section Cut, |Ψ|^2 vs y/λ at x/λ=1.88 at two times τ=t/T =5.5 and 6.0