# Part FIVE

## Quantum Mechanics and the Nuclear Structure

from **On the Studies of Physics and Her Axillary Studies** by Shing Hin (John) Yeung

# Chapter 50

# Properties of Schroedinger's Equation

**What is in this chapter?**

Schroedinger's Equation is central to quantum mechanics, while analyses the nature of wave functions on different physical systems.

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## 50.1 Motivation of using Schroedinger's Equation upon Wave-particle Duality

Wave-particle duality links between wave and particle properties of any physical objects. So the particle can be described by a fictitious wavelength $\lambda$. In fact, particles move and this has found Newton's First Law of Motion. If a particle collides with another, it slows down, means of changing magnitude of speed $v$.

Indeed that de Broglie's relation eq. (49.17) in page 270 takes snapshots of $p = mv$, hence only one value of $v$ survives here. If one ought for changing speeds, here is the complication: How may one encounter a wave with different crest-to-crest (or trough-to-trough) distances, hence correlate the observed non-sinusoidal wave for each physical system?

So here comes Schroedinger's Equation.

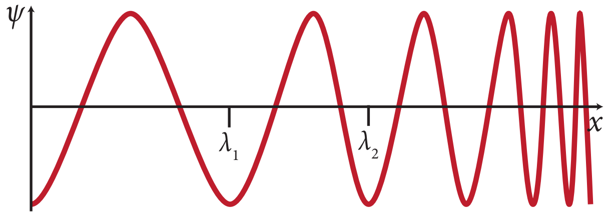


Figure 50.1: Wave functions when the corresponding particle is changing speed. In the graph of wave-function-amplitude versus displacement, the earlier trough-to-trough distance, say $\lambda_1 = \frac{h}{p(\dot{x})}$, is longer than the next one $\lambda_2 = \frac{h}{p(\dot{x})}$. So from eq. (49.17) in page 270, the earlier has a smaller speed than latter. de Broglie's relation cannot say anything of how to encounter this difference since, one value of speed maps to its unique wavelength (or trough-to-trough distance in this case).

## 50.2 Wave Function

Since de Broglie's principle cannot map out wavelengths, what if a spatial map of wave packets (see section 50.2.3)? So that at each spatial point, we know that there might be an electron, for example. In 1926, Erwin Schroedinger published a wave equation that corresponds to de Broglie's principle. Schroedinger Equation has the following format:

$$\hat{\mathscr{H}}\, \psi(\mathbf{r}) = E\, \psi(\mathbf{r}) \tag{50.1}$$

where $\hat{\mathscr{H}}$ is the Hamiltonian operator (or shorten as "Hamiltonian"). While $\psi$ is the solution of the Schroedinger Equation, called **wave function**. Equation (50.1) is called **Time-independent Schroedinger Equation**, and

$$\hat{\mathscr{H}}\,\psi(\mathbf{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) \tag{50.2}$$

namely the **Time-dependent Schroedinger Equation**. Equation (50.2) is essentially a linear partial equation, with $\psi$ as its solution. After Schroedinger invented his Nobel Prize Equation (Nobel Media AB 2014), much discussion are around the solution, and this made more discoveries about our quantum systems.

Meanwhile, wave functions are defined as:

**50.2.1 Definition (Wave Function)**
A wave function is a complex (number) valued probability amplitude which contains the information of quantum states of any physical systems.

Wave functions are denoted as $\psi$, psi in Greek.

## 50.2.1 Mathematical Forms of Wave Functions

The definition definition 50.2.1 raises two (i.e. 2) novel approach:

- complex valued
- probabilistic approach on describing physical systems

The first point is easily understood by means of sinusoidal wave. A sine or cosine curve can be written as a complex exponential function such as

$$\mathrm{e}^{i(k\mathbf{x} - \omega t)} \tag{50.3}$$

or

$$\mathrm{e}^{i\left(\frac{1}{\hbar}\mathbf{p}\cdot\mathbf{x} - \omega t\right)} \tag{50.4}$$

Equations (50.3) and (50.4) are form of travelling waves and we then append a normalisation constant, which is the amplitude of wave functions.

Equations (50.3) and (50.4) are important while interpreting the wave functions in physical space. However, there are no special envelope shapes for those two equations eqs. (50.3) and (50.4), and this is uninteresting. Since, this argues that one may find an electron if she points to anywhere. In fact, electrons likely to stay say, ground state of an atom. Equation (50.3) means of spatial (i.e. $x$) and temporal (i.e. $t$) observables from one quantum state. These solutions are possible to add together, we called this in terms of wave mechanics as **superposition**. Classically, when waves intersect, they are not guaranteed to add the amplitudes higher[1]. Rather at a (spatial or temporal) point:

- When one has positive amplitude while one is negative, when added hence destructing the resultant amplitude (i.e. destructive interference).

[1] It depends on the frequencies of both input waves.

- When both amplitudes are positive or negative, hence enhanced the magnitude of the resultant amplitude at such point (i.e. constructive interference).

This can be corresponded to particle view of physical systems, classically the Young's Double Slit Experiment. While one picked on one point and ask what the intensity could be. The intensity of that spatial point is the sum of two (i.e 2) electric fields from each slits:

$$\mathbf{E}(\mathbf{x}, t) = \mathbf{E}_1(\mathbf{x}, t) + \mathbf{E}_2(\mathbf{x}, t) \tag{50.5}$$

Hence

$$I = |\mathbf{E}(\mathbf{x}, t)|^2 = |\mathbf{E}_1(\mathbf{x}, t)|^2 + |\mathbf{E}_2(\mathbf{x}, t)|^2 + 2\,\mathrm{Re}\,(\mathbf{E}_1{}^* \cdot \mathbf{E}_1) \tag{50.6}$$

Which the last term is due to interference of the two electric fields. We may mimic eq. (50.6) upon the regime of wave functions. Since electric fields mathematically the form of wave-alike, so one may substitute wave function as the electric field as in eq. (50.6), which is $|\psi(\mathbf{x}, t)|^2$. The meaning of $|\psi(\mathbf{x}, t)|^2$ is central to interpreting quantum systems, and we would leave this discussion later.

### 50.2.2 Superposition of Wave Functions

However, there is something that seems more urgent: Superposing wave functions. In a mathematical point of view, one may commit the same. First, we would ask if superposing wave functions would work in Schroedinger Equation, which appears below in Exercise 50.2.1.

**Exercise 50.2.1: Proving that Linear Combinations of Wave Functions fulfils Schroedinger Equation**

Proving that any linear combinations of wave functions, that is

$$\psi(\mathbf{x}, t) = \sum_i c_i\, \psi_i(\mathbf{x}, t) \tag{50.7}$$

where $c_i$ is a constant for each corresponding wave function $\psi_i(\mathbf{x}, t)$. Which $\psi(\mathbf{x}, t)$ still fulfils (time dependent) Schroedinger Equation eq. (50.2).

**Solution:**
By substituting eq. (50.7) into eq. (50.2), we have

$$\sum_k \hat{\mathscr{H}}\, c_i\, \psi_i(\mathbf{r}, t) = \sum_k i\hbar \frac{\partial}{\partial t} c_i\, \psi_i(\mathbf{r}, t) \tag{50.8}$$

So that we ought to use index as $k$ to avoid confusion with imaginary number $i$ above. Equation (50.8) is a consequence of summing the Schroedinger Equations for each individual solutions. Our strategy is to factor eq. (50.8) into the form that a Schroedinger Equation with the solution of $\psi$ in eq. (50.7). Hence,

$$\sum_k \hat{\mathscr{H}}\, c_k\, \psi_k(\mathbf{r}, t) = \sum_k i\hbar \frac{\partial}{\partial t} c_k\, \psi_k(\mathbf{r}, t) \qquad \text{(Original)}$$

$$\sum_k \frac{\hbar^2}{2m}\nabla^2 c_k\, \psi_k(\mathbf{r}, t) + V(\mathbf{r})\, c_i\, \psi_k(\mathbf{r}, t) = \sum_k i\hbar \frac{\partial}{\partial t} c_k\, \psi_k(\mathbf{r}, t) \qquad \text{(Expansion of Hamiltonian operator)}$$

$$\frac{\hbar^2}{2m}\sum_k \nabla^2 c_k\, \psi_k(\mathbf{r}, t) + V(\mathbf{r}) \sum_k c_k\, \psi_k(\mathbf{r}, t) = i\hbar \sum_k \frac{\partial}{\partial t} c_k\, \psi_k(\mathbf{r}, t) \qquad \text{(Factoring the constants)}$$

Where $V(\mathbf{r})$ is irrelevant to the index $k$, hence factorisable.
The differential operators $\nabla^2$ and $\frac{\partial}{\partial t}$ are factorisable here. Where the operators have no preference upon which solution, either acting on the linear combinations or each of the individual solutions. The final result is

$$\frac{\hbar^2}{2m}\nabla^2 \sum_k c_k\, \psi_k(\mathbf{r}, t) + V(\mathbf{r}) \sum_k c_k\, \psi_k(\mathbf{r}, t) = i\hbar \frac{\partial}{\partial t} \sum_k c_k\, \psi_k(\mathbf{r}, t) \qquad \text{(Factoring the operators)} \tag{50.9}$$

Equation (50.7) comes along when substituting the summations, and this is essentially eq. (50.2).

Exercise 50.2.1 make possible to superposing wave functions. The superposition of wave functions is in form of

$$\psi(\mathbf{x}, t) = \frac{1}{\sqrt{(2\pi)^3}} \int \hat{\psi}(\mathbf{k})\, e^{i(k\mathbf{x} - \omega t)}\, d^3 k \tag{50.10}$$

Which

1. the normalisation constant $\frac{1}{\sqrt{(2\pi)^3}}$ allows eq. (50.10) to return to a central value. We will be using $\mathbf{k}_0$ at this time.
2. $\hat{\psi}(\mathbf{k})$ indeed means eq. (50.10) a Fourier Transform. We are transforming the Fourier transform $\hat{\psi}(\mathbf{k})$ to map the wave function in terms of time $t$ and $\mathbf{x}$.

The expansion is aimed for relating the angular momentum $\omega$ and wave vector $\mathbf{k}$.

Integrating eq. (50.10) has an obstacle: The dispersion relation $\omega(k)$ requires attention, since this general function is indecision for integrations. Instead, one may expand the relation, around the central value $k_0$ the magnitude of what was specified, as:

$$\begin{aligned}\omega(k) &\simeq \omega(k_0) + (\mathbf{k} - \mathbf{k}_0) \cdot \nabla_k\, \omega(k)\big|_{k=k_0} \\ &= \omega(k_0) + (\mathbf{k} - \mathbf{k}_0) \cdot \hat{\mathbf{k}} \frac{\mathrm{d}}{\mathrm{d}k}\, \omega(k)\big|_{k=k_0} \\ &= \omega_0 + \frac{(\mathbf{k} - \mathbf{k}_0) \cdot \mathbf{k}_0}{k_0} \left.\frac{\mathrm{d}\omega}{\mathrm{d}k}\right|_{k=k_0}\end{aligned} \tag{50.11}$$

From here, there are three (i.e. 3) points to consider. Firstly, we set $\omega(k_0)$ as a constant $\omega_0$. Secondly, the gradient operator $\nabla_k$ means of differentiating the dispersion relation $\omega(\mathbf{k})$ due to the parameter of $k$. The second line of eq. (50.11) means of the definition of a gradient operator. Which ends in substituting the central value $\kappa_0$ into the unit vector $\hat{\mathbf{k}}$. Finally, term $\frac{\mathrm{d}\omega}{\mathrm{d}k}\big|_{k=k_0}$ is known as the group velocity of the wave function. In classical mechanics, this is the speed where the shape of the wave form travels. In this topic, it means the speed of the wave packet (see section 50.2.3) (Baily 2003). From de Broglie's Principle eq. (49.8), the dispersion relation therefore have its explicit form which relates to the wave number $k_0$ by

$$\begin{aligned}v_0 &= \frac{p_0}{m} \\ &= \frac{\hbar k_0}{m}\end{aligned} \tag{50.12}$$

While in general

$$\omega(k_0) = \frac{\hbar \mathbf{k}^2}{2m} \tag{50.13}$$

or

$$E = \hbar\,\omega(k_0) = \frac{(\hbar \mathbf{k})^2}{2m} \tag{50.14}$$

For wave vector $\mathbf{k} \cdot \mathbf{x}$ around the central value $\mathbf{k}_0$. One may expand it into a vector addition:

$$\mathbf{k} \cdot \mathbf{x} = (\mathbf{k} - \mathbf{k}_0) \cdot \mathbf{x} + \mathbf{k}_0 \cdot \mathbf{x} \tag{50.15}$$

The final product of expansions is

$$\psi(\mathbf{x}, t) = \frac{1}{\sqrt{(2\pi)^3}} \mathrm{e}^{i(\mathbf{k}_0 \cdot \mathbf{x} - \omega_0 t)}\, \mathscr{A}\left(\mathbf{x} - \hat{\mathbf{k}}_0 v_0 t\right) \tag{50.16}$$

where

$$\mathscr{A}\left(\mathbf{x} - \hat{\mathbf{k}}_0 v_0 t\right) = \int \hat{\psi}(\mathbf{k})\, \mathrm{e}^{i(\mathbf{k} - \mathbf{k}_0)\left(\mathbf{x} - \hat{\mathbf{k}}_0 v_0 t\right)}\, \mathrm{d}^3 k \tag{50.17}$$

eq. (50.16) is produced after the substitution of eqs. (50.11) and (50.15). Where the particle (i.e. left) and quantum wave (i.e. right) informations are therefore separated.

### 50.2.3 Wave Packet

The superposition of wave functions leads to a term of wave packets. A wave packet is a short burst which a wave with localised envelope emitted. Which is desirable for particle-like structures, so that we have a spatial point that is more probable to find the particle we after.

In order to find the (furthermore) explicit form of eq. (50.16), which is to compute eq. (50.17). The Fourier transform function $\hat{\psi}$, must normalise with when intersect with its conjugate function $\psi$. Given from the hint of Fourier transform, if $\psi$ has a form of

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int \hat{\psi}(k) \mathrm{e}^{i(kx - \omega t)}\, \mathrm{d}k \tag{50.18}$$

then $\hat{\psi}$ has a form of

$$\hat{\psi}(k) = \frac{1}{\sqrt{2\pi}} \int \psi(x, t) \mathrm{e}^{i(kx - \omega t)}\, \mathrm{d}x \tag{50.19}$$

At $t = 0$, the initial time, the wave function is assumed to have form as a Gaussian wave packet such that

$$\psi(x, t = 0) = \alpha\, \mathrm{e}^{-\frac{x^2}{2b^2}}\, \mathrm{e}^{i k_0 x} \tag{50.20}$$

where $\alpha$ is a constant defined as

$$\alpha = \frac{1}{\sqrt{b \sqrt[4]{\pi}}} \mathrm{e}^{i \varphi_\alpha} \tag{50.21}$$

for the sake of normalisation. The width of the wave packet initially is

$$2b\sqrt{\ln 2} \tag{50.22}$$

The generalisation into the temporal regime is therefore,

$$\psi(x,t) = \frac{\alpha\, b}{\sqrt{b^2 + \frac{i\hbar t}{m}}}\, \mathrm{e}^{\frac{x^2}{2\left(b^2 + i\frac{\hbar t}{m}\right)}}\, \mathrm{e}^{i\frac{k_0 x - \frac{\hbar k_0^2 t}{2m}}{1 + i\frac{i\hbar t}{mb^2}}} \tag{50.23}$$

and this is cumbersome to remember. However, the absolute square of the wave function is easier to analyse.

$$|\psi(x,t)|^2 = \frac{|\alpha|^2}{\sqrt{1 + \frac{\hbar^2 t^2}{m^2 b^4}}}\, \mathrm{e}^{\frac{\left(x - \frac{\hbar k_0 t}{m}\right)^2}{b^2\left(1 + i\frac{\hbar^2 t^2}{m^2 b^4}\right)}} \tag{50.24}$$

The reason for eq. (50.24) would become easier to analyse is if we suppose the wave packet is now defined in the momentum space. We now then use the phase velocity defined as $\frac{\hbar k_0}{m}$, in which the wave packet is moving at this velocity. Next, use eq. (50.21) and hence derive

$$|\alpha|^2 = \frac{1}{b\sqrt{\pi}} \tag{50.25}$$

The width of the wave packet in the coordinate space is

$$b\sqrt{1 + \frac{\hbar^2 t^2}{m^2 b^4}} \tag{50.26}$$

or while in momentum space it is a constant of

$$\frac{1}{b} \tag{50.27}$$

## 50.3 Expectation of Observables

Given that the wave packets are in Gaussian Distribution, then there must be the peak which is its expected value. In terms of Physics, it is said that the expected location to find the particle is the mean point. Recall that

$$\langle X \rangle = \int x\, f_X(x)\, \mathrm{d}x \tag{50.28}$$

and the notation of expected value $\langle X \rangle$ is related to the bra-ket notation.

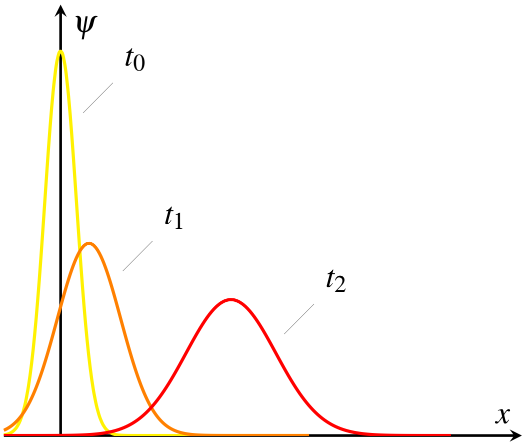


Figure 50.2: Wave packets will flatten out in long term. The initial wave packet we were interested namely $t_0$, then $t_1$ and $t_2$. The width of $t_0$ has the form of eq. (50.22), and from what eq. (50.26) states that the width of the wave packets are enlarging. The normalisation constraint means the peak of the wave packet is falling.

### 50.3.1 Expectation of Position

Suppose a wave packet is moving, as per eq. (50.26) states. Wave packets spreads out on the run, while the wave packet is travelling at the group speed $v$. The expectation of the wave packet, is the expectation value of the Gaussian curve, which is its peak as well. In order to compute the expectation value of the position (of the wave packet), which is

$$\langle X \rangle = \int x \left| \psi \left( x, t \right) \right|^2 \mathrm{d}x \tag{50.29}$$

Since the squared wave function $\left| \psi \left( x, t \right) \right|^2$ is a general function of the variable of interest $x$. There is no explicit form when computing the integral eq. (50.29) directly. However, we knew a hint which is the wave packet travels in the group velocity $v$. While $vt$ constitutes the dimension of the position $x$, we may do the trick of cancellation on the variable $x$, so

$$\langle X \rangle = \int \left( x - vt \right) \left| \psi \left( x, t \right) \right|^2 \mathrm{d}x + \int vt \left| \psi \left( x, t \right) \right|^2 \mathrm{d}x \tag{50.30}$$

The first term in eq. (50.30) is vanished since the position $x$ is equivalent to the product term $vt$, hence it is a term of integrating zeros. The latter term is independent to the integrating variable. Hence we may separate the term $vt$ from the integral

$$\langle X \rangle = vt \int \left| \psi \left( x, t \right) \right|^2 \mathrm{d}x \tag{50.31}$$

and the integral means one (i.e. 1). Hence the expectation value of position $\langle X \rangle$ is

$$\langle X \rangle = vt \tag{50.32}$$

Which is one of the kinetic equations in Classical Mechanics.

# Bibliography

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# Appendix 50.A Working Diary

## 50.A.1 04/12/2016

Aim: What is SE and the properties of solutions that fulfils SE.

## 50.A.2 16/12/2016

Continue from Wave-particle duality and set the foundation of SE. Which explains why we should move on from de Broglie's theory.

## 50.A.3 01/01/2017

Made a breakthrough in the new year. Section 50.2.1 is extended from eq. (50.3), and referenced through Scheck (2013).

## 50.A.4 04/01/2017

Still doing the section 50.2.1.

## 50.A.5 06/01/2017

Section 50.2.2 is a separation from section 50.2.1, while the heading is resumed from what I have proposed in 16 December 2016.

Started section 50.2.3.

### 50.A.6 19/01/2017

Finished section 50.2.3, although I just put the equations from Scheck (2013). Haven't understand them fully yet, maybe after this sem?

### 50.A.7 01/02/2017

Started section 50.3. The equation of expectation value comes from eq. (37.6), in which the Hilbert Space is continuous.

### 50.A.8 13/02/2017

Started section 50.3.1.

## Appendix 50.B Selected Readings and their Reviews

## Appendix 50.C Connections to Other Topics

## Appendix 50.D Documentations