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

Problem Set 1, University of Waterloo, Winter 2013

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Problem 1- (15 marks) Starting from relativistic equation, $E^2 = m_o^2 c^4 + |\mathbf{p}|^2 c^2$, for the energy of a free relativistic object, where m_o is the rest mass, $\mathbf{p}$ is the momentum and c is the speed of light,

a) Derive the Klein-Gordon equation describing the wavefunction of the free particle and compare it with Schrödinger. (5 marks)

b) By setting up the current continuity equation, find the probability current density, $\mathbf{J_p}$ and probability density, ρ. (10 marks)

Problem 2- (10 marks) Calculate the rate of change in the expectation value of a momentum for an elementary object in light of Schrodinger equation.

Discuss the result and show that the expectation value of a momentum in quantum mechanics obey Newtonian laws of classical mechanics. This is the special case of **Ehrenfest's Theorem**.

Problem 3- (15 marks) Consider a physical object that can be fully described by its wavefunction, $\Psi(\mathbf{r}, t)$. Suppose you would like to describe a nonequilibrium situation, in which the object spontaneously disintegrates with a "life time", τ. This situation might occur for a paired electron that is decomposed to one electron due to impulse-type external excitation such as a photon with enough energy. In this case, the probability of finding the object should not be constant but can be modeled to be decreasing with an exponential rate as:

$$P(t) = \int_{-\infty}^{+\infty} |\Psi(\mathbf{r}, t)|^2 dV = \exp(-\frac{t}{\tau}) \tag{1}$$

One way to justify this physical situation is to assign a complex potential energy in the Schrödinger equation, i.e. $V = V_0 - i\Gamma$, where V_0 is a real potential and Γ is a positive potential to model the nonequilibrium situation.

a) Find the rate of the temporal change in the probability, $P(t)$, as a function of Γ. Note that this rate of change in equilibrium reduces to the well-known relation $\dfrac{dP(t)}{dt} = 0$. (10 marks)

b) Solve the equation found in part a) and determine the life time in terms of Γ. (5 marks)

Problem 4- (20 marsk) An object is described by the initial momentum wavefunction $\Phi(k) = A(a - |k|)$ for $|k| \leq a$, and is zero elsewhere, where A and a are real positive parameters.

a) Determine the normalization factor A. (5 marks)

b) Calculate the uncertainty in z.(5 marks)

c) Calculate the uncertainty in p.(5 marks)

d) Check the Heisenberg uncertainty principle by calculating the product of the uncertainties in position and momentum. (5 marks)

Problem 5 (40 marks)- A wave function of an object, i.e. an electron, can be numerically simulated through a *Finite-Difference Time-Domain* (FDTD) technique. Consider the one-dimensional Schrödinger Equation (SE) and decompose the wave function to its real and imaginary parts as $\Psi(z,t) = \Psi_r(z,t) + i\Psi_i(z,t)$.

a)Find the coupled equations relating real and imaginary parts of the wavefunction. (2 marks)

Now discretize the space and time as $z = s\Delta z$ and $t = n\Delta t$ where s and n are integers, i.e. $\Psi(z,t) = \Psi(s\Delta z, n\Delta t) = \Psi^n(s)$.

b) Apply the following difference equations for time-derivative and second space-derivative to the coupled equations found in part a). (3 marks)

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

$$\frac{\partial^2}{\partial z^2}\Psi_i(z,t) = \frac{\Psi_i\big((s+1)\Delta z, n\Delta t\big) - 2\Psi_i(s\Delta z, n\Delta t) + \Psi_i\big((s-1)\Delta z, n\Delta t\big)}{(\Delta z)^2} \tag{3}$$

You may have equations at your disposal that the value of Ψ at time $(n+1)\Delta t$ can be calculated from the previous value and the surrounding values. Notice that the Ψ_r are calculated at integer values of n while Ψ_i are calculated at the half-integer values of n. This represents the *leapfrog* technique between the real and imaginary parts of the wavefunction.

c) Consider an electron traveling in free-space with initial wavefunction

$\Psi(z,t=0) \propto \exp(\frac{-(z-z_0)^2}{\sigma^2})\exp(\frac{2\pi i(z-z_0)}{\lambda_e})$, where z_0 is the electron's initial position and λ_e is the electron de Broglie's wavelength. Using $\Delta z = 0.1$ nm, $\Delta t = 0.02$ femtoseconds (fs), $\sigma = \lambda_e = 5nm$, simulate the motion of the electron in time, specifically plot the presence of the electron after 34 fs and 68 fs in space. (20 marks)

Note 1) The normalization condition of the $|\Psi|^2$ has to preserve in time, so this can be used as a sanity check for your computer program.

Note 2) The choices of the numerical values of Δt and Δz are a bit tricky depending on the problem at hand and stability condition for the FDTD method. In the case of SE, usually the parameter $\frac{\hbar}{2m_e}\frac{\Delta t}{(\Delta z)^2}$ must be small enough, practically less than 0.15.

d) First derive an equation and then compute the expectation value of the kinetic energy of the electron using the developed FDTD method. (10 marks)

e) Compare your results with classical mechanics and justify your numerical simulation. (5 marks)

Due: Wednesday Jan 30, 2013. (before starting the class)