
Quantum Notes

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Lei Ma

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Some notes for quantum

INTRODUCTION

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

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2.1 Vocabulary

Vocabulary of physics, the fountain of research ideas.

0. Fine Structure Constant

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

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

Some of the calculable 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.

Procedure

1. Pick a trial function.

Note: How to pick a trial function? For ground state energy, we should pick a function that has the same property as the real ground state. This requires some understanding of the problem we are dealing with.

Things to consider:

- (a) The new problem is just a modification of a known solved problem. Then we can easily find out what really is different and interpret the new problem in terms of the old one.
 - (b) If the Hamiltonian have definite parity, the ground state wave function should pick up some parity which is usually even to make it the lowest energy.
 - (c) Continuous function? A C^∞ Hamiltonian can only have continuous functions as solutions for a finite system.
 - (d) Nodes determines the kinetic energy so check the nodes for ground state wave function.
 - (e) Check the behavior of the wave function at different limits. In most cases, the Schrödinger equation can be reduced to something solvable at some limits.
 - (f) **One more thing, the trial function should make the problem calculable.**
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Why Not General Variational Method

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 Schrödinger 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 ψ^* ,

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

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.

Virial theorem is pretty interesting. It shares the same math with equipartition theorem.

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 Schrödinger 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, near 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](#).

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