

Chapter 20

Single Particle Quantum Mechanics

20.1 Single Particle Quantum Mechanics for Massive Particles

20.1.1 Introduction

The implications of Planck's and Einstein's inferences when dealing with the interactions of electrons and light were incredibly far reaching. Planck's realization that the structure of the spectrum of the emissions of a black body cavity required that light had a discretely countable constituent that was identified by its energy content which was given by the light's frequency, $\epsilon = hf$, and that these constituent elements were strangely indistinguishable. The person who recognized the far reaching implications of Planck's work was Einstein. He connected Planck's black body processes with any energy exchange processes between electrons and light. He realized that these process could be observed in the photoelectric process described in Section 19.3 on page 423. Analysis of the operation of the photo cell showed that the process of energy transfer from the light to the electrons was local but stochastic in both space and time within the illumination pattern of the light.

It is important to realize that this will not be our final theory of energy and matter. In this section, we are restricting ourselves to the case of low energy processes with a fixed number of massive objects. In fact, our entities are basically light and electrons. These are processes in which the scales of energies are small compared to a few $m_e c^2$ where m_e is the mass of the

electron, see Section 15.2 on page 334. The theory that is applicable at all energies will be constructed using the insights of the few electron low energy models.

20.1.2 Implications of Young's Double Slit with Electrons

From the observation that both light, historically considered a field object, and electrons, historically considered a particle, exhibit interference phenomena in Young's double slit experiment; the patterns of bright and dark occur whether the beam is electrons or light.¹

When dealing with light, we were convinced that this pattern of bright and dark spots of illumination can only be interpreted by having the light be composed of causal agents that add on superposition but can not be directly observable, their squares representing the brightness defined as the energy per unit area per unit time. Light was a field object. Replacing the screen with Einsteinian photo cells and running the system at very low detection rates, the pattern of clicks on the detectors built up ultimately to follow the illumination pattern of the classical Young experiment with the relation $I(x)A = n(x)hf$, where $I(x)$ is the brightness of the light, A is the area of the individual photo cells and $n(x)$ is the number of photons detected at the place x on the screen.

For light, following Maxwell, we can develop an action that produces via the process of minimization Maxwell's equations for the evolution of the light. Since the Maxwell equations are time and space translation symmetric, there are conserved energy and momentum constructs. It is a traveler field and the frequency and wavelength are related by $\lambda = \frac{c}{f}$ where c is the speed of light. This action also will be space and time translation symmetric and thus there has to be a classical momentum and energy. For a beam of light, the classical momentum, p and the classical energy, E of the beam satisfies $p = \frac{E}{c}$. If $p = \frac{E}{c}$ for light and the constituents have an energy content $\epsilon = hf$ then the momentum of each constituent is $p = \frac{hf}{c} = \frac{h}{\lambda}$. Thus since the pattern on the screen is determined by a wavelength for the Einsteinian photodetector case we can say that it is determined by the momentum of the constituents.

¹Actually, it is not true that we can do a Young's double slit experiment with electrons. The electron in this context is a non-relativistic object whereas light is intrinsically relativistic at all energies including the low energies available to Young. The wavelength which we assign to electrons is so small there is no material that could serve as a slitted screen. Regardless, for the sake of simple pedagogy, we will use this gedanken or thought experiment.

For light, Maxwell discovered that the field is the electromagnetic field. Since we have similar patterns for electron or light we need that field construct for electrons which could account for the pattern in our Young's experiment with electron beams and a detector that indicates the presence of an electron. This new causal agent again has to work similar to the one we have for light; it is additive on superposition and it is local. Following the Einstein's interpretation of the process by which the photo cell operates its square is the probability of finding the electron at a place \vec{x} at a time t . The field is designated $\Psi(\vec{x}, t)$.

20.1.3 The Schrödinger Probability Amplitude Field*

The $\Psi(\vec{x}, t)$ field has a local dynamic. The dynamic contains an evolution, a part telling how as time advances the field changes, and the local dynamic which states how this evolution develops from the conditions at any place. The dynamic for particles and, at low energy large mass, appropriate to a low energy electron, is the Schrödinger equation of tee shirt fame² or

$$i\hbar \frac{\partial \Psi}{\partial t}(\vec{x}, t) = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{x}, t) + V(\vec{x}) \Psi(\vec{x}, t). \quad (20.1)$$

This certainly appears to be a rather large leap in technical complications but we are now equipped to at least interpret it since we have been indoctrinated into the mysteries of field theory. Many of the symbols are obvious. m is the mass of the electron. \hbar is $\frac{h}{2\pi}$ where h is Planck's constant. $V(\vec{x})$ is the energy at the place \vec{x} . i is that magic number whose square is -1 . There are three positional dimensions and thus the \vec{x} is our place labels. Of course, Ψ is our field; the amplitude for the measurable probability of the electron being at the place \vec{x} at time t , $n(\vec{x}, t) = \Psi^*(\vec{x}, t) \Psi(\vec{x}, t)$. The idea of the amplitude squared being the measured entity is expanded by the use of the complex number system. The ∇^2 is short hand for $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$. Finally, ∂ is what we have been writing as Δ . In other words, if we reduce our space to one dimension, x , and revert to our notation the tee shirt equation reduces to

$$i\hbar \frac{\Delta \Psi}{\Delta t}(x, t) = -\frac{\hbar^2}{2m} \frac{\Delta}{\Delta x} \left(\frac{\Delta \Psi}{\Delta x} \right) (x, t) + V(x) \Psi(x, t). \quad (20.2)$$

²This is the usual tee shirt example. Actually, there are two fields and two evolution equations. Equation (20.1) has a partner equation that is the equation for the complex conjugate field. Complex conjugation is the process changing all the i to $-i$. For reasons that I do not understand, many physicists act and think that there is only one relevant field in this system.

Except for the magic i , we have seen field dynamics like this one before. The first term in the dynamic contains the construction $\frac{\Delta}{\Delta x} \left(\frac{\Delta \Psi}{\Delta x} \right) (x, t)$. Read directly in our vocabulary, this is the slope of the slope of Ψ at (x, t) . This is what for want of a better name we have called the ‘Bendy’, see 5.3 on page 128 operator on $\Psi(x, t)$. In this sense our dynamic is now

$$i\hbar \frac{\Delta \Psi}{\Delta t}(x, t) = -\frac{\hbar^2}{2m} (\text{Bendy}(\Psi))(x, t) + V(x)\Psi(x, t). \quad (20.3)$$

We can handle the i problem by realizing that this is actually a two field problem and this single evolution equation evolves both of these fields. If we define $\Psi_R(x, t) \equiv \frac{\Psi(x, t) + \Psi^*(x, t)}{2}$ and $\Psi_I(x, t) \equiv \frac{\Psi(x, t) - \Psi^*(x, t)}{2i}$. Both of these fields are real, $\Psi_R^* = \Psi_R$ and $\Psi_I^* = \Psi_I$. The final form of our dynamic is this coupled field dynamic

$$\begin{aligned} -\hbar \frac{\Delta \Psi_I}{\Delta t}(x, t) &= -\frac{\hbar^2}{2m} (\text{Bendy}(\Psi_R))(x, t) + V(x)\Psi_R(x, t) \\ \hbar \frac{\Delta \Psi_R}{\Delta t}(x, t) &= -\frac{\hbar^2}{2m} (\text{Bendy}(\Psi_I))(x, t) + V(x)\Psi_I(x, t). \end{aligned} \quad (20.4)$$

This separation argument is true in any number of spatial dimensions. In other words, the use of the i is a convenient notational tool for combining two real fields into one complex field.

The Schrödinger field is the amplitude for the probability of finding the electron at the place x at time t . The probability of finding the electron at x at time t is the absolute value of the amplitude which in the case of a complex field is

$$n(x, t) = \Psi^*(x, t)\Psi(x, t) = \Psi_R^2(x, t) + \Psi_I^2(x, t). \quad (20.5)$$

We can find the mean position of the electron by multiplying the place x by the probability of the electron being at the place x and summing over all places,

$$\langle x \rangle (t) = \sum_{\text{all places}} x n(x, t) \Delta x \quad (20.6)$$

$$= \sum_{\text{all places}} \Psi^*(x, t) x \Psi(x, t) \Delta x \quad (20.7)$$

$$= \sum_{\text{all places}} x (\Psi_R^2(x, t) + \Psi_I^2(x, t)) \Delta x. \quad (20.8)$$

Beside the convenience of a single evolution equation there is an important symmetry that is at the heart of the nature of quantum mechanics. Any complex $\Psi(x, 0)$ can be replaced by

$$e^{i\theta}\Psi(x, 0) = \sin\theta\Psi_R(x, 0) + i\cos\theta\Psi_I(x, 0) \quad (20.9)$$

and this new field has the same evolution as the original. In our notation, we are saying that initial $\Psi_R(x, 0)$ and $\Psi_I(x, 0)$ that we start with that is consistent with observables like $n(x, 0)$ can be replaced by $\Psi_R(x, 0) = \sin\theta\Psi_R(x, 0)$ and $\Psi_I(x, 0) = \cos\theta\Psi_I(x, 0)$ for any θ and this will not change the physics of the problem. This result is a consequence of the fundamental process for the evolution of massive quantum objects³. It is also the source of the ability to expand computational capabilities as in quantum computation, quantum cryptography, and quantum teleportation.

20.1.4 The Field as a Causal Agent

The idea of Causal Agent was first introduced in Section 6.1 and described in an “Aside” on page 6. The Schrödinger field is the probability amplitude for finding an electron at the position x at time t .

20.1.5 The Magic of Separable Field Configurations

For any field evolution, there are special solutions called separable. These are solutions of the evolution equations that take the form $\Psi(\vec{x}, t) = \Psi_x(\vec{x})\Psi_T(t)$; the field solution $\Psi(\vec{x}, t)$ splits into the product of two functions, $\Psi_x(\vec{x})$ and $\Psi_T(t)$ each of which depend only on the spatial variables and time respectively.

20.1.6 Dimensional Considerations in Single Electron Quantum Mechanics

As expected the Schrödinger equation contains \hbar . The presence of \hbar is the signal that we are dealing with a quantum phenomena. Also since it is the appropriate field for a massive particle. From these two parameters, it is impossible to establish a complete set of measurable constants; a mass

³Note that in Equation 20.1 and its derivative equations you cannot put $m = 0$. Massless particles cannot be described by Schrödinger evolution. The reason is that for those particles there is no non-relativistic domain of motion. Note also that this means that for energetic electrons we cannot use the Schrödinger equation for evolution and must use relativistic quantum field theory, a theory that allows particle creation.

M, a length L and a time T. Of course, $V(x)$ could and likely will contain parameters with a length dimension. Notice that for the free particle, $V(x) = 0$, and thus there is no length or time and, particularly, no velocity and thus the evolution of the system with $V(x) = 0$ is not a pure wave system with travelers independent of the shape of the initial disturbance. The particular case of the localized electron does not have $V(x) = 0$ everywhere but has non-zero potential for all points outside the box. It is hard walled if that potential is very large compared to the energy range of the electron being localized, basically infinite, or soft walled for cases in which the electron can be found outside the box. Also note that $\frac{\hbar}{E} \stackrel{\text{dim}}{=} T$

20.1.7 More than One Low Energy Electron

Our first realization is that the field for the case of m electrons must now be described by a

20.2 Examples

20.2.1 Free Particle

20.2.2 Particle in the box

Another simple system that we can deal with is a localized particle. In the extreme ‘spherical cow’ sense, the ideal particle in an ideal box. Let’s go even one step further by working in one spatial dimension, the real line. It is obvious that if we want to restrict the electron to a segment of the line, we can do so by having $V(x) = \infty$ for all the places outside that region. This will force $\Psi(x, t) = 0$ outside that region and thus $\Psi^*(x, t)\Psi(x, t) = 0$ for all places outside the allowed region. This is the idea of a hard walled box. It can only be considered an approximation to any realistic situation such as an electron localized in an atom. Our purpose here is to show the intrinsic features of quantum systems and using simple confinement protocols to do so. For now, we are also requiring that we have one electron in the box. This requires that the sum on $n(x, t)$ over the length of our box equal 1 for all times since we must find our electron in the box or

$$\sum_0^L n(x, t)\Delta x = \sum_0^L \Psi^*(x, t)\Psi(x, t)\Delta x = \sum_0^L (\Psi_R^2(x, t) + \Psi_I^2(x, t)) \Delta x = 1$$

There are two approaches to this analysis. Have some $\Psi(x, 0)$ that is normalized, $\sum_0^L n(x, t)\Delta x = 1$ and then evolve it forward in time. This

would be the standard field approach. The alternative is to find the separable solutions and use their completeness to represent the original field configuration

