Quantum Notes

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Some notes for quantum

CHAPTER

ONE

INTRODUCTION

Some notes continued from the full theoretical physics notes are here.

CHAPTER

TWO

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2.1 Vocabulary

Vocabulary of physics, the fountain of research ideas.

0. Fine Structure Constant

:math:‘ alpha = frac{k_mathrm{e} e^2}{hbar c} = frac{1}{(4 pi varepsilon_0)} frac{e^2}{hbar c} = frac{e^2 c mu_0}{2 h}‘

In electrostatic cgs units, :math‘alpha = frac{e^2}{hbar c}‘.

In natural units, :math:‘ alpha = frac{e^2}{4 pi}‘ .

1. Hydrogen Atom

Potential $V(r) = -fracZe^2 4\pi\epsilon_0 r$.

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

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 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.

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 $A(x)$ $\frac{1}{\sqrt{k(x)}}$. 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 bouldary: However, this method requires that the potential varies slowly or equivalently the wave number varies slowly. Basicly we are just using the following approximation:

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

For example when taking the derivative of wave function,

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

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 condtion, 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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