Time Dependent Dirac Equation FEM Solutions for Relativistic Quantum Mechanics

A. J. Kalinowski[1]
1. Consultant/, East Lyme, CT, USA

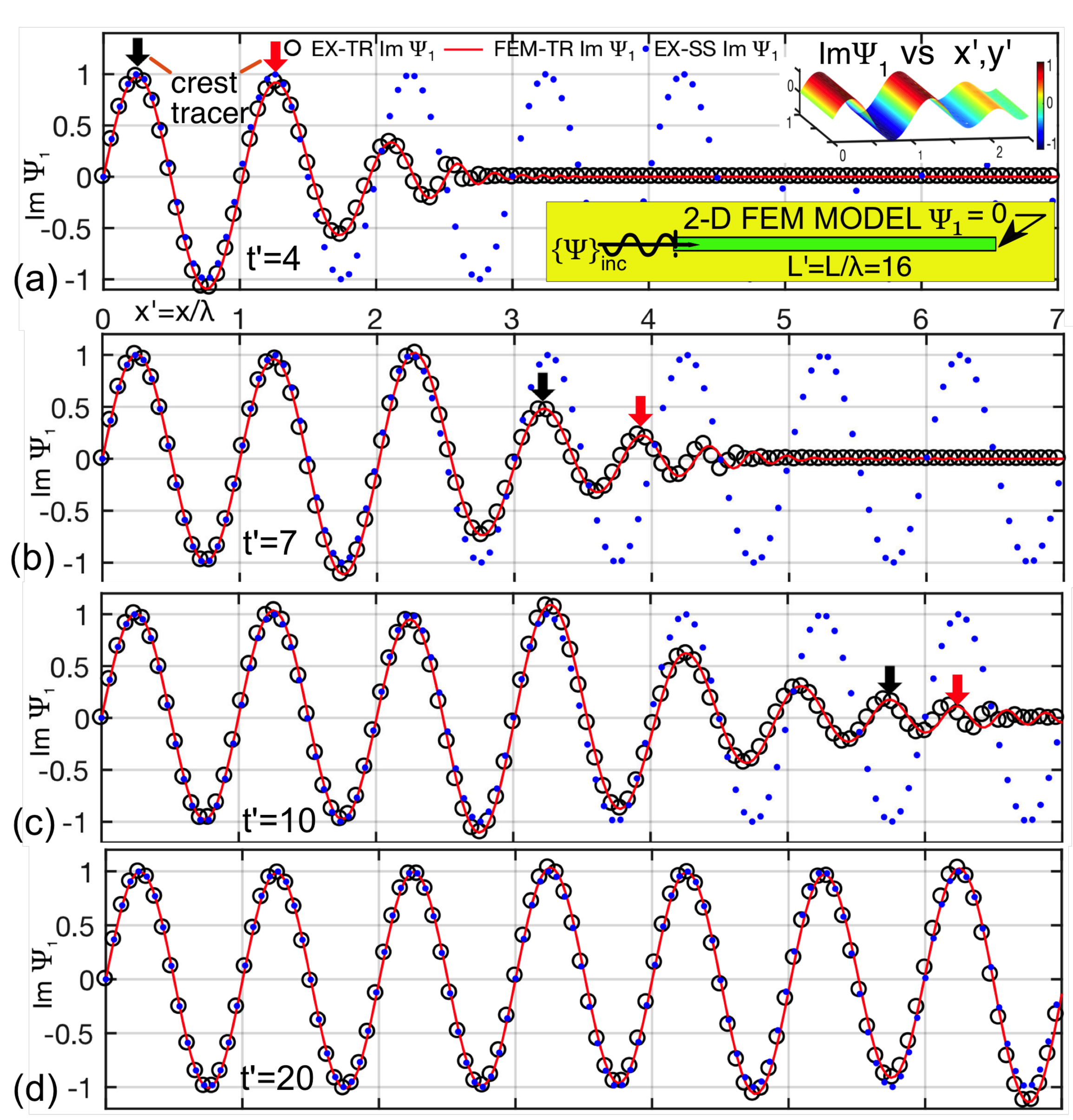
Introduction: COMSOL is used for obtaining the relativistic quantum mechanics wave function $\Psi_m(x,y,z,t)$ as a solution to the *time dependent* Dirac equation. The probability density, ρ_d, evaluation of a particle is extracted from $\rho_d=\Sigma|\Psi_m|^2$ @x,y,z, m=1..4

Computational Methods: The Dirac equations [1] for the behavior of a free particle of mass *m* with $M=mc/\hbar$, c= speed of light, $\hbar$=Planck's constant, are:

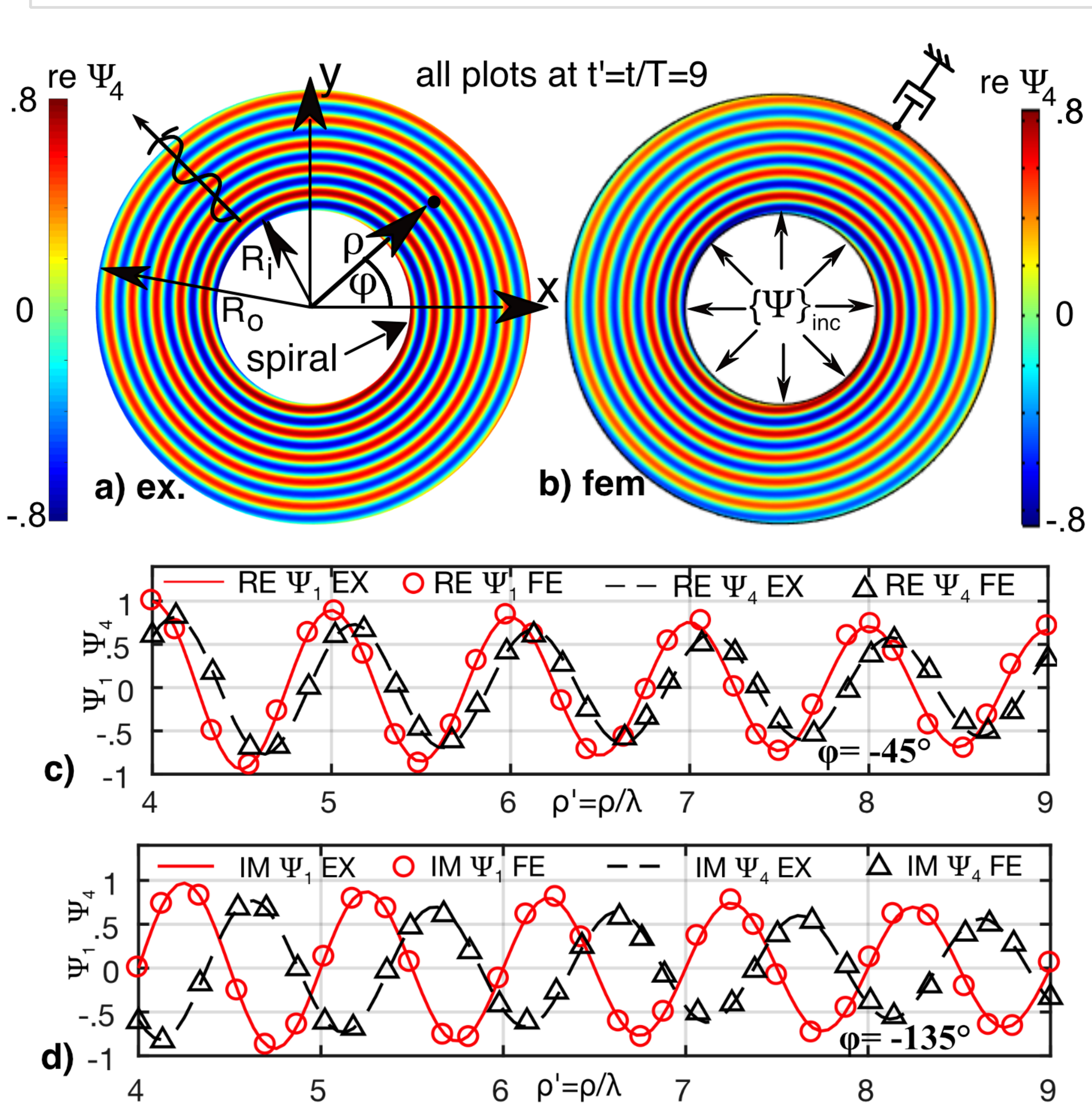
$$\frac{1}{c}\frac{\partial\Psi_1}{\partial t}+\frac{\partial\Psi_4}{\partial x}-i\frac{\partial\Psi_4}{\partial y}+\frac{\partial\Psi_3}{\partial z}+iM\Psi_1=0$$
$$\frac{1}{c}\frac{\partial\Psi_2}{\partial t}+\frac{\partial\Psi_3}{\partial x}+i\frac{\partial\Psi_3}{\partial y}-\frac{\partial\Psi_4}{\partial z}+iM\Psi_2=0$$
$$\frac{1}{c}\frac{\partial\Psi_3}{\partial t}+\frac{\partial\Psi_2}{\partial x}-i\frac{\partial\Psi_2}{\partial y}+\frac{\partial\Psi_1}{\partial z}-iM\Psi_3=0$$
$$\frac{1}{c}\frac{\partial\Psi_4}{\partial t}+\frac{\partial\Psi_1}{\partial x}+i\frac{\partial\Psi_1}{\partial y}-\frac{\partial\Psi_2}{\partial z}-iM\Psi_4=0$$

and are solved with the *"Coefficient-Form PDE"*. When the wave vector ***k*** is in the xy plane, $\partial\Psi_m/\partial z$ terms drop out and the 1st & 4th eqs. decouple, where Ψ_1,Ψ_4 and are solved alone.

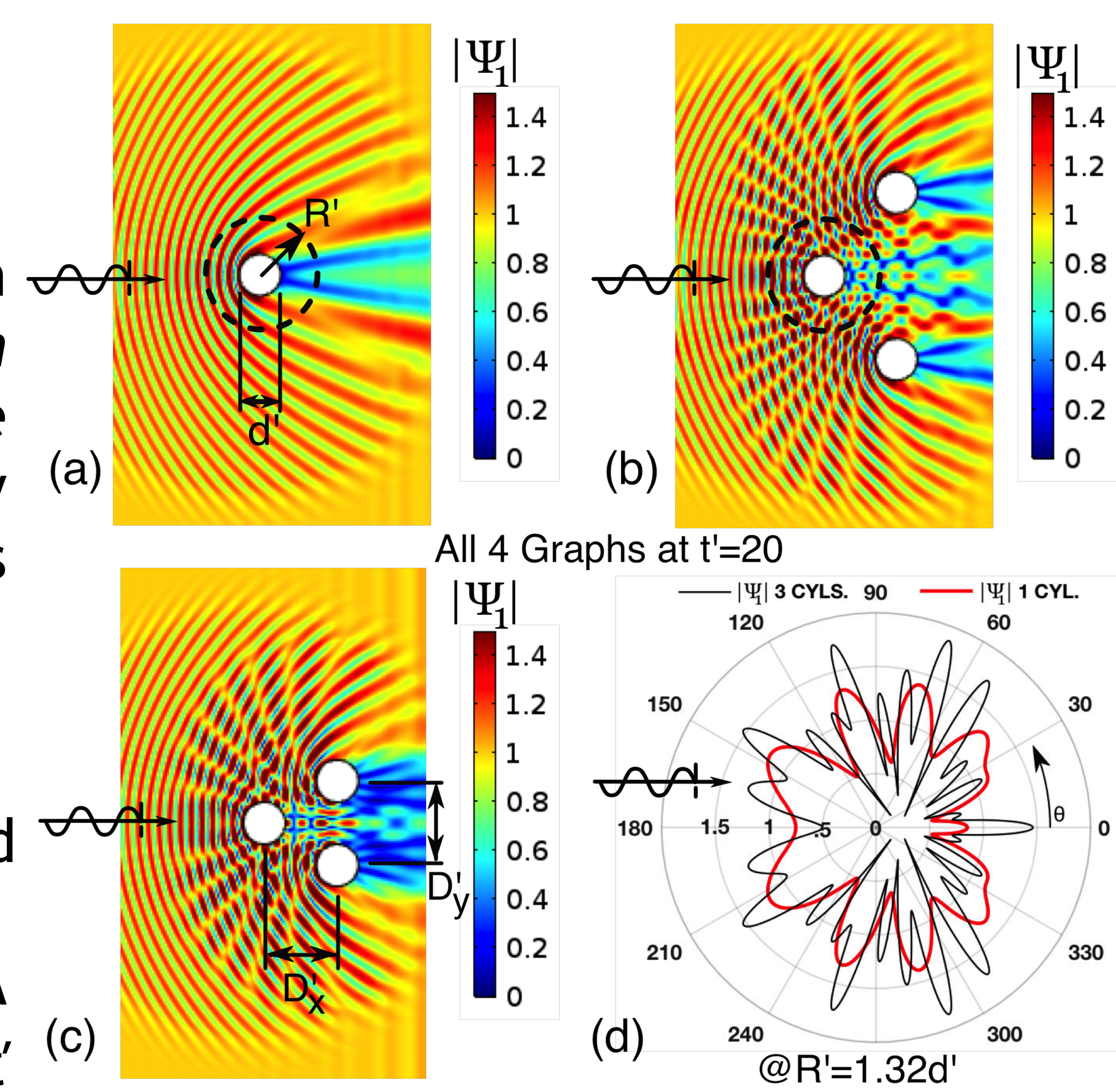
Results: • **Fig.1** below validates the $\Psi_1=1e^{-i\omega' t'}$ end driven *transient* plane wave FEM↔Exact solution. Wave evolution vs $x'=x/\lambda$ is shown at times $t'=t/T=\{4,7,10,20\}$. Dispersion is noted by tracking the crest-to-crest peaks denoted by tracers ⬇ ⬇. These tracer amplitudes reduce in magnitude and change in wavelength with increasing t′.



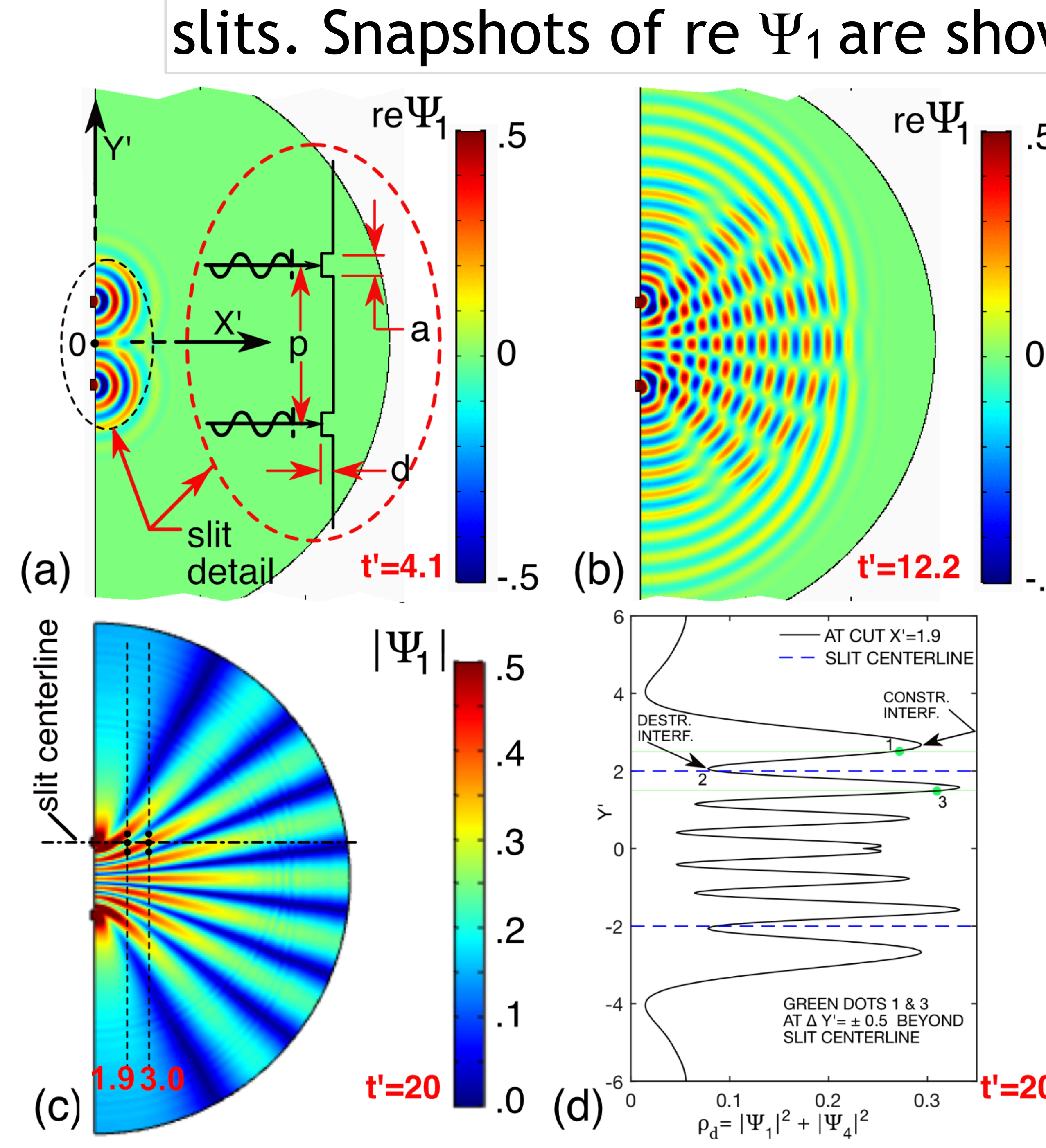
• **Fig.2** below validates re Ψ_4 *transient* cylindrical wave (2a)Exact SS↔(2b)FEM sol. for t′=9, driven at R_i with $\Psi_1=1e^{-i\omega' t'}$. Plot (1c) shows the Exact SS↔FEM sol. vs radial variation $\rho'=\rho/\lambda$ at cut $\varphi=-45°$ and Plot (1d) shows the Exact SS↔FEM sol. vs radial variation $\rho'=\rho/\lambda$ at cut $\varphi=-135°$. Spiral Ψ_4 var. in φ is nicely validated.



• **Fig.3** below illustrates the FEM transient response to a plane wave incident upon a cluster of d′=2 reflecting cylinders, initiated by driving the left surface with $\Psi_1=1e^{-i\omega' t'}$. A one cyl. $|\Psi_1|$ response is shown in (3a) as compared to: the three cyl. $D_y'=4d'$ case shown in (3b) -or- to the three cyl. $D_y'=2d'$ case shown in (3c). Polar plots at $R'=1.32d'$ of case (3a) vs (3b) is given in (3d).



• **Fig.4** Particles fired at 2 slits, is a classic quantum mechanics demo, represented by a $\Psi_1=1e^{-i\omega' t'}$ PW wave function incident upon the slits. Snapshots of re Ψ_1 are shown in (4a) &(4b). Bands of $|\Psi_1|$ constuctive and destructive interference are in (4c). A vertical x′=1.9 cut in (4c) is used to make (4d) probability density ρ_d. Note probability of a particle being in line with the slit is ≈0.272 times smaller than off line @ $\Delta y'=\pm.5$!



Conclusions: The *Coefficient-Form PDE* option successfully validated the time dependent Dirac equation solutions. In the 2 slit demo, banded downfield groupings of particle locations, as inferred by (4d), are also observed experimentally.

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