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% This is a 1D FDTD simulation of psi.

clear all, close all, clc

datetime(clock)

NN = 400;           % Number of points in the problem space.
hbar = 1.054e-34;   % Plank's constant
m0 = 9.1e-31;       % Free space mass of an electron
meff = 1.0;         % Effective mass: Si is 1.08, Ge is 0.067, GaAs is 0.55
melec = meff*m0;    % Mass of an electron
eV2J = 1.6e-19;     % Energy conversion factors
J2eV = 1/eV2J;

dx = .1e-9;         % The cell size
dt = 2e-17;         % Time steps
ra = (0.5*hbar/melec)*(dt/dx^2); % ra must be < .15
DX = dx*1e9;        % Cell size in nm.
XX = (DX:DX:DX*NN); % Length in nm for plotting

% --- Specify the potential -----

V=zeros(1,NN);

% -----
% Initialize a sine wave in a gaussian envelope

lambda = 50;        % Pulse wavelength
sigma = 50;         % Pulse width
nc = 150;           % Starting position
prl = zeros(1,NN);  % The real part of the state variable
pim = zeros(1,NN);  % The imaginary part of the state variable
ptot = 0.;

%
n=2:NN-1;
prl = exp(-1.*((n-nc)./sigma).^2).*cos(2*pi.*(n-nc)./lambda) ;
pim = exp(-1.*((n-nc)./sigma).^2).*sin(2*pi.*(n-nc)./lambda) ;
ptot = sum(prl.^2 + pim.^2);
%
pnorm = sqrt(ptot); % Normalization constant

% Normalize and check
ptot = 0.;
prl = prl./pnorm;
pim = pim./pnorm;
ptot = ptot + sum(prl.^2 + pim.^2);

ptot % This should have the value 1

T = 0;
n_step = 1;

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count = 1;
prl = [0, prl, 0];
pim = [0, pim, 0];
asked = false;

while count < 4
    if asked == false
        n_step = input('How many time steps -->');
        asked = true;
    end
    if n_step < 0
        return
    end
    % -----This is the core FDTD program -----

    T = T + 1;
    mid=2:NN-1;
    left = mid - 1;
    right = mid + 1;

    prl(mid) = prl(mid) - ra.*(pim(left) -2.*pim(mid) + pim(right)) ...
        + (dt/hbar).*V(mid).*pim(mid);

    pim(mid) = pim(mid) + ra.*(prl(left) -2.*prl(mid) + prl(right)) ...
        - (dt/hbar).*V(mid).*prl(mid);

    % -----

    % Calculate the expected values
    if n_step == 1
        PE = 0.;
        psi = prl + i*pim;    % Write as a complex function
        PE = PE + sum(psi.*transpose(psi').*V);

        psi*psi'              % This checks normalization
        PE = PE*J2eV;          % Potential energy

        ke = 0. + j*0.;
        lap_p = psi(right) - 2*psi(mid) + psi(left);
        ke = ke + sum(lap_p*psi(mid)');
        KE = -J2eV*((hbar/dx)^2/(2*melec))*real(ke); % Kinetic energy

        subplot(3,1,count)
        plot(XX,prl,'k')
        hold on
        plot(XX,pim,'-r')
        plot(XX,J2eV*V,'--k')
        hold off
        axis( [ 1 DX*NN -.2 .3 ])
        TT = text(5,.15,sprintf('%7.0f fs',T*dt*1e15));
        set(TT,'fontsize',12)
        TT = text(5,-.15,sprintf('KE = %5.3f eV',KE));

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        set(TT,'fontsize',12)
        TT = text(25,-.15,sprintf('PE = %5.3f eV',PE));
        set(TT,'fontsize',12)
        TT = text(25,.13,sprintf('E_t_o_t = %5.3f eV',KE+PE));
        set(TT,'fontsize',12)
        xlabel('nm')
        set(gca,'fontsize',12)
        T

        count = count + 1;
        asked = false;

    end
    n_step = n_step - 1;
end

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ans =
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```
datetime
```

```
24-Nov-2023 20:34:42
```

```
ptot =
```

```
1.0000
```

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Error using input
Cannot call INPUT from EVALC.

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Error in L08_20231111_FDTD (line 61)
    n_step = input('How many time steps -->');

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