Relativistic Quantum Mechanics Applications Using the Time Independent Dirac Equation in COMSOL Multiphysics® Software

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Introduction: COMSOL is used for obtaining the relativistic quantum mechanics wave function $\Psi_m(x,y,z,t)$ as a solution to the time independent Dirac equation. The steady state probability density (i.e. ρ′) evaluation of a particle being at a spatial point is extracted from $\rho' = \sum |\psi_m|^2$ at point x,y,z, m=1..4 .

Computational Methods: The equations for the behavior of a free particle of mass *m* with $M' = mc/\hbar$, c= speed of light, $\hbar = h/(8\pi)$, (where *h* is Plank's constant) are given by the Dirac pde equations [1]:

$$\frac{1}{c}\frac{\partial\Psi_1}{\partial t}+\frac{\partial\Psi_4}{\partial x}-i\frac{\partial\Psi_4}{\partial y}+\frac{\partial\Psi_3}{\partial z}+iM'\Psi_1=0$$
$$\frac{1}{c}\frac{\partial\Psi_2}{\partial t}+\frac{\partial\Psi_3}{\partial x}+i\frac{\partial\Psi_3}{\partial y}-\frac{\partial\Psi_4}{\partial z}+iM'\Psi_2=0 \qquad (1)$$
$$\frac{1}{c}\frac{\partial\Psi_3}{\partial t}+\frac{\partial\Psi_2}{\partial x}-i\frac{\partial\Psi_2}{\partial y}+\frac{\partial\Psi_1}{\partial z}-iM'\Psi_3=0$$
$$\frac{1}{c}\frac{\partial\Psi_4}{\partial t}+\frac{\partial\Psi_1}{\partial x}+i\frac{\partial\Psi_1}{\partial y}-\frac{\partial\Psi_2}{\partial z}-iM'\Psi_4=0$$

and are solved with the *"Coefficient-Form PDE"*. When the wave vector ***k*** lies in the xy plane, $\partial\Psi_m/\partial z$ terms drop out and the 1st and 4th eqs. decouple, where Ψ_1,Ψ_4 and are solved alone. The *time independent* solution form of Eq(1) use $\Psi_m=\psi_m(x,y)e^{-i\omega t}$, m=1;4.

Results: • Fig.1 validates the plane wave wave Eigenvalue solution of COMSOL compared to an exact solution.

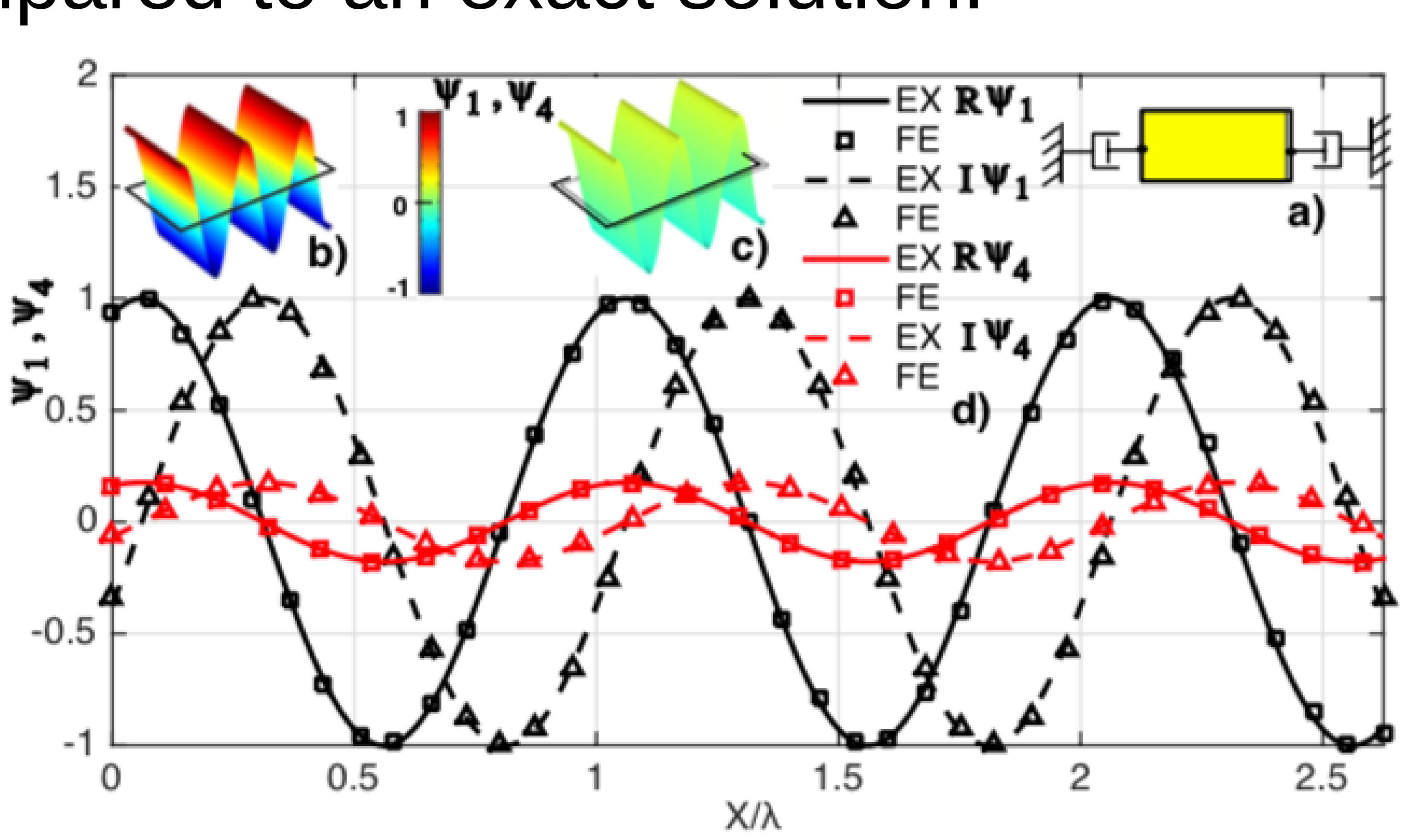

Figure 1 Wave Function Eigenvector ψ_1, ψ_4 vs. Normalized x/λ Coordinate ; (a) Simulated Infinite Domain FEM Model, (b) FEM Real ψ_1 vs. x,y, (c) FEM Real ψ_4 vs. x,y, (d) Real and Imag. ψ_1, ψ_4 of FEM ↔ Exact Comparison Solutions @ Mid Line y=0

• Fig.2 validates the radiating steady state cylindrical wave; inner surface is driven with a cylindrical Eigenfunction.

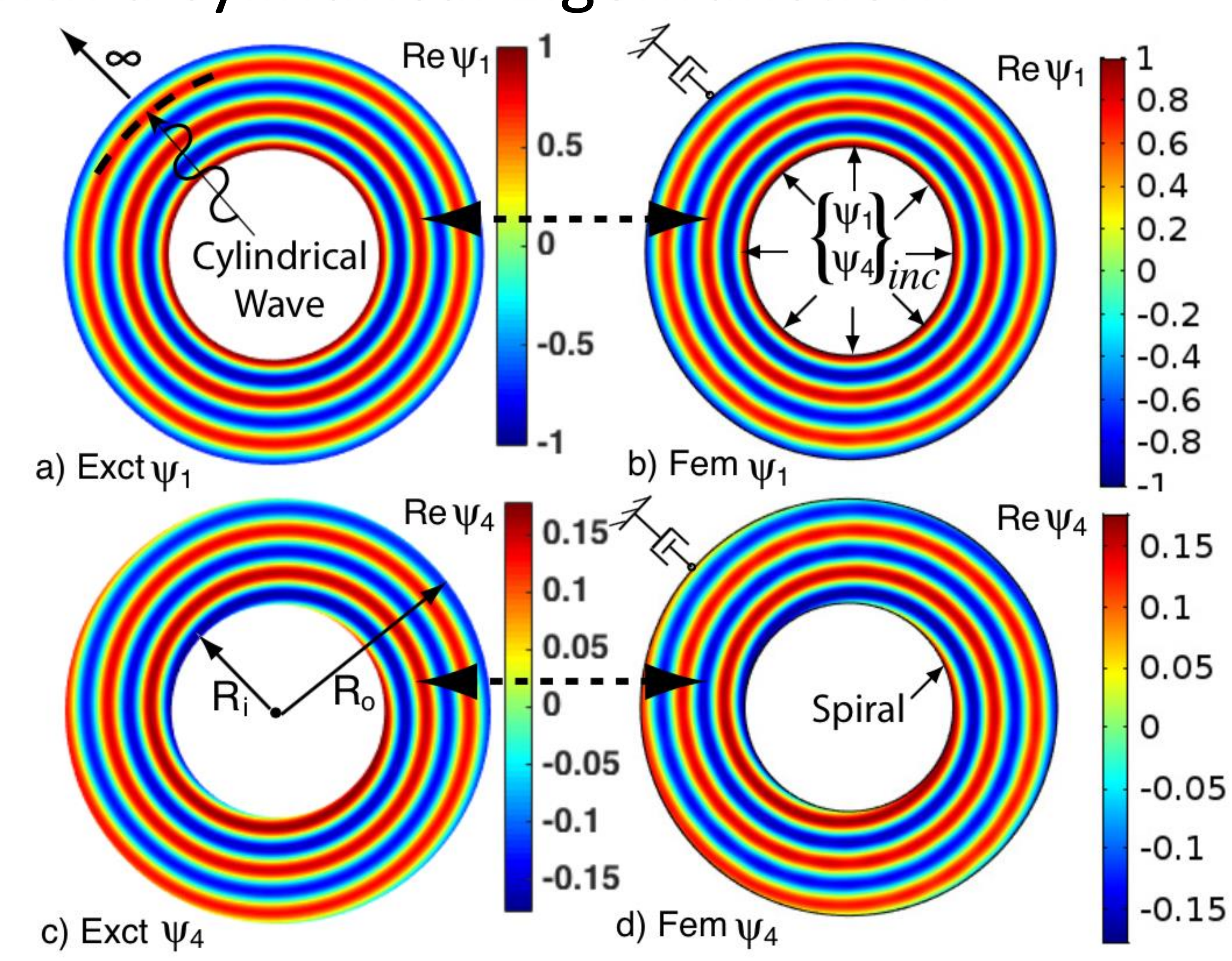

Figure 2 Dirac Cylindrical Wave : (a) Exact Real ψ_1 , (b) FEM Real ψ_1 , (c) Exact Real ψ_4 , (d) FEM Real ψ_4

• Fig.3 An incident PW enters an infinite domain via two slits (Fig.3a.). We observe that waves emerging from the slits interact, forming bands of constructive (orange) and destructive (green) interference. Fig.3 b-c shows that in close at cut1, probability density ρ′ is .067 time smaller above the slit than in line with the slit, yet back at cut 2, ρ′ is 18.9 times bigger above the slit than in line.

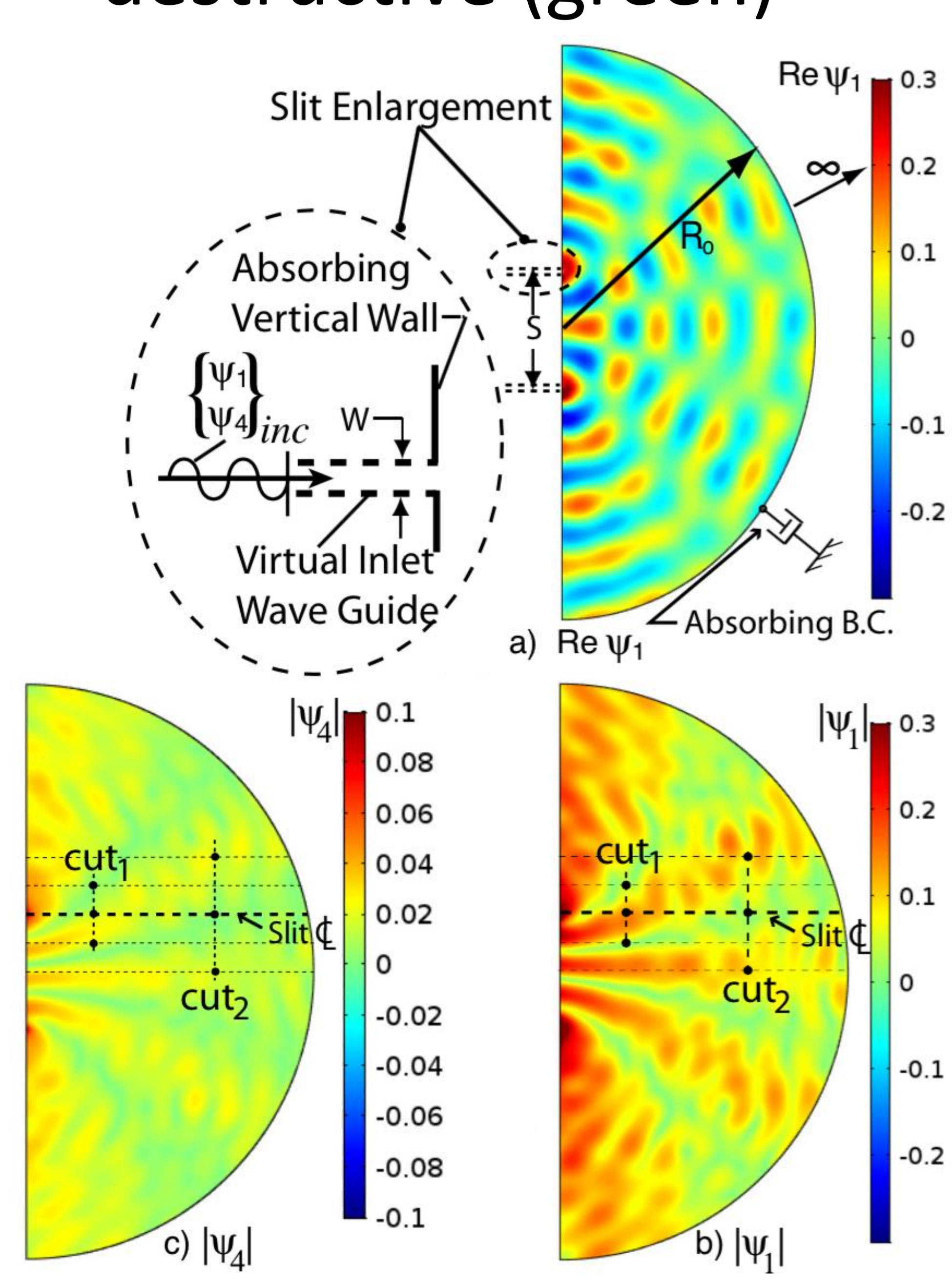

Figure 3 Two Slit Interference Pattern

Conclusions: The *Coefficient-Form PDE* option successfully solved the time independent Dirac equation. Banded groupings of particle locations as inferred by Fig.3 are also observed experimentally.

References:1. P. Strange, Relativistic Quantum Mech., Camb. Univ. Press 1998

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