ECE 770-T14/ QIC 885: Quantum Electronics & Photonics

Solution of Problem Set 1, University of Waterloo, Winter 2013

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Problem 1-

a- We start by the following relativistic energy-momentum relationship:

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

Now, we are using the following operators to get the new energy statement using wavefunction notion:

$$\hat{\mathbf{p}} = -i\hbar\nabla \tag{2}$$

$$\hat{E} = i\hbar\frac{\partial}{\partial t} \tag{3}$$

As a consequence, we yield:

$$E^2 = m_o^2 c^4 + \mathbf{p}^2 c^2 \Leftrightarrow \left(i\hbar\frac{\partial}{\partial t}\right)^2 \Psi = \left[\left(-i\hbar\nabla^2\right) c^2 + m_o^2 c^4\right]$$
$$\Leftrightarrow -\hbar^2 c^2 \nabla^2 \Psi + m_o^2 c^4 \Psi = -\hbar^2 \frac{\partial^2 \Psi}{\partial t^2}$$

Whence:

$$\boxed{\nabla^2\Psi - \frac{1}{c^2}\frac{\partial^2\Psi}{\partial t^2} = \frac{m_o^2 c^2}{\hbar^2}\Psi} \tag{4}$$

This is the relativistic Schrodinger equation or Kelin-Gordon equation. Note the second order time derivative in equation (4) rather than first order time-derivative in the Schrodinger equation.

b- In order to get to the probability current continuity equation, we multiply (4) by Ψ^*:

$$\Psi^*\nabla^2\Psi - \frac{1}{c^2}\Psi^*\frac{\partial^2}{\partial t^2}\Psi = \frac{m_o^2 c^2}{\hbar^2}\Psi^*\Psi \tag{5}$$

and the conjugate of the equation (4) by Ψ

$$\Psi\nabla^2\Psi^* - \frac{1}{c^2}\Psi\frac{\partial^2}{\partial t^2}\Psi^* = \frac{m_o^2c^2}{\hbar^2}\Psi\Psi^* \tag{6}$$

one can find the following equation by subtracting (5) by (6):

$$\Psi^*\nabla^2\Psi - \Psi\nabla^2\Psi^* = \frac{1}{c^2}\Big[\Psi^*\frac{\partial^2}{\partial t^2}\Psi - \Psi\frac{\partial^2}{\partial t^2}\Psi^*\Big] \tag{7}$$

Equation (7) can be written as:

$$\nabla\cdot\Big[\Psi^*(\nabla\Psi) - (\nabla\Psi^*)\Psi\Big] = \frac{1}{c^2}\frac{\partial}{\partial t}\Big(\Psi^*\frac{\partial\Psi}{\partial t} - \frac{\partial\Psi^*}{\partial t}\Psi\Big) \tag{8}$$

By multiplying both sides of equation (8) by $\frac{-\hbar}{2im_o}$ and in light of $\nabla\cdot J_p + \frac{\partial}{\partial t}\rho = 0$, one can arrive at:

$$J_p = \frac{\hbar}{2im_o}\Big[\Psi^*(\nabla\Psi) - (\nabla\Psi^*)\Psi\Big] \tag{9}$$

and

$$\rho = -\frac{\hbar}{2im_oc^2}\Big(\Psi^*\frac{\partial\Psi}{\partial t} - \frac{\partial\Psi^*}{\partial t}\Psi\Big) \tag{10}$$

Note that the choice of prefactor is stemming from the fact that the integration of probability current over space should be related to the expectation value of velocity, i.e. $\int J_p(\mathbf{r},t)dV = \frac{<|p(t)|>}{m_o}$. Note that the probability density is quite different from the non-relativistic Schrodinger equation.

Problem 2-

Note that:

$$\hat{\mathbf{p}} = -i\hbar\nabla \tag{11}$$

$$\text{So, } \frac{d\hat{\mathbf{p}}}{dt} = 0 \tag{12}$$

As a consequence, one can write :

$$\frac{d}{dt}\langle\hat{\mathbf{p}}\rangle = \frac{d}{dt}\int \Psi^*\hat{\mathbf{p}}\Psi dr^3 \tag{13}$$

$$= \int \frac{\partial\Psi^*}{\partial t}\hat{\mathbf{p}}\Psi dr^3 + \cancel{\int \Psi^* \frac{d\hat{\mathbf{p}}}{dt}\Psi dr^3} + \int \Psi^*\hat{\mathbf{p}}\frac{\partial\Psi}{\partial t}dr^3 \tag{14}$$

$$= \int \frac{\partial\Psi^*}{\partial t}\hat{\mathbf{p}}\Psi dr^3 + \int \Psi^*\hat{\mathbf{p}}\frac{\partial\Psi}{\partial t}dr^3 \tag{15}$$

Using Schrodinger equation and knowing the fact that potential energy is time-independent, we know that $\frac{\partial\Psi}{\partial t} = \frac{i\hbar}{2m}\nabla^2\Psi - i\frac{V(\mathbf{r})}{\hbar}\Psi$ and $\frac{\partial\Psi^*}{\partial t} = -\frac{i\hbar}{2m}\nabla^2\Psi^* + i\frac{V(\mathbf{r})}{\hbar}\Psi^*$. As a result, we get :

$$\frac{d}{dt}\langle\hat{\mathbf{p}}\rangle = \int \frac{\partial\Psi^*}{\partial t}\hat{\mathbf{p}}\Psi dr^3 + \int \Psi^*\hat{\mathbf{p}}\frac{\partial\Psi}{\partial t}dr^3 \tag{16}$$

$$= -i\hbar\left[\int \Psi^*\left(-\frac{i\hbar}{2m}\nabla^2 + i\frac{V}{\hbar}\right)\nabla\Psi dr^3 + \int \Psi^*\nabla\left(\frac{i\hbar}{2m}\nabla^2 - i\frac{V}{\hbar}\right)\Psi dr^3\right] \tag{17}$$

$$= -i\hbar\int \Psi^*\left[\left(\cancel{-\frac{i\hbar}{2m}\nabla^2} + i\frac{V}{\hbar}\right)\nabla + \nabla\left(\cancel{\frac{i\hbar}{2m}\nabla^2} - i\frac{V}{\hbar}\right)\right]\Psi dr^3 \tag{18}$$

$$= \int \Psi^*\left(V\nabla - \nabla V\right)\Psi dr^3 \tag{19}$$

$$= \int \Psi^* V\nabla\Psi dr^3 - \int \Psi^*\nabla(V\Psi)dr^3 \tag{20}$$

$$= \cancel{\int \Psi^* V\nabla\Psi dr^3} - \int \Psi^*(\nabla V)\Psi dr^3 - \cancel{\int \Psi^* V\nabla\Psi dr^3} \tag{21}$$

$$= \int \Psi^*(-\nabla V)\Psi dr^3 \tag{22}$$

$$= \langle -\nabla V\rangle \tag{23}$$

As a consequence, we can conclude that the expectation value of the momentum behaves like the momentum in classical mechanics, obeying Newtonian mechanics:

$$\boxed{\frac{d}{dt}\langle\hat{\mathbf{p}}\rangle = \langle -\nabla V(\mathbf{r})\rangle = \langle\mathbf{F}\rangle} \tag{24}$$

Problem 3-

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

$$\frac{d}{dt}\int |\Psi(\mathbf{r},t)|^2 dv = \int dv \left(\Psi^* \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t}\Psi\right) \tag{25}$$

Using Schrodinger's equation the right hand side of equation (25) can be simplified. We first decompose Hamiltonian ($\hat{H}$) operator into (Hermitian) ($\hat{H}_0$) and (anti-Hermitian) ($\hat{H}_a$) parts:

$$\hat{H} = \hat{H}_0 + \hat{H}_a \tag{26}$$

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\nabla^2 + V_0 \tag{27}$$

$$\hat{H}_a = -i\Gamma \tag{28}$$

It's straightforwad to show:

$$\Psi^* \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t}\Psi = \frac{1}{i\hbar}\left\{\Psi^* \hat{H}_0 \Psi - \Psi \hat{H}_0 \Psi^*\right\} + \frac{1}{i\hbar}\left\{\Psi^* \hat{H}_a \Psi + \Psi \hat{H}_a \Psi^*\right\} \tag{29}$$

Combining (25) and (29) leads to the following equation:

$$\frac{dP(t)}{dt} = -\frac{2\Gamma}{\hbar}\int |\Psi|^2 \, dv = -\frac{2\Gamma}{\hbar}P(t) \tag{30}$$

Note that the integration of the first term on the right hand side of equation vanishes and just the second term remains. The simple algebraic steps are:

$$\int dv \left\{\Psi^* \left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi - \Psi\left(-\frac{\hbar^2}{2m}\nabla^2 + V\right)\Psi^*\right\} = -\frac{\hbar^2}{2m}\int dv \nabla.\left(\Psi^*\nabla\Psi - \Psi\nabla\Psi^*\right) = 0 \tag{31}$$

b-

The solution of the first order differential equation (30) is simply an exponential function:

$$\frac{dP(t)}{dt} = -\frac{2\Gamma}{\hbar}P(t) \Longrightarrow P(t) = P(0)\exp(-\frac{2\Gamma}{\hbar}t) \tag{32}$$

The life time is $\tau = \dfrac{\hbar}{2\Gamma}$.

Problem 4-

Initial momentum wave function is :

$$\Phi(k) = \begin{cases} A\,(a - |k|) & |k| < a \\ 0 & \text{elsewhere} \end{cases} \tag{33}$$

a-

Momentum space wave function should be normalized so that:

$$\int_{-\infty}^{+\infty} |\Phi(k)|^2\, dk = 1 \tag{34}$$

therefore:

$$|A|^2 \int_{-a}^{a} (a - |k|)^2 dk = 1 \Longrightarrow |A|^2 = \frac{3}{2a^3} \Longrightarrow A = \sqrt{\frac{3}{2a^3}} \tag{35}$$

b-

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

$$\langle (\Delta z)^2 \rangle = \langle (z - \langle z \rangle)^2 \rangle = \langle z^2 \rangle - 2\langle z \rangle \langle z \rangle + \langle z \rangle^2 = \langle z^2 \rangle - \langle z \rangle^2 \tag{36}$$

z acts like an operator in momentum space and we should substitute $z \leftrightarrow i\frac{\partial}{\partial k}$ in k-space. Using this, we can write:

$$\langle z \rangle = \int_{-\infty}^{+\infty} \Psi^*(z) z \Psi(z) dz = \int_{-\infty}^{+\infty} \Phi^*(k) \hat{z} \Phi(k) dk \tag{37}$$

In the above equation $\hat{z} = i\frac{\partial}{\partial k}$, thus:

$$\langle z \rangle = i \int_{-\infty}^{+\infty} \Phi^* \frac{\partial \Phi}{\partial k} dk = 0 \tag{38}$$

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:

$$\langle z^2 \rangle = -\int_{-\infty}^{+\infty} dk \Phi^*(k) \frac{\partial^2 \Phi}{\partial k^2} \tag{39}$$

$$= \Phi^* \frac{\partial \Phi}{\partial k} - \int \frac{\partial \Phi^*}{\partial k} \frac{\partial \Phi}{\partial k} dk \tag{40}$$

$$\frac{\partial^2 \Phi}{\partial k^2} = A\left[\delta(k + a) - 2\delta(k) + \delta(k - a)\right] \tag{41}$$

Combining equations (39) and (41) one obtains:

$$\langle z^2 \rangle = 2 \left| A \right|^2 a \tag{42}$$

and uncertainty in z is:

$$\langle (\Delta z)^2 \rangle = 2a \left| A \right|^2 = \frac{3}{a^2} \tag{43}$$

c-

The calculation of the uncertainty in p is straightforward. we should calculate these integrals:

$$\langle p \rangle = \int_{-\infty}^{+\infty} dk \Phi^*(k) \hbar k \Psi = 0 \tag{44}$$

$$\langle p^2 \rangle = \int_{-\infty}^{+\infty} dk \Phi^*(k) \left(\hbar k \right)^2 \Phi(k) = 2\hbar^2 \left| A \right|^2 \int_0^{+a} dk \left(a^2 k^2 + k^4 - 2ak^3 \right) = \frac{\hbar^2 a^2}{10} \tag{45}$$

Hence:

$$\langle (\Delta p)^2 \rangle = \langle p^2 \rangle - \langle p \rangle^2 = \frac{\hbar^2 a^2}{10} \tag{46}$$

d-

$$\langle (\Delta z)^2 \rangle = \frac{3}{a^2} \quad , \quad \langle (\Delta p)^2 \rangle = \frac{\hbar^2 a^2}{10} \Longrightarrow \quad \sigma_z \sigma_p = \frac{2\sqrt{3}}{\sqrt{10}} \frac{\hbar}{2} > \frac{\hbar}{2} \tag{47}$$

Problem 5-

a-

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

$$i\hbar\frac{\partial\Psi(z,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(z,t)}{\partial z^2} + V(z)\Psi(z,t) \tag{48}$$

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:

$$\frac{\partial\Psi_i(z,t)}{\partial t} = \frac{\hbar}{2m}\frac{\partial^2\Psi_r(z,t)}{\partial z^2} - \frac{1}{\hbar}V(z)\Psi_r(z,t) \tag{49}$$

$$\frac{\partial\Psi_r(z,t)}{\partial t} = -\frac{\hbar}{2m}\frac{\partial^2\Psi_i(z,t)}{\partial z^2} + \frac{1}{\hbar}V(z)\Psi_i(z,t) \tag{50}$$

b-

Now we use the following equation as we need:

$$\frac{\partial}{\partial t}\Psi_r(z,t) = \frac{\Psi_r\big(z,(n+1)\Delta t\big) - \Psi_r(z,n\Delta t)}{\Delta t} \tag{51}$$

$$\frac{\partial^2}{\partial z^2}\Psi_i(z,t) = \frac{\Psi_i\big((s+1)\Delta z, n\Delta t\big) - 2\Psi_i(s\Delta z, n\Delta t) + \Psi_i\big((s-1)\Delta z, n\Delta t\big)}{(\Delta z)^2} \tag{52}$$

With some algebraic manipulation, we arrive at the following equations:

$$\begin{aligned}\Psi_r(s,n+1) &= \Psi_r(s,n) - \xi\Big[\Psi_i(s+1,n+1/2) - 2\Psi_i(s,n+1/2) + \Psi_i(s-1,n+1/2)\Big] \\ &+ \frac{\Delta t}{\hbar}V(s)\Psi_i(s,n+1/2)\end{aligned} \tag{53}$$

$$\begin{aligned}\Psi_i(s,n+3/2) &= \Psi_i(s,n+1/2) + \xi\Big[\Psi_r(s+1,n+1) - 2\Psi_i(s,n+1) + \Psi_i(s-1,n+1)\Big] \\ &- \frac{\Delta t}{\hbar}V(s)\Psi_r(s,n+1)\end{aligned} \tag{54}$$

where

$$\xi \triangleq \frac{\hbar}{2m}\frac{\Delta t}{(\Delta z)^2} \tag{55}$$

Equations (53) and (54) return the value of Ψ at time $(n+1)\Delta t$ from the previous value and surrounding values. Leapfrogging techniques is implemented here by having the real values of the

wavefunction at the integer values of n while the imaginary parts at the half-integer values of n.

c-

It's assumed that the wave function is a Gaussian wave packet at $t = 0$ this wave function evolves in the light of Schrodinger's equation. The initial normalized wave function is:

$$\Psi(z, t = 0) = \left(\frac{2}{\pi\sigma^2}\right)^{\frac{1}{4}} \exp\left(\frac{-(z - z_0)^2}{\sigma^2}\right) \exp\left(\frac{2\pi i(z - z_0)}{\lambda_e}\right) \tag{56}$$

wherein z_0 is the electron's initial position. It is set that $z_0 = 0$ in the simulations. λ_e is the electron de Broglie's wave length. We choose $\Delta z = 0.1\text{nm}$, $\Delta t = 0.02\text{fs}$, $\sigma = \lambda_e = 5\text{nm}$.

The following simulation shows that the object moves 5 nm at 34 fs and 10 nm at 68 fs.

d-

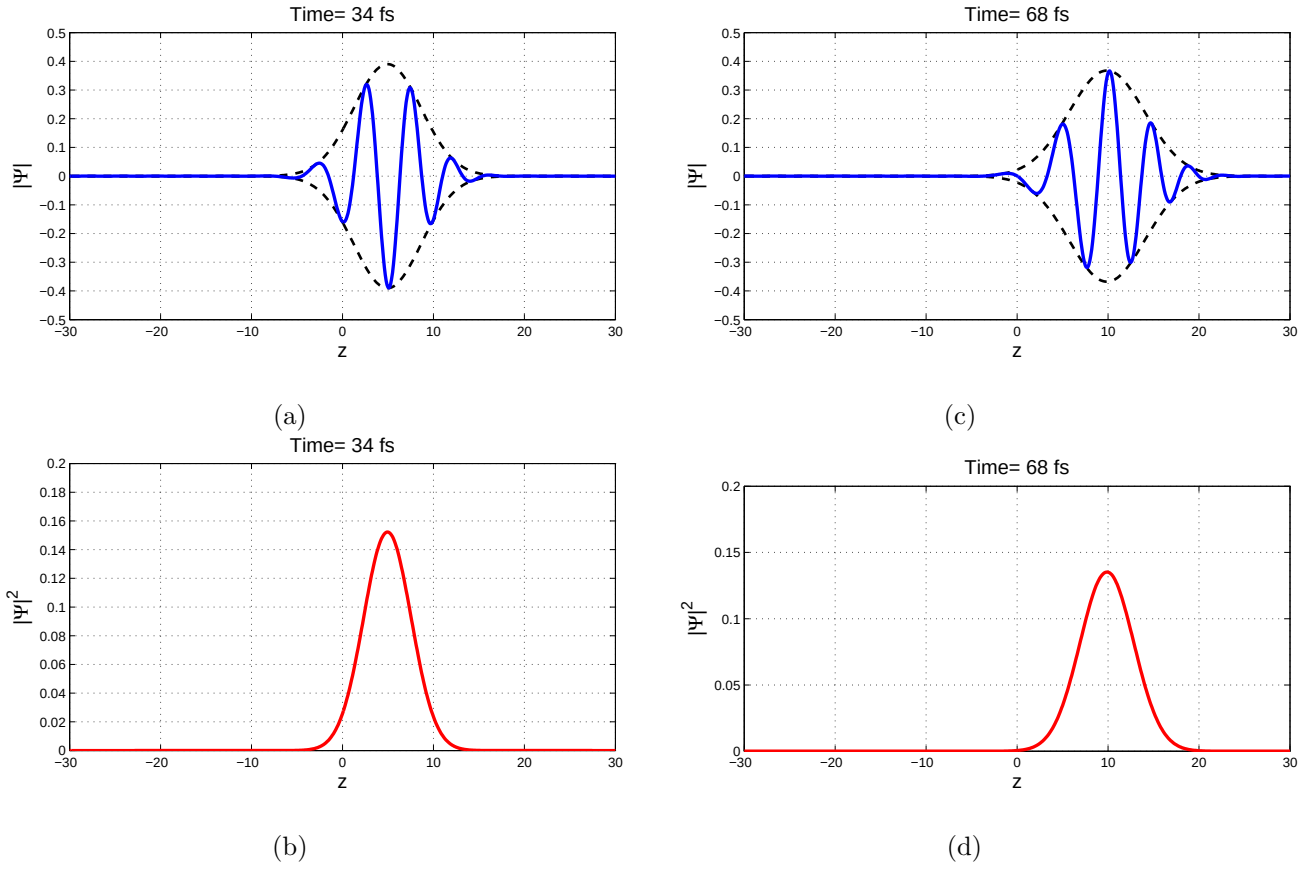


Figure 1: (a) the carrier frequency that is modulated by Gaussian at $t = 34\text{fs}$ (b) $|\Psi(r, t)|^2$ at $t = 34\text{fs}$ (c) the carrier frequency that is modulated by Gaussian at $t = 68\text{fs}$ (d) $|\Psi(r, t)|^2$ at $t = 68\text{fs}$

The expectation value of the **kinetic energy** of the electron can be readily calculated in our FDTD

simulation. The expectation value of the kinetic energy is :

$$\langle K\rangle = -\frac{\hbar^2}{2m}\int_{-\infty}^{+\infty}\Psi^*(z,t)\frac{\partial^2\Psi(z,t)}{\partial z^2} \tag{57}$$

This expression can be numerically implemented as below:

$$\langle K\rangle_{n\Delta t} \approx -\frac{\hbar^2}{2m}\sum_s \Psi^*(s,n)\frac{\Psi(s+1,n)-2\Psi(s,n)+\Psi(s-1,n)}{(\Delta z)^2} \tag{58}$$

$$\Psi(s,n) = \Psi_r(s,n) + i\frac{1}{2}\left[\Psi_i(s,n+1/2)+\Psi_i(s,n-1/2)\right] \tag{59}$$

The expectation value of the kinetic energy is about 0.062 eV based on FDTD calculation.

e-

First the wave function in the momentum space can be evaluated using basic properties of the Fourier transformation:

$$\Phi(k) = \int_{-\infty}^{+\infty}\Psi(z,0)\exp\left(-ikz\right)dz \tag{60}$$

After some simple algebraic steps:

$$\Phi(k) = \left(\frac{\sigma^2}{2\pi}\right)^{\frac{1}{4}}\exp\left[-\frac{(k-2\pi/\lambda_e)^2\sigma^2}{4}\right] \tag{61}$$

The expectation value of the electron's kinetic energy can be determined by the initial momentum-space wavefunction:

$$\langle K\rangle = \int_{-\infty}^{+\infty} dk\frac{\hbar^2k^2}{2m}\left|\Phi(k)\right|^2 = \frac{\sigma\hbar^2}{2m\sqrt{2\pi}}\int_{-\infty}^{+\infty}k^2\exp\left[\frac{1}{2}\sigma^2(k-k_0)^2\right]dk \tag{62}$$

After some simple algebraic steps we get:

$$\langle K\rangle = \frac{\hbar^2k_0^2}{2m} + \frac{\hbar^2}{2m\sigma^2} = \frac{1}{2}mv_g^2 + \frac{\hbar^2}{2m\sigma^2} \tag{63}$$

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:

$$\langle K\rangle = K_{classic} + \frac{\hbar^2}{2m\sigma^2} \tag{64}$$

Note 1- **Stability Analysis**

Time discretization Δt is a successive time increment between two wave functions in the numerical approach. The choice of Δt is critical in the FDTD simulation. Computational cost decreases as Δt increases. However it is shown 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. The best time step would be the longer one so that the algorithm stability is maintained.

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 Schrodinger's equation. A numerical scheme determines a specific growth factor of the eigenfunction components. In the free space problem plane wave propagating function (eigenfunctions) is:

$$\widetilde{\Psi}(k,t,z) = \exp\left(i\omega t - kz\right) \tag{65}$$

The discrete version of the Schrodinger's equation can be used to determine the *growth factor* of each wave component. In this case the time evolution of the plane wave functions can be described by a growth factor (q) that is defined as:

$$q \triangleq \exp(j\widetilde{\omega}\Delta t) = \frac{\widetilde{\Psi}(k,(n+1)\Delta t, s\Delta z)}{\widetilde{\Psi}(k,n\Delta t, s\Delta z)} \tag{66}$$

In above equation $\widetilde{\omega}$ is a complex number which represents the numerical error accumulation in the discrete Schrodinger'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 (53) and (54) we get (for free particle):

$$\left(1-q^{-1}\right)\widetilde{\Psi}_i(k,s,n+1/2) = 2\xi\left[\cos(k\Delta z)-1\right]\widetilde{\Psi}_r(k,s,n) \tag{67}$$

$$(q-1)\,\widetilde{\Psi}_r(k,s,n) = -2\xi\left[\cos(k\Delta z)-1\right]\widetilde{\Psi}_i(k,s,n+1/2) \tag{68}$$

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

$$\det\begin{bmatrix} 1-q^{-1} & 4\xi\sin^2\left(\frac{k\Delta z}{2}\right) \\ -4\xi\sin^2\left(\frac{k\Delta z}{2}\right) & q-1 \end{bmatrix} = 0 \Longrightarrow q^2 - 2\alpha q + 1 = 0 \tag{69}$$

wherein

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

To satisfy the stability condition α should vary as:

$$|q| \leq 1 \Longrightarrow |\alpha| \leq 1 \qquad \text{for all } k \tag{70}$$

This constraint leads to the following bound for ξ:

$$\xi = \frac{\hbar \Delta t}{2m(\Delta x)^2} \leq \frac{1}{2} \tag{71}$$

To check the stability condition in the FDTD analysis one can calculate the probability density of the wave function inside the integration region as:

$$P = \int |\Psi(z,t)|^2 \, dz \tag{72}$$

This parameter can be used to show whether the algorithm is stable or not.

Note 2- **Absorbing Boundary Conditions**

A number of techniques have been considered for boundary conditions which would alleviate spurious reflection from artificial boundaries during the numerical solution of the one-dimensional Schrodinger's equation. For example Kosloff and Kosloff [4] used an enlarged computational domain and then applied a damping in artificial part of the domain to decrease the amplitude of outgoing wave. Although this method can produce reliable results, the enlarged domain is costly, especially for extensions to higher dimensions. Another method is Shibata's absorbing boundary condition [3]. This work is based on the work of Enquist and Majd [5] which leads to one-way absorbing boundary conditions for the Schrodinger's equation. From the basic principle of the quantum mechanics k and ω satisfy the dispersion relation:

$$\hbar^2 k^2 = 2m\left(\hbar\omega - V\right) \tag{73}$$

Solving (73) in terms of $\hbar k$, we get:

$$\hbar k = \pm\sqrt{2m(\hbar\omega - V)} \tag{74}$$

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 plus-signed dispersion equation (74) at the boundary at right and the minus-signed equation (74) at the left boundary. These are the one-way equations for the wave function. Unfortunately, function (74) is not rational and con not be converted into a partial differential equation. We can just make an approximation [3]:

$$\hbar k = \pm\frac{\sqrt{2m\alpha_2} - \sqrt{2m\alpha_1}}{\alpha_2 - \alpha_1}(\hbar\omega - V) \pm \frac{\alpha_2\sqrt{2m\alpha_1} - \alpha_1\sqrt{2m\alpha_2}}{\alpha_2 - \alpha_1} \tag{75}$$

where α_1 and α_2 are adjustable parameters. Equation (75) is a straight line interpolation of equation (74), which intersects the dispersion relations at two points. The correspondence of $\frac{\partial}{\partial t} \Leftrightarrow -i\omega$ and $\frac{\partial}{\partial z} \Leftrightarrow ik$ leads us to write this partial differential equation [3]:

$$i\hbar\frac{\partial\Psi(z,t)}{\partial t}\left[-i\hbar\frac{1}{g_1}\frac{\partial}{\partial z} - \frac{g_2}{g_1}\right]\Psi(z,t) \tag{76}$$

This equation has be written for free particle. In his equation g_1 and g_2 are [3]:

$$g_1 = \pm\frac{\sqrt{2m\alpha_2} - \sqrt{2m\alpha_1}}{\alpha_2 - \alpha_1} \tag{77}$$

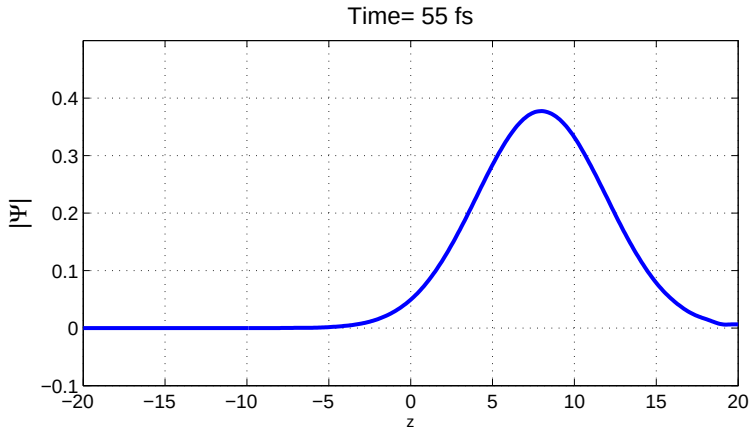
$$g_2 = \pm\frac{\alpha_2\sqrt{2m\alpha_1} - \alpha_1\sqrt{2m\alpha_2}}{\alpha_2 - \alpha_1} \tag{78}$$

Equation (76) 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 2 shows the wave reflection from the boundary. As we can see the wave absorption is not complete however it's acceptable for practical simulations.

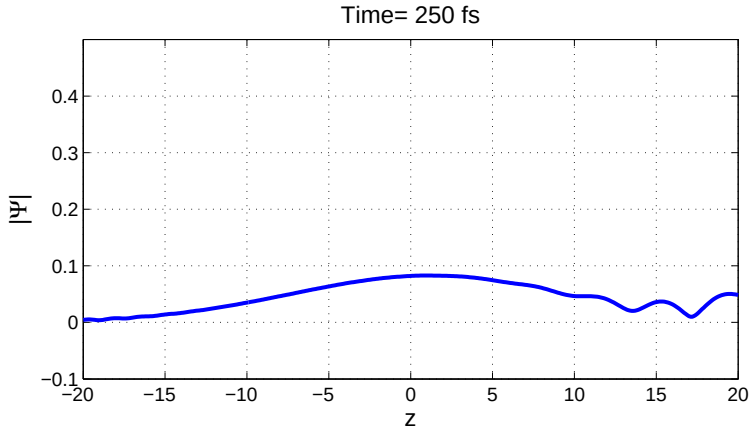
Parameter P defined in (79) is also plotted in Figure 3. This parameter shows how much power reflects back to the region of integration.

$$P = \int_{z_l}^{z_r} |\Psi|^2\, dz \tag{79}$$

As it's shown in figure 3 energy of wave function is conspicuously reduced after reflection. This shows that the wave has been absorbed by the boundary.



(a)



(b)

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

References

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[2] A. Soriano et.al, *Analysis of the finite difference time domain technique to solve the Schrödinger's equation for quantum devices* Journal of App. Phys, vol 95,N 12,2004.

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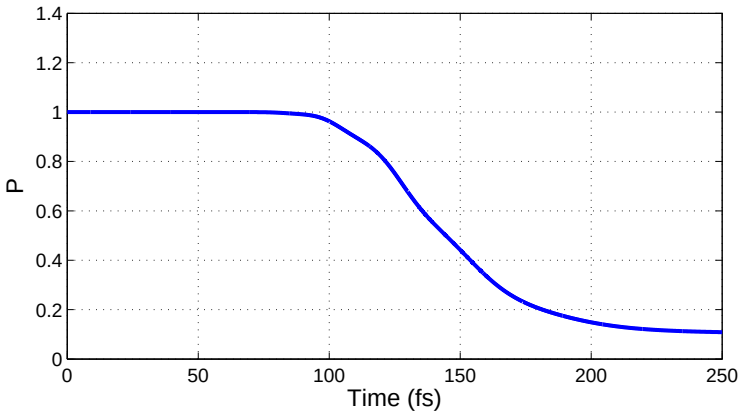

Figure 3: Energy of the wave function inside the region. Total probability (energy) is constant before impinging to the boundary and reduces after reflection

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[5] B. Engquist and A. Majd *Absorbing boundaries for numerical solutions of the waves*. Math of Computation, vol 31, N 139, 1977.