

---

# Quantum Notes

*Release 1.38*

**Lei Ma**

February 04, 2014



## CONTENTS

<b>1</b>	<b>Introduction</b>	<b>3</b>
<b>2</b>	<b>Table of Contents</b>	<b>5</b>
2.1	Vocabulary . . . . .	5
2.2	Approximation Methods . . . . .	5



Some notes for quantum



## INTRODUCTION

Some notes continued from the full theoretical physics notes are [here](#).





## TABLE OF CONTENTS

## 2.1 Vocabulary

Vocabulary of physics, the fountain of research ideas.

### 0. Fine Structure Constant

$$\alpha = \frac{k_e e^2}{\hbar c} = \frac{1}{(4\pi\epsilon_0)} \frac{e^2}{\hbar c} = \frac{e^2 c \mu_0}{2\hbar}$$

In electrostatic cgs units,  $\alpha = \frac{e^2}{\hbar c}$ .

In natural units,  $\alpha = \frac{e^2}{4\pi}$ .

### 1. Hydrogen Atom

$$\text{Potential } V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r}.$$

$$\text{Energy levels: } E_n = -\left(\frac{Z^2 \mu e^4}{32\pi^2 \epsilon_0^2 \hbar^2}\right) \frac{1}{n^2} = -\left(\frac{Z^2 \hbar^2}{2\mu a_\mu^2}\right) \frac{1}{n^2} = \frac{\mu c^2 Z^2 \alpha^2}{2n^2}.$$

$$\text{Ground state of hydrogen atom } \psi_{100}(r) = \frac{1}{\sqrt{\pi}} \frac{1}{a^{3/2}} e^{-Zr/a}.$$

## 2.2 Approximation Methods

### 2.2.1 Variational Method

#### Trial functions

1.  $\psi(x) = \cos \alpha x$ , for  $|\alpha x| < \pi/2$ , otherwise 0.
2.  $\psi(x) = \alpha^2 - x^2$ , for  $|x| < \alpha$ , otherwise 0.
3.  $\psi(x) = C \exp(-\alpha x^2/2)$ .
4.  $\psi(x) = C(\alpha - |x|)$ , for  $|x| < \alpha$ , otherwise 0.
5.  $\psi(x) = C \sin \alpha x$ , for  $|\alpha x| < \pi$ , otherwise 0.

Why don't we just use a most general variational method to find out the ground state? Because we will eventually come back to the time-independent Shrodinger equation.

Suppose we have a functional form

$$E(\psi^*, \psi, \lambda) = \int dx \psi^* H \psi - \lambda \left( \int dx \psi^* \psi - 1 \right)$$

The reason we have this Lagrange multiplier method is that the wave function should be normalized and this multiplier provides the degree of freedom. We would only get a wrong result if we don't include this DoF.

Variation of  $\psi^*$ ,

$$\delta E = \int dx \delta \psi^* H \psi - \int dx \delta \psi^* \psi = 0$$

Now what?

$$H\psi - \lambda\psi = 0$$

Not helpful.

## 2.2.2 Variational Method and Virial Theorem

For a potential  $V(x) = bx^n$ , we can prove that virial theorem is valid for ground state if we use Gaussian trial function  $e^{-\alpha x^2/2}$ .

A MMA proof is here.

## 2.2.3 WKB

This is a semi-classical method. It is semi classical because we will use the classical momentum

$$\hbar k(x) = \sqrt{2m(E - V(x))}$$

The following points are important for this method.

0. WKB start from a classical estimation of wave number at a certain energy  $E$  which is later quantified by the Bohr-Sommerfeld quantization rule.
1. Conservation law:

$$\frac{\partial}{\partial t} \rho + \nabla \cdot \vec{j} = 0$$

where  $\rho = \psi^* \psi$ ,  $\vec{j} = -\frac{\hbar}{2mi} (\psi \nabla \psi^* - \psi^* \nabla \psi)$ . This can be derived from Shrodinger equation easily.

2. Phase: Wave function is generally  $A(x) \exp(\phi(x))$ . However,  $\phi(x)$  should be the area of the phase function starting from some initial point. For example in WKB,  $k(x) = \phi'(x)$  and  $\phi(x) = \int \phi'(x') dx' = \int k(x') dx'$ .

Using this general wave function and conservation law we find out that  $A(x) \propto \frac{1}{\sqrt{k(x)}}$ . Then we can apply the two boundary conditions. However we will find two different wave functions given by two boundary conditions. Now we should connect them because  $\psi(a) = \psi(b)$  exactly. By comparing the two wave functions we can find something like Bohr-Sommerfeld quantization rule.

3. Correction at boundary: However, this method requires that the potential varies slowly or equivalently the wave number varies slowly. Basically we are just using the following approximation:

$$A'(x) = 0, k'(x) = 0$$

For example when taking the derivative of wave function,

$$\psi'(x) = A'(x)e^{i\int \dots} + A(x)k(x)e^{i\int \dots} \approx A(x)k(x)e^{i\int \dots}$$

where we drop the term with  $A'(x)$ . That is to say

$$|A'| \ll |Ak| \Rightarrow |k'| \ll k^2$$

But at boundary where  $E = V$ , this is obviously not valid because  $k = 0$ . So we need to fix this problem.

The solution is to use first order of the potential in a Taylor expansion. Then solve the problem exactly. Finally we connect regions that is far out from the boundary, need the boundary and between the boundary.

If we can have a good boundary condition, then the energy spectrum given by WKB can be very good. Even we don't have a good boundary condition, the excited states given by this method are always close to the exact ones.

---



---

This open source project is hosted on GitHub: [quantum](#) .

[Latest PDF here](#).