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

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Introduction: COMSOL is used for obtaining the quantum mechanics wave function $\Psi(x,y,z,t)$ as a solution to the time dependent Schrödinger equation. The probability determination of a particle being at a spatial point is extracted from $\int|\Psi|^2\,dA$ over finite box zone ΔA; as shown in Fig.2d.

Computational Methods:The governing equation for the behavior of a particle of mass *m* in the presence of a potential field V, is represented by the time dependent Schrödinger p.d.e. equation :

$$\nabla^2\Psi + i\underbrace{\frac{2m}{\hbar}}_{a}\frac{\partial\Psi}{\partial t} - \frac{2mi}{\hbar^2}V\Psi = 0 \qquad (1)$$

In the paper we consider only nonrelativistic "free particles", where V=0. Models are end driven by $\Psi_0 Exp(-i\omega t)$ where Ψ_0 is slowly increased from ε to 1.0 over 2 cycles to avoid a sudden startup. A traveling wave of wave number $k=\sqrt{(a\omega)}$ (Wave Length $\lambda=2\pi/k$; Per. $T=2\pi/\omega$) is created at the inlet.

Results: ● Fig.1 validates the wave guide solution of COMSOL compared to an exact solution obtained with Laplace transforms.

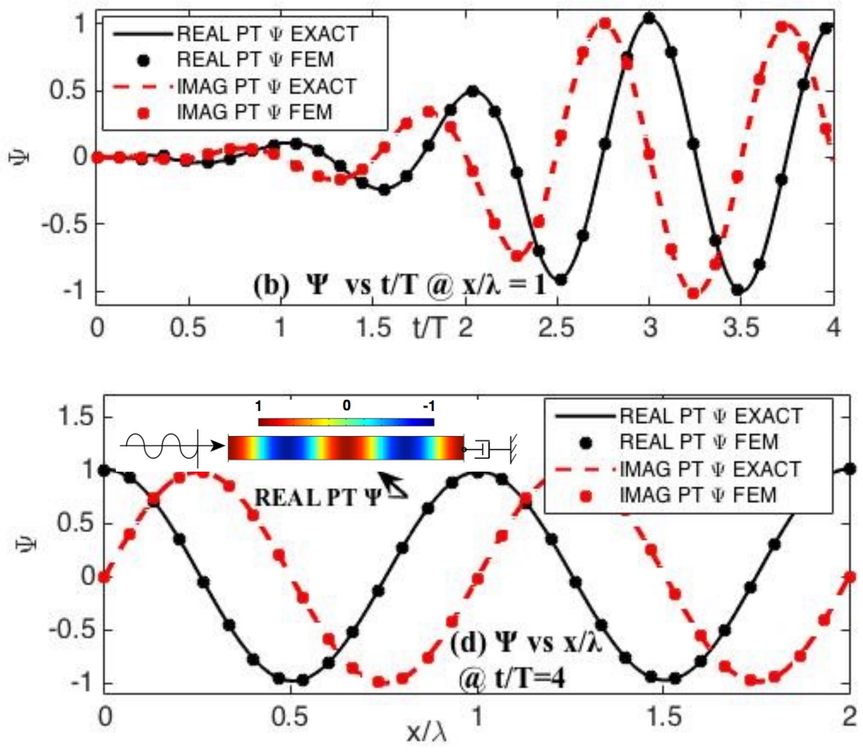

Figure 1.Waveguide Validation Bar Model

● Fig.2 considers a stream of particles impinging upon the two slit model. Fig.2 a-c shows the Ψ traveling wave constructive and destructive interference after it passes through the slits and d) is the resulting banded $|\Psi|^2$ (probability density function).

Fig.3a resolves a bigger model, and 3b shows that at the cut, the probability density is lower in-line with the slit, than say above or below it. Evaluating $\int|\Psi|^2\,dA_U \div \int|\Psi|^2\,dA_M$ implies it is 1.74 times more probable that a particle is found in the Fig.2d Upper zone box than in the in-line Mid zone box.

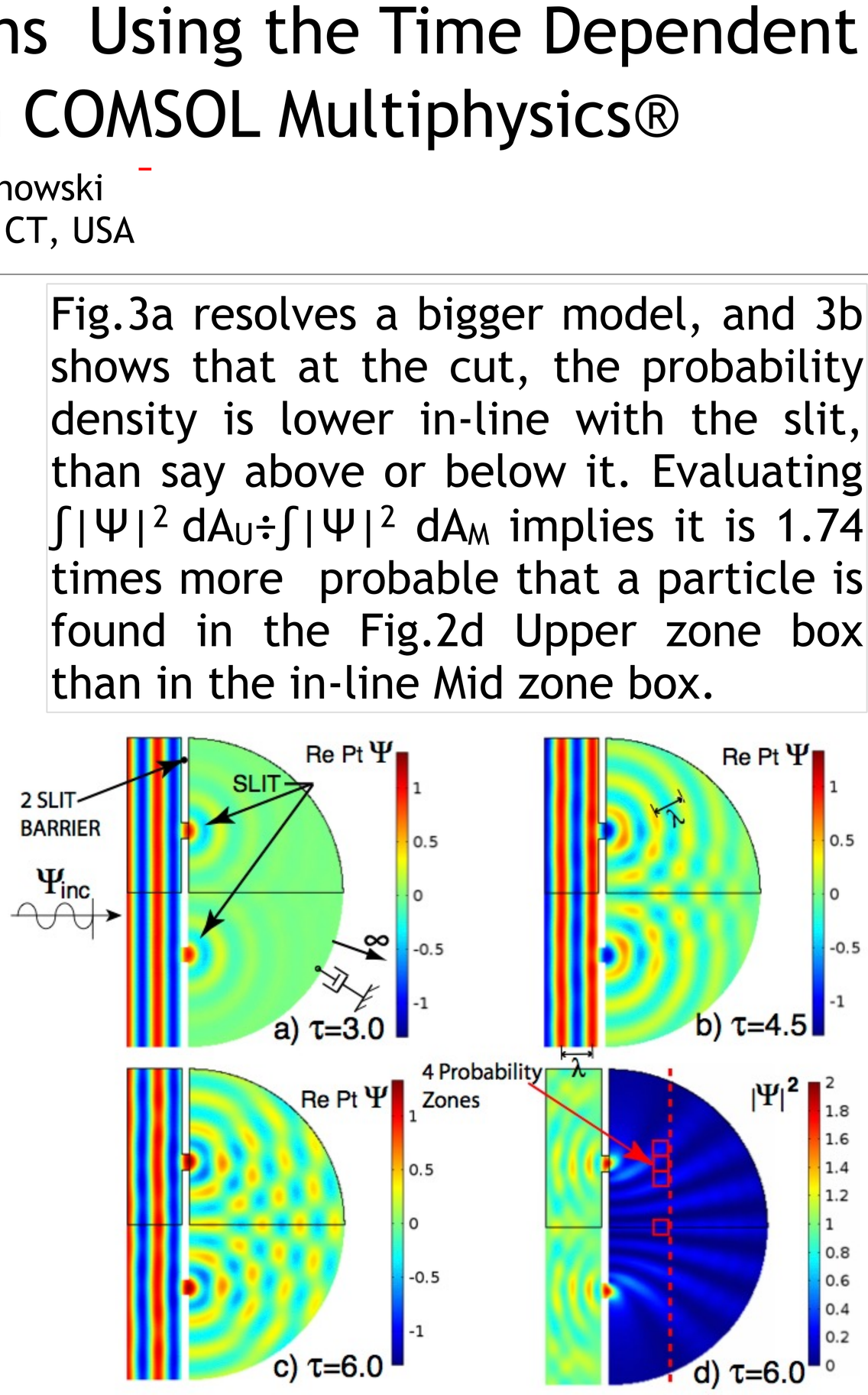

Figure 2. Base Two Slit Model at 3 fixed times τ=t/T

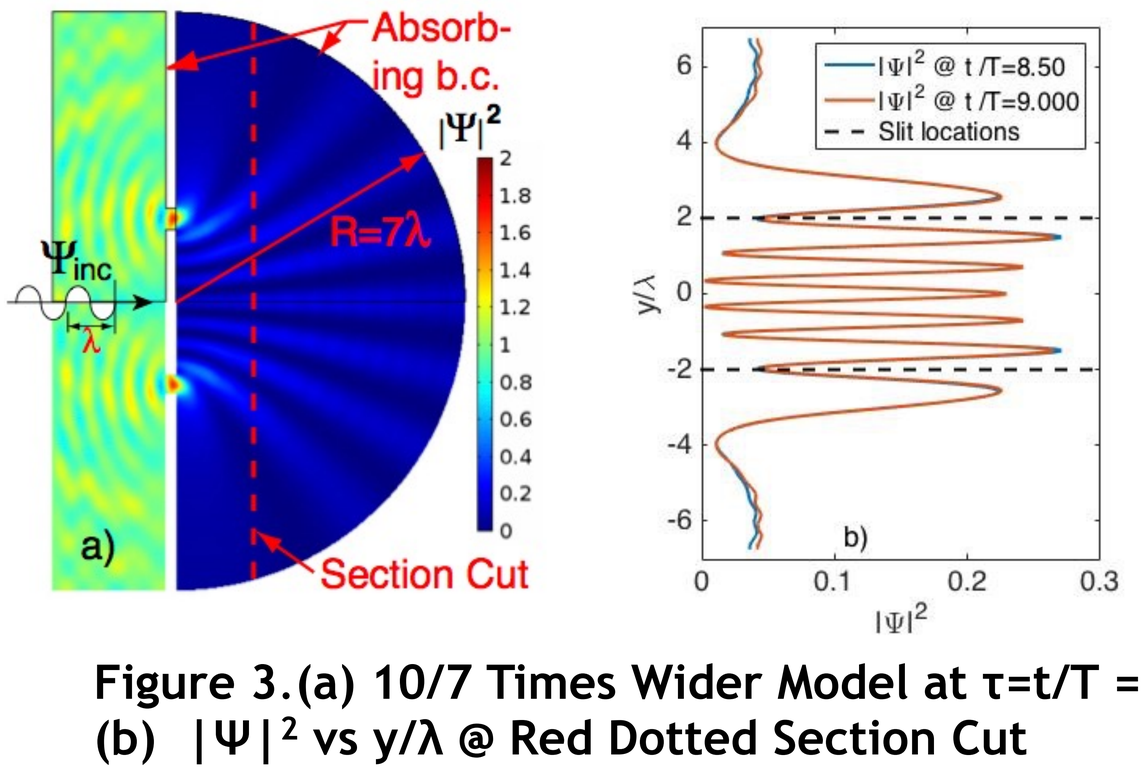

Figure 3.(a) 10/7 Times Wider Model at τ=t/T = 9
(b) $|\Psi|^2$ vs y/λ @ Red Dotted Section Cut

Conclusions: The *General Form PDE* option successfully solved the time dependent Schrödinger equation. Banded groupings of particle locations as inferred by Fig3b are observed experimentally [1].

References:1. K. W. Ford, "101 Quantum Questions", Harv. Univ. Pr., Camb. MA