Quantum Electronics and Photonics

Assignment 1

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Contents

Problem 1

(a)

From the Einstein's theory of special relativity total energy of a particle (including rest mass energy) can be expressed as an elliptic equation:

$$E^2 = m_0^2 c^4 + |\mathbf{p}|^2 c^2 \tag{1}$$

According to the basic principles of the quantum mechanics momentum is a generator of space translation and Hamiltonian is just a generator of time translation [1]. So we can replace E with $i\hbar\frac{\partial}{\partial t}$ and $\mathbf{p}$ with $-i\hbar\nabla$. Those substitutions lead to the following wave equation:

$$-\hbar^2\frac{\partial^2\Psi}{\partial t^2} = m_0^2 c^4\Psi - \hbar^2 c^2\nabla^2\Psi \tag{2}$$

or simply:

$$\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2 + \left(\frac{m_0 c}{\hbar}\right)^2\right]\Psi = 0 \tag{3}$$

This equation can be expressed in a more fancy way using four-vector formulation:

$$\left[\Box + \left(\frac{m_0 c}{\hbar}\right)^2\right]\Psi = 0 \tag{4}$$

in above equation $\Box = \partial_\mu\partial^\mu$. In four-vector formulation we use minkowski metric i.e.

$$\partial_\mu\partial^\mu = \partial_0^2 - \partial_1^2 - \partial_2^2 - \partial_3^2$$

wherein ∂_0 represents covariant normalized time derivative and covariante spacal derivatives are

$$\partial_\mu = \frac{\partial}{\partial x^\mu}$$

Klein-Gordon equation fulfills special relativity but contains two fundamental problems, which have to be taken care of for the equation to be physically meaningful. The first problem associated with this equation originates from possibility of negative energies as the solution of the wave equation. Equation (1) has lost the information about the sign of energy. Completeness of the solutions can not be satisfied without considering negative-energy eigenfunctions and consequently there is the problem of physical interpretation of negative energy solutions. Actually the solutions yielding to negative energy are physically connected with antiparticles [2]. the second problem is discussed in part (b).

(b)

In this part we build up a conservative quantity and corresponding flux vector. Continuity equation relates flux vector of an arbitrary conservative fluid to the density of the carriers:

$$\nabla.\mathbf{J} + \frac{\partial\rho}{\partial t} = 0 \tag{5}$$

In non-relativistic Schrödinger's equation the probablity density and the corresponding flux vector are:

$$\rho_{sch} = |\Psi|^2 \tag{6}$$

$$\mathbf{J}_{sch} = -\frac{\hbar}{2mi}\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right) \tag{7}$$

It can be readily shown that $\int_{V_\infty}\rho_{sch}dv$ is independent of time (conservative) in Schrödinger's dynamic (time evolution governed by Schrödinger's equation) and the equation (7) reflects this simple fact. However ρ_{sch}

Problem 1 continued on next page...

defined in this equation is not conservative in Klein-Gordon equation and consequently we have to define a new density.
If we follow the four-vector generalization we can define a new flux vector which describes a conservative quantity. Using the wave equation (4) one obtains:

$$\Psi^*\Box\Psi - \Psi\Box\Psi^* = -\left(\frac{m_0 c}{\hbar}\right)^2 \left[|\Psi|^2 - |\Psi|^2\right] = 0 \tag{8}$$

This equation can be rewritten as below:

$$\frac{1}{c^2}\left[\Psi^*\frac{\partial^2\Psi}{\partial t^2} - \Psi\frac{\partial^2\Psi^*}{\partial t^2}\right] = \Psi^*\nabla^2\Psi - \Psi\nabla^2\Psi^* \tag{9}$$

Using the simple divergence identity

$$\nabla.(\phi\mathbf{V}) = \nabla\phi.\mathbf{V} + \phi\nabla.\mathbf{V}$$

we obtain:

$$\frac{1}{c^2}\frac{\partial}{\partial t}\left(\Psi^*\frac{\partial\Psi}{\partial t} - \Psi\frac{\partial^2\Psi^*}{\partial t^2}\right) = \nabla.(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*) \tag{10}$$

This equation described a continuity equation. So we can define *probability current density* and *probability density* as below:

$$\rho = \frac{\zeta}{c^2}\frac{\partial}{\partial t}\left(\Psi^*\frac{\partial\Psi}{\partial t} - \Psi\frac{\partial\Psi^*}{\partial t}\right) \tag{11}$$

$$\mathbf{J}_p = -\zeta\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right) \tag{12}$$

In above equations ζ is an arbitrary proportionality factor. To make $\mathbf{J}_p$ agree with $\mathbf{J}_{sch}$, ζ is chosen to be $-\frac{\hbar}{2im}$. We may intuitively expect that the probability flux ($\mathbf{J}_p$) is related to mpmentum. This is indeed the case for $\mathbf{J}_p$ integarted over all space. In both Schrödinger's equation and Klein-Gordon's equation we have:

$$\int dv\mathbf{J}_p(\mathbf{r},t) = \frac{\langle\mathbf{p}\rangle_t}{m} \tag{13}$$

where $\langle\mathbf{p}\rangle_t$ is the expectation value of momentum operator at time t. This is one of the reasons why we choose similar expressions for the flux vector in both non-relativistic and relativistic quantum dynamics.
The probability density defined in the equation (11) contains the second fundamental problem. Actually ρ can be positive or negative and interpretation of ρ as a probability density would mean that the theory allows the negative probability. This is the problem of indefinite probability [2].

Problem 2

To calculate the expectation value of momentum operator evolving in the light of Schrödinger's equation, we first prove a simple and important dynamic equation. Assume that observable A evolves under the dynamics imposed by Hamiltonian $\hat{H}$. From the Schrödinger's equation we can write:

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi \tag{1}$$

The rate of change in the expectation value of observable A can be calculated as below:

$$\frac{d}{dt}\langle A\rangle = \frac{d}{dt}\int dv\Psi^* A\Psi dv = \int dv\Psi^*(\mathbf{r},t)\frac{\partial A}{\partial t}\Psi + \int dv\left(\Psi^* A\frac{\partial\Psi}{\partial t} + \frac{\partial\Psi^*}{\partial t}A\Psi\right) \tag{2}$$

Problem 2 continued on next page...

Using (1) left hand side of (2) can be simplified as below:

$$\frac{d}{dt}\langle A\rangle = \langle\frac{\partial A}{\partial t}\rangle + \frac{1}{i\hbar}\int dv\Psi^*\left(A\hat{H} - \hat{H}A\right)\Psi \tag{3}$$

Please note that Hamiltonian ($\hat{H}$) is a hermitian operator and we have utilized this fact in equation (3). this equation can be rewritten in a more convenient form:

$$\frac{d}{dt}\langle A\rangle = \langle\frac{\partial A}{\partial t}\rangle + \frac{1}{i\hbar}\int dv\Psi^*\left[A,\hat{H}\right]\Psi \tag{4}$$

In order to evaluate the rate of change in the expectation value of momentum we can simply substitute momentum operator ($\mathbf{p}$) for A in equation (4). Since there is no explicit time dependent in the momentum operator the first term on the right hand side of equation (4) will vanish and :

$$\frac{d}{dt}\langle\mathbf{p}\rangle = \frac{1}{i\hbar}\langle\left[\mathbf{p}, -\frac{\hbar^2}{2m}\mathbf{p}^2 + V(\mathbf{r})\right]\rangle \tag{5}$$

This equation can be simplified more using basic properties of commutators [1]:

$$\langle\left[\mathbf{p}, -\frac{\hbar^2}{2m}\mathbf{p}^2 + V(\mathbf{r})\right]\rangle = -\frac{\hbar^2}{2m}\langle\left[\mathbf{p},\mathbf{p}^2\right]\rangle + \langle[\mathbf{p},V(\mathbf{r})]\rangle \tag{6}$$

It's evident that $\mathbf{p}$ and $\mathbf{p}^2$ commutate and consequently the first term in the right hand side of equation (6) vanishes. the second term can be simply calculated by substituating $-i\hbar\nabla$ in $\mathbf{p}$:

$$\frac{1}{i\hbar}\langle[\mathbf{p},V(\mathbf{r})]\rangle = -\int dv\left(\Psi^*\nabla\left(V(\mathbf{r})\Psi\right) - \Psi^*V(\mathbf{r})\nabla\Psi\right) = \int dv\left|\Psi\right|^2\left(-\nabla V\right) = \langle-\nabla V\rangle \tag{7}$$

Combining equations (6) and (7) the following semi-classical equation will be obtained:

$$\frac{d}{dt}\langle\mathbf{p}\rangle = \langle-\nabla V(\mathbf{r})\rangle \tag{8}$$

Problem 3

(a)

The rate of change in the total probability in nonequilibrium situation can be readily evaluated using Schröinger's dynamics. by applying time derivative operator on the total probability we obtain:

$$\frac{d}{dt}\int\left|\Psi(\mathbf{r},t)\right|^2 dv = \int dv\left(\Psi^*\frac{\partial\Psi}{\partial t} + \frac{\partial\Psi^*}{\partial t}\Psi\right) \tag{1}$$

Using Schrödinger's equation the right hand side of equation (1) can be simplified. We first decompose Hamiltonian ($\hat{H}$) operator into hermitian ($\hat{H}_0$) and anti-hermitian ($\hat{H}_a$) parts:

$$\hat{H} = \hat{H}_0 + \hat{H}_a \tag{2}$$

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\nabla^2 + V_0 \tag{3}$$

$$\hat{H}_a = -i\Gamma \tag{4}$$

It's straightforwad to show:

$$\Psi^*\frac{\partial\Psi}{\partial t} + \frac{\partial\Psi^*}{\partial t}\Psi = \frac{1}{i\hbar}\left\{\Psi^*\hat{H}_0\Psi - \Psi\hat{H}_0\Psi^*\right\} + \frac{1}{i\hbar}\left\{\Psi^*\hat{H}_a\Psi + \Psi\hat{H}_a\Psi^*\right\} \tag{5}$$

Problem 3 continued on next page...

Combining (1) and (5) leads to the following equation:

$$\frac{dP(t)}{dt} = -\frac{2\Gamma}{\hbar}\int |\Psi|^2 \, dv = -\frac{2\Gamma}{\hbar}P(t) \tag{6}$$

Note that the integaration of first term in righ hand side of equation vanishes and just the second term remains. The simple algebraic steps are given here:

$$\int dv \left\{ \Psi^* \left(-\frac{\hbar^2}{2m}\nabla^2 + V \right) \Psi - \Psi \left(-\frac{\hbar^2}{2m}\nabla^2 + V \right) \Psi^* \right\} = -\frac{\hbar^2}{2m}\int dv \nabla.\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right) = 0 \tag{7}$$

(b)

The solution of fisrt order differential equation (6) is simplely an exponential function:

$$\frac{dP(t)}{dt} = -\frac{2\Gamma}{\hbar}P(t) \Longrightarrow P(t) = P(0)\exp(-\frac{2\Gamma}{\hbar}t) \tag{8}$$

It's evident that the total pobability is constant when $\Gamma = 0$.

Problem 4

Initial momentum wave function is :

$$\Phi(k) = \begin{cases} A\left(a - |k|\right) & |k| < a \\ 0 & \text{elsewhere} \end{cases} \tag{1}$$

or explicitly in the term of p:

$$\widetilde{\Phi}(p) = \begin{cases} A'\left(a - |p/\hbar|\right) & |p| < a \\ 0 & \text{elsewhere} \end{cases} \tag{2}$$

(a)

Conventionally momentum space wave function should be normalized so that:

$$\int_{-\infty}^{+\infty} |\Phi(k)|^2 \, dk = 1 \tag{3}$$

Hence:

$$|A|^2 \int_{-a}^{a} (a - |k|)^2 dk = 1 \Longrightarrow |A|^2 = \frac{3}{2a^3} \Longrightarrow A = \sqrt{\frac{3}{2a^3}} \tag{4}$$

(b)

Calculation of the uncertaintly in z can be accomplished by evaluating the expectation value of $(\Delta z)^2 = (z - \langle z\rangle)^2$. First note that:

$$\langle(\Delta z)^2\rangle = \langle(z - \langle z\rangle)^2\rangle = \langle z^2\rangle - 2\langle z\rangle\langle z\rangle + \langle z\rangle^2 = \langle z^2\rangle - \langle z\rangle^2 \tag{5}$$

We can simply utilized p and z commutation relation. z acts like an operator in momentum space and we should substitute $z \leftrightarrow i\frac{\partial}{\partial k}$ in k-space. Using this simple theory we can write:

$$\langle z\rangle = \int_{-\infty}^{+\infty} \Psi^*(z) z \Psi(z) dz = \int_{-\infty}^{+\infty} \Phi^*(k)\hat{z}\Phi(k) dk \tag{6}$$

Problem 4 continued on next page...

In above equation $\hat{z} = i\frac{\partial}{\partial k}$ hence:

$$\langle z \rangle = i \int_{-\infty}^{+\infty} \Phi^* \frac{\partial \Phi}{\partial k} dk = 0 \tag{7}$$

Note that since $\Phi(k)$ is a real even function $\dfrac{\partial \Phi}{\partial k}$ is an odd function, so the integrant is odd in the symmetric integration interval. In order to evaluate the expectation of $\langle z^2 \rangle$ we follow the same method:

$$\langle z^2 \rangle = -\int_{-\infty}^{+\infty} dk \Phi(k)^* \frac{\partial^2 \Phi}{\partial k^2} \tag{8}$$

$$\frac{\partial^2 \Phi}{\partial k^2} = A\left[\delta(k+a) - 2\delta(k) + \delta(k-a)\right] \tag{9}$$

Combining equations (8) and (9) one obtaines:

$$\langle z^2 \rangle = 2\left|A\right|^2 a \tag{10}$$

and uncertainty in z is:

$$\langle (\Delta z)^2 \rangle = 2a\left|A\right|^2 = \frac{3}{a^2} \tag{11}$$

(c)

The calaculation of the uncertainty in p is straightforward. we should calculate these integarls:

$$\langle p \rangle = \int_{-\infty}^{+\infty} dk \Phi^*(k) \hbar k \Psi = 0 \tag{12}$$

$$\langle p^2 \rangle = \int_{-\infty}^{+\infty} dk \Phi^*(k) \left(\hbar k\right)^2 \Phi(k) = 2\hbar^2 \left|A\right|^2 \int_0^{+a} dk \left(a^2k^2 + k^4 - 2ak^3\right) = 0.1\hbar^2 a^2 \tag{13}$$

Hence:

$$\langle (\Delta p)^2 \rangle = \langle p^2 \rangle - \langle p \rangle^2 = 0.1\hbar^2 a^2 \tag{14}$$

(d)

Heisenberg uncertainty principle which prohibits arbitrary exactness in measuring the both momentum and location of an object can be checked here. Quite generally consider two incompatible observable A and B:

$$\langle (\Delta A)^2 \rangle \langle (\Delta B)^2 \rangle \geq \frac{1}{4} \langle [A, B]^2 \rangle \tag{15}$$

Specifically in the case of momentum and space:

$$\langle (\Delta z)^2 \rangle \langle (\Delta p)^2 \rangle \geq \frac{\hbar^2}{4} \tag{16}$$

We can readily check the uncertainty in this problem:

$$\langle (\Delta z)^2 \rangle = \frac{3}{a^2} \quad , \quad \langle (\Delta p)^2 \rangle = 0.1\hbar^2 a^2 \Longrightarrow \quad \langle (\Delta z)^2 \rangle \langle (\Delta p)^2 \rangle = 0.3\hbar^2 > 0.25\hbar^2 \tag{17}$$

Problem 5

The *finite difference time domain (FDTD)* is a widely used tool in electromagnetics [3]. The FDTD method solves Maxwell's equations using discrete derivative operators. In the same way FDTD method can be applied to solve Schrödinger's equation. The numerical scheme used to solve the Schrödinger's equation differs from the scheme found in electromagnetics. In this project, a simple discretization of the one-dimensional Schrödinger's equation is presented and numerical results are compared with theoretical calculations.
The FDTD technique simulates the time revolution of the wave function in the space where the potential could be any arbitrary function. The stability of time-marching FDTD scheme is analyzed and a bound for the time step is given. The maximum bound step is a bound which avoids the accumulation of the numerical errors [4].
In practical calculations, because of the finite capacity of the memories, the area of computation must be limited to appropriate size. When the natural domain for the problem being solved is infinite the use of absorbing (transparent) boundary conditions are necessitated to eliminate undesirable spurious reflections at boundaries [5, 6].
In the successive sections first the discrete version of the Schrödinger's equation is given and then the theoretical and numerical evolution of a normalized one-dimensional wave packet is presented. Stability analysis and approximate artificial boundary conditions and the corresponding update equations are given afterwards.

FDTD Calculation of 1D Schrödinger's Equation

One dimensional Schrödinger's equation for a real potential is:

$$i\hbar\frac{\partial\Psi(z,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(z,t)}{\partial z^2} + V(z)\Psi(z,t) \tag{1}$$

Assume that we decompose the wave function to its real and imaginary parts as:

$$\Psi(z,t) = \Psi_r(z,t) + i\Psi_i(z,t)$$

then:

$$-\hbar\frac{\partial\Psi_i(z,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi_r(z,t)}{\partial z^2} + V(z)\Psi_r(z,t) \tag{2}$$

$$\hbar\frac{\partial\Psi_r(z,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi_i(z,t)}{\partial z^2} + V(z)\Psi_i(z,t) \tag{3}$$

Two couple partial differential equations can be numerically analyzed using FDTD method. If we discretize the space and time as $z = s\Delta z$ and $t = n\Delta t$ and using central difference scheme for the ordinary spatial nodes the desired update equations can be obtained. In order to set up two implementable update equations we have to calculate Ψ_r at integer values of n while Ψ_i are calculated at the half-integer values of n. The discredited version of the equation (2) at $t = n\Delta t$ and $z = s\Delta z$ is given below. For convenience we use $\Psi(s,n)$ instead of $\Psi(s\Delta z, n\Delta t)$ in the rest of this report:

$$\hbar\frac{\Psi_i(s,n+0.5) - \Psi_i(s,n-0.5)}{\Delta t} = \frac{\hbar^2}{2m}\frac{\Psi_r(s+1,n) - 2\Psi_r(s,n) + \Psi_r(s,n-1)}{(\Delta z)^2} - V(s\Delta z)\Psi_r(s,n) \tag{4}$$

Discretization of the equation (3) at $t = (n+0.5)\Delta t$ and $z = s\Delta z$ leads to the following equation:

$$\hbar\frac{\Psi_r(s,n+1) - \Psi_r(s,n)}{\Delta t} = - \frac{\hbar^2}{2m}\frac{\Psi_i(s+1,n+0.5) - 2\Psi_i(s,n+0.5) + \Psi_i(s-1,n+0.5)}{(\Delta z)^2} + V(s\Delta z)\Psi_i(s,n+0.5) \tag{5}$$

Problem 5 continued on next page...

The equations (4) and (5) can be rewritten in a more convenient form:

$$\Psi_i(s, n+0.5) = \Psi_i(s, n-0.5) + \xi\left[\Psi_r(s+1, n) - 2\Psi_r(s, n) + \Psi_r(s, n)\right] - \frac{\Delta t V(s\Delta z)}{\hbar}\Psi_r(s, n) \tag{6}$$

$$\Psi_r(s, n+1) = \Psi_r(s, n) - \xi\left[\Psi_i(s+1, n+0.5) - 2\Psi_i(s, n+0.5) + \Psi_i(s, n+0.5)\right] + \frac{\Delta t V(s\Delta z)}{\hbar}\Psi_i(s, n) \tag{7}$$

In above equations ξ is defined as:

$$\xi = \frac{\hbar\Delta t}{2m(\Delta x)^2}$$

In this project Drichlet boundary condition for initial wave function is chosen. It's assumed that the wave function is a Gaussian wave packet at $t = 0$ this wave function evolves in the light of Schrödinger's equation. The initial normalized wave function is:

$$\Psi(z, t=0) = \left(\frac{2}{\pi\sigma^2}\right)^{\frac{1}{4}} \exp\left(\frac{-(z-z_0)^2}{\sigma^2}\right) \exp\left(\frac{2\pi i(z-z_0)}{\lambda_e}\right) \tag{8}$$

wherein z_0 is electron's initial position . we choose $z_0 = 0$ in our simulations. λ_e is the electron de Broglie's wave length. We choose $\Delta z = 0.1$nm , $\Delta t = 0.02$fs , $\sigma = \lambda_e = 5$nm. In our computer program we use nm and fs as the unites of length and time respectively. The mass of electron is expressed in the term of em. Electron's rest mass is 0.511Mev . In this case reduced Planck's constant is $\hbar \approx 0.658$eV.fs. This wave packet propagates in the free space ($V = 0$) .

Time Revolution of the Wave Function

The evolution of the wave packet in free space can be simply calculated using basic principles of the quantum mechanics. In this section we first present an abstract formulation for quantum dynamics. We use time evolution operator and Dirac's notations to simplify the expressions. Assume that $|\alpha, t\rangle$ represents quantum state of the particle at time t. Hamiltonian as the generator of time translation is responsible for infinitesimal time evolution [1]. It can be shown that finite time evolution operator is [1]:

$$|\alpha, t\rangle = \exp\left[\frac{-i\hat{H}t}{\hbar}\right]|\alpha, 0\rangle \tag{9}$$

Free space Hamiltonian is :

$$\hat{H} = \frac{\hat{p}^2}{2m} \tag{10}$$

Completness of the momentum and space eigen functions allows us to write:

$$\Psi(z, t) = \int_{-\infty}^{+\infty} dp \int_{-\infty}^{+\infty} dz' \langle z| \exp\left[\frac{-i\hat{H}t}{\hbar}\right] |p\rangle\langle p|z'\rangle\langle z'|\alpha, t=0\rangle \tag{11}$$

In above equation $|p\rangle$ and $|z\rangle$ stand for momentum and space eigen functions repectively. This equation can be simplified more :

$$\langle z| \exp\left[\frac{-i\hat{H}t}{\hbar}\right] |p\rangle = \exp\left[-i\frac{p^2 t}{2m\hbar}\right]\langle z|p\rangle \tag{12}$$

$$\langle z|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} \exp\left(\frac{ipz}{\hbar}\right) \tag{13}$$

Combining all, one obtains:

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$$\Psi(z,t) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} dp \int_{-\infty}^{+\infty} dz' \Psi(z',0) \exp\left[\frac{-ip^2 t}{2m\hbar} + \frac{ip(z-z')}{\hbar}\right] \tag{14}$$

Equation (14) is used to justify our FDTD simulation. Please note that evaluation of the double integrals appeared on the right hand side of equation (14) is numerically expensive and extremely time-consuming. However some approximations can be used to analyze wave function behavior. First the wave function in the momentum space can be evaluated using basic properties of the Fourier transformation:

$$\Phi(k) = \int_{-\infty}^{+\infty} \Psi(z',0) \exp\left(-ikz'\right) \tag{15}$$

After some simple algebraic steps:

$$\Phi(k) = \left(\frac{\sigma^2}{2\pi}\right)^{\frac{1}{4}} \exp\left[-\frac{(k-2\pi/\lambda_e)^2\sigma^2}{4}\right] \tag{16}$$

It's assumed that $z_0 = 0$ in all equations. From the elementary wave theory we know that the relationship between ω and k is called dispersion relation. It's straightforward to show that the wave packet moves with the group velocity

$$v_g \approx \left(\frac{\partial\omega(k)}{\partial k}\right)_{k=k_0} = \frac{\hbar k_0}{m} \tag{17}$$

wherein $k_0 = \frac{2\pi}{\lambda_e}$. It's assumed that the wavefunction is somewhat localized in momentum space. i.e. it's sharply peaked about the value of $k = k_0$. We may make the approximation:

$$\omega(k) \approx \omega(k_0) + (k-k_0)\left(\frac{\partial\omega}{\partial k}\right)_{k=k_0} + \frac{1}{2}(k-k_0)^2\left(\frac{\partial^2\omega}{\partial k^2}\right)_{k=k_0} \tag{18}$$

Note that

$$\hbar\omega = \frac{p^2}{2m}$$

so if we insert ω from the equation (18) into the equation (14) and after some algebraic manipulations the following approximation will be derived:

$$\Psi(z,t) \approx \left[\frac{2}{\pi(\sigma^2 + 4i\gamma t)}\right]^{\frac{1}{4}} \exp i(k_0 z - \omega_0 t) \exp\left[-\frac{(z-v_g t)}{\sigma^2 + 4i\gamma t}\right] \tag{19}$$

wherein:

$$\gamma = \left(\frac{\partial^2\omega}{\partial k^2}\right)_{k=k_0}$$

This is a rather untransparent expression, involving a complex function of x and t. If we calculate absolute magnetude of the wave function we get:

$$|\Psi(x,t)|^2 = \left[\frac{4}{\pi\left(\sigma^4 + 16\gamma^2 t^2\right)}\right]^{\frac{1}{4}} \exp\left[-\frac{2\sigma^2(z-v_g t)}{\sigma^2 + 16\gamma^2 t^2}\right]$$

As it's anticipated from the classical physics the peak of wave function moves with the group velocity. Wave traveling with speed v_g spreads as time increases.
The expectation value of the **kinetic energy** of the electron can be readily calculated in our FDTD simulatation. The expectation value of the kinetic energy is :

$$\langle K\rangle_t = \langle\alpha,t|\frac{p^2}{2m}|\alpha,t\rangle = -\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty} \Psi^*(z,t)\frac{\partial^2\Psi(z,t)}{\partial z^2} \tag{21}$$

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This expression can be numerically implemented as below:

$$\langle \widetilde{K} \rangle_{n\Delta t} \approx -\frac{\hbar^2}{2m} \sum_s \Psi^*(s,n) \frac{\Psi(s+1,n) - 2\Psi(s,n) + \Psi(s-1,n)}{\Delta z} \tag{22}$$

$$\Psi(s,n) = \Psi_r(s,n) + i\frac{1}{2}\left[\Psi_i(s,n+0.5) + \Psi_i(s,n-0.5)\right] \tag{23}$$

From the classical physics the kinetic energy of a free particle should be constant. As it's anticipated we will show that the kinetic energy is a *constant of motion* in quantum mechanics (in free particle problem) as well. It has been shown in problem 2 that the rate of change in the expectation value of any time-independent operator (in Schrödinger picture) can be calculated by a simple commutation relation. Using this theory we can write:

$$\frac{d\langle K \rangle_t}{dt} = \frac{1}{i\hbar}\left[H, H\right] = 0 \tag{24}$$

So the kinetic energy is a constant of motion and it can just be evaluated in the initial state. However it can be used to check the validity of our numerical results. The expectation value of the electron can be theoretically calculated in the initial momentum-space wavefunction:

$$\langle K \rangle = \int_{-\infty}^{+\infty} dk \frac{\hbar^2 k^2}{2m} \left|\Phi(k)\right|^2 = \frac{\sigma\hbar^2}{2m\sqrt{2\pi}} \int_{-\infty}^{+\infty} k^2 \exp\left[\frac{1}{2}\sigma^2(k-k_0)^2\right] dk \tag{25}$$

After some simple allgebraic steps we get:

$$\langle K \rangle = \frac{\hbar^2 k_0^2}{2m} + \frac{\hbar^2}{2m\sigma^2} = \frac{1}{2}mv_g^2 + \frac{\hbar^2}{2m\sigma^2} \tag{26}$$

As we can see there is a relatively small term which makes the expectation value of the kinetic energy a bit different from what is expected from the classical mechanics, however this term is small as long as the wave function is not sharply localized in the space:

$$\langle K \rangle = K_{classic} + \frac{\hbar^2}{2m\sigma^2} \tag{27}$$

Numerical Results

In this section the numerical results of our FDTD simulation is presented. figure 1 shows the magnitude of the wave function at two distinct time. The solid lines are obtained from FDTD analysis and the circles are corresponding theoretical values derived from (14) using direct numerical integration. The excellent agreement between our FDTD simulation and the theoretical prediction is undeniable.
The normalization condition of the $|\Psi|^2$ has to preserve in time. Total probability of finding the is plotted in figure 2. Obviously this quantity is preserved while the wave packet is inside the integration region. Please note that to clarify the details of the figure **total probability is plotted in** dB **scale**. Maximum relative error is:

$$e_{\max} = \left|P - 1\right|_{\max} \times 100\% \approx 1.65 \times 10^{-4}\% \tag{28}$$

The another quantity that should be preserved in time is the expectation value of the kinetic energy of the particle. As discussed in the previous section it's anticipated that the kinetic energy to be so close to the classical value calculated based on the group velocity of the wave packet. Hhowever there may be a small deviation which is purely quantum mechanical (since it's a quadric function of $\hbar$). Figure 3 shows the expectation value of the kinetic energy (solid line)in time. First, as it can be observed the kinetic energy is a constant of motion and very small fluctuations originate from the numerical errors. The classical prediction is also shown in the same figure (dash line). As it's anticipated from the equation (27) classical value of the kinetic energy is a bit smaller than the the expectation value in the real quantum state. The difference

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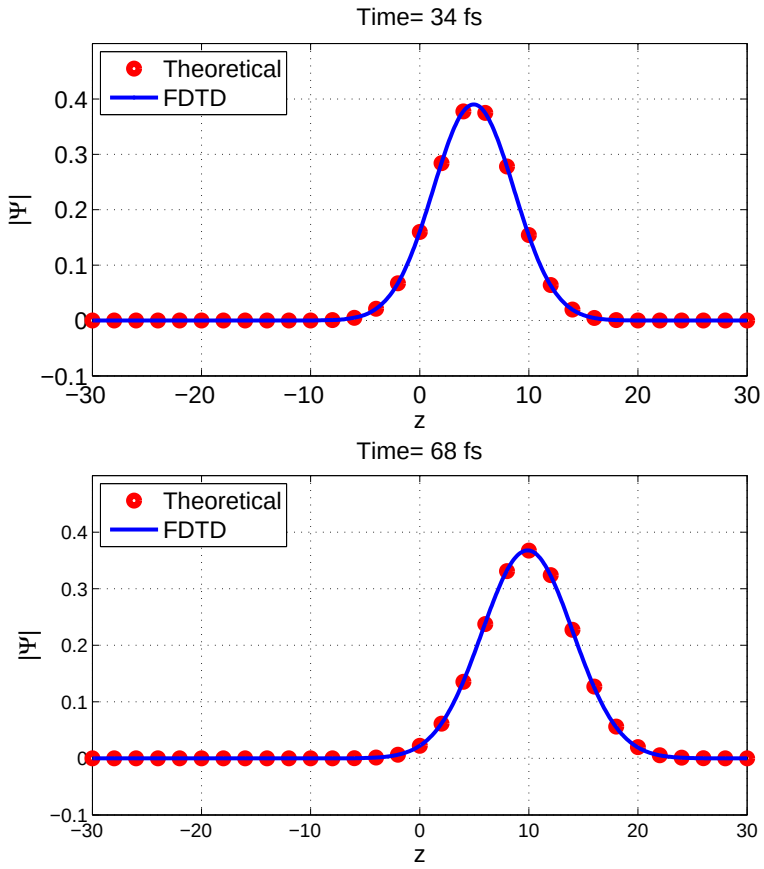

Figure 1: $|\Psi(r,t)|$ for two time steps. The solid lines show our FDTD analysis and the the circles are the theoretical results obtained from (14)

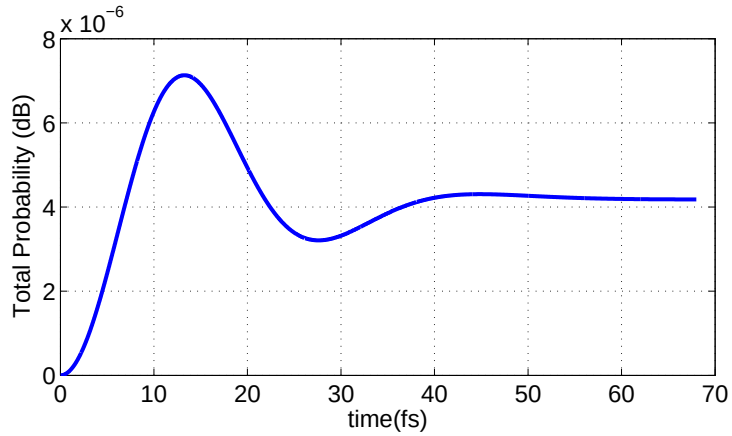

Figure 2: Total probability in dB scale versus time. The normalization condition of the $|\Psi|^2$ is preserved in time.

of these quantities is also plotted in figure 4. Amazingly the difference agrees well with the equation (27). Equation (27) predicts that the difference is:

$$\langle K \rangle - K_{classic} = \frac{\hbar^2}{2m\sigma^2} \approx 0.0015\text{ev}$$

All data on the vertical axis in figure 4 are in the same order of the predicted value.

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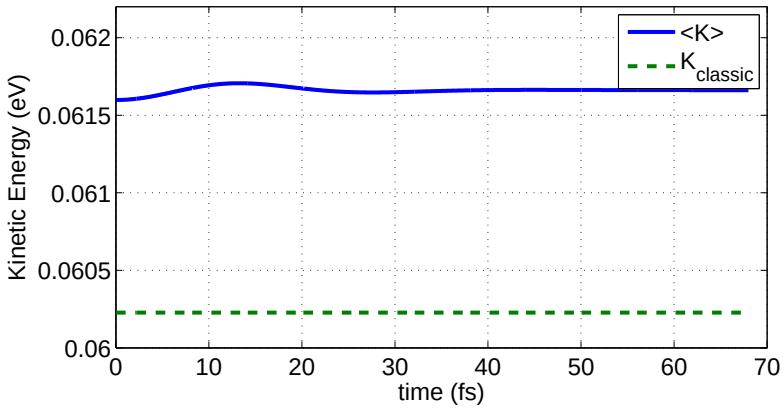

Figure 3: Expectation value of the kinetic energy (solid line) and classically expected value (dash-line).

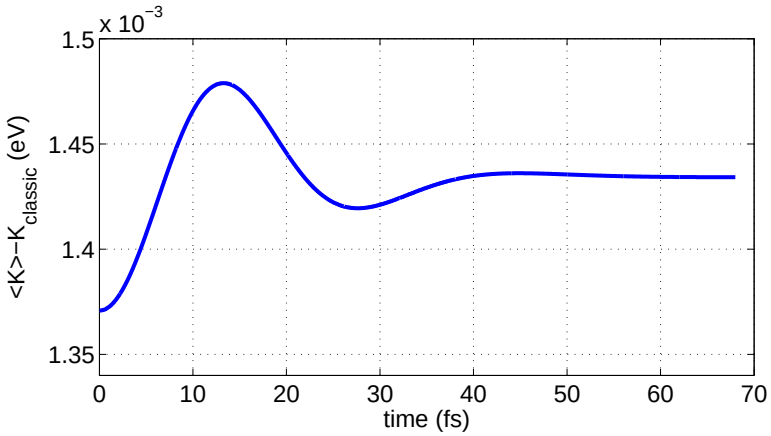

Figure 4: $\langle K \rangle - \frac{1}{2} m v_g^2$

Stability Analysis

Time dicretization Δt is time increment between consecutively calculated wave function in the numerical approach. The choice of Δt is critical is the FDTD simulation. Undoubtedly, computation cost decreases as Δt increases. However it is shown here that there is an upper bound for Δt which ensures stability and prevents numerical error accumulation. As a matter of the fact, the time step should be chosen as a balance between computational cost and stability. Of course , the best time step would be the longer one so that the algorithm stability is maintained [3].
The study of the numerical stability is analytically feasible through the eigenfunction decomposition technique. The wave function can be expressed as a continuous spectrum of the plane-wave functions satisfying Schrödinger's equation. Our numerical scheme determines a specific growth factor the eigenfunction components. In the free space problem plane wave propagating functions (eigenfunctions) are:

$$\widetilde{\Psi}(k,t,z) = \exp\left(i\omega t - kz\right) \tag{29}$$

The discrete version of the Schrödinger's equation can be used to determine the *growth factor* of each wave component. Actually the numerical discretization of the determines the time evolution of the wave components and naturally the eigenfunctions are numerically subject to a special temporal dependence. In this case the time evolution of the plane wave functions can be described by a growth factor (q). The growth

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factor is defined as :

$$q = \exp(j\widetilde{\omega}\Delta t) = \frac{\widetilde{\Psi}(k,(n+1)\Delta t, sz)}{\widetilde{\Psi}(k,n\Delta t, sz)} \tag{30}$$

In above equation $\widetilde{\omega}$ is a complex number which represents the numerical error accumulation in the discrete Schrödinger's equation. The numerical scheme is generally stable if and only if $|q| \leq 1$ for all wave components. If we apply this theory to the couple equations (6) and (7) we get (for free particle):

$$\left(1 - q^{-1}\right) \widetilde{\Psi}_i(k,s,n+0.5) = 2\xi \left[\cos(k\Delta z) - 1\right] \widetilde{\Psi}_r(k,s,n) \tag{31}$$

$$(q-1)\, \widetilde{\Psi}_r(k,s,n) = -2\xi \left[\cos(k\Delta z) - 1\right] \widetilde{\Psi}_i(k,s,n+0.5) \tag{32}$$

To have non-zero solution we should put the determinant of the coefficents to zero:

$$\det \begin{bmatrix} 1-q^{-1} & 4\xi \sin^2\left(\frac{k\Delta z}{2}\right) \\ -4\xi \sin^2\left(\frac{k\Delta z}{2}\right) & q-1 \end{bmatrix} = 0 \Longrightarrow q^2 - 2\alpha q + 1 = 0 \tag{33}$$

wherein

$$\alpha = 1 - 8\xi^2 \sin^4\left(\frac{k\Delta z}{4}\right)$$

To satisfy the stability condition α should varies as:

$$|q| \leq 1 \Longrightarrow |\alpha| \leq 1 \qquad \text{for all } k \tag{34}$$

This constraint leads to the following bound for ξ:

$$\xi = \frac{\hbar \Delta t}{2m(\Delta x)^2} \leq \frac{1}{2} \tag{35}$$

To check the stability condition in our FDTD analysis we first define the energy of the wave function inside the integration region as:

$$P = \int |\Psi(z,t)|^2 \, dz \tag{36}$$

This parameter can be used to show whether the algorithm is stable or not. In the figure (5) P is plotted for four different values of ξ. Vertical axises show P defined in (36) **in dB scale**. Obviously for $\xi = 0.15$ and $\xi = 0.5$ which are below the critical value (0.5) the algoithm is stable but for $\xi = 0.51$ and $\xi = 0.7$ FDTD analysis is conspecuously unstable and diverges.

Absorbing Boundary Condition

A number of techniques have been considered for boundary conditions which would remove spurious reflection from artificial boundaries during the numerical solution of the one-dimensional Schrödinger's equation. For example Kosloff and Kosloff [6] used an enlarged computational domain and then applied a damping in arificial part of the domain to decrease the amplitude of outgoing wave. Although this method can produce good results, the enlarged domain is costly, especially for extensions to higher dimensions. In this project we have implementted Shibata's absorbing boundary condition [5]. This work is based primarily one the work of Enquist and Majd [7] which leads to one-way absorbing boundary conditions for the Schrödinger's equation. From the basic principle of the quantum mechanics k and ω satisfy the dispersion relation:

$$\hbar^2 k^2 = 2m\left(\hbar\omega - V\right) \tag{37}$$

Solving (37) in terms of $\hbar k$, we get:

$$\hbar k = \pm\sqrt{2m(\hbar\omega - V)} \tag{38}$$

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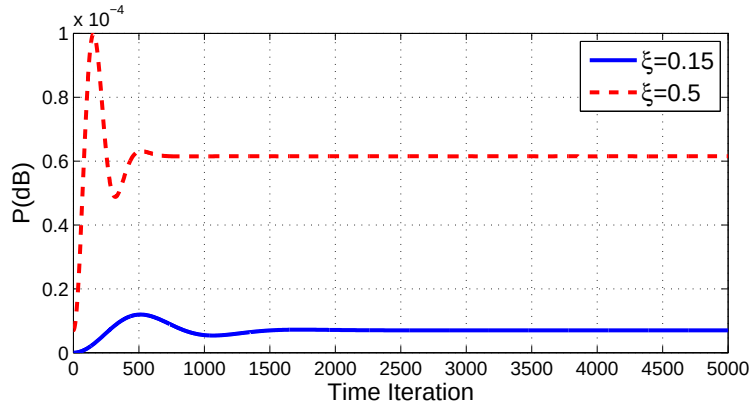
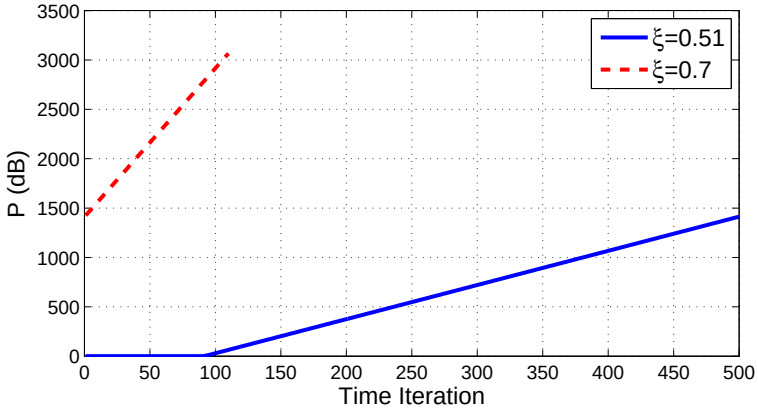


(a)



(b)

Figure 5: (a) Two stable FDTD simulations for $\xi = 0.15$ and $\xi = 0.5$. Both are smaller than the critical value. (b) Two unstable FDTD simulations for $\xi = 0.51$ and $\xi = 0.7$. Both don't satisfy stability condition

In this equation, plus and minus signs means the right going and left-going waves, respectively. Thus, the absorbing boundary conditions should be designed to satisfy the dispersion relation given by the plused-signed equation (38) at the boundary at right and the minus-signed equation (38) at the left boundary. These are the one-way equations for the wave function. Unfortunately, function (38) is not rational and connot be converted into a partial differential equation. We can just make an approximation [5]:

$$\hbar k \approx \pm \frac{\sqrt{2m\alpha_2} - \sqrt{2m\alpha_1}}{\alpha_2 - \alpha_1}(\hbar\omega - V) \pm \frac{\alpha_2\sqrt{2m\alpha_1} -_1 \sqrt{2m\alpha_2}}{\alpha_2 - \alpha_1} \tag{39}$$

where α_1 and α_2 are adjustable parameters. Equation (39) is a straight line interpolation of equation (38), which intersects the dispersion relations at two points. The correspondance of $\frac{\partial}{\partial t} \Leftrightarrow -i\omega$ and $\frac{\partial}{\partial z} \Leftrightarrow ik$ leads us to write this partial differential equation [5]:

$$i\hbar\frac{\partial\Psi(z,t)}{\partial t} = \left[-i\hbar\frac{1}{g_1}\frac{\partial}{\partial z} - \frac{g_2}{g_1}\right]\Psi(z,t) \tag{40}$$

This equation has be written for free particle. In his equation g_1 and g_2 are [5]:

$$g_1 = \pm\frac{\sqrt{2m\alpha_2} - \sqrt{2m\alpha_1}}{\alpha_2 - \alpha_1} \tag{41}$$

$$g_2 = \pm\frac{\alpha_2\sqrt{2m\alpha_1} -_1 \sqrt{2m\alpha_2}}{\alpha_2 - \alpha_1} \tag{42}$$

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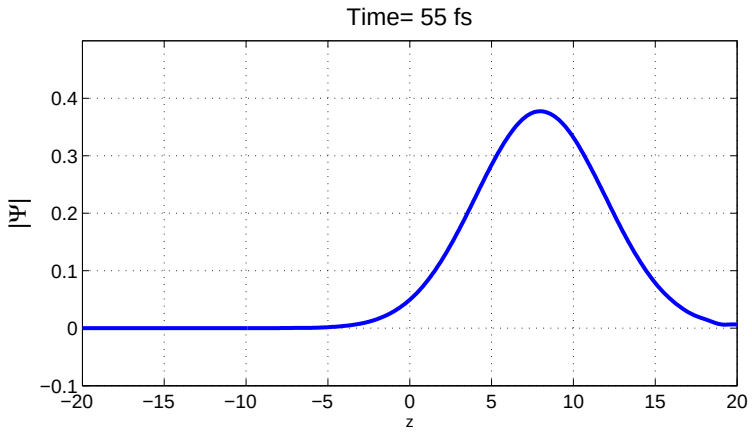
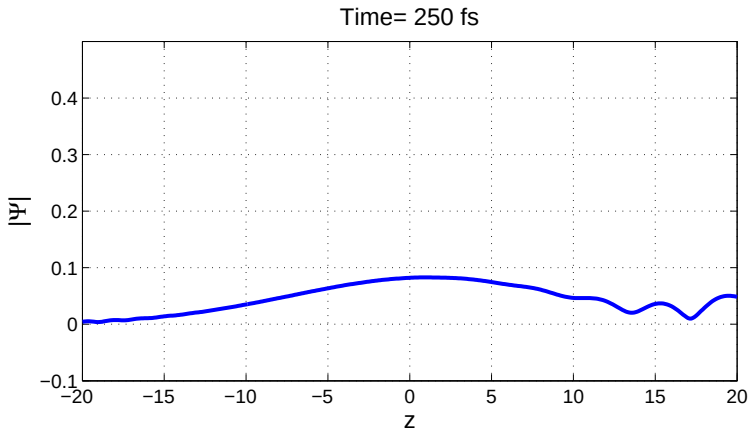
Equation (40) has been implemented in FDTD simulation and the result is plotted here. $\alpha_1 = k_0\hbar/m$ and $\alpha_2 = 10k_0\hbar/m$ are chosen for adjustable parameters.
Figure 6 shows the wave reflection from the boundary. As we can see the wave absorption is not complete however it's acceptable for practical simulations.



(a)



(b)

Figure 6: $|\Psi|^2$ (a) before the wave impinges to the boundary . (b) after reflection

Parameter P defined in (43) is also plotted in Figure 7. This parameter shows how much power reflects back to the region of integration.

$$P = \int_{z_l}^{z_r} |\Psi|^2 \, dz \tag{43}$$

As it's shown in figure 7 energy of wave function is conspicuously reduced after reflection. This shows that the wave has been absorbed by the boundary.

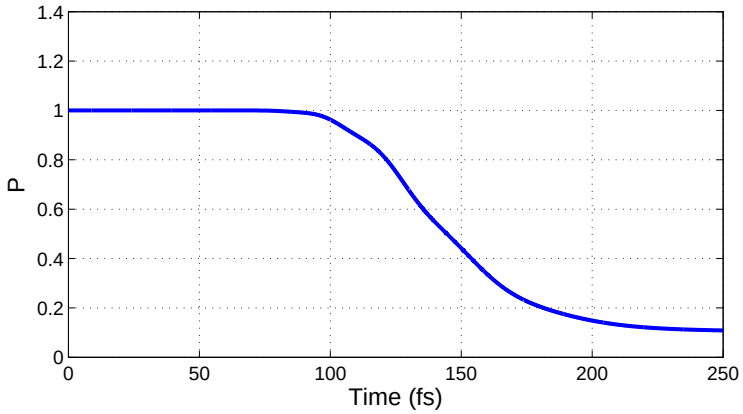


Figure 7: Energy of the wave function inside the region. Total probability (energy) is constant befor impinging to the boundary and reduces after reflection

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