

Guided Study Log on Quantum Mechanics

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Abstract

This is a record of my Guided Study on Quantum Mechanics during the 2022 fall semester, under the supervision of Prof. Hui Pak Ming. My studies contains the most part of the PHYS3021 and some part of PHYS3022 in CUHK, both of which are taught by Prof. Hui.

Note: Prof. Hui has given some typical problems, which have highly programmed, step-by-step recipes. Their positions are:

1. Recipe 1: General Initial Value Problems in Quantum Mechanics
2. Recipe 2: Think classically first, then go quantum

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1 PHYS3021

1.1 chapter 1

Chapter 1 has been skipped.

1.2 chapter 2

This chapter is about **how to connect the wave** presented in Chapter 1 **to our real world**. In my first time touching the Quantum Mechanics, I found it messy about the **FORMALISM** part. They seemed to be too abstract than the actual cases in TISE part, but without an understanding of it, I found the things became harder and harder in the later studies of QM. I need lots of time to memorize those properties, which is not a "natural" thing for me. After learning from Prof. Hui, I found this chapter is about connecting the real world(the measurement, the observations) and the theory. And surprisingly, we could find everything in the **FORMALISM** part have a real world corresponding.

1.2.1 Why we need a complex form wave function?

One thing the following pdf have not introduced is the necessity of a complex form wave function. Actually there are also some work have shown that it is possible to only use real number to simulate quantum system [1].

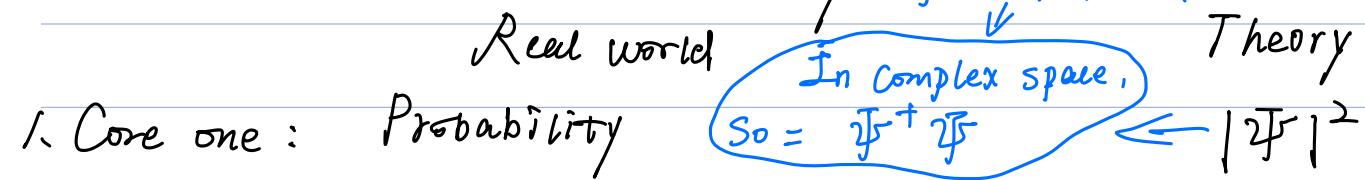
But some experiments have shown that complex number could simulate the quantum system better [2]:

1. From academic view, Bell game under photonic and the superconducting environments have been carried out to test the performance of complex and real players. Both of the environments have shown that complex performs better than real.
2. From industry view, new work points to there being real advantages to developing protocols for quantum networks based on complex-valued, instead of real-valued, quantum theory.

Chapter 2 How to connect the "wave" to our real world?

Namely the interpretation of "wave function"

So this chapter is all about finding corresponding relations between the two: Real world , and Theory Definition in math!



But why in Complex space? See the text part before this pdf page

1.1 The probability in a certain position (x, y, z) $|\bar{\psi}|^2$ is single at some time t is certain value

1.2 Same reason as 1.1, if $\bar{\psi}$ is not continuous $|\bar{\psi}|^2$ is continuous at some position, it would have 2 probabilities at this position, which conflicts the single-value principle.

1.3 Probability needs to have a sum = 1 among Normalization:
the whole available space $\int |\bar{\psi}|^2 d\tau = 1$

1 is the core one, telling us Probability = $|\bar{\psi}|^2$.

and 1.1 - 1.3 are deduced by the inner properties of probability

But since it is a statistical problem (probability),

it is easy to think of what we could do use the probability .

And they are the following two things , 2 and 3, expectation value and variance. Why we put "expectation" before "variance"?

Still based on statistical knowledge, we could use expectation to calculate variance.

$$\begin{aligned} \text{Here comes : Variance of } x = \sigma^2 &= E \left[[x - E(x)]^2 \right] = E [x^2 + E^2(x) - 2x E(x)] \\ &= E(x^2) + E(x)E(x) - 2E(x)E(x) = E(x^2) - E(x)E(x) = \langle x^2 \rangle - \langle x \rangle^2 \end{aligned}$$

Real World

Theory

2. Expectation Value

$$\langle \hat{A} \rangle = \int \bar{\psi}^* \hat{A} \psi d\tau$$

I know that usually we write it as $\int \bar{\psi}^* \hat{A} \psi d\tau$, but based on the definition of Hermitian operator, it seems more suitable to use $\bar{\psi}^*$ and just regard the $\int \bar{\psi}^* \hat{A} \psi d\tau$ form is the special case under the differential form of QM. But under Matrix form, to make sure the Matrix multiplication could be down, we need to use "+" rather than "*"
 $(m_A, n_A) (m_B, n_B)$ $A \times B$, then $n_A = m_B$ is needed.

2.1 Expectation of a physics quantity
should be a real number

The operator of a physics quantity should be Hermitian

$\int \bar{\psi}^* \hat{A} \psi d\tau$ needs to be real, that is

$$\underbrace{\int \bar{\psi}^* \hat{A} \psi d\tau}_{\text{||}} = (\int \bar{\psi}^* \hat{A} \psi d\tau)^+$$

$$\downarrow \quad (\int \bar{\psi}^* \hat{A}^T (\hat{A}^*)^T \psi d\tau)^*$$

The only difference

$$\text{is } \hat{A} \rightarrow \hat{A}^T \quad \leftarrow \underbrace{\int \bar{\psi}^* A^T \psi d\tau}_{\text{||}}$$

So $\hat{A} = \hat{A}^T \Rightarrow \int \bar{\psi}^* \hat{A} \psi d\tau$ is real

Besides, it is real under any wave functions $\Rightarrow \hat{A} = \hat{A}^T$

As a result, the two are equivalent, and we give a name to this property ($\hat{A} = \hat{A}^T$), Hermitian Operator

Real World

3. Variance

Theory

Since we have expressed variance

in terms of expectation, and we also give the solution of expectation, we could calculate variance

3.1

During the experiments, we found the uncertainty relation, that is, the multiplication of two physics quantities' standard variance have to be larger than a certain positive constant. In the case of x and p , we have

$$(\Delta x)(\Delta p) \geq \frac{1}{2}\hbar$$

Generalized Uncertainty:

$$(\Delta A)(\Delta B) \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle|$$

reason would be explained
in later chapter

$$\text{For } \hat{x} \text{ and } \hat{p}, [\hat{x}, \hat{p}] = i\hbar$$

$$(\Delta x)(\Delta p) \geq \frac{1}{2} \sqrt{(i\hbar)(-i\hbar)} = \frac{1}{2}\hbar$$

Proof of 3.1

Suppose \hat{A} and \hat{B} are the physical quantities we are concerned with.

From 2.1, we know \hat{A}, \hat{B} are all Hermitians

$$\text{Name } \hat{A}' = \hat{A} - \langle \hat{A} \rangle \quad \hat{B}' = \hat{B} - \langle \hat{B} \rangle$$

Hermitian Operator plus a constant is still a Hermitian. i.e. \hat{A}', \hat{B}' Hermitian

$$(\Delta \hat{A})^2 = \int \psi^+ \hat{A}'^2 \psi d\tau \stackrel{\text{why?}}{=} \int \psi^+ \hat{A}' + \hat{A}' \hat{A}' \psi d\tau = \int (\hat{A}' \psi)^+ (\hat{A}' \psi) d\tau$$

$$= \int |\hat{A}' \psi|^2 d\tau$$

$$(\Delta \hat{B})^2 = \int |\hat{B}' \psi|^2 d\tau$$

$$\therefore (\Delta A)^2 (\Delta B)^2 = \int |\hat{A}' \psi|^2 d\tau \cdot \int |\hat{B}' \psi|^2 d\tau$$

$$\text{Then, a math fact: } \int |f|^2 d\tau \cdot \int |g|^2 d\tau \geq \left| \int f^* g d\tau \right|^2$$

(Schwartz's Inequality)

$$\begin{aligned}
 \therefore (\Delta A)^2 (\Delta B)^2 &= \int |\hat{A}' \hat{\psi}|^2 d\tau \cdot \int |\hat{B}' \hat{\psi}|^2 d\tau \\
 &\geq \left| \int (\hat{A}' \hat{\psi})^\dagger \hat{B}' \hat{\psi} d\tau \right|^2 \\
 &= \left| \int \hat{\psi}^\dagger \hat{A}'^\dagger \hat{B}' \hat{\psi} d\tau \right|^2 \quad \hat{A}' \text{ is Hermitian} \\
 &= \left| \int \hat{\psi}^\dagger \hat{A}' \hat{B}' \hat{\psi} d\tau \right|^2
 \end{aligned}$$

Now our main job is to separate $(\hat{\psi})$ to the form $\underbrace{x + yi}_{\text{all real numbers}}$, then we could calculate it easily. The part under square

But for an integral, it's hard to separate it directly.

However, Hermitian operator's expectation is real.

So if we could divide the part between $\hat{\psi}^\dagger$ and $\hat{\psi}$ to 2 parts, one of which is $\hat{\psi}^\dagger$ Hermitian, the other is Hermitian, then ok!

So we could focus on $\hat{A}' \hat{B}'$, there is a plan:

$$\begin{aligned}
 \hat{A}' \hat{B}' &= \frac{1}{2} \hat{A}' \hat{B}' + \frac{1}{2} \hat{A}' \hat{B}'^\dagger + \frac{1}{2} \hat{B}' \hat{A}' - \frac{1}{2} \hat{B}' \hat{A}'^\dagger \\
 &= \frac{1}{2} (\hat{A}' \hat{B}' - \hat{B}' \hat{A}') + \frac{1}{2} (\hat{A}' \hat{B}'^\dagger + \hat{B}' \hat{A}'^\dagger) \\
 &= \underbrace{\frac{1}{2} (-i) \hat{\psi}}_{\downarrow} (\hat{A}' \hat{B}' - \hat{B}' \hat{A}') + \underbrace{\frac{1}{2} (\hat{A}' \hat{B}'^\dagger + \hat{B}' \hat{A}'^\dagger)}_{\swarrow}
 \end{aligned}$$

This two are Hermitian. the proofs are:

$$\begin{aligned}
 [i(\hat{A}' \hat{B}' - \hat{B}' \hat{A}')]^\dagger &= [-i(\hat{A}' \hat{B}' - \hat{B}' \hat{A}')^\dagger] \\
 &= -i(\hat{B}'^\dagger \hat{A}'^\dagger - \hat{A}'^\dagger \hat{B}'^\dagger) \\
 &= -i(\hat{B}' \hat{A}' - \hat{A}' \hat{B}') \\
 &= i(\hat{A}' \hat{B}' - \hat{B}' \hat{A}'^\dagger)
 \end{aligned}$$

$$\begin{aligned}
 [\hat{A}' \hat{B}'^\dagger + \hat{B}' \hat{A}']^\dagger &= (\hat{A}' \hat{B}')^\dagger + (\hat{B}' \hat{A}')^\dagger \\
 &= \hat{B}'^\dagger \hat{A}'^\dagger + \hat{A}'^\dagger \hat{B}'^\dagger
 \end{aligned}$$

$$= \hat{B}'\hat{A}' + \hat{A}'\hat{B}'$$

$$= \hat{A}'\hat{B}' + \hat{B}'\hat{A}'$$

$$\text{Great! So } (\Delta A)^2 (\Delta B)^2 = \left| \int \bar{\psi}^\dagger \hat{A}' \hat{B}' \bar{\psi} d\tau \right|^2$$

$$= \left| \int \bar{\psi}^\dagger \left[\frac{1}{2}(-i) \bar{\psi} (\hat{A}'\hat{B}' - \hat{B}'\hat{A}') + \frac{1}{2}(\hat{A}'\hat{B}' + \hat{B}'\hat{A}') \right] \bar{\psi} d\tau \right|^2$$

$$= \left| \int \bar{\psi}^\dagger \frac{1}{2}(-i) \bar{\psi} (\hat{A}'\hat{B}' - \hat{B}'\hat{A}') \bar{\psi} d\tau + \int \bar{\psi}^\dagger \frac{1}{2}(\hat{A}'\hat{B}' + \hat{B}'\hat{A}') \bar{\psi} d\tau \right|^2$$

$$= \left| \frac{i}{2} \left(\int \bar{\psi}^\dagger \frac{1}{2}(-i) \bar{\psi} (\hat{A}'\hat{B}' - \hat{B}'\hat{A}') \bar{\psi} d\tau \right) + \frac{1}{2} \left(\int \bar{\psi}^\dagger (\hat{A}'\hat{B}' + \hat{B}'\hat{A}') \bar{\psi} d\tau \right) \right|^2$$

two real numbers R_1'' R_2''

$$= \frac{1}{4} R_1^2 + \frac{1}{4} R_2^2$$

$$= \frac{1}{4} \left| \int \bar{\psi}^\dagger [\hat{A}', \hat{B}'] \bar{\psi} d\tau \right|^2 + \frac{1}{4} \left| \int \bar{\psi}^\dagger (\hat{A}'\hat{B}' + \hat{B}'\hat{A}') \bar{\psi} d\tau \right|^2$$

Now it is only a math structure called commutator to express $\hat{A}'\hat{B}' - \hat{B}'\hat{A}'$
but in the future chapter we would see it again

$$\text{The second term is } \geq 0, \text{ so } (\Delta A)^2 (\Delta B)^2 \geq \frac{1}{4} \left| \int \bar{\psi}^\dagger [\hat{A}', \hat{B}'] \bar{\psi} d\tau \right|^2$$

$$(\Delta A)(\Delta B) \geq \frac{1}{2} \left| \int \bar{\psi}^\dagger [\hat{A}', \hat{B}'] \bar{\psi} d\tau \right|$$

$$\text{And } [\hat{A}', \hat{B}'] = [\hat{A} - \langle \hat{A} \rangle, \hat{B} - \langle \hat{B} \rangle] = [\hat{A}, \hat{B}]$$

$$\begin{aligned} \text{So } (\Delta A)(\Delta B) &\geq \frac{1}{2} \left| \int \bar{\psi}^\dagger [\hat{A}, \hat{B}] \bar{\psi} d\tau \right| \\ &= \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle| \end{aligned}$$

1.3 chapter 3

The previous chapter has discussed wave function's corresponding in actual world, but we need to know what equation it satisfies, thus we could find the solution of wave function, namely the explicit form of it. That is the Schrodinger equation, which we do not know the derivation of, but it could explain the experimental data so it must be true.

Firstly let me give Some notations:

$$\text{Nabla operator: } \nabla \quad \text{In 2D cartesian: } \nabla = \frac{\partial}{\partial x} \hat{i} + \frac{\partial}{\partial y} \hat{j}$$

$$\text{In 3D cartesian: } \nabla = \frac{\partial}{\partial x} \hat{i} + \frac{\partial}{\partial y} \hat{j} + \frac{\partial}{\partial z} \hat{k}$$

Laplace operator: $\Delta = \nabla^2 = \nabla \cdot \nabla$, giving the divergence of the

gradient of a function $\text{In 2D cartesian: } \Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}$

$$\text{In 3D cartesian: } \Delta f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

So actually we can get Laplace from Nabla — Nabla is the only one to remember

Besides, these two are both operators for space, not including time!

Schrodinger Equation: General form: $-\frac{\hbar^2}{2m} \Delta \Psi + U \Psi = i\hbar \frac{\partial}{\partial t} \Psi$

Then 2 things make it be able to vary: { Coordinate system
number of dimension

Figure 1: Schrodinger Equation

After giving the form of Schrodinger Equation, we found it hard to solve. But can we at least solve some simplified form of it? Here comes TISE(time independent Schrodinger Equation), a special type of the general Schrodinger Equation(also known as TDSE, time dependent Schrodinger Equation). The main idea here is, if the potential is independent of time, then we could treat this problem by **Variable Separation Method**. The following is about how we found this condition could make it possible to separate variables.

No. _____

Date _____

How to get TISE from TDSE? (Take 1D for example)

Firstly: TDSE is $-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x,t) \psi(x,t) = i\hbar \frac{\partial \psi}{\partial t}$

Suppose that $\psi(x,t)$ could be written as:

$$\psi(x,t) = \Psi(x) \Psi(t) \quad (\text{Variable separation})$$

then: $-\frac{\hbar^2}{2m} \Psi(t) \frac{\partial^2 \Psi(x)}{\partial x^2} + V(x,t) \Psi(x) \Psi(t) = i\hbar \Psi(x) \frac{\partial \Psi}{\partial t}$

$$-\frac{\hbar^2}{2m} \frac{1}{\Psi(x)} \frac{\partial^2 \Psi(x)}{\partial x^2} + V(x,t) = i\hbar \frac{1}{\Psi(t)} \frac{\partial \Psi(t)}{\partial t}$$

(divided by $\Psi(x) \Psi(t)$)

Since now $\Psi(x)$ only depends on x

$\Psi(t)$ only depends on t

we could write $\frac{\partial}{\partial x} \rightarrow \frac{d}{dx}$

$$-\frac{\hbar^2}{2m} \frac{1}{\Psi(x)} \frac{\partial^2 \Psi(x)}{\partial x^2} \frac{d^2 \Psi(x)}{dx^2} + V(x,t) = i\hbar \frac{1}{\Psi(t)} \frac{d \Psi(t)}{dt}$$

In this case, if $V(x,t)$ only depends on x

then LHS = only dep on x

RHS = only $\sim +$

So we got a constant, by which we can make the equation still equal, we call it E

$$-\frac{\hbar^2}{2m} \frac{1}{\Psi(x)} \frac{d^2 \Psi(x)}{dx^2} + V(x) = E \Rightarrow -\frac{\hbar^2}{2m} \frac{d^2 \Psi(x)}{dx^2} + V \Psi(x) = E \Psi(x)$$

(TISE)

$$i\hbar \frac{1}{\Psi(t)} \frac{d \Psi(t)}{dt} = E \Rightarrow \frac{d \Psi(t)}{dt} = -\frac{i\hbar E}{\hbar} \Psi(t)$$

Figure 2: from TDSE to TISE

1.3.1 Recipe 1: General Initial Value Problems in Quantum Mechanics

Still we are working on the cases U is only dependent on position, but even in this case, we could get the wave function at a given time t .

1. Solve the time-independent Schrodinger Equation
2. Expand given initial wave function in terms of states of definite energies
3. Let each definite energy state evolve with its own time part $e^{\frac{-iE_i t}{\hbar}}$

1.4 chapter 4

After separating the variables, what we have is not only the general form in figure 1, but two single equations on the bottom of figure 2. The second one is easy to deal with, whose solution could be written as $\phi(t) = e^{\frac{-iE_i t}{\hbar}}$. But the first one, also known as TISE, seems hard to solve. So in this chapter, we have introduced some math tools for solving TISE, that is, using the concept of operator to transform TISE problem to a eigenvalue problem. Then based on the fundamental commutation relationship given by Dirac(which Prof. Hui said we could regard as a fact, and do not need to know how it is imposed now), we found operator \hat{H} in TISE just corresponds to Hamiltonian of a one particle system. It gave us a more general method to solve any problems in quantum: firstly think classical and secondly go quantum.

1.4.1 Operators-from the perspective of math

Definition operator represents a mathematical operation that acts on whatever comes behind it.

For example, we call $\hat{A}f(x) = g(x)$: the operator \hat{A} acts on $f(x)$ and then returns some function $g(x)$.

What kind of operators we would use in Quantum Mechanics? Firstly, as we have discussed in chapter 2, it needs to be Hermitian operator. Secondly, the operators need to satisfy the property: $\hat{A}[c_1f_1(x) + c_2f_2(x)] = c_1\hat{A}f_1(x) + c_2\hat{A}f_2(x)$, which is called *linear*.

operator's property 1: The ordering of two operators is a serious matter

Take operators \hat{A}, \hat{B} as examples, $\hat{A}\hat{B}f(x) \text{may } \neq \hat{B}\hat{A}f(x)$. To better describe this property, we introduced the concept of commutator and commute.

commutator it is an operator needing two operators as input. Its symbol is $[\quad , \quad]$. Its definition is: $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

commute it is a term describing a property of two operators. If the commutator taking in the two operators equals to zero, then we say the two operators *commute* with each other.

So finally we know, although look similar, they are two different things. For every two operators, they would have a commutator, but only some of them would commute (the commutator equals to zero).

operator's property 2 : For an operator \hat{A} , there is an special set of functions called Eigenfunctions As we know in 1.4.1, $f(x)$ and $g(x)$ are usually different functions. But if $g(x)$ is just equal to constant times(this constant could be complex, let us name it a) as $f(x)$, then we call $f(x)$ is the eigenfunction of this operator \hat{A} , and a is the eigenvalue corresponding to this eigenfunction for \hat{A} .

So the picture for this problem is: for a given operator \hat{A} , there are n pairs of eigenvalues and eigenfunctions(from 1, 2, 3 to n), which could be written as,

$$\hat{A}\phi_i(x) = a_i\phi_i(x), i = 1, 2, 3 \dots n \quad (1)$$

properties about eigenfunctions

1: $[\hat{A}, \hat{B}] = 0 \Leftrightarrow \hat{A}\hat{B}$ share common set of eigenstates this is the reason why we would introduce the concepts of commute and commutator ahead of eigenvalues and eigenfunctions
The proof is waited to be completed in the future

operator's property 3 : Ehrenfest theorem

The proof of this theorem is shown in the next page pdf. Let us see the result of it:

$$\frac{d}{dt} \langle \hat{A} \rangle = \frac{1}{i\hbar} \langle [\hat{A}, \hat{H}] \rangle + \frac{\partial \hat{A}}{\partial t} \quad (2)$$

When the operator is independent of time, it becomes:

$$\frac{d}{dt} \langle \hat{A} \rangle = \frac{1}{i\hbar} \langle [\hat{A}, \hat{H}] \rangle \quad (3)$$

In language, it means if an time-independent operator commutes with the Hamiltonian, then it does not evolve through time.

Proof of Ehrenfest theorem:

$\Psi(x, t)$ is the wave function of a physics system,

\hat{A} is an operator,

$$\text{then: } \frac{d}{dt} \langle \hat{A} \rangle = \frac{d}{dt} \int \Psi^+ \hat{A} \Psi dx$$

$$= \int \frac{\partial}{\partial t} (\Psi^+) \hat{A} \Psi dx + \int \Psi^+ \frac{\partial}{\partial t} (\hat{A} \Psi) dx$$

$$= \int \frac{\partial}{\partial t} (\Psi^+) \hat{A} \Psi dx + \int \Psi^+ \left[\frac{\partial}{\partial t} \hat{A} \cdot \Psi + \hat{A} \frac{\partial \Psi}{\partial t} \right] dx$$

$$= \int \frac{\partial \Psi^+}{\partial t} \hat{A} \Psi dx + \int \Psi^+ \left(\frac{\partial \hat{A}}{\partial t} \right) \Psi dx + \int \Psi^+ \hat{A} \frac{\partial \Psi}{\partial t} dx$$

$$= \int \frac{\partial \Psi^+}{\partial t} \hat{A} \Psi dx + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \int \Psi^+ \hat{A} \frac{\partial \Psi}{\partial t} dx \quad (*)$$

The only QM knowledge we use

Here we need to use the time part of TDSE

\downarrow

TDSE

$$\hat{A} \Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad \textcircled{1}$$

as Hermitian Conjugate still holds: $(\hat{A} \Psi)^+ = (i\hbar \frac{\partial \Psi}{\partial t})^+$

$$\text{LHS} = \Psi^+ \hat{A}^+ = \Psi^+ \hat{A} \quad \text{RHS} = -i\hbar \frac{\partial \Psi^+}{\partial t}$$

$$\downarrow \Psi^+ \hat{A} = -i\hbar \frac{\partial \Psi^+}{\partial t} \quad \textcircled{2}$$

Substitute \textcircled{1} \textcircled{2} to (*) we have:

$$= \int \frac{i}{\hbar} \Psi^+ \hat{A} \hat{A} \Psi dx + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \int \Psi^+ \hat{A} \frac{\hat{H} \Psi}{i\hbar} dx$$

$$= \int \left[\frac{i}{\hbar} \Psi^+ \hat{A} \hat{A} \Psi - \frac{i}{\hbar} \Psi^+ \hat{A} \hat{H} \Psi \right] dx + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle$$

$$= \frac{i}{\hbar} \int [\hat{A} \hat{A} \Psi - \hat{A} \hat{H} \Psi] dx + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle$$

$$= -\frac{i}{\hbar} \int \hat{A} (\hat{A} \hat{H} - \hat{H} \hat{A}) \Psi dx + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle$$

$$= \frac{1}{i\hbar} \langle [\hat{A}, \hat{H}] \rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle$$

1.4.2 $[\hat{x}, \hat{p}] = i\hbar$, then everything follows

From classical mechanics we have a basic relationship for the coordinate x and momentum p: $\{x, p\} = 1$, where $\{ \ , \ \}$ means Poisson Bracket.

Poisson Bracket For some functions $F(x, p)$, $G(x, p)$, $\{F, G\} = \frac{\partial F}{\partial x} \cdot \frac{\partial G}{\partial p} - \frac{\partial F}{\partial p} \cdot \frac{\partial G}{\partial x}$

So my understanding for $\{x, p\} = 1$ is, under this condition the coordinate and momentum could be regarded as *not interfering with each other*, thus could be used to express the most number of probabilities in the phase space.

And to get the same fundamental argument in quantum mechanics, Dirac has imposed: $[\hat{x}, \hat{p}] = i\hbar$. Although we don't need to know how it comes now [The proof is waited to be completed in the future](#), but we should know if it is true, then everything could appear:

1. Then we could know the operator in the TISE is just the Hamiltonian operator of a single particle. If $[\hat{x}, \hat{p}] = i\hbar$ needs to be satisfied, then we could get $\hat{p} = -i\hbar \frac{\partial}{\partial x}$. Then TISE could be written as:

$$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) \right] \Psi(x) = E \Psi(x)$$

↓

$$\left[\frac{1}{2m} - \hbar^2 \frac{d^2}{dx^2} + U(x) \right] \Psi(x) = E \Psi(x)$$

↓

$$\left[\frac{1}{2m} (-i\hbar \frac{d}{dx}) (i\hbar \frac{d}{dx}) + U(x) \right] \Psi(x) = E \Psi(x)$$

↓

$$\left[\frac{1}{2m} \hat{P} \hat{P}^+ + U(x) \right] \Psi(x) = E \Psi(x)$$

↓

$$\underbrace{\left[\frac{1}{2m} \hat{P}^2 + U(x) \right]}_{\text{Kinetic Energy} + \text{potential energy}} \Psi(x) = E \Psi(x)$$

Kinetic Energy + potential energy (or to be more specific, $T_2 + U$)

In most cases, $T_2 + U = H$, so we could regard the part before $\Psi(x)$ as Hamiltonian

Figure 3: from commuting relation to Hamiltonian in QM

Now we have proved the relationship between Hamiltonian and TISE, but it is under the suppose of kinetic energy only consists of second order item. Luckily that is the most cases we are discussing, but the further explanation could be found in 4.

About when $T_2 + U$ would equal H

$$\left. \begin{array}{l} L = T - U \\ H = \sum_{\alpha=1}^S p_\alpha q'_\alpha - L \end{array} \right\}$$

True for all the time

Based on Euler's principle for homogeneous function:

If $f(x_1, x_2, \dots, x_n)$ is n -order homogeneous function, then we have

$$\sum_{\alpha=1}^n \frac{\partial f}{\partial x_\alpha} \cdot x_\alpha = nf$$

$$p_\alpha = \frac{\partial L}{\partial q'_\alpha} = \frac{\partial I}{\partial q'_\alpha}$$

$$\text{So } \sum_{\alpha=1}^S p_\alpha \cdot q'_\alpha = \sum_{\alpha=1}^S \frac{\partial I}{\partial q'_\alpha} q'_\alpha = 0T_0 + 1T_1 + 2T_2$$

$$\begin{aligned} H &= \sum_{\alpha=1}^S p_\alpha \cdot q'_\alpha - L = 0T_0 + 1T_1 + 2T_2 - (T_0 - T_1 - T_2 + U) \\ &= 0T_0 + 1T_1 + 2T_2 - T_0 + T_1 + T_2 - U \\ &= T_2 - T_0 + U \end{aligned}$$

What's more, $\frac{\partial H}{\partial t} = -\frac{\partial L}{\partial t}$ → given by Hamilton Canonical Equation

So our conclusion: 1. if $\frac{\partial L}{\partial t} = 0$, then $\frac{\partial H}{\partial t} = 0$, so H is a constant
 2. if $T_0 = 0$, then $H = T_2 + U$

Figure 4: when $T_2 + U = H$

2. Then we get the basic recipe to treat QM problem: think classically to get the classical Hamiltonian of the system, and then substitute the operators in the classical Hamiltonian to get the Quantum-version Hamiltonian to go quantum. (Actually in this document there are many examples of application of this recipe in energy, but still we have application in other physical quantities, like angular momentum, which is shown in 1.8.2)

But a new problem would be proposed: if the basic relationship we need to meet is 1.4.2, is the form of x and p only?

A:

No!

We could find $\hat{x} \rightarrow i\hbar \frac{\partial}{\partial p}$, $\hat{p} \rightarrow p$ also satisfies the relation:

$$\begin{aligned} [\hat{x}, \hat{p}] f(p) &= \hat{x} \hat{p} f(p) - \hat{p} \hat{x} f(p) \\ &= i\hbar \frac{\partial}{\partial p} [p f(p)] - p i\hbar \frac{\partial}{\partial p} f(p) \\ &= i\hbar [f(p) + p \frac{\partial f(p)}{\partial p}] - p i\hbar \frac{\partial f(p)}{\partial p} \\ &= i\hbar f(p) + i\hbar p \frac{\partial f(p)}{\partial p} - p i\hbar \frac{\partial f(p)}{\partial p} \\ &= i\hbar f(p) \end{aligned}$$

$$[\hat{x}, \hat{p}] f(p) = i\hbar f(p) \text{ for all } f(p)$$

So this one is also ok! The only difference is that all the unknowns we see in the equation would be about p instead of x , but whether it is good would depend on what you want to focus on!

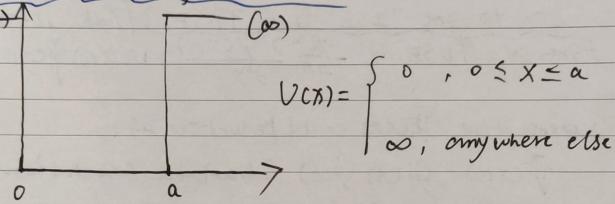
Figure 5: select operator majoring in momentum

1.5 chapter 5

This chapter we use the simplest example, 1D infinite well, to illustrate how a QM problem is solved. Firstly, the problem description and the process of solving this question is shown in the following 1 page pdf. Secondly I would explain the result from two perspectives: the eigenvalues and the eigenfunctions. Thirdly, we could get some common properties from this typical problem, which also work for all the QM problems however.

1.5.1 1D infinite potential well: problem description and solving process

How to solve 1D infinite well?



Firstly, $V(x)$ only depends on x (I mean, position)

So we could use TISE

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2} + V(x)\Psi(x) = E\Psi(x)$$

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2} = [E - V(x)]\Psi(x)$$

$$\frac{d^2\Psi(x)}{dx^2} = \frac{2m}{\hbar^2} [V(x) - E]\Psi(x)$$

When [anywhere else] $\Psi(x) = 0$

why? From two perspectives:

① Mathematically:

The second order of $\Psi(x)$ need to be ∞
derivation

Then it could not satisfy Normalization Condition

② Physical Situation (David Griffiths):

You regard the "wall" as a real wall (very high),
then the particle could not appear on the walls.

Next for $0 \leq x \leq a$

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi(x)}{dx^2} = E\Psi(x)$$

$$\frac{d^2\Psi(x)}{dx^2} = -\frac{2mE}{\hbar^2}\Psi(x)$$

Firstly, we could assume $E > 0$ (why?)

$$\text{In TISE: } \frac{d^2\Psi(x)}{dx^2} = \frac{2m}{\hbar^2} [V(x) - E]\Psi(x)$$

If $E < V_{\min}$ then Ψ and its second order derivative holds the same sign, which makes it impossible to do Normalization.

As a result, we could use: $k^2 = \frac{2mE}{\hbar^2}$

$$k = \sqrt{\frac{2mE}{\hbar^2}} = \frac{\sqrt{2mE}}{\hbar}$$

$$\text{TISE in this case becomes: } \frac{d^2\Psi(x)}{dx^2} = -k^2\Psi(x)$$

Sin and Cos just have this property: 2nd order derivative holds a "minus" sign.

So why not $\Psi(x) = A\sin kx + B\cos kx$.

Finally we could add Boundary Conditions on it: ① $\Psi(0) = 0 \Rightarrow B\cos kx = 0$ for all the time

Only $B = 0$ So now $\Psi(x) = A\sin kx$

② $\Psi(a) = 0 \Rightarrow A\sin ka = 0 \Rightarrow \sin ka = 0 \Rightarrow ka = n\pi, n = 0, \pm\pi, \pm 2\pi, \pm 3\pi, \dots$

$$\text{But } a \neq 0, i.e. 0, \pm \frac{\pi}{a}, \pm \frac{2\pi}{a}, \dots$$

$$\text{Meanwhile if } k=0 \quad A\sin kx = 0$$

$$\Psi(x) = 0, \text{ Not Satisfying Normalization}$$

Besides, $k = \frac{\sqrt{2mE}}{\hbar}$, this is a value > 0

$$\therefore k = \frac{\pi}{a}, \frac{2\pi}{a}, \dots$$

$$k = \frac{n\pi}{a}, n = 1, 2, 3, \dots$$

$$E = \frac{(kn)^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2}{2ma^2} n^2$$

$$\text{So } \Psi(x) = A\sin\left(\frac{n\pi}{a}x\right)$$

Normalization:

$$\int_0^a A^2 \sin^2\left(\frac{n\pi}{a}x\right) dx = A^2 \int_0^a \frac{1 - \cos 2\left(\frac{n\pi}{a}x\right)}{2} dx = A^2 \left[\frac{1}{2}x - \frac{\sin 2\left(\frac{n\pi}{a}x\right)}{4n\pi} \right]_0^a$$

$$= A^2 \left[\frac{1}{2}a - \frac{1}{2}a \right] = A^2 \cdot \frac{1}{2}a = 1$$

$$A = \sqrt{\frac{2}{a}}$$

$$\text{Finally: } \Psi(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right), & 0 \leq x \leq a \\ 0, & \text{else} \end{cases}$$

1.5.2 How to understand the result

1. About eigenvalues $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$

(a) from n^2

the available energies are discrete; there is a lowest energy called ground state energy when $n=1$

(b) from $\frac{1}{m}$:

Smaller mass particle has more noticeable discrete-energy effect. For example, the lightest particle is electron. When one electron is confined to the vicinity of nucleus, the energy would be as large as noticeable.

(c) from $\frac{1}{a^2}$:

a corresponds to the width of potential well, when a is larger, the state energy for every state would be lower. Besides, $k = \frac{n\pi}{a}$ so we could observe the behavior of k to induce the behavior of a.

2. About eigenfunctions

(a) from $k=\sqrt{\frac{2mE}{\hbar^2}}$, the coefficient before x

$E \rightarrow k \rightarrow$ the ratio we stretch the sine function along the x axis. But the continuity condition on the boundary let us only select the “k” that could make the wave function’s graph just ends its half integer period or integer period, thus only part of E is permitted.

(b) from its second order derivative

We could know that $-\frac{\hbar^2}{2m} \cdot \frac{d^2}{dx^2}$ is the kinetic term of Hamiltonian, so we could get: **kinetic energy** $\propto \frac{d^2}{dx^2}\psi$. For sine function, if the “twist number” in the well is more, then the second derivative for each position is higher, thus the expectation of kinetic energy is higher. Besides, in the well we know the potential energy is always zero, so the total energy E would also be higher.

And as we said in the last item, $k=\sqrt{\frac{2mE}{\hbar^2}}$ means the ratio we stretch the sine function along the x axis. So when k is higher $\uparrow \Rightarrow$ twist number $\uparrow \Rightarrow$ kinetic energy $\uparrow \Rightarrow$ total energy \uparrow , which just meets our knowledge that k would increase when E increases.

Above discussion only talks about the relationship between k and E, but who could result in the increasing of E or k? We need to turn back to 1 to explore deeper. Then we know: the twist number theory only works for the case where n is the only thing changing. But if n is constant, why could the changing of a, width of potential well result in the energy’s

changing? It decreased the length of a period for sine function-when the height of the sine function stays unchanged the second order derivative is already increasing, not to mention that the height also needs to increase to ensure the total Normalization result is 1(since the width is smaller). Thus it would definitely increased the expectation value of the second order derivative.

To conclude, the width is smaller could let the energy for every states(from 1 to n) increase, but when the width a is settled down, we could only see the energy increasing when n increases.

(c) from its symmetry

From the graph of wave function we know it is symmetric or anti-symmetric, accordingly corresponding to the function has just half-integer or integer period in the well.

So we could give it an explanation: that's because the potential function is symmetric, but how could a symmetric property result two sides, symmetry and anti-symmetry?

A: because what matters in QM is not the wave function, but the square of wave function. And anti-symmetric wave function's square is also symmetric, resulting in the feasibility of anti-symmetric wave functions.

1.5.3 Some general properties from the easiest problem

1. The continuity of the Wave function's 1st derivative is up to whether the potential has a infinite break point

For 1D infinite well problem, we found that the 1st order derivative of wave function is not continuous. However, this is only a special property for the problems with a potential which may be **infinite** somewhere. So, if the potential function does not have a infinite break point(even a finite break point is still okay), then we could get one more condition to solve the problem: the 1st order derivative of the wave function is continuous.

2. Energy eigenfunctions corresponding to different eigenvalues are orthogonal

We could found that for the 1D infinite potential well's eigenfunctions, they have this property:

$$\int_{-\infty}^{\infty} \psi_i^*(x)\psi_j(x)dx = 0, \text{ for } i \neq j \quad (4)$$

And this property is in fact general for all Hermitian operators. To describe both the situations $i = j$ and $i \neq j$, we have:

$$\int_{-\infty}^{\infty} \psi_i^*(x)\psi_j(x)dx = \delta_{ij} \quad (5)$$

PROOF

Suppose there are two eigenstates:

$$\hat{A}\psi_m = a_m\psi_m \quad (6)$$

$$\hat{A}\psi_n = a_n\psi_n \quad (7)$$

From the definition of Hermitian operator, we have on the one hand:

$$\int \psi_m^\dagger \hat{A} \psi_n d\tau = \int \psi_m^\dagger a_n \psi_n d\tau = a_n \int \psi_m^\dagger \psi_n d\tau \quad (8)$$

On the other hand because \hat{A} is an Hermitian Operator:

$$\begin{aligned} \int \psi_m^\dagger \hat{A} \psi_n d\tau &\stackrel{\substack{\hat{A} \text{ is} \\ \text{Hermitian}}}{=} \int \psi_m^\dagger \hat{A}^\dagger \psi_n d\tau = \int (\hat{A}\psi_m)^\dagger \psi_n d\tau = \int (a_m\psi_m)^\dagger \psi_n d\tau \\ &\stackrel{\substack{\text{Hermitian} \\ \text{operator's} \\ \text{are} \\ \text{real} \\ \text{eigenvalues} \\ \text{number}}}{=} \int a_m(\psi_m)^\dagger \psi_n d\tau = a_m \int (\psi_m)^\dagger \psi_n d\tau = a_m \int \psi_m^\dagger \psi_n d\tau \end{aligned} \quad (9)$$

Since the above two equations have the same left hand side item, their results are equal:

$$a_n \int \psi_m^\dagger \psi_n d\tau = a_m \int \psi_m^\dagger \psi_n d\tau \quad (10)$$

Then we could have an important argument:

$$(a_m - a_n) \int \psi_m^\dagger \psi_n d\tau = 0 \quad (11)$$

So if $(a_m - a_n) \neq 0$ then we must have $\int \psi_m^\dagger \psi_n d\tau = 0$, Q.E.D.

Actually **corresponding to different eigenvalues is not a necessary condition**, we talked about the **degenerate**^{1.7.2} case in 1.10.1.

3. Completeness

If any function $\psi(x)$ could be expanded to $\psi(x) = \sum C_n \phi_n(x)$, then we call the set

$$\phi_1(x), \phi_2(x), \dots, \phi_n(x), \dots \quad (12)$$

a **complete set**. And the eigenfunctions set given by TISE is always a complete set.

(a) How to get the coefficient C_n ?

$$C_n = \int_{-\infty}^{\infty} \phi_n^*(x) \psi(x) dx \quad (13)$$

(b) What is the physical meaning of C_n ?

Actually C_n could not been “measured”, what we could see directly is its square $|C_n|^2$, it is the probability of an eigenvalue appearing when we measured the state $\psi(x)$. Figure 6 below is the proof:

Let $\Psi(x) = \sum C_i \phi_i(x)$, $\phi_i(x) \Leftrightarrow E_i, \phi_i(x)$ is the eigenfunctions of \hat{A} ($\hat{A} \phi_i = E_i \phi_i$)

$$\text{Then } \langle \Psi | \hat{A} | \Psi \rangle = \langle \Psi | \hat{A} \Psi \rangle = \langle \Psi | \hat{A} \sum_i C_i \phi_i \rangle$$

$$= \langle \Psi | \sum_i C_i \hat{A} \phi_i \rangle = \langle \Psi | \sum_i C_i E_i \phi_i \rangle$$

$$= \langle \sum_j C_j \phi_j | \sum_i C_i E_i \phi_i \rangle = \sum_j \sum_i C_j^* C_i E_i \langle \phi_j | \phi_i \rangle$$

$$= \sum_j \sum_i C_j^* C_i E_i \delta_{ji} = \sum_i C_i^* C_i E_i$$

$$= \sum_i |C_i|^2 E_i$$

Figure 6: proof of physical meaning of C_n^2

1.6 chapter 6

1.6.1 1D finite square well

Two approaches to solving 1D finite well: analytical and computational The following 3 pages are analytical method, while the fourth page is the computational method.

How to solve the 1D finite well?
Problem description:

$$V(x) = \begin{cases} -V_0, & -a \leq x \leq a \\ 0, & |x| > a \end{cases}$$

$$(V_0 > 0)$$

Considering the physics truth, unlike 1D infinite well, here E could be < 0 or ≥ 0

We gave them names: bound scattering
State

1. Bound state ($E < 0$)

1.1 when $x < -a$: $V = 0$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2} \psi \stackrel{\downarrow}{=} k^2 \psi, \quad k = \sqrt{-\frac{2mE}{\hbar^2}}$$

because $E < 0$: $-\frac{2mE}{\hbar^2} > 0$

So ψ should be a function whose 2-nd derivative holds the same sign.

$$\psi = Ae^{-kx} + Be^{kx}$$

But when $x \rightarrow -\infty$ the $\psi(x)$ would explode, to prevent this, $B = 0$, $A \neq 0$

Actually it's what we could get so far. Waiting for 1.3 to give boundary conditions.

1.3 when $x > a$

Totally like 1.1, the only diff - is "-"

$$\psi = Fe^{kx} + Ge^{-kx}, \quad x > a$$

$x \rightarrow \infty$ Fe^{kx} explode

$$\text{So } F = 0, \psi = Ge^{-kx}, \quad x > a$$

ψ BC

Now we could add B C.

Thanks to the symmetry we discussed in 1.2

we could classify it by 2 cases:

1. ψ odd function
even

then $C = 0$ since \cos is even

$$\text{the total solution: } \psi(x) = \begin{cases} Pe^{-kx}, & x > a \\ D \cos kx, & -a < x < a \\ Be^{kx}, & x < -a \end{cases}$$

What "even" could bring us is not only $C = 0$, but also $B = F$, then it becomes

$$\begin{cases} Be^{-kx}, & x > a \\ D \cos kx, & -a < x < a \\ Be^{kx}, & x < -a \end{cases}$$

Then the result is $\psi = B e^{kx}$

1.2 when $-a < x < a$

$$V(x) = -V_0 \quad \text{TISE is:}$$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - V_0\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} = -\frac{(V_0+E)\cdot 2m}{\hbar^2} \psi = -k^2 \psi, \quad k = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$$

Why we could be sure $E+V_0 \geq 0$?

Considering the physics fact:

$$E = k + V, \quad \text{where } V = -V_0$$

that is $E = k - V_0$. but $k \geq 0$?, $E + V_0 \geq 0$

Like what we did in 1.1, we could let $\psi = C'e^{-ikx} + D'e^{+ikx}$ (using exponential form).

the only diff - is "i"
But in this case, $|x| < a$, the potential function is symmetric, so the wave function should be odd or even. To express odd/even function, the \sin/\cos functions are more convenient.

Next, I would try the two cases →

$$\text{case 1: } C'e^{-ikx} + D'e^{+ikx}$$

$$\psi = C \sin kx + D \cos kx$$

$\psi =$

Then if one side meet BC, the other side would meet it spontaneously, so we only add it for

① ψ BC ② ψ' BC one side

$$\psi(a) = \psi'(a) \quad \psi'(ca) = \psi(a)$$

$$Be^{-ka} = D \cos ka \quad -KB e^{-ka} = -CD \sin ka \quad \Rightarrow \quad D \cos ka$$

$$\text{then } KD \cos ka = CD \sin ka$$

$$K \cos ka = \sin ka$$

$$k = \tan(ka) \quad \frac{1}{\sqrt{\frac{-2m}{\hbar^2}}} \quad \frac{\sqrt{2m(E+V_0)}}{\hbar} \quad a$$

$$\frac{\sqrt{-2mE}}{\hbar} = \frac{\sqrt{2m(E+V_0)}}{\hbar} a$$

So the only unknown here is E , this equation actually gives a restriction on E .

$$\frac{\sqrt{-2mE}}{\hbar} = \tan\left(\frac{\sqrt{2m(E+V_0)}}{\hbar} a\right) \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

$$\frac{\sqrt{E+V_0}}{\sqrt{E+V_0} - E} = \sqrt{\frac{-E}{E+V_0}} = \tan\left(\frac{\sqrt{2m(E+V_0)}}{\hbar} a\right)$$

$$\sqrt{\frac{-E}{E+V_0}} = \tan z \quad \text{giving a name: } z \text{ to it}$$

To fully change this

rewrite this formula, we need another variable (since $E, a \Rightarrow 2$ another variables)

Combining the meaning of E : it's a variable

We could make it zero in z to give a z_0 that is $z_0 = \frac{\sqrt{2mV_0}}{\hbar}$

then $\sqrt{\frac{-E}{E+V_0}}$ could be represented by z_0 and z

$$z_0^2 = (2mV_0) \frac{a^2}{\hbar^2}$$

$$z^2 = 2m(E+V_0) \frac{a^2}{\hbar^2} \quad \text{Subtract}$$

$$z^2 - z_0^2 = 2mE \frac{a^2}{\hbar^2} \Rightarrow E = \frac{\hbar^2(z^2 - z_0^2)}{2ma^2}$$

$$\sqrt{\frac{-E}{E+V_0}} = \sqrt{\frac{\hbar^2(z_0^2 - z^2)}{2ma^2}} / \left(\frac{\hbar^2(z^2 - z_0^2)}{2ma^2} + V_0 \right)$$

$$= \sqrt{\frac{\hbar^2(z_0^2 - z^2)}{\hbar^2(z^2 - z_0^2) + 2ma^2V_0}}$$

$$= \sqrt{\frac{(z_0^2 - z^2)}{(z^2 - z_0^2) + \left(\frac{2ma^2V_0}{\hbar^2}\right)}}$$

$$= \sqrt{\frac{z_0^2 - z^2}{z^2 - z_0^2 + z_0^2}}$$

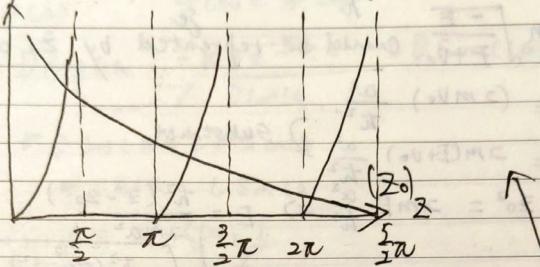
$$= \sqrt{\frac{z_0^2 - z^2}{z^2}} = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$

$$\text{As a result: } \tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$$

No.

Date

So the problem has been converted to find the value of E on the intersection of the two functions



$\tan z$ is very easy

But for $\sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$ we need to investigate

z_0 and z 's relationship:

$$z = (a = \frac{a}{\hbar} \sqrt{2m(E+V_0)})$$

$$z_0 = \frac{a}{\hbar} \sqrt{2mV_0}$$

$$\text{So as } E \rightarrow 0 \rightarrow z_0 \rightarrow \infty \quad \sqrt{\left(\frac{z_0}{z}\right)^2 - 1} \rightarrow 0$$

Then we could add it!

z_0 is a constant, z is a variable representing E .

No matter how small z_0 is,

there would always exist one intersection!

1.6.2 odd function

Firstly $x \in [-a, a]$, f needs to be odd

$$f(x) = c \sin kx \quad \text{So:}$$

$$f(x) = \begin{cases} Fe^{-kx}, & x > a \\ c \sin kx, & -a \leq x \leq a \\ Be^{kx}, & x < -a \end{cases}$$

Secondly, $x < -a$ & $x > a$ needs to be symmetric

$$Fe^{-kx} = -Be^{-kx} \quad B = -F$$

$$f(-x) = -f(x)$$

$$\text{So it becomes: } f(x) = \begin{cases} -Be^{-kx}, & x > a \\ c \sin kx, & -a \leq x \leq a \\ Be^{kx}, & x < -a \end{cases}$$

add

$$\Rightarrow BC =$$

$$\textcircled{1} \quad f(x)BC$$

$$-Be^{-ka} = c \sin ka \quad B k e^{-kka} = c k \cos ka$$

$$\text{We can get: } -ka \sin ka = k \cos ka$$

$$\tan(a) = -\frac{1}{k}$$

No.

Date

Like what we did, let $(a = z = \frac{a}{\hbar} \sqrt{2m(E+V_0)})$

$$z_0 = \frac{a}{\hbar} \sqrt{2mV_0}$$

$$\text{then } \tan(z) = -\frac{1}{k} = -\frac{\sqrt{2m(E+V_0)}}{\sqrt{-2mE}}$$

$$= -\sqrt{\frac{E+V_0}{-E}}$$

let it to be Q

For this part, we have:

$$\frac{z}{z_0} = \sqrt{\frac{E+V_0}{V_0}}$$

$$\text{then } \frac{1}{Q} = -\sqrt{\frac{-E}{E+V_0}} \quad \frac{z_0}{z} = \sqrt{\frac{V_0}{E+V_0}}$$

$$-\frac{1}{Q^2} + \frac{z_0^2}{z^2} = 1$$

$$\cancel{Q^2} = \frac{z_0^2}{z^2} - 1 \quad Q^2 = \frac{z^2}{z_0^2 - z^2} \cancel{Q^2} = \frac{z^2}{z_0^2 - z^2} \quad Q = \sqrt{\frac{z^2}{z_0^2 - z^2}}$$

$$\text{So finally: } \tan z = \frac{z}{z_0} - \sqrt{\frac{z^2}{z_0^2 - z^2}}$$

$$= -\sqrt{\frac{z^2 - z_0^2 + z_0^2}{z_0^2 - z^2}} = -\sqrt{-1 + \frac{z_0^2}{z_0^2 - z^2}}$$

In this part, we try to, but we failed

because there are z_0 and z in the below

which is no methods unless we get a reciprocal.
Luckily, $\overline{tcm} = \cot$, it has a meaning.

$$\text{So we could: } \cot(z) = -\sqrt{\frac{-E}{E+V_0}}$$

$$\frac{z_0}{z} = \sqrt{\frac{V_0}{E+V_0}} - \sqrt{\frac{-E}{E+V_0}} = \frac{1 - \cancel{\frac{z_0^2}{z^2}}}{-\sqrt{\frac{z_0^2}{z^2} - 1}}$$

$$\Rightarrow \cot(z) = -\sqrt{\frac{z_0^2}{z^2} - 1}$$

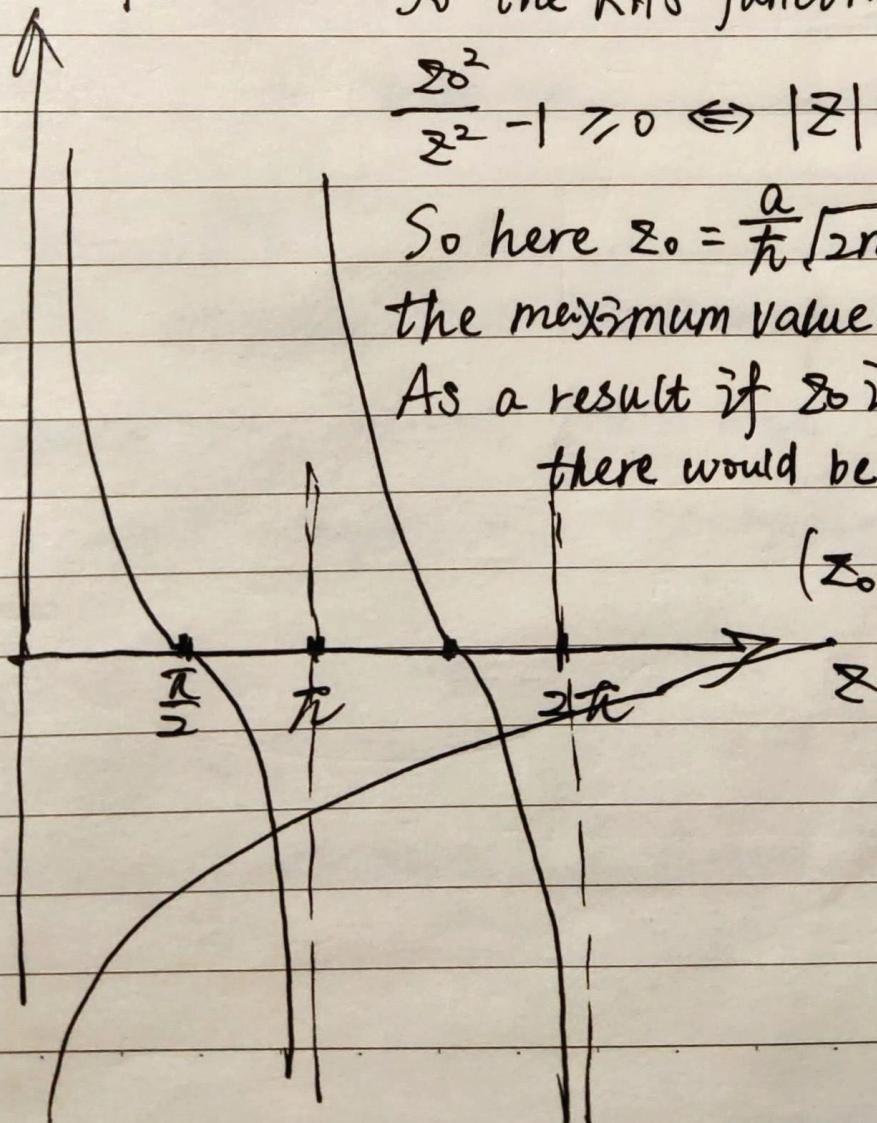
Let us Plot: So the RHS function should meet:

$$\frac{z_0^2}{z^2} - 1 \geq 0 \Leftrightarrow |z| \leq |z_0|$$

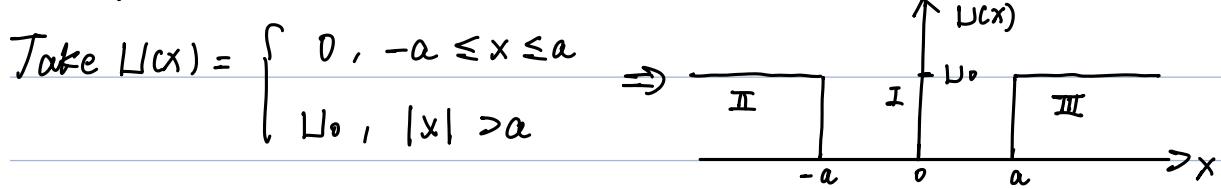
So here $z_0 = \frac{a}{\hbar} \sqrt{2mV_0}$ decided the maximum value of z .

As a result if z_0 is small enough there would be no intersection

(z_0) thus solution.
no



1D finite potential well — Matrix or Computer approach



Then we can discuss the solutions to different regions:

For II and III, they are similar:

$$\text{Get the general form } \psi(x) = \text{Constant}_1 e^{-kx} + \text{Constant}_2 \cdot e^{kx}$$

Then consider the infinity and avoid explosion

$$\text{The final result for II is: } \psi_{\text{II}}(x) = C e^{kx} \quad (x < -a) \quad \textcircled{1}$$

$$\text{for III is: } \psi_{\text{III}}(x) = F e^{-kx} \quad (x > a) \quad \textcircled{2}$$

For I, there are many solution candidates, but the symmetric $U(x)$ suggests us the wave function should be symmetric / anti-symmetric. So \sin/\cos would be better.

$$\psi_I(x) = A \cos(kx) + B \sin(kx) \quad (-a < x < +a) \quad \textcircled{3}$$

$\textcircled{1}$ $\textcircled{2}$ $\textcircled{3}$ are possible solutions, and we could add 4 Boundary Conditions on them:

$$x = +a$$

$$x = -a$$

$$\psi \text{ Continuous } A \cos(ka) + B \sin(ka) = F e^{-ka} \quad (4) \quad A \cos(ka) - B \sin(ka) = C e^{-ka} \quad (6)$$

$$\psi' \text{ Continuous } -A k \sin(ka) + B k \cos(ka) = -k F e^{-ka} \quad (5) \quad A k \sin(ka) + B k \cos(ka) = k C e^{-ka} \quad (7)$$

(4-7) could be written as matrix form:

$$\begin{pmatrix} \cos(ka) & \sin(ka) & 0 & -e^{-ka} \\ -k \sin(ka) & k \cos(ka) & 0 & k e^{-ka} \\ \cos(ka) & -\sin(ka) & -e^{-ka} & 0 \\ k \sin(ka) & k \cos(ka) & -k e^{-ka} & 0 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ F \end{pmatrix} = 0 \quad (8)$$

To get a non-trivial solution, we need the determinant of first Matrix = 0

which is equivalent to $J(E, a, U_0) = 0$

Namely: for given constants a, U_0 , find the permitted E . It's a "zero question"!

Some key feature of 1D finite well

1. The number of bound states are finite: symmetric, anti-symmetric, symmetric, anti-symmetric, ...
2. At least one symmetric bound state even U_0 is very shallow.

All the features could be read from Figure 7, which I drew it based on the analytical method's solution.

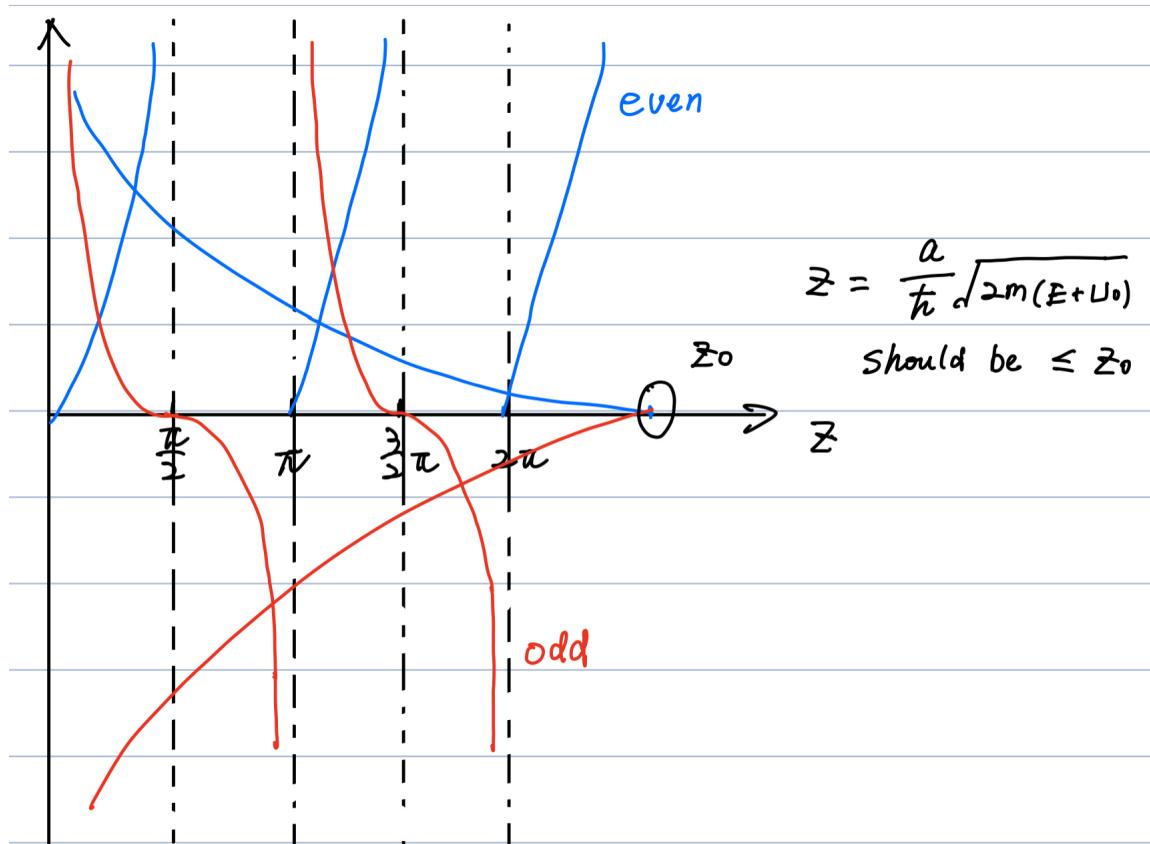


Figure 7: 1D finite well key features

1.6.2 1D harmonic oscillator

First we need to answer a question: **Why 1D harmonic oscillator so important?**

A: Physics around a equilibrium position is oscillator physics. Equilibrium position means:

$$\frac{dU}{dx}|_{x_0} = 0 \quad (14)$$

Then we could expand the potential energy near the equilibrium position to:

$$U(x) = U(x_0) + \frac{dU}{dx}|_{x_0} \cdot (x - x_0) + \frac{d^2U}{dx^2}|_{x_0} \cdot \frac{(x - x_0)^2}{2} \quad (15)$$

Use the Equation 14 condition:

$$U(x) = U(x_0) + \frac{d^2U}{dx^2}|_{x_0} \cdot \frac{(x - x_0)^2}{2} \quad (16)$$

If we only consider the behavior near the equilibrium position, then we could regard the second derivative of the potential energy here is a constant, name it k . Then the potential energy becomes:

$$U(x) = U(x_0) + \frac{1}{2}k(x - x_0)^2 \quad (17)$$

which has the same form as harmonic oscillator.

1. series method

The following two pdf pages has shown the series solution to 1D harmonic oscillator. I actually followed the process of [3]. However a question has come out(see the bottom of sub-page 2 of pdf page 1), then Prof. Hui's notes taught me how to solve it(see the sub-pages 3 and 4 of pdf page 1).

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How to solve 1D Harmonic oscillator? (with series solution)

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2} k x^2 \psi = E \psi$$

\Downarrow
 $\Downarrow \omega^2 m$

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{1}{2} m \omega^2 x^2 \psi = E \psi$$

Introducing one variable:

$$\xi = \sqrt{\frac{m\omega}{\hbar}} x \quad \text{But why is it no-unit?}$$

$$= \sqrt{\frac{m\omega x^2}{\hbar}} = \sqrt{\frac{m\omega^2 x^2}{\hbar\omega}} = \sqrt{\frac{m\omega^2 x}{\hbar\omega}} \sqrt{x}$$

I think the first part
is no-unit.

Then $x = \sqrt{\frac{\hbar}{m\omega}} \xi$, into it:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = (E - \frac{1}{2} m \omega^2 x^2) \psi$$

$$-\frac{\hbar^2}{2m} \frac{m\omega}{\hbar} \frac{d^2\psi}{d\xi^2} = (E - \frac{1}{2} m \omega^2 \frac{\hbar}{m\omega} \xi^2) \psi$$

$$-\frac{1}{2} \hbar \omega \frac{d^2\psi}{d\xi^2} = (E - \frac{1}{2} \hbar \omega \xi^2) \psi$$

$$\frac{d^2\psi}{d\xi^2} = (\xi^2 - \left(\frac{E}{\frac{1}{2}\hbar\omega}\right)) \psi$$

giving a result. ↗

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$$\text{So it becomes: } \frac{d^2\psi}{d\xi^2} = (\xi^2 - k) \psi \quad (2.72)$$

We noticed that if $\xi \rightarrow$ a large number,

$\xi^2 \gg k$. ξ^2 would dominate

$$\text{namely: } \frac{d^2\psi}{d\xi^2} = \xi^2 \psi \quad (2.74)$$

There is a solution: $A e^{-\frac{\xi^2}{2}} + B e^{\frac{\xi^2}{2}}$

Substituting it to verify:

$$\frac{d^2(A e^{-\frac{\xi^2}{2}})}{d\xi^2} = A (\xi^2 - 1) e^{-\frac{\xi^2}{2}} \approx A \xi^2 e^{-\frac{\xi^2}{2}}$$

$$\frac{d^2(B e^{\frac{\xi^2}{2}})}{d\xi^2} = B (\xi^2 + 1) e^{-\frac{\xi^2}{2}} \approx B \xi^2 e^{-\frac{\xi^2}{2}}$$

Since we have assumed

ξ^2 is a large number

But $B e^{\frac{\xi^2}{2}}$ is not able to be normalized.

So it becomes: $\psi(\xi) = f(\xi) e^{-\frac{\xi^2}{2}}$, when ξ is large
why this part changes from a constant $h(\xi)$
to a function of ξ

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$$\begin{aligned} &= e^{-\frac{1}{2}\xi^2} [\xi^{m+2} - (2m+1)\xi^m + m(m-1)\xi^{m-2}] \\ &= (e^{-\frac{1}{2}\xi^2} \cdot \xi^m) \cdot [\xi^2 - (2m+1) + m(m-1)\xi^{-2}] \\ &\approx (e^{-\frac{1}{2}\xi^2} \cdot \xi^m) \cdot \xi^2 \quad \text{Q.E.D.} \end{aligned}$$

So combining the both sides:

for the $h(\xi)$ in $\psi = h(\xi) e^{-\frac{1}{2}\xi^2}$

we have: $\begin{cases} h(\xi) \rightarrow A + B\xi^2 + O(\xi^2) & \text{when } \xi \rightarrow 0 \\ h(\xi) \rightarrow \xi^m & \text{when } \xi \rightarrow \infty \end{cases}$

Thus we have proved its feasibility of being solved by series method.

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Because the textbook is not too clear here.

① Firstly, it only discussed the situation of ∞ ,
but we could discuss when $\xi \rightarrow 0$:

The (2.72) becomes: $\frac{d^2\psi}{d\xi^2} = (\xi^2 - k) \psi = -k \psi$

$$\frac{d^2\psi}{d\xi^2} + k\psi = 0$$

That is, do derivative twice would give a minus constant multiplying itself.

Similars could do it!

So $\psi(\xi) = A \cos(\sqrt{k}\xi) + B \sin(\sqrt{k}\xi)$

$$\sim A[1 + O(\xi^2)] + B[\sqrt{k}\xi + O(\xi^3)]$$

$$\sim A + B'\xi + O(\xi^2) \dots$$

$$\sim [A + B'\xi + O(\xi^2)] \cdot e^{-\frac{1}{2}\xi^2}$$

② Secondly, it has lost a part for " ∞ ":

For large ξ , not only $e^{-\frac{1}{2}\xi^2}$ would satisfy,
 $\xi^m \cdot e^{-\frac{1}{2}\xi^2}$ would also satisfy.

We could try it:

$$\begin{aligned} (\xi^m \cdot e^{-\frac{1}{2}\xi^2})' &= m\xi^{m-1} \cdot e^{-\frac{1}{2}\xi^2} + e^{-\frac{1}{2}\xi^2} (-\xi) \xi^m \\ &= e^{-\frac{1}{2}\xi^2} (m\xi^{m-1} - \xi^{m+1}) \\ -\xi^m \cdot e^{-\frac{1}{2}\xi^2})'' &= e^{-\frac{1}{2}\xi^2} (-\xi)(m\xi^{m-1} - \xi^{m+1}) \\ &+ e^{-\frac{1}{2}\xi^2} [m(m-1)\xi^{m-2} - (m+1)\xi^m] \\ &= e^{-\frac{1}{2}\xi^2} [-m\xi^m + \xi^{m+2} + m(m-1)\xi^{m-2} - (m+1)\xi^m] \end{aligned}$$

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For the above equation:

$$C) \frac{d^4}{d\zeta^4} = (\frac{dh}{d\zeta} - \zeta h) e^{-\frac{\zeta^2}{2}}$$

$$C) \frac{d^4 h}{d\zeta^4} = (\frac{d^2 h}{d\zeta^2} - 2\zeta \frac{dh}{d\zeta} + (\zeta^2 - 1) h) e^{-\frac{\zeta^2}{2}}$$

Then back to (2.72) (Note: Let 2.74)

$$\frac{d^2 h}{d\zeta^2} - 2\zeta \frac{dh}{d\zeta} + (k-1) h = 0 \quad (2.78)$$

We assume $h(\zeta) = a_0 + a_1 \zeta + \dots$

$$= \sum_{j=0}^{\infty} a_j \zeta^j$$

$$C) \frac{dh}{d\zeta} = a_1 + 2a_2 \zeta + \dots = \sum_{j=0}^{\infty} j a_j \zeta^{j-1}$$

$$C) \frac{d^2 h}{d\zeta^2} = 2a_2 + 2 \times j a_j \zeta^j + \dots = \sum_{j=0}^{\infty} (j+1)(j+2) a_{j+2} \zeta^j$$

Back to (2.78), we get:

$$\sum_{j=0}^{\infty} [(j+1)(j+2) a_{j+2} - 2j a_j + (k-1) a_j] \zeta^j = 0$$

To make this eq. correct,

then the coefficient of every term needs to be zero:

That is, $(j+1)(j+2) a_{j+2} - 2j a_j + (k-1) a_j = 0$

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A max n $\alpha_{n+2} = 0$

What's more, if n is odd, $a_0 = 0$

if n is even, $a_0 \neq 0$

So we could use $k = 2n+1$ in a_{j+2} :

$$a_{j+2} = \frac{[2j+1 - (2n+1)]}{(j+1)(j+2)} a_j$$

$$\text{And: } k = \frac{E}{\frac{1}{2} \hbar \omega}$$

$$\text{So } E = \frac{1}{2} \hbar \omega (2n+1) !$$

$$= (n+\frac{1}{2}) \hbar \omega, n=0, 1, 2, \dots$$

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$$a_{j+2} = \frac{(2j+1-k)}{(j+1)(j+2)} a_j$$

This Eq contains all the information from the S-E in the beginning

$$h(\zeta) = h_{\text{even}}(\zeta) + h_{\text{odd}}(\zeta)$$

$$a_0 + a_2 \zeta^2 + a_4 \zeta^4 + \dots + a_1 \zeta + a_3 \zeta^3 + \dots$$

The only two unknowns here is a_0 & a_1

when $j \rightarrow \text{large}$, the $\frac{2j+1-k}{(j+1)(j+2)} \rightarrow \frac{2j}{j \cdot j} = \frac{2}{j}$

so the approximate solution for large j

$$a_j = C - \text{a const}$$

if $a_j = \frac{C}{(j/2)!}$ why the "C" here is same for even and odd?

$$h(\zeta) = C \sum \frac{1}{(j/2)!} \zeta^j$$

$$= C \sum \frac{1}{j!} \zeta^{2j} = C e^{\zeta^2}$$

So ζ should be $e^{\frac{\zeta^2}{2}}$, which could explode.

The only way to solve is: having a break point

Now we have solved 1D harmonic oscillator analytically, thus it is possible to get the explicit form of a few eigenfunctions and their graphs like Figure 8. **We could read some features from it:**

- (a) The even and odd functions would alternatively appear.

Like what we wrote in subsubsection 1.5.2, we know that the more “turns” indicates larger kinetic energy. So it is not strange the number of turns in Figure 8 would increase as the Energy eigenvalue increases. Thus we may get a not so arbitrary conclusion: **if the potential function is symmetric, then the eigenfunctions would behave as even and odd alternatively.** Since we have known that symmetric potential would result in even or odd wave function from 1.5.2, and from the view of turn number increasing, even and odd should appear alternatively.

- (b) As n increases, the width of the function would be wider.

We know that for oscillator, the potential energy would be larger in the region x is big. So if the total energy is increasing which indicating the potential energy should also increase, then the wave function should tend to the x -big-region to make more probability there, then get a larger expectation value of potential energy.

- (c) There are two vertical line in every state. It is corresponding to the classical turning point-the region further than the turning points are classically forbidden. So it is not strange for the higher energy states to have further turning points.

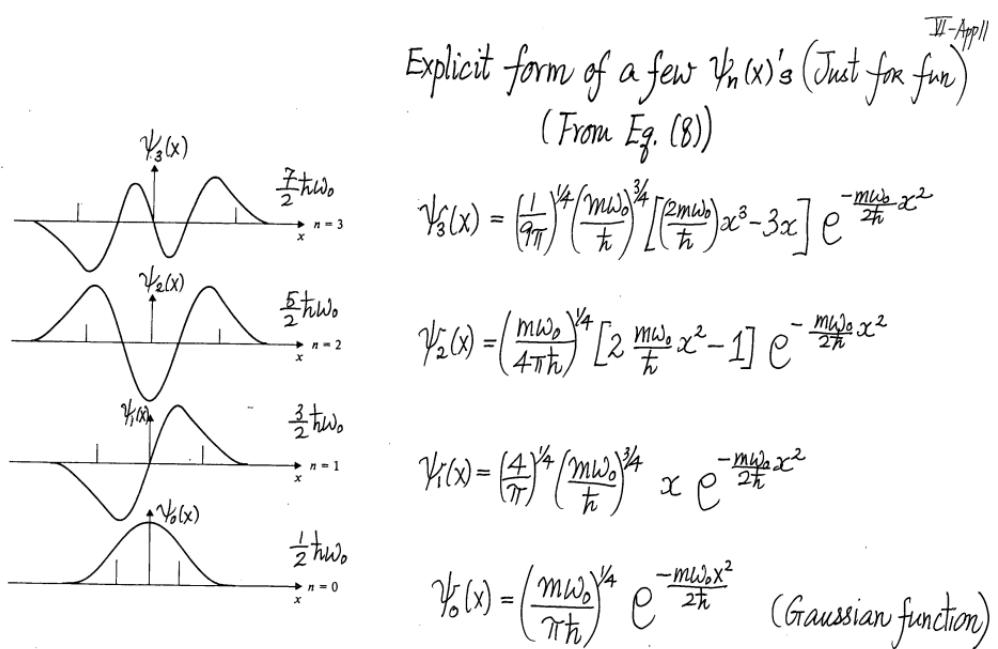


Figure 8: 1D harmonic key features

2. **Operator Method** Operator method is a method with inspiration. My process of solving is in the following two pages pdf. Now let me talk about the result and some by-products we could get from the operator method.

(a) **About the result:** the key idea is, if $|n\rangle$ is an eigenstate, then $\hat{a}^-|n\rangle$ and $\hat{a}^+|n\rangle$ generate other energy eigenstates.

(b) **By-product 1: selection Rule**

See the 3rd page of the following pdf.

(c) **By-product 2: $\infty \times \infty$ matrices in Oscillator Problem** Please see Figure 15 and the following several pages pdf.

Chapter 6 operator method

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2} m \omega_0^2 \hat{x}^2$$

Introduce two operators: $\hat{a}^- = \sqrt{\frac{m\omega_0}{2\hbar}} \hat{x} + i\sqrt{\frac{1}{2\hbar m\omega_0}} \hat{P} = \sqrt{\frac{m\omega_0}{2\hbar}} (\hat{x} + \frac{i}{m\omega_0} \hat{P})$

$$\hat{a}^+ = \sqrt{\frac{m\omega_0}{2\hbar}} \hat{x} - i\sqrt{\frac{1}{2\hbar m\omega_0}} \hat{P} = \sqrt{\frac{m\omega_0}{2\hbar}} (\hat{x} - \frac{i}{m\omega_0} \hat{P})$$

Why this form? Because they satisfy:

$$\hat{a}^+ \hat{a}^- = \frac{1}{\hbar \omega_0} \hat{H} - \frac{1}{2} \quad ; \quad \hat{H} = \hbar \omega_0 (\hat{a}^+ \hat{a}^- + \frac{1}{2})$$

cost of change order: +1

it means they could change order

Test some properties: $[\hat{a}^-, \hat{a}^+] = 1 \quad [\hat{a}^-, \hat{a}^-] = 0, [\hat{a}^+, \hat{a}^+] = 0$

We have a new combination $(\hat{a}^+ \hat{a}^-)$, test it:

$$[\hat{a}^-, \hat{a}^+ \hat{a}^-] = \hat{a}^- \hat{a}^+ \hat{a}^- - \hat{a}^+ \hat{a}^- \hat{a}^- = (\hat{a}^+ \hat{a}^- + 1) \hat{a}^- - \hat{a}^+ \hat{a}^- \hat{a}^- = \hat{a}^- \quad \textcircled{7}$$

$$[\hat{a}^+, \hat{a}^+ \hat{a}^-] = \hat{a}^+ \hat{a}^+ \hat{a}^- - \hat{a}^+ \hat{a}^- \hat{a}^+ = \hat{a}^+ \hat{a}^+ \hat{a}^- - \hat{a}^+ (\hat{a}^+ \hat{a}^- + 1) = -\hat{a}^+ \quad \textcircled{8}$$

They are far beyond this form: $[\hat{a}^-, \hat{a}^+ \hat{a}^-] = [\hat{a}^-, \frac{1}{\hbar \omega_0} \hat{H}]$

$$[\hat{a}^+, \hat{a}^+ \hat{a}^-] = [\hat{a}^+, \frac{1}{\hbar \omega_0} \hat{H}]$$

Define $\hat{a}^+ \hat{a}^- = \hat{N}$, then $\hat{H} = \hbar \omega_0 (\hat{N} + \frac{1}{2})$

\hat{N} has its own eigenvalue problem: its eigenvalues are numbers

$$\hat{N} |n\rangle = n |n\rangle$$

So for \hat{H} : $\hat{H} |n\rangle = \hbar \omega_0 (\hat{N} + \frac{1}{2}) |n\rangle = \underbrace{\hbar \omega_0 (n + \frac{1}{2})}_{\text{So } E_n = (n + \frac{1}{2}) \hbar \omega_0} |n\rangle = E_n |n\rangle$

$$E_n = (n + \frac{1}{2}) \hbar \omega_0$$

Now use $\textcircled{7}$ and $\textcircled{8}$ $\hat{H} (\hat{a}^- |n\rangle) = \hat{a}^- \hat{H} |n\rangle - [\hat{a}^-, \hat{H}] |n\rangle$

$$= \hat{a}^- E_n |n\rangle - \hbar \omega_0 \hat{a}^- |n\rangle$$

$$= (E_n - \hbar \omega_0) (\hat{a}^- |n\rangle) \quad \textcircled{13}$$

It means if \hat{a}^- acts on an eigenstate, then it would convert it into the lower eigenstate (lower $\hbar \omega_0$ in eigenvalue)

For \hat{a}^+ : $\hat{H} (\hat{a}^+ |n\rangle) = E_n \hat{a}^+ |n\rangle - [\hat{a}^+, \hat{H}] |n\rangle = E_n \hat{a}^+ |n\rangle - (-\hbar \omega_0 \hat{a}^+) |n\rangle$

$$= (E_n + \hbar \omega_0) (\hat{a}^+ |n\rangle) \quad \textcircled{15}$$

It means if \hat{a}^+ acts on an eigenstate, then it would convert it into the higher eigenstate (higher two in eigenvalue)

Note! Above we say they are converted to the higher or lower eigenstate, means they are parallel to the new state not equal to. So there must be some constants we need to solve!

$$\text{And the result is: } \hat{a}^- |n\rangle = C_1 |n-1\rangle = \sqrt{n} |n-1\rangle$$

$$\hat{a}^+ |n\rangle = C'_1 |n+1\rangle = \sqrt{n+1} |n+1\rangle$$

Finally we need a cut off!

Because for "Energy of oscillator", it could not be negative!

So there must be a $|n_{\min}\rangle$ satisfying:

$$\hat{a}^- |n_{\min}\rangle = 0$$

Then no matter how many \hat{a}^- are going to apply, it would stay zero!

And: $|n\rangle$ is the eigenstate of $\hat{N} = \hat{a}^+ \hat{a}^-$

So we can construct $\hat{a}^+ \hat{a}^- |n_{\min}\rangle = 0$ to get:

\hat{N} has 0 as its minimum eigenvalue.

So it is naturally to label $|n_{\min}\rangle = |0\rangle$

And what we are interested in is $\hat{H} = \hbar\omega_0(\hat{N} + \frac{1}{2})$

$$\hat{H} |0\rangle = \hbar\omega_0(\hat{a}^+ \hat{a}^- + \frac{1}{2}) |0\rangle = \frac{1}{2} \hbar\omega_0 |0\rangle$$

And from ⑯ we could calculate the eigenvalue for \hat{H} :

$$E_n = (\frac{1}{2} + n) \hbar\omega_0$$

To express the eigenfunction from operator's method:

$$|n\rangle = \frac{1}{\sqrt{n!}} (\hat{a}^+)^n |0\rangle$$

By-product 1 : Selection Rule

Let the notation of $\int_{-\infty}^{\infty} \psi_1^*(x) \times \psi_0(x) dx$ be $\langle \hat{x} | 0 \rangle$

$\int_{-\infty}^{\infty} \psi_1^*(x) \psi_0(x) dx$ be $\langle 1 | 0 \rangle$

Then for \hat{a}^+ and \hat{a}^- we have : $\langle n' | \hat{a}^- | n \rangle = \sqrt{n} \langle n' | n-1 \rangle$

$$= \sqrt{n} \delta_{n', n-1}$$

$$\langle n' | \hat{a}^+ | n \rangle = \sqrt{n+1} \delta_{n', n+1}$$

And $\hat{x} = \sqrt{\frac{\hbar}{2m\omega_0}} (\hat{a}^- + \hat{a}^+) \quad \hat{p} = -i\sqrt{\frac{\hbar m\omega_0}{2}} (\hat{a}^- - \hat{a}^+)$

||

We could calculate $\langle n' | \hat{x} | n \rangle$ or $\langle n' | \hat{p} | n \rangle$

$$\sqrt{\frac{\hbar}{2m\omega_0}} [\sqrt{n} \delta_{n', n-1} + \sqrt{n+1} \delta_{n', n+1}] - i\sqrt{\frac{\hbar m\omega_0}{2}} [\sqrt{n} \delta_{n', n-1} - \sqrt{n+1} \delta_{n', n+1}]$$

the "δ" here indicates the transition is allowed only when $\Delta n = \pm 1$

1.7 chapter 7

This chapter is very short, as a preparation chapter for the Spherically Symmetric Problems, which is also the preparation chapter for H atom chapter.

1.7.1 The feasibility of variable separation comes from the special form of potential energy

This chapter's major idea is: **the feasibility of variable separation comes from the special form of potential energy**, that is, could be written as the sum of the potential energies from different dimensions. My example of 2D infinite square well is shown in figures 9 and 10. There would be some questions and they are answered below:

1. **Q: A question from chapter 9: why variable separation could also work on H atom, since its potential energy only relies on its r coordinate?**

A: Only relies on one coordinate, means the potential energy from other coordinates is zero, thus it could also be written as $U = U(r) = U(r) + U(\phi) + U(\theta)$ where $U(\phi) = u(\theta) = 0$. So our deduction still works. **Another thing we could know is that this principle is not only valid in Cartesian coordinates, but also other coordinates like spherically coordinates.**

2. **Q: A question from Physics Of Atoms: when treating the multi-electron atom problem(to be more precise, 2-electron problem) by perturbation method, we used a Hamiltonian without the electron-electron term to be the H^0 , so how could we decide the wave function corresponding to H^0 is just the multiplication of two single-electron wave functions?**

A: The same reason! Also because the total potential term is the addition of two separate potential terms. Actually when Prof. Hui asked me this question for the first time, I am a little suspicious of it, because what I saw is not only the potential terms of them are added, their kinetic terms are also added. But back to the examples in this chapter, we could see actually the for this example, the kinetic terms are also added. So I guess maybe we could say "**if the Hamiltonian could be written as the addition of Hamiltonians from different dimensions, then the total problem could be solved by variables separation method**". It's just that the kinetic terms always could be written as the addition of different particles or dimensions' kinetic terms, so actually if the total potential term is the

addition of the separate potential terms, then the total Hamiltonian is always the addition of separate Hamiltonians.

1.7.2 degenerate and degeneracy

Besides, this chapter also introduces the concept of **degenerate/degeneracy**, which would also be seen in H Atom. **Degeneracy** is the number of different eigenstates corresponding to a certain energy eigenvalue. If one eigenvalue's degeneracy is more than 1, then we call it **degenerate**; if more than 1(2 or more), it is called **non-degenerate**.

Degenerate/degeneracy also came from the feasibility of variable separation: in many cases the potential energies from different dimensions hold the same format, thus causing the possibility of degeneracy easily. For example, on the bottom of figure 10 comes the formula of eigenvalues of 2D infinite square well, where n_x n_y have the same status, that is, at least $n_x = i, n_y = j$ and $n_x = j, n_y = i$ would have the same eigenvalues thus be degenerate.

2D infinite square well

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \Psi(x, y, t) + V(x, y) \Psi(x, y, t) = i\hbar \frac{\partial}{\partial t} \Psi(x, y, t)$$

$$V(x, y) = \begin{cases} 0 & , x \in [0, a] \text{ & } y \in [0, a] \\ \infty & , \text{ else} \end{cases}$$

$$\tilde{\Psi}(x, y, t) = \Psi(x, y) T(t)$$

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \Psi(x, y) T(t) + V(x, y) \Psi(x, y) T(t) = i\hbar \frac{\partial}{\partial t} \Psi(x, y) T(t)$$

$$-\frac{\hbar^2}{2m} T(t) \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \Psi(x, y) + V(x, y) \Psi(x, y) T(t)$$

$$= \Psi(x, y) T(t) \frac{\partial T(t)}{\partial t}$$

$$-\frac{\hbar^2}{2m} \frac{1}{\Psi(x, y)} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \Psi(x, y) + V(x, y) = \frac{1}{T(t)} \frac{\partial T(t)}{\partial t}$$

For the first part

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \Psi(x, y) + V(x, y) \Psi(x, y) = E \Psi(x, y)$$

Separate variables again:

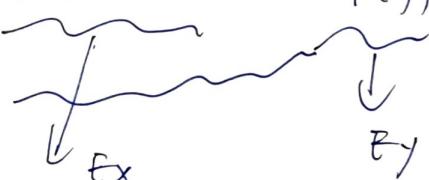
$$\Psi(x, y) = X(x) Y(y) : -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) X(x) Y(y) + V(x, y) X(x) Y(y) = E X(x) Y(y)$$

When $V(x, y) = 0$

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) X(x) Y(y) = E X(x) Y(y)$$

Figure 9: 2D infinite square well page 1

$$-\frac{\hbar^2}{2m} [Y(y) X''(x) + X(x) Y''(y)] = E X(x) Y(y)$$

$$-\frac{\hbar^2}{2m} \left[\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} \right] = E$$


$$Ex + Ey = E$$

Then for x, y :

$$\begin{cases} -\frac{\hbar^2}{2m} \frac{\partial^2 X}{\partial x^2} = Ex X \\ -\frac{\hbar^2}{2m} \frac{\partial^2 Y}{\partial y^2} = Ey Y \end{cases}$$

We could just use the conclusion of 1D infinite well:

$$X_{nx}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n_x \pi x}{a}\right), \quad Y_{ny}(y) = \sqrt{\frac{2}{b}} \sin\left(\frac{n_y \pi y}{b}\right)$$

$$\Psi_{n_x, n_y} = \sqrt{\frac{4}{ab}} \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{b}\right)$$

$$E_{n_x, n_y} = \cancel{\text{Add } E \text{ to } X(x) Y(y)}$$

$$\begin{aligned} -\frac{\hbar^2}{2m} \left[\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} \right] &= +\frac{\hbar^2}{2m} \left[\left(\frac{n_x \pi}{a}\right)^2 + \left(\frac{n_y \pi}{b}\right)^2 \right] \\ &= \frac{\hbar^2 \pi^2}{2m} \left[\left(\frac{n_x}{a}\right)^2 + \left(\frac{n_y}{b}\right)^2 \right] \end{aligned}$$

Figure 10: 2D infinite square well page 2

1.8 chapter 8

Chapter 8 is the basis of chapter 9. Since H atom problem is a special case of the “**potential only depends on r spherical problem**”. We have discussed all the things we could get without considering the Coulomb potential.

Firstly, since the angular part is not related to the radial part, we could discuss its solution

totally even without considering Coulomb potential.

Secondly, orbital angular momentum is also something we could get without knowing the explicit form of radial part solution. We got its analytical form operator and found it is similar to the angular part equation. So we use the solution we derived for the angular part equation to get the eigenvalues and eigenfunctions of orbital angular momentum. And this try actually helps us get the physical meaning of two quantum number(l, m_l) obtained in the first part!

1.8.1 Angular part of spherical problem

In conclusion, we have use variable separation to get the (Angular part equation),

$$\left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} (\sin\theta \frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] Y_{lm_l} = -l(l+1)Y_{lm_l} \quad (\text{Angular part equation})$$

and then found the solution to Y_{lm_l} , which is shown in 13:

$$Y_{lm_l}(\theta, \phi) = A_{lm_l} P_l^{m_l}(\cos\theta) e^{im_l\phi} \quad (\text{Angular part solution})$$

where A_{lm_l} is the Normalization constant.

$$-\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] + V \psi = E \psi \quad (4.14)$$

This is the 3D spherical TDSE for all problems

The following would only specify on H-atom.

Let

$$\psi(r, \theta, \phi) = R(r) Y(\theta, \phi)$$

then (4.14) becomes

only reduced to

$$\left\{ \frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) - \frac{2mr^2}{\hbar^2} [V(r) - E] \right\} +$$

$$+ \frac{1}{r^2} \left\{ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 Y}{\partial \phi^2} \right\} = 0$$

$\theta \& \phi$

Because we need to use "Legendre polynomials" for $Y(\theta, \phi)$, so the constant is a bit complex:

$$L(L+1) - L(L+1)$$

Part 1 $Y(\theta, \phi)$

$$\sin \theta \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + \frac{\partial^2 Y}{\partial \phi^2} = -L(L+1) \sin^2 \theta Y$$

$$Y(\theta, \phi) = R(r) E(\phi) \text{, then}$$

Figure 11: Spherical problem angular part solution 1

No. _____
 Date _____

$\left\{ \frac{1}{\theta} [I \sin \theta \frac{d}{d\theta} (\sin \theta \frac{d\psi}{d\theta})] + ((l+1) \sin^2 \theta \right\}$

$+ \left(\frac{1}{\theta} \frac{d^2 \psi}{d\theta^2} \right) = 0$

Now we can separate again.

$-m^2$

It's the simplest one:

$\Psi(\theta) = e^{im\theta}$

For ϕ :

$[\sin \theta \frac{d}{d\theta} (\sin \theta \frac{d\psi}{d\theta})] + ((l+1) \sin^2 \theta \psi - m^2 \psi) = 0$

After changing variables, $\begin{cases} v = \cos \theta \\ \theta \rightarrow PV \end{cases}$

we could get a form like $\frac{d}{dv} [(1-v^2) \frac{dp}{dv}] + [A - \frac{m^2}{1-v^2}] p = 0$

And for this equation,

we have a solution:

$P_l^m(\cos \theta) = (1 - \cos^2 \theta)^{\frac{|m|}{2}} \left(\frac{d}{dv} \right)^{|m|} P_l(v \cos \theta)$

And for every l , m could be $\underbrace{-l, -l+1, \dots, 0, \dots, l}_{(2l+1)}$

Figure 12: Spherical problem angular part solution 2

So finally we have
 $Y_{lm}(\theta, \phi) \sim P_l^{|m|}(\cos\theta) \cdot e^{im\phi}$

Figure 13: Spherical problem angular part solution 3: result

1.8.2 Orbital angular momentum

We naturally would consider the orbit angular momentum since angular momentum is another important physical quantity just like energy. So like the idea in recipe 2, we could **think classically** first:

In Cartesian coordinate, the orbital momentum operator is easy to get:, **waiting for further completing**. And by Chain rule, which also works for partial derivative, we could get the angular momentum operator in spherical coordinate:

$$\hat{L}_x = i\hbar(\sin\phi \frac{\partial}{\partial\theta} + \cot\theta \cos\phi \frac{\partial}{\partial\phi}) \quad (18)$$

$$\hat{L}_y = i\hbar(-\cos\phi \frac{\partial}{\partial\theta} + \cot\theta \sin\phi \frac{\partial}{\partial\phi}) \quad (19)$$

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial\phi} \quad (20)$$

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} (\sin\theta \frac{\partial}{\partial\theta}) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \quad (21)$$

Then we need to **go quantum**, but unlike the cases where we need to find the eigenfunction with lots of efforts, here we could notice the 21 firstly, since it looks similar to the Angular part equation. It could even be written as:

$$\frac{\hat{L}^2}{\hbar^2} Y_{lm_l} = l(l+1) Y_{lm_l} \quad (22)$$

thus

$$\hat{L}^2 Y_{lm_l} = l(l+1)\hbar^2 Y_{lm_l} \quad (23)$$

So we found the physical meaning of the quantum number $l : l(l+1)\hbar^2$ is the eigenvalue of the square of the total orbit angular momentum.

And we also could notice the form of 20 is very simple, only has derivative of ϕ . And actually in the Angular part solution, the ϕ part is also very special, which is exponential function. It implies us to try:

$$\hat{L}_z Y_{lm_l}(\theta, \phi) = -i\hbar A_{lm_l} P_l^{m_l}(\cos\theta) \frac{\partial}{\partial\phi} e^{im_l\phi} = m_l \hbar Y_l^{m_l}(\theta, \phi) \quad (24)$$

So we luckily got the physical meaning of m_l too! $m_l\hbar$ means the eigenvalue of the z direction orbit angular momentum.

Combining the physical meaning-the z direction component $m_l\hbar$ should not be greater than the total orbit angular momentum $\sqrt{l(l+1)\hbar}$, we could get the value range for m_l :

$$m_l = -l, -l+1, \dots, 0, \dots, l-1, l \quad (25)$$

0 could be achieved since m_l is an integer. The integer property comes from:

$$\Phi(\phi) = \Phi(\phi + 2\pi) \quad (26)$$

Here are some additional properties for orbital angular momentum:

1. $[\hat{L}^2, \hat{L}_x] = [\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z] = 0$ and $[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z \quad [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x \quad [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$

2. Commute with Hamiltonian

Based on 1: $[\hat{A}, \hat{B}] = 0 \Leftrightarrow \hat{A}\hat{B}$ share common set of eigenstates we could know we can find who shares the same eigenfunctions with the orbital angular momentum operator to decide the commutation. But we only know Y_{lm_l} is the eigenfunctions of \hat{L}^2 , it is only part of the eigenfunction of the Hamiltonian!

However, if an operator is not dependent on some variables, then it could exchange with the function dependent on those variables:

$$\hat{L}^2 Y_{lm_l} = l(l+1)\hbar^2 Y_{lm_l} \quad (23 \text{ revisited})$$

$$\begin{aligned} R(r)\hat{L}^2 Y_{lm_l} &= R(r)l(l+1)\hbar^2 Y_{lm_l} \\ \Leftrightarrow R(r)\hat{L}^2 Y_{lm_l} &= l(l+1)\hbar^2 R(r)Y_{lm_l} \\ \Leftrightarrow \hat{L}^2 R(r)Y_{lm_l} &= l(l+1)\hbar^2 R(r)Y_{lm_l} \end{aligned} \quad (27)$$

where $R(r)Y_{lm_l}$ is the eigenfunction of H atom's Hamiltonian. As a result:

$$[\hat{H}, \hat{L}^2] = [\hat{H}, \hat{L}_x] = [\hat{H}, \hat{L}_y] = [\hat{H}, \hat{L}_z] = 0 \quad (28)$$

1.9 chapter 9

1.9.1 How to get the radial part

Let me do some advanced operation for the original problem in 14.

Part 2. Radial Part $R(r)$

$$\frac{d}{dr} \left(r^2 \frac{\partial R}{\partial r} \right) - \frac{2m r^2}{\hbar^2} [V(r) - E] R = U(l) R$$

With $u(r) = R(r) \cdot r$, it could be simpler.

$$-\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \left[V + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \right] u = Eu$$

That's ~~the~~ difference with

1D TISE

Let κ be "Effective Potential"

$$V = -\frac{e^2}{4\pi\epsilon_0 r} \quad \text{For A-atom.}$$

κ
 bound -cuss
 scattering

Name $\frac{1-2mE}{\hbar^2}$ as K

Since $E < 0$ for Bound state

$$\frac{1}{K^2} \frac{d^2 u}{dr^2} = 1 - \left(\frac{me^2}{2\pi\epsilon_0\hbar^2} \right) \frac{1}{(Kr)} + \frac{U(l)}{(Kr)^2} u$$

Figure 14: H atom radial part 1

After get some variables replaced, the equation becomes:

$$\frac{d^2 u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2} \right] u \quad (\text{radial equation after processed})$$

Then consider two limiting cases:

1. when $\rho \rightarrow \infty$ (radial equation after processed) becomes:

$$\frac{d^2 u}{d\rho^2} = u \quad (29)$$

The solution is:

$$u(\rho) = Ae^{-\rho} + Be^{\rho} \quad (30)$$

To avoid explode, B should equal to zero. So the final solution is:

$$u(\rho) = Ae^{-\rho} \quad (31)$$

2. when $\rho \rightarrow 0$ (radial equation after processed) becomes:

$$\frac{d^2u}{d\rho^2} = \frac{l(l+1)}{\rho^2}u \quad (32)$$

whose solution should be:

$$u(\rho) = C\rho^{l+1} + D\rho^{-l} \quad (33)$$

This one is not too obvious as the former one, but just do second derivative for the solution, we will find it just satisfies (32). maybe waiting for future completing

And to avoid explosion, D needs to be zero, so the final solution becomes:

$$u(\rho) = C\rho^{l+1} \quad (34)$$

Considering both two cases, the final complete solution should be:

$$u(\rho) = \rho^{l+1}e^{-\rho}v(\rho) \quad (35)$$

Then the (radial equation after processed) becomes:

$$\rho \frac{d^2v}{d\rho^2} + 2(l+1-\rho) \frac{dv}{d\rho} + [\rho_0 - 2(l+1)]v = 0 \quad (\text{radial equation in terms of } v(\rho))$$

We could try to see whether the $v(\rho)$ could be expressed in a series:

$$v(\rho) = \sum_{j=0}^{\infty} c_j \rho^j \quad (36)$$

Then calculate the first order and second order derivatives and substitute them into (radial equation in terms of $v(\rho)$), we could get this relationship by comparing the items with same order:

$$c_{j+1} = \left\{ \frac{2(j+l+1) - \rho_0}{(j+1)(j+2l+2)} \right\} c_j \quad (\text{recurrence relation})$$

With this Recurrence relation, we could find that if we know c_0 then every item is known, thus the whole $v(\rho)$ is known. But c_0 could be got through Normalization, so everything has been ensured now.

But we want to get a formula rather than a recurrence relation, so let us consider when the **j is very large**.

Then the (recurrence relation) becomes:

$$c_{j+1} \simeq \frac{2j}{(j+1)j} c_j = \frac{2}{j+1} c_j \quad (37)$$

which is equivalent to

$$c_j = \frac{2^j}{j!} c_0 \quad (38)$$

It is just the Taylor's Formula for exponential function:

$$v(\rho) = c_0 \sum_{j=0}^{\infty} \frac{2^j}{j!} \rho^j = c_0 e^{2\rho} \quad (39)$$

As we said, we are considering j is very large, so to avoid explosion, we need to add cutoff: for a certain max integer j_{max} , it must have $c_{j_{max}+1}$. And back to the (recurrence relation), we could have:

$$2(j_{max} + l + 1) - \rho_0 = 0 \quad (40)$$

Here we define n, the principal quantum number, please note, although we know there is a "n" from senior high, but here we defined it for the first time, we have never seen it before:

$$n = j_{max} + l + 1 \quad (41)$$

And it is also the origin of the quantum number l's value range: since j starts from 0, so $l_{max} = n - 1$; as a result the value range is from 0 to n-1.

Considering Equation 40 and Equation 41, we have:

$$\rho_0 = 2n \quad (42)$$

As ρ_0 is connected to energy, then n would also connect the energy:

$$E = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2} = \frac{E_1}{n^2}, n = 1, 2, 3, \dots \quad (43)$$

Summary of the result

Combining (35) and $u = R(r) \cdot r$, we have:

$$R_{nl}(r) = \frac{1}{r} \rho^{l+1} e^{-\rho} v(\rho) = c_0 \frac{1}{r} \rho^{l+1} e^{\rho} \quad (44)$$

But do the normalization to get c_0 is kind of tiring, more importantly even we do the normalization here, we need to do normalization again for the whole solution, so why not just leave the

normalization step to the end? Now we could use some functions given by mathematician here **firstly-associated Laguerre function**:

$$v(\rho) = L_{n-l-1}^{2l+1}(2\rho) \quad (45)$$

which is associated with the quantum number n and l.

then the final result could be written as:

$$R_{nl}(r) = \frac{1}{r} \rho^{l+1} e^{-\rho} L_{n-l-1}^{2l+1}(2\rho) \quad (46)$$

Several questions may be asked by readers

1. **This part's derivation seems similar to the series method for 1D harmonic oscillator, right?**

A: Yes! And we would find many things in common: both studying the behavior at ∞ and 0 to get the asymptotic solution, both needing series method, both needing cutoff from physics background, both using some math work(Hermite polynomials/Laguerre function)

2. **You have mentioned *Normalization* when getting Equation 45, so what is the Normalization formula for the H atom question?**

A: it should be

$$\int |\psi|^2 r^2 \sin\theta dr d\theta d\phi = 1 \quad (47)$$

And we also have:

$$\int |\psi|^2 r^2 \sin\theta dr d\theta d\phi = \int |R|^2 r^2 dr \int |Y|^2 \sin\theta d\theta d\phi \quad (48)$$

It means we only need to ensure the multiplication of the two parts is equal to 1, because what matters is the total result. For example, trying to normalize the two parts to 0.5 and 2 would also work for our problem.

But for convenience, normalize both the two parts to 1 is a good choice. So the final normalization condition becomes:

$$\int_0^{+\infty} |R|^2 r^2 dr = \int_0^{2\pi} \int_0^\pi |Y|^2 \sin\theta d\theta d\phi = 1 \quad (49)$$

1.9.2 How to understand the whole solution of H atom

Combining chapter 8 and 9, we could get the total solution of H atom:

$$\psi_{nlm_l} = R_{nl}(r) Y_{lm_l}(\theta, \phi) \quad (50)$$

So in total, $R_{nl}(r)$ would govern the radial dependence, while $Y_{lm_l}(\theta, \phi)$ governs the angular dependence.

Take ψ_{100} as an example, now it is composed of:

$$Y_{00}(\theta, \phi) = \text{constant} \cdot \frac{1}{\sqrt{4\pi}} \quad (51)$$

which means every direction has a same value, that is, isotropic or no preferred direction and

$$R_{10}(r) = \frac{1}{a_0^{\frac{3}{2}} \sqrt{\pi}} e^{\frac{-r}{a_0}} \quad (52)$$

which indicates the dropping trend with the radius.

The radius part is easy to understand, let me take another example of the angular part to show the case of an-isotropic:

$$Y_{10} = \sqrt{\frac{3}{4\pi}} \cos\theta \quad (53)$$

which means it only depends on θ .

Several important things we could extract from H atom problem

1. **Probability corresponds to a differential, rather than a derivative**(for the Chinese readers who have a problem of those terminology, there is a web page 为什么导数和微分的英日文术语如此混乱? - 知乎)

We often said the probability is the square of wave function, but in fact the precise description should be: **The probability of finding the electron in a volume element $d\tau$ is dP** , which is:

$$dP = |\psi_{nlm_l}(r, \theta, \phi)|^2 d\tau = |\psi_{nlm_l}(r, \theta, \phi)|^2 \cdot r^2 \sin\theta dr d\theta d\phi \quad (54)$$

The spherical system is a good example for us, since in Cartesian coordinates, $d\tau$ is always $dx dy dz$, which would easily be neglected.

- (a) **To calculate the probability in one dimension, we need to integrate all the other dimensions**

It is actually the integration of Equation 54

$$dP(r \rightarrow r + dr) = \int_0^{2\pi} \int_0^\pi dP = \int_0^{2\pi} \int_0^\pi |\psi_{nlm_l}(r, \theta, \phi)|^2 \cdot r^2 \sin\theta dr d\theta d\phi \quad (55)$$

Then extract the part independent of θ or ϕ :

$$dP(r \rightarrow r + dr) = r^2 |R_{nl}(r)|^2 dr \cdot \int_0^{2\pi} d\phi \int_0^\pi d\theta |Y_{lm_l}(\theta, \phi)|^2 \sin\theta \quad (56)$$

And luckily we have talked about the second part in last chapter, that is Equation 49, which is equal to 1. So:

$$dP(r \rightarrow r + dr) = r^2|R_{nl}(r)|^2dr \cdot 1 = r^2|R_{nl}(r)|^2dr \quad (57)$$

2. The probability distribution function corresponds to the derivative, that is, no “d something” part in it

For the two probabilities we discussed above, their distribution functions are accordingly:

$$P = \frac{dP}{drd\theta d\phi} = |\psi_{nlm_l}(r, \theta, \phi)|^2 \cdot r^2 \sin\theta \quad (58)$$

$$P(r) = \frac{dP(r)}{dr} = r^2|R_{nl}(r)|^2 \quad (59)$$

3. A serious question comes: from what we learnt in Recipe 1: General Initial Value Problems in Quantum Mechanics, if the H atom is in a eigenstate, it could not evolve to other eigenstates. But we know the atom could de-excite to a lower energy state and emit a photon, is there anything wrong with QM?

Actually the Hamiltonian we used is just the one for H atom itself, so it only means if we could find a environment without other things, it would not evolve to other eigenstates. But actually even in the vacuum it is still not totally isolated. In the formula's way:

$$\hat{H}_{whole} = \hat{H}_{H-atom} + \hat{H}_{photon} + \hat{H}_{interaction} \quad (60)$$

it means it is impossible to eliminate the $\hat{H}_{interaction}$, which is not zero even in the vacuum.

Further discussion could be found in Atomic Transitions, Light-Matter Interaction And Approximation.

1.10 chapter 10: More on Operators and some Formal Results

As the title *chapter 10: More on Operators and some Formal Results* suggested: The first part is about some additional knowledge on operators. Actually I just want to put all the knowledge about operators in one place like 1.4, to be more concentrated, for example I put Ehrenfest theorem in 1.4. But when writing this chapter I found Prof. Hui's purpose: there are some knowledge on operators could not be introduced until some background was introduced, for example the paragraph *More on orthogonal* has involved the concept degenerate, so we could not discuss it earlier than *degenerate and degeneracy*. As a result: in 1.10.1 I only discussed the content not has been covered previously; 1.10.2 is a totally strange topic, it introduced the relationship between orbital angular

momentum and spin-they are just twins from the same mathematical origin-in the discussion of the origin(1.10.2), no additional physics background is needed, so the discoveries of the two became very natural!

1.10.1 More on Operators

More on orthogonal : even the degenerate states could be orthogonal

Back to page 20, we could have this result:

$$(a_m - a_n) \int \psi_m^\dagger \psi_n d\tau = 0 \quad ((11) \text{ revisited})$$

So even the eigenvalues is equal, it does not mean the eigenfunctions have to be non-orthogonal. Actually, for the degenerate eigenstates(suppose the total number is n), we always have a method to construct n new orthogonal eigenfunctions to replace them. The new n eigenfunctions would be orthogonal to each other and share the same eigenvalues as the former ones. So they could play the role of the old ones totally.

The method is what we learnt in Linear Algebra, Gram–Schmidt process.

One question may be asked by readers: does it mean the parallel eigenfunctions would be constructed to be orthogonal? Since it seems too “easy” to construct two orthogonal eigenfunctions from above discussion.

A: No! The reason remains in the part I have not expanded, that is, the Gram–Schmidt process. Let us take the two eigenfunctions situation as an example, there are two eigenfunctions $\psi_{n1}, \psi_{n2} \leftrightarrow a_n$, then the construction process would be:

$$\psi_{n2}^{new} = [\int \psi_{n1}^* \psi_{n2} d\tau] \psi_{n1} - \psi_{n2} \quad (61)$$

So if ψ_{n1}, ψ_{n2} is parallel, then the result ψ_{n2}^{new} is also parallel to the former two, then this method would lose its effectiveness-could not construct orthogonal eigenvectors.

$\langle \hat{A}^2 \rangle \geq 0$ for Hermitian \hat{A}

$$\begin{aligned} \langle \hat{A}^2 \rangle &= \langle \hat{A}\hat{A} \rangle = \int \psi^\dagger \hat{A}\hat{A}\psi d\tau = \int \psi^\dagger \hat{A}^\dagger \hat{A}\psi d\tau \\ &= \int \hat{A}\psi^\dagger \hat{A}\psi d\tau = \int (\hat{A}\psi)^\dagger (\hat{A}\psi) d\tau = \int |\hat{A}\psi|^2 d\tau \geq 0 \end{aligned} \quad (62)$$

1.10.2 some Formal Results: General Solution to Angular Momentum Eigenvalue Problem

Since we have already introduced the orbit angular momentum, which is represented by L . Actually the physics on L is dependent on its 6 commutation relationships, so let us use J to obtain a general solution to angular momentum problem, where:

$$\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 \quad (63)$$

Originating from Page 44 the six commutation relationships become:

$$[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z \quad (64a)$$

$$[\hat{J}_y, \hat{J}_z] = i\hbar\hat{J}_x \quad (64b)$$

$$[\hat{J}_z, \hat{J}_x] = i\hbar\hat{J}_y \quad (64c)$$

$$[\hat{J}^2, \hat{J}_x] = 0 \quad (64d)$$

$$[\hat{J}^2, \hat{J}_y] = 0 \quad (64e)$$

$$[\hat{J}^2, \hat{J}_z] = 0 \quad (64f)$$

Take ϕ be the eigenstate of \hat{J}^2 then it must be the eigenstate of \hat{J}_z . Let α and β be their eigenvalues separately, then based on Equation 63 and the conclusion $\langle \hat{A}^2 \rangle \geq 0$ for Hermitian \hat{A} we have:

$$\alpha \geq \beta^2 \quad (65)$$

Note: here we do not introduce any new hypothesis! All we hypothesized are the six commutation relationships.

Then we need to draw support from two operators, who can help to raise or lower the eigenfunctions to another eigenfunctions corresponding to the eigenvalues \hbar higher or lower:

$$\hat{J}_z(\hat{J}_+\phi) = (\beta + \hbar)(\hat{J}_+\phi) \quad (66a)$$

$$\hat{J}_z(\hat{J}_-\phi) = (\beta - \hbar)(\hat{J}_-\phi) \quad (66b)$$

And we could find the solutions to \hat{J}_+ and \hat{J}_- :

$$\hat{J}_+ = \hat{J}_x + i\hat{J}_y \quad (67a)$$

$$\hat{J}_- = \hat{J}_x - i\hat{J}_y \quad (67b)$$

Since we define the raising or lower operators with \hat{J}_z , let us see what would happen when they are applied to \hat{J}^2

When we are trying to see something about raising or lower operators, we usually calculate the commutation firstly:

$$[\hat{J}^2, \hat{J}_{\pm}] = [\hat{J}^2, \hat{J}_x \pm i\hat{J}_y] = [\hat{J}^2, \hat{J}_x] \pm i[\hat{J}^2, \hat{J}_y] = 0 \quad (68)$$

$$\hat{J}^2(\hat{J}_+ \phi) = \hat{J}_+(\hat{J}^2 \phi) = \alpha(\hat{J}_+ \phi) \quad (69a)$$

$$\hat{J}^2(\hat{J}_- \phi) = \hat{J}_-(\hat{J}^2 \phi) = \alpha(\hat{J}_- \phi) \quad (69b)$$

So the result is: after the raising or lower operators' effect, the eigenfunctions of \hat{J}^2 are still the eigenfunctions of \hat{J}^2 .

It means if we have a state which is the eigenstate of \hat{J}^2 and \hat{J}_z simultaneously(from (64f)), and use the raising or lower operators to produce new eigenstates, we could get a pairs of them like this:

$$\alpha \leftrightarrow \beta_0 \quad \alpha \leftrightarrow \beta_1 \quad \alpha \leftrightarrow \beta_2 \quad \dots \quad (70)$$

And we also have:

$$\alpha \geq \beta^2 \quad ((65) \text{ revisited})$$

So there must be some boundaries for β :

$$\hat{J}_+ \phi_{\beta_{max}} = 0 \quad (71a)$$

$$\hat{J}_- \phi_{\beta_{min}} = 0 \quad (71b)$$

Then we could have two more equations—one operator adding on zero would still return zero:

$$\begin{aligned} & \hat{J}_-(\hat{J}_+ \phi_{\beta_{max}}) = 0 \\ &= (\hat{J}^2 - \hat{J}_z^2 - \hbar \hat{J}_z) \phi_{\beta_{max}} \\ &= (\alpha - \beta_{max}^2 - \hbar \beta_{max}) \phi_{\beta_{max}} \\ &\iff \alpha - \beta_{max}(\beta_{max} + \hbar) = 0 \\ &\iff \alpha = \beta_{max}(\beta_{max} + \hbar) \end{aligned} \quad (72)$$

$$\begin{aligned} & \hat{J}_+(\hat{J}_- \phi_{\beta_{min}}) = 0 \\ &= (\hat{J}^2 - \hat{J}_z^2 + \hbar \hat{J}_z) \phi_{\beta_{min}} \\ &= (\alpha - \beta_{min}^2 + \hbar \beta_{min}) \phi_{\beta_{min}} \\ &\iff \alpha - \beta_{min}(\beta_{min} - \hbar) = 0 \\ &\iff \alpha = \beta_{min}(\beta_{min} - \hbar) \end{aligned} \quad (73)$$

Combining the results of (73) and (72), we could have:

$$\beta_{min} = -\beta_{max} \quad (74)$$

which could be called **the symmetry about zero point**. And considering the raising and lowering operation's step is \hbar , there are two plans:

1. **Permit zero as a candidate value, then every candidates become integers** here comes the same conclusion as (25), so now we have derived the orbital angular momentum from the way of math.
2. **Not including zero, but we still have a method to make sure the symmetry about zero point: regarding it as the middle point of one step, so $\pm\frac{1}{2}\hbar$ are chosen, then all the permitted values are half-integers** This what we are talking about in chapter 11, spin.

A question may be proposed naturally: **How to add spin and orbital angular momentum?** Actually, adding angular momentums are not only for spin and orbital one, we even could add the angular momentum from different particles in one system, such as spin from proton and spin from electron in one atom.

A new question: how to add two angular momentums

1.11 chapter 11

1.11.1 Discovery process of spin

How to measure orbital angular momentum The discovery of spin originates from scientist's measurement of orbital momentum.

We want to find some physical quantities which could be measured. Firstly, we have known that magnetic dipole is a typical model, of which once we know the magnetic moment μ then we could know the exerted energy as:

$$U = -\vec{\mu} \cdot \vec{B} \quad (75)$$

And energy could be “seen” by light spectrum, so we could add a magnetic field on it to see the orbital angular momentum.

From the definition of magnetic moment:

$$|\hat{\mu}_L| = |i| \cdot \pi r^2 = e \cdot \frac{v}{2\pi r} = \frac{1}{2}evr \quad (76)$$

And for the direction, the magnetic moment's direction should be the opposite direction as the orbital angular momentum:

$$\vec{\mu}_L \propto -\vec{L} \quad (77)$$

$$|L| = rm_e v \quad (78)$$

Combining the above three equations, we could write:

$$\vec{\mu}_L = -\frac{e}{2m_e} \vec{L} \quad (79)$$

And we do know the value of orbital angular momentum, thus we could know the value of magnetic moment:

$$|\vec{\mu}_L| = \frac{e}{2m_e} |\vec{L}| = \frac{e\hbar}{2m_e} \sqrt{l(l+1)} \quad (80)$$

if we let:

$$\mu_B = \frac{e\hbar}{2m_e} \quad (81)$$

Then:

$$|\vec{\mu}_L| = \mu_B \sqrt{l(l+1)} \quad (82)$$

Unexpected result: Stern-Gerlach Experiment S-G experiment is designed to detect the orbital angular momentum. From (75) we could know the potential energy, so adding a gradient operator we could get the force:

$$\vec{F} = -\vec{\nabla}(-\vec{\mu} \cdot \vec{B}) = (\vec{\mu} \cdot \vec{\nabla}) \vec{B} \quad (83)$$

It implied that we could use a same in-homogeneous magnetic field to add different force for the atoms with different orbital angular momentum, thus they would have different moving tracks.

It is the original idea of the experimental device of S-G experiment, but not the classic results of S-G experiment in 1922.

They have used Ag atom, which only have 1 outer-electron in s-orbital. So it was expected to see no atoms changing their tracks. But we have found nearly half of the atoms a little up while the rest a little down, namely two slits, compared the situation without B field, which is only one slit.(Here if the B field is a homogeneous one, it still should be one slit-although the Hamiltonian would be changed, we are not detecting its energy, but only using the force to see the tracks)

So there must be something other than orbital AM, which also have interactions with the in-homogeneous magnetic field. What's more, at least for Ag, there must be only two possible states as there are only two slits. It let us introduce spin, because as we talked in 1.10.2, there is another angular momentum in atom, whose candidates are even number, and the simplest case is two candidates.

1.11.2 How to explain spin

So from S-G experiment, we have found spin **for electron**, then we could use the result of 1.10.2 to explain:

Every electron has a spin angular momentum \vec{S} , there are two properties:

1. \hat{S}^2 has only one eigenvalue $\frac{3}{4}\hbar^2$

2. \hat{S}_z takes on only $+\frac{1}{2}\hbar$ and $-\frac{1}{2}\hbar$

But there may be other particles also having spin, so the general form is:

1. \hat{S}^2 has one eigenvalue $s(s+1)\hbar^2$

2. \hat{S}_z takes on $-s\hbar, (-s + \frac{1}{2})\hbar, \dots, -\frac{1}{2}\hbar, \frac{1}{2}\hbar, \dots, (s + \frac{1}{2})\hbar, s\hbar$

where s is positive half integer. And we gave a name to the eigenvalue of \hat{S}_z , m_s .

Schrodinger Equation can't explain it We could not get spin from Schrodinger Equation, because **Spin angular momentum is a relativistic effect**, which is solved by **Dirac**.

We would not talk about how to derive it, but we could give some conclusions:

Spin angular momentum eigenstates cannot be expressed as a wave function of space (x, y, z)

Electron's spin is a property of electron itself. It would not be dependent on which atom energy level it is on.

Electron's spin is unrelated to electron's probability density.

Matrix representation of spin As we said in 1.11.2, spin could not be represented in a wave function of space (x, y, z) , so we should give it a representation in matrix.

But the 6 commutation relations still hold(64a)-(64f) even in the matrix representation.

Actually x, y, z directions are in the same status, but we select z as the mostly used one, thus giving its operator the simplest form: diagonal matrix. Then based on the eigenvalues $\frac{\hbar}{2}$ and $-\frac{\hbar}{2}$ we could simply construct it:

$$\hat{S}_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (84)$$

Let χ_+ and χ_- represent the eigenfunctions of the z direction spin operator \hat{S}_z :

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (85)$$

$$\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad (86)$$

Then the general form wave function χ could be represented as the linear combination of the above two.

$$\chi = a\chi_+ + b\chi_- \quad (87)$$

Actually the above two eigenvectors multiplied by any constant is still working, but we choose to normalize them. Then we could calculate the matrix form of \hat{S}^2 operator by (64f):

$$\hat{S}^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (88)$$

Then based on the commutation relations (64a) - (64c), we could get:

$$\hat{S}_x = \frac{1}{2}\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (89)$$

$$\hat{S}_y = \frac{1}{2}\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (90)$$

Since we choose z direction to have the simplest form eigenfunctions and matrix form operator, x and y directions could also have their own eigenfunctions, but in a more complex form: take x direction as an example:

$$\chi_+^x = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \quad (91)$$

$$\chi_-^x = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} \quad (92)$$

We could still express the general form in terms of the eigenfunctions on x direction to read the probability more easily:

$$\chi = \left(\frac{a+b}{\sqrt{2}}\right)\chi_+^x + \left(\frac{a-b}{\sqrt{2}}\right)\chi_-^x \quad (93)$$

Pauli matrix For (89) (90) (84), we could use another way to represent them, which are proposed by Pauli:

$$\hat{S}_x = \frac{\hbar}{2}[\sigma_x] \quad \hat{S}_y = \frac{\hbar}{2}[\sigma_y] \quad \hat{S}_z = \frac{\hbar}{2}[\sigma_z] \quad (94)$$

where:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (95)$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (96)$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (97)$$

And we could get some more properties on Pauli matrix:

The process of getting Pauli matrix's commutator, the square, the product See the problem 6.1 on next several pages' pdf for detail.

The process of getting Pauli matrix's eigenvalues, eigenfunctions, trace and determinant

See the problem 6.2 on next several pages' pdf for detail.

Matrix representation for spin operator in any direction $\hat{S}_{\theta,\phi}$ See the problem 6.3 on next several pages' pdf for detail.

Matrix representation for the mean spin angular momentum operator $\langle \hat{\vec{S}} \rangle$ The above discussion only includes the square of \hat{S} operator. But we could construct $\hat{\vec{S}} = \hat{S}_x \hat{i} + \hat{S}_y \hat{j} + \hat{S}_z \hat{k}$ and see its property. See the problem 6.4 on next several pages' pdf for detail.

PHYS3021 Quantum Mechanics I Problem Set 6

Due: 4 December 2017 (Monday)

"T+2" = 6 December 2017 (Wednesday)

All problem sets should be handed in not later than 5pm on the due date. Drop your assignments into the PHYS3021 box outside Rm.213.

Please work out the steps of the calculations in detail. Discussions among students are highly encouraged, yet it is expected that we do your homework independently.

6.0 Reading Assignment. (Don't need to hand in everything for this item.)

Chapter X goes back to some formal QM. First, Hermitian operators, which carry real expectation values $\langle \hat{A} \rangle$ for any state, real eigenvalues, orthogonal eigenstates, non-negative $\langle \hat{A}^2 \rangle$ for any state, and many more useful properties are introduced. Obviously, the properties are perfect for physical quantities in QM. Thus, all physical quantities in QM are represented by Hermitian operators. This statement is a postulate of QM. Chapter X explores the properties that are most relevant to QM, including simultaneous eigenstates of two commuting operators. A **general uncertain relation** concerning two operators will be derived. Operator method can also give us general results for **general QM angular momentum eigenvalue problems**. The results cover the orbital angular momentum already discussed and also the spin angular momentum to be covered in the next chapter. Chapter XI discussed spin angular momentum or simply spin. It is another example of general angular momentum with $s = 1/2$, and thus only two values for its component at any direction. The Stern-Gerlach experiment, nearly 100 years old, remains a useful set up for learning and investigating QM. A matrix representation is convenient, because the size is only 2×2 . Matrices representing \hat{S}_x , \hat{S}_y , and \hat{S}_z are introduced. Using their eigenvectors and eigenvalues, the general mathematical structure of QM and the measurement theory can be illustrated. After spin, we will go back to Chapter X to summarize the course with a few QM postulates.

Chapters in Rae's *Quantum Mechanics*, Griffiths' *An introduction to quantum mechanics*, McQuarrie's *Quantum Chemistry*, Engels' *Quantum Chemistry and Spectroscopy*, and Bransden and Joachain's —e, Quantum Mechanics are good places to look up more discussion. The chemistry books are better illustrations of the hydrogen atomic orbitals.

6.1 Having fun with the Pauli Matrices

We introduced the matrices for \hat{S}_x , \hat{S}_y and \hat{S}_z . It turns out that they are closely related to the Pauli matrices σ_x , σ_y , and σ_z , only off by a factor of $\hbar/2$. The Pauli matrices are

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad (1)$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad (2)$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (3)$$

Here, you will explore some properties of the Pauli matrices.

- (a) Find the commutator $[\sigma_x, \sigma_y]$ by playing with the matrices.
- (b) Find the commutator $[\sigma_x, \sigma_y]$ without playing with the matrices, but simply using the commutators between the spin components (the definition of angular momentum in QM).
- (c) Find σ_x^2 by playing with the matrices.
- (d) Realizing that a general spin-half state χ can be written in the form of

$$\chi = c_1 \alpha_x + c_2 \beta_x$$

where α_x (β_x) is the eigenstate of \hat{S}_x with eigenvalue $+\hbar/2$ ($-\hbar/2$). By operating \hat{S}_x^2 on χ , find \hat{S}_x^2 and hence identify σ_x^2 . [Remark: Compare result with part (c).]

- (e) Find the product $\sigma_x \sigma_y$ and relate the result to σ_z .
- [Remark: You may want to explore a cyclic pattern of this result.]

- (f) While $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ is the **commutator**, $\{\hat{A}, \hat{B}\} = [\hat{A}, \hat{B}]_+ \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$ is the **anti-commutator** of two operators. Find $\{\sigma_x, \sigma_y\}$.
 (g) What is $\{\sigma_i, \sigma_i\}$, for $i = x, y$, and z ? [Note: Answer in part (c) will be useful.]

6.2 Eigenvalues and Eigenvectors of Pauli Matrices

- (a) Find the eigenvalues and eigenvectors of the three Pauli matrices.
- (b) Find the trace of the Pauli matrices. [Hint: Very easy if you know the relation between the trace of a matrix and its eigenvalues.]
- (c) Find the determinant of the Pauli matrices.

6.3 The most general operator for a “component” of spin

After we draw some axes for the x , y , and z directions, we then have S_x , S_y , and S_z for the spin angular momentum \vec{S} . These directions, however, are nothing special.

Therefore, one can look at the component of spin along any direction. In 3D, a direction can be specified by two angles θ and ϕ . Just think about the spherical coordinates. When θ and ϕ are given, a direction is given.

- (a) Now we want to construct the operator $\hat{S}_{\theta, \phi}$ corresponding to the component of \vec{S} in that direction. Following **think classical and go quantum**, show that the operator is given by

$$\hat{S}_{\theta, \phi} = \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix} \quad (4)$$

- (b) As a quick check, show that Eq. (4) reduces to the matrices for \hat{S}_x , \hat{S}_y , and \hat{S}_z , when the corresponding angles are chosen.
 (c) Find the eigenvalues and normalized eigenvectors of $\hat{S}_{\theta, \phi}$.
 [Remark: Now you see that if you have done this part first, 6.2(a) will be trivial.]
 (d) Let's have some fun with measurements. Let $\beta_{\theta, \phi}$ be the eigenvector corresponding to the eigenvalue $-\hbar/2$. If a beam of particles prepared to be in this state is sent into a Stern-Gerlach experiment measuring the x -component of spin, i.e., SGX, what could you say about the outcomes? Now take the exiting beam corresponding to the measured result of $+\hbar/2$ in SGX and then send the beam again into a Stern-Gerlach experiment SG(θ, ϕ). what could you say about the outcomes?

6.4 The mean spin angular momentum ($\hat{\vec{S}}$)

Recall that an expectation value involves two ingredients: a quantity (an operator) and a state.

There is a quantity called spin, which is a vector $\hat{\vec{S}} = \hat{S}_x \hat{i} + \hat{S}_y \hat{j} + \hat{S}_z \hat{k}$. Given a state, one can calculate the expectation value $\langle \hat{\vec{S}} \rangle$ by calculating the expectation value of each component.

- (a) Warming up! Take the state to be the eigenvector β_z of \hat{S}_z corresponding to the eigenvalue $-\hbar/2$. Find the expectation values $\langle \hat{S}_x \rangle$, $\langle \hat{S}_y \rangle$, and $\langle \hat{S}_z \rangle$. If we think about a mean spin angular momentum $\langle \hat{\vec{S}} \rangle$ as $\langle \hat{\vec{S}} \rangle = \langle \hat{S}_x \rangle \hat{i} + \langle \hat{S}_y \rangle \hat{j} + \langle \hat{S}_z \rangle \hat{k}$, what would you say about the direction of $\langle \hat{\vec{S}} \rangle$?
- (b) Go back to 6.3(d). Take the state to be the eigenvector of $\hat{S}_{\theta, \phi}$ corresponding to the eigenvalue $-\hbar/2$, i.e. the state is $\beta_{\theta, \phi}$ in 6.3(d) again. Take this state, calculate the expectation values $\langle \hat{S}_x \rangle$, $\langle \hat{S}_y \rangle$, and $\langle \hat{S}_z \rangle$. From the results, what would you say about the direction of $\langle \hat{\vec{S}} \rangle$?

6.5 Matrix formulation of QM harmonic oscillator

We discussed in class that every QM problem can be turned into a big matrix (sometimes small such as spin) problem. This problem is to illustrate that even one can do the 1D harmonic oscillator problem by matrices.

Problem Set 6

6.1

$$(a) [6x, 6y] = 6x \cdot 6y - 6y \cdot 6x$$

$$= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -3 \\ 2 & 0 \end{pmatrix} - \begin{pmatrix} 0 & -3 \\ 2 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} -3 & 0 \\ 0 & -2 \end{pmatrix} - \begin{pmatrix} -3 & 0 \\ 0 & 2 \end{pmatrix}$$

$$= \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix}$$

$$(b) \hat{s}_x = \frac{\hbar}{2} 6x, \hat{s}_y = \frac{\hbar}{2} 6y$$

$$[6x, 6y] = \left(\frac{2}{\hbar}\right)^2 [\hat{s}_x, \hat{s}_y] = \left(\frac{2}{\hbar}\right)^2 \frac{\hbar}{2} \hat{s}_z$$

$$= \frac{-i \cdot \frac{1}{2}}{\hbar^2} \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= 2i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix}$$

$$(c) 6x^2 = 6x \cdot 6x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$(d) \hat{s}_x^2 x = \hat{s}_x \hat{s}_x x = \hat{s}_x \hat{s}_x (c_1 \alpha x + c_2 \beta x)$$

$$\text{We know } \hat{s}_x \alpha x = \frac{1}{2} \hbar \alpha x, \hat{s}_x \beta x = -\frac{1}{2} \hbar \beta x$$

$$\begin{aligned} \text{So the above becomes:} &= \hat{s}_x (c_1 \hat{s}_x \alpha x + c_2 \hat{s}_x \beta x) \\ &= \hat{s}_x [c_1 \cdot \frac{1}{2} \hbar \alpha x + c_2 \cdot (-\frac{1}{2} \hbar \beta x)] \\ &= \hat{s}_x \frac{1}{2} \hbar (c_1 \alpha x + c_2 \beta x) \\ &= \frac{1}{2} \hbar (c_1 \hat{s}_x \alpha x - \hat{s}_x \beta x) = \frac{1}{2} \hbar (c_1 \frac{1}{2} \hbar \alpha x + c_2 \frac{1}{2} \hbar \beta x) \end{aligned}$$

$$\begin{aligned} i\hbar \frac{\partial \Psi}{\partial t} &= -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V \Psi \\ \hat{p} &= \frac{i\hbar}{\tau} \frac{d}{dx} \\ [\hat{s}_x, \hat{s}_y] &= i\hbar \hat{s}_z \end{aligned}$$

$$= \left(\frac{1}{2}\pi\right)^2 (c_1 \alpha x + c_2 \beta x)$$

$$= \left(\frac{1}{2}\pi\right)^2 X$$

Because there is a mistake

We know $\hat{S}_X = \frac{1}{2} \hat{B}_X^2$ \Rightarrow Should be: $\left(\frac{1}{2}\pi\right)^2 \hat{B}_X^2 X = \left(\frac{1}{2}\pi\right)^2 X$
 $\therefore \left(\frac{1}{2}\pi\right)^2 \hat{B}_X^2 = \left(\frac{1}{2}\pi\right)^2 X$ \nearrow i.e. $\hat{B}_X^2 = I$
 the same result in (e)!

$$\hat{B}_X^2 = X \quad \text{----} \quad \text{Why? It is different from (e)'s result}$$

(e)

$$B_X B_Y = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = i B_Z$$

Try to explore a cyclic pattern:

$$B_Y B_Z = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = -i B_X$$

$$B_Z B_X = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = -i \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = -i B_Y$$

(f)

$$\{B_X, B_Y\} = [B_X, B_Y]_+ = B_X B_Y + B_Y B_X$$

$$= -i B_Z + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} + \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} = 0$$

$$(g) = B_Z B_Z + B_Z B_Z$$

$$= 2 B_Z^2 \quad \text{For } i=x, 2 B_X^2 = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

$$\text{For } i=y, 2 B_Y^2 = 2 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = 2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

$$\text{For } i=z, 2 B_Z^2 = 2 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = 2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

They are
the same

6.2

$$(a) \quad \cancel{\text{Sx} = f}$$

$$6x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad 6y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad 6z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

For x :

$$6x \cdot \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix} \Rightarrow \begin{pmatrix} b \\ a \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix} \Rightarrow \begin{pmatrix} b - \lambda a \\ a - \lambda b \end{pmatrix} = 0$$

$$\begin{array}{l} b = \lambda a \\ a = \lambda b \end{array} \quad b = \lambda^2 b \quad \lambda^2 = 1 \quad \lambda = \pm 1 \Rightarrow \begin{array}{l} b = a \\ b = -a \end{array}$$

→ Add normalization condition:

$$b = a = \frac{\sqrt{2}}{2} \quad / -b = +a = \frac{\sqrt{2}}{2}$$

$$\lambda = 1 \quad \begin{pmatrix} \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} \end{pmatrix}$$

$$\lambda = -1 \quad \begin{pmatrix} \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2} \end{pmatrix}$$

For y :

$$\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix} \Rightarrow \begin{pmatrix} -bi \\ ai \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\begin{pmatrix} -bi - \lambda a \\ ai - \lambda b \end{pmatrix} = 0 \quad \begin{array}{l} b = \frac{-\lambda a}{i} = \bar{i}\lambda a \\ a = \frac{\lambda b}{i} = -i\lambda b \end{array} \quad b = \bar{i}\lambda (-i\lambda b) = \lambda^2 b$$

$$\lambda^2 = 1 \quad \lambda = \pm 1 \Rightarrow \begin{array}{l} b = \bar{i}a \\ b = -\bar{i}a \end{array}$$

Add normalization: $a = \frac{1}{\sqrt{2}}$ $b = \frac{1}{\sqrt{2}}i \quad / \quad a = \frac{1}{\sqrt{2}}$

$$\text{Result: } \lambda = 1 \quad \begin{pmatrix} \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2}i \end{pmatrix} \quad \lambda = -1 \quad \begin{pmatrix} \frac{\sqrt{2}}{2} \\ -\frac{\sqrt{2}}{2}i \end{pmatrix} \quad b = -\frac{\sqrt{2}}{2}$$

$$\text{For } z: \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix} \Rightarrow \begin{pmatrix} a \\ -b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix} \Rightarrow \begin{cases} a = \lambda a \\ b = -\lambda b \end{cases}$$

$$\lambda = \pm 1 \Rightarrow \begin{array}{l} a = a \\ b = -b \end{array} \quad / \quad \begin{array}{l} a = -a \\ b = b \end{array} \Rightarrow \begin{array}{l} a = a \\ b = b \end{array} \quad / \quad \begin{array}{l} \text{Add Normalization} \\ a \neq 0 \end{array} \Rightarrow \begin{array}{l} a = 1 \\ b = 0 \end{array} \quad / \quad \begin{array}{l} a = 0 \\ b = 1 \end{array}$$

$$\text{Result: } \lambda = 1 \quad \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \lambda = -1 \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

(b) Trace Trace is the multiplication of all the elements on the diagonal. And the ~~max~~^{tr} could be written as $\begin{pmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_n \end{pmatrix}$ so $\text{tr} \sum \lambda_i$

So for three pauli matrixes = trace = $c(-1) \cdot c(i) = -1$

$$(c) b_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad |b_x| = 0 - 1 \times 1 = -1$$

$$b_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad |b_y| = 0 - (-i) \times i = -1$$

$$b_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad |b_z| = -1 - 0 = -1$$

6.3

(a)



We adopted the Right-Hand Coordinate:

$$\begin{aligned} S_{\theta, \phi} &= \cos \theta \hat{S}_z + \sin \theta [\cos \phi \hat{S}_x + \sin \phi \hat{S}_y] \\ &= \frac{1}{2} \hbar [\cos \theta \left(\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) + \sin \theta \cos \phi \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right) + \sin \theta \sin \phi \left(\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \right)] \\ &= \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta [\cos \phi - \sin \phi i] \\ \sin \theta (\cos \phi + \sin \phi i) & -\cos \theta \end{pmatrix} \\ &= \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix} \end{aligned}$$

(b)

$$\begin{aligned} X_2: \theta = 0 &\quad \theta = \frac{\pi}{2} \quad Y_2: \theta = \frac{\pi}{2} \quad \theta = \frac{\pi}{3} \quad Z_2: \theta = 0 \quad (\phi \text{ doesn't matter}) \\ \Downarrow \quad \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} &\quad \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \end{aligned}$$

$$(c) \frac{1}{2}t \begin{pmatrix} \cos\theta & \sin\theta e^{-i\phi} \\ \sin\theta e^{i\phi} & -\cos\theta \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\frac{1}{2}t \begin{pmatrix} a\cos\theta + b\sin\theta e^{-i\phi} \\ a\sin\theta e^{i\phi} - b\cos\theta \end{pmatrix} = \begin{pmatrix} \lambda a \\ \lambda b \end{pmatrix}$$

$$\begin{cases} a\cos\theta + b\sin\theta e^{-i\phi} = \frac{2\lambda a}{t} \quad (1) \\ a\sin\theta e^{i\phi} - b\cos\theta = \frac{2\lambda b}{t} \quad (2) \end{cases}$$

then $a\sin^2\theta = \left(\frac{2\lambda}{t} + \omega_0\right)\left(\frac{2\lambda}{t} - \omega_0\right)a$

If $a=0$ then $b=0$, it is not acceptable

so $\sin^2\theta = \frac{4\lambda^2}{t^2} - \omega_0^2 \Rightarrow \lambda^2 = \frac{1}{4}t^2 \Rightarrow \lambda_1 = \frac{1}{2}t$
 $\lambda_2 = -\frac{1}{2}t$

When $\lambda = \lambda_1 = \frac{1}{2}t \Rightarrow b = (1 - \cos\theta) \frac{e^{i\phi}}{\sin\theta} a = \tan\frac{\theta}{2} e^{i\phi} \cdot a$

Normalization: $a^* \cdot a + b^* \cdot b = 1$

$$|a|^2 + \tan^2\frac{\theta}{2} e^{i\phi} \cdot a \cdot \tan^2\frac{\theta}{2} e^{-i\phi} \cdot a^* = 1$$

$$|a|^2 + \tan^2\frac{\theta}{2} |a|^2 = 1 \Rightarrow |a|^2 = \frac{1}{1 + \tan^2\frac{\theta}{2}} = \cos^2\frac{\theta}{2}$$

~~for~~ a could be $\cos\frac{\theta}{2}$ And I found why A problem here:

then b could be $\sin\frac{\theta}{2} e^{i\phi}$ instead of ~~Normalization~~; where $x^2 + y^2$

When $\lambda = \lambda_2 = -\frac{1}{2}t \Rightarrow b = (1 - \cos\theta) \frac{e^{i\phi}}{\sin\theta} a$ has less information. $= \cos^2\frac{\theta}{2}$

~~② $a \sin\theta e^{i\phi} = (0.50 + \frac{1}{2}i) b$~~ we have: ~~$a \sin\theta e^{i\phi} = \frac{(0.50 + \frac{1}{2}i)}{\sin\theta} b$~~

$$b = -\frac{\cos\frac{\theta}{2}}{\sin\frac{\theta}{2}} \frac{e^{i\phi}}{\sin\frac{\theta}{2} \cos\frac{\theta}{2}} a$$

$$= -\cot\frac{\theta}{2} e^{i\phi} a$$

Normalize: $b^* \cdot b + a^* \cdot a = 1$

$$\frac{(1 - \cos^2\theta) e^{i\phi}}{\sin\theta} \cdot$$

$$-\cot^2\frac{\theta}{2} e^{-i\phi} a^* \cdot \frac{(-\cot\frac{\theta}{2})}{(1 - \cos^2\theta) e^{i\phi}} + a^* a = 1 \Rightarrow |a|^2 = \sin^2\frac{\theta}{2}.$$

a could be $\sin \frac{\theta}{2}$ b could be $-\cos \frac{\theta}{2} e^{i\phi}$

$$\text{Result: } \lambda_1 = \frac{1}{2}h \quad \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} e^{i\phi} \end{pmatrix}$$

$$\lambda_2 = -\frac{1}{2}h \quad \begin{pmatrix} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} e^{i\phi} \end{pmatrix}$$

(d)

so $\beta_{0,\phi} = \begin{pmatrix} \sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} e^{i\phi} \end{pmatrix}$ is the $|1\rangle$, into SGX so we need to expand

it in α_x, β_x
 $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$ that is $\begin{pmatrix} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} e^{i\phi} \end{pmatrix} = c_1 \alpha_x + c_2 \beta_x$

$$c_1 = \alpha_x^+ \cdot \beta_{0,\phi} = \frac{1}{\sqrt{2}} (1 \ 1) \begin{pmatrix} \sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} e^{i\phi} \end{pmatrix} = \frac{1}{\sqrt{2}} (\sin \frac{\theta}{2} + \cos \frac{\theta}{2}) = \sin(\frac{\theta}{2} + \frac{\pi}{4})$$

$$|c_1|^2 = c_1^* \cdot c_1 = \sin^2(\frac{\theta}{2} + \frac{\pi}{4}) \frac{1}{\sqrt{2}} (\sin \frac{\theta}{2} - e^{-i\phi} \cos \frac{\theta}{2}) \cdot \frac{1}{\sqrt{2}} (\sin \frac{\theta}{2} - e^{i\phi} \cos \frac{\theta}{2})$$

$$c_2 = \beta_x^+ \cdot \beta_{0,\phi} = \frac{1}{\sqrt{2}} (-1 \ 1) \begin{pmatrix} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} e^{i\phi} \end{pmatrix} = \frac{1}{\sqrt{2}} (-\sin \frac{\theta}{2} - \cos \frac{\theta}{2})$$

$$|c_2|^2 = c_2^* \cdot c_2 = \cos^2(\frac{\theta}{2} + \frac{\pi}{4}) = \frac{1}{2} (1 + \sin \theta \cos \phi)$$

I could say we have $\frac{1}{2}(1 - \sin \theta \cos \phi)$ probability to get $\frac{1}{2}h$ from SGX

$\cos^2(\frac{\theta}{2} + \frac{\pi}{4})$ probability to get $-\frac{1}{2}h$ from SGX

If select the $\frac{1}{2}h$ beam from SGX, then the $|1\rangle$ becomes $\alpha_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

Expand it in $\alpha_{0,\phi}$ and $\beta_{0,\phi}$

$$|\alpha_x|^2 = \begin{pmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} e^{i\phi} \end{pmatrix} \begin{pmatrix} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} e^{i\phi} \end{pmatrix} = \frac{1}{2} (\cos \frac{\theta}{2} + \sin \frac{\theta}{2})^2 = \frac{1}{2} (1 + \sin \theta \cos \phi)$$

$$c_1' = \alpha_x^* \cdot \beta_{0,\phi} = (\sin \frac{\theta}{2} - e^{-i\phi} \cos \frac{\theta}{2}) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} (\sin \frac{\theta}{2} + \cos \frac{\theta}{2})$$

$$C_2' = \beta_{\theta, \phi} + \cdot \alpha_X = (\sin \frac{\theta}{2} - \cos \frac{\theta}{2} e^{-i\phi}) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}} (\sin \frac{\theta}{2} - \cos \frac{\theta}{2} e^{-i\phi})$$

$$|C_2'|^2 = C_2'^* \cdot C_2' = \frac{1}{2} (\sin \frac{\theta}{2} - \cos \frac{\theta}{2} e^{i\phi}) (\sin \frac{\theta}{2} - \cos \frac{\theta}{2} e^{-i\phi})$$

$$= \frac{1}{2} [\sin^2 \frac{\theta}{2} + \cos^2 \frac{\theta}{2} - \sin \frac{\theta}{2} \cos \frac{\theta}{2} (e^{i\phi} + e^{-i\phi})]$$

$$= \frac{1}{2} (1 - \sin \theta \cos \phi)$$

I could say the $\frac{1}{2}\hbar$ beam from SGX, could get the following result from $\frac{1}{2}(1 + \sin \theta \cos \phi)$ probability to get $\frac{1}{2}\hbar$

$$\frac{1}{2}(1 - \sin \theta \cos \phi) \sim -\frac{1}{2}\hbar$$

6.4 All "*" in 6.4 should be replaced by "+"

$$(a) \Psi = \beta_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\langle \hat{S}_X \rangle = \Psi^* \hat{S}_X \Psi = (0 \ 1) \frac{1}{2}\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$$

$$\langle \hat{S}_Y \rangle = \Psi^* \hat{S}_Y \Psi = (0 \ 1) \frac{1}{2}\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$$

$$\langle \hat{S}_Z \rangle = \Psi^* \hat{S}_Z \Psi = (0 \ 1) \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{1}{2}\hbar$$

$$\langle \hat{S} \rangle = \langle \hat{S}_X \rangle \hat{i} + \langle \hat{S}_Y \rangle \hat{j} + \langle \hat{S}_Z \rangle \hat{k}$$

$$= -\frac{1}{2}\hbar \hat{k}$$

$$(b) \Psi = \beta_{\theta, \phi} = \begin{pmatrix} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} e^{i\phi} \end{pmatrix}$$

$$\langle \hat{S}_X \rangle = \Psi^* \hat{S}_X \Psi = (\sin \frac{\theta}{2} - \cos \frac{\theta}{2} e^{-i\phi}) \frac{1}{2}\hbar \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} e^{i\phi} \end{pmatrix} = \frac{\hbar}{2} \sin \theta \cos \phi$$

$$\langle \hat{S}_Y \rangle = \Psi^* \hat{S}_Y \Psi = (\sin \frac{\theta}{2} - \cos \frac{\theta}{2} e^{-i\phi}) \frac{1}{2}\hbar \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} e^{i\phi} \end{pmatrix} = -\frac{\hbar}{2} \sin \theta \sin \phi$$

$$\langle \hat{S}_Z \rangle = \Psi^* \hat{S}_Z \Psi = (\sin \frac{\theta}{2} - \cos \frac{\theta}{2} e^{-i\phi}) \frac{1}{2}\hbar \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \sin \frac{\theta}{2} \\ -\cos \frac{\theta}{2} e^{i\phi} \end{pmatrix} = -\frac{\hbar}{2} \cos \theta$$

it is just the projection of $C - \frac{1}{2}\hbar$.

 And its direction is the same as (r, θ, ϕ) point's opposite direction

2 PHYS3022

2.1 Three Methods (Mostly Approximations) In QM

All the three methods could be used to solve TISE, but only the perturbation theory could solve TDSE. Here we only talk about how the three methods treat TISE.

2.1.1 An Exact Approach - Turning TISE into a huge matrix problem

This part gave an exact approach to solve TISE, however, we could still get an approximation method. The following two pages are the details of derivations.

A Formal and Exact Approach — Huge matrix

Our question is still : $\hat{H}\psi = E\psi$ (A1)

And we could select a group of basis : $\{\phi_1, \phi_2, \dots, \phi_i, \phi_j, \dots\}$ to express : $\psi = \sum_i a_i \phi_i$

Then (A1) becomes : $\sum_i a_i \hat{H} \phi_i = E \sum_i a_i \phi_i$

Left multiply ϕ_j^+ , and then integrate : $\int \sum_i a_i \phi_j^+ \hat{H} \phi_i d\tau = \int E \sum_i a_i \phi_j^+ \phi_i d\tau$

$$\underbrace{\sum_i a_i \int \phi_j^+ \hat{H} \phi_i d\tau}_{S_{ji}} = E \underbrace{\sum_i a_i \int \phi_j^+ \phi_i d\tau}_{H_{ji}} \quad (\text{A3})$$

It seems then we should use the orthogonal property, but

For TISE problems, Orthogonal is sometimes invalid.

So let us see what general conclusion we can draw: Give a name:

$$S_{ji} = \langle \phi_j | \phi_i \rangle = \int \phi_j^+ \phi_i d\tau$$

$$H_{ji} = \langle \phi_j | \hat{H} | \phi_i \rangle = \int \phi_j^+ \hat{H} \phi_i d\tau$$

Then (A3) becomes: $\sum_j H_{ji} a_i = E \sum_j S_{ji} a_i \Rightarrow \sum_j (H_{ji} - E S_{ji}) a_i = 0$, which could be written in matrix:

$$\begin{pmatrix} H_{11} - ES_{11} & H_{12} - ES_{12} & H_{13} - ES_{13} & \dots \\ H_{21} - ES_{21} & H_{22} - ES_{22} & H_{23} - ES_{23} & \dots \\ H_{31} - ES_{31} & H_{32} - ES_{32} & H_{33} - ES_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} = 0 \quad (\text{A7})$$

At first we want to get $E - \psi$ pairs

Now we have established the relationship between ψ and $\{\phi_1, \phi_2, \dots, \phi_i, \phi_j, \dots\}$

So now we are looking for $E - \begin{pmatrix} a_1 \\ a_2 \\ \vdots \end{pmatrix}$ pairs

To solve (A7), $\begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix}$ is definitely common solution for any E , but it is not what we want, since the wave function should not be zero

So we turn (A7) to :

$$\begin{array}{cccc|c}
 H_{11} - ES_{11} & H_{12} - ES_{12} & H_{13} - ES_{13} & \cdots & \\
 H_{21} - ES_{21} & H_{22} - ES_{22} & H_{23} - ES_{23} & \cdots & = 0 \quad (A8) \\
 H_{31} - ES_{31} & H_{32} - ES_{32} & H_{33} - ES_{33} & \cdots & \\
 \vdots & \vdots & \vdots & \ddots &
 \end{array}$$

Now actually we could try different \mathcal{E} to get the correct result

but we could use QM's property to get some simplification:

① In QM we are studying Hermitian Operator, so if \hat{H} is Hermitian then $\int \phi_j^* \hat{H} \phi_j d\tau = (\int \phi_j^* \hat{H} \phi_j d\tau)^*$
 it means \downarrow

$$H_{ji} = (H_{ij})^* = H_{ij}^*$$

1st Special Case: $H_{ii} = H_{ii}^* (= H_{ii}^*)$, so the diagonal elements are real

2nd Special Case: $S_{ji} = (S_{ij})^* = S_{ij}^*$

② For the case $\int \int \phi_j^* \phi_i d\tau = 0 \text{ or } \approx 0$

$$\int \phi_j^* \phi_i d\tau = 1$$

$$(A7) \text{ becomes: } \begin{pmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} & H_{23} & \cdots \\ H_{31} & H_{32} & H_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} = \mathcal{E} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ \vdots \end{pmatrix} \quad (A11)$$

③

And one approximation method has appeared: truncate into $N \times N$ size from the $\infty \times \infty$ one. (if we want the lowest 10 eigenvalues, truncate it into 500×500 may not affect)

Let us give some conclusions based on the last three points in the pdf.

1. The 1st point is correct for all the Hermitian operators. It is not about approximation. Here comes an example of application. The problem is about Matrix formulation of QM harmonic oscillator, whose description is in Figure 15. **Note: actually we could get the matrix form of the coordinate and momentum operators by choosing the eigenfunctions of 1D harmonic oscillator as the basis** We could express \hat{x} and \hat{p} by using the raising and lower operators, which have selection rules to connect different eigenfunctions of 1D harmonic oscillator, thus being able to help construct the matrix.

6.5 Matrix formulation of QM harmonic oscillator

We discussed in class that every QM problem can be turned into a big matrix (sometimes small such as spin) problem. This problem is to illustrate that even one can do the 1D harmonic oscillator problem by matrices.

2

Once upon a time, some clever physicists (meaning: Heisenberg, Born) found that the momentum operator and the position operator in the 1D harmonic oscillator problem of characteristic angular frequency ω are given by an infinite by infinite matrices of the form

$$\hat{x} = \left(\frac{1}{2} \frac{\hbar}{m\omega}\right)^{1/2} \begin{pmatrix} 0 & 1 & 0 & 0 & \dots \\ 1 & 0 & \sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \dots \end{pmatrix} \quad (5)$$

$$\hat{p} = \left(\frac{1}{2} m\hbar\omega\right)^{1/2} \begin{pmatrix} 0 & -i & 0 & 0 & \dots \\ i & 0 & -i\sqrt{2} & 0 & \dots \\ 0 & i\sqrt{2} & 0 & -i\sqrt{3} & \dots \\ 0 & 0 & i\sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \dots \end{pmatrix} \quad (6)$$

[Don't worry how these matrices are obtained. For those really wanted to do, read optional set of class notes on the operator method in harmonic oscillator.]

- (a) By multiplying matrices, **show** that the given \hat{x} and \hat{p} give the correct commutation relation.
- (b) **Construct** the Hamiltonian, which is now an infinite by infinite matrix, and **find** the eigenvalues of a 1D harmonic oscillator.

Figure 15: Matrix formulation of QM harmonic oscillator

The solution is in the following two pages pdf.

6.5

$$(a) \text{ in normal case: } \hat{x} = x \quad \hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = x \frac{\hbar}{i} \frac{\partial}{\partial x} - \frac{\hbar}{i} \frac{\partial}{\partial x} (x)$$

$$[\hat{x}, \hat{p}] f = x \frac{\hbar}{i} \frac{\partial f}{\partial x} - \frac{\hbar}{i} \frac{\partial}{\partial x} (xf) = x \frac{\hbar}{i} \frac{\partial f}{\partial x} - \frac{\hbar}{i} (f + x \frac{\partial f}{\partial x}) \\ = \frac{\hbar}{i} (x \frac{\partial f}{\partial x} - f - x \frac{\partial f}{\partial x}) = -\frac{\hbar}{i} f = i\hbar f$$

$$[\hat{x}, \hat{p}] = i\hbar$$

in matrix form:

$$\hat{x}\hat{p} = \frac{1}{2}\hbar \begin{pmatrix} 2 & 0 & -\sqrt{2} & 0 & \dots \\ 0 & 2 & 0 & -\sqrt{6} & \dots \\ \sqrt{2} & 0 & 2 & 0 & \dots \\ 0 & \sqrt{6} & 0 & 2 & \dots \\ \vdots & \vdots & \ddots & \ddots & \ddots \end{pmatrix}$$

$$\hat{p}\hat{x} = \frac{1}{2}\hbar \begin{pmatrix} -i & 0 & -i\sqrt{2} & 0 & \dots \\ 0 & -i & 0 & -i\sqrt{6} & \dots \\ i\sqrt{2} & 0 & -i & 0 & \dots \\ 0 & i\sqrt{6} & 0 & -i & \dots \\ \vdots & \vdots & \ddots & \ddots & \ddots \end{pmatrix}$$

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = \frac{1}{2}\hbar \begin{pmatrix} 2i & 0 & 0 & 0 & \dots \\ 0 & 2i & 0 & 0 & \dots \\ 0 & 0 & 2i & 0 & \dots \\ 0 & 0 & 0 & -2i & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \\ = \hbar \begin{pmatrix} i & & & & \\ & i & & & \\ & & \ddots & & \\ & & & i & \\ & & & & i \end{pmatrix} \quad \begin{array}{l} \text{other elements other than} \\ \text{the ones on diagonal are all "zero"} \end{array}$$

The same as the derivative form.

$$(b) \hat{H} = \frac{\hat{P}^2}{2m} + \frac{1}{2} m \omega^2 \hat{x}^2$$

$$\frac{\hat{P}^2}{2m} = \frac{1}{2} m \hbar \omega \underbrace{\frac{1}{m}}_{\frac{1}{2} \hbar \omega} \begin{pmatrix} 1 & 0 & -\sqrt{2} & 0 & \dots \\ 0 & 3 & 0 & -\sqrt{6} & \dots \\ -\sqrt{2} & 0 & 5 & 0 & \dots \\ 0 & -\sqrt{6} & 0 & 7 & \dots \\ \vdots & \ddots & \ddots & \ddots & \dots \end{pmatrix}$$

$$\left(\frac{1}{2} m \omega^2\right) \hat{x}^2 = \frac{1}{2} \frac{\hbar}{m} \omega \underbrace{\frac{1}{m} \hbar \omega}_{\frac{1}{2} \hbar \omega} \begin{pmatrix} 1 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 3 & 0 & \sqrt{6} & \dots \\ \sqrt{2} & 0 & 5 & 0 & \dots \\ 0 & \sqrt{6} & 0 & 7 & \dots \\ \vdots & \ddots & \ddots & \ddots & \dots \end{pmatrix}$$

$$\hat{H} = \frac{1}{2} \hbar \omega \begin{pmatrix} 2 & & & & \dots \\ & 6 & & & \dots \\ & & 10 & & \dots \\ & & & 14 & \dots \\ & & & & \dots \end{pmatrix} = \frac{1}{2} \hbar \omega \begin{pmatrix} 1 & & & & \\ & 3 & & & \\ & & 5 & & \\ & & & 7 & \dots \\ & & & & \dots \end{pmatrix}$$

Other Elements are all zero!

For the eigenvalues, since it is a Diagonal-Matrix, the elements on the diagonal are the eigenvalues.

They are $\frac{1}{2} \hbar \omega, \frac{3}{2} \hbar \omega, \frac{5}{2} \hbar \omega, \frac{7}{2} \hbar \omega \dots$

2. The 2nd and 3rd points are approximations.

(a) If we use the 3rd point solely in a simplest way: 2 by 2, then we could get:

$$\begin{pmatrix} H_{ii} - ES_{ii} & H_{ij} - ES_{ij} \\ H_{ji} - ES_{ji} & H_{jj} - ES_{jj} \end{pmatrix} \quad (98)$$

(b) If we use the 2nd and 3rd points together, then we could simplify more:

$$\begin{pmatrix} H_{ii} - ES_{ii} & H_{ij} \\ H_{ji} & H_{jj} - ES_{jj} \end{pmatrix} \quad (99)$$

And for the form in (99), we often call it **the eigenvalue problem of:**

$$\begin{pmatrix} H_{ii} & H_{ij} \\ H_{ji} & H_{jj} \end{pmatrix} \quad (100)$$

A question may be proposed: since in this point we have used the hypothesis that the basis are orthogonal, why $H_{ij} = \delta_{ij}E_j$ could not be used? Then it would get a more simplified form.

Answer: $H_{ij} = \delta_{ij}E_j$ could only be derived when the basis is the eigenstates of the operator! So our conditions used are not enough for this conclusion!

2.1.2 Variational Method

Variational Method is often used when the TISE is hard to solve, then we could guess some wave functions as answer candidate. We could know that all the guess functions would give a expectation value of the Hamiltonian higher than the real ground state eigenfunction(101), so here comes a method to evaluate “how good” our guess function is: the one with lower expectation value must be closer to the expectation value under the real ground state.

Proof of (101):

$$E_{gs} \leq \langle \psi | \hat{H} | \psi \rangle = \langle \hat{H} \rangle \quad (101)$$

Here ψ is our guess wave function. Because of the completeness of the real eigenfunctions of the Hamiltonian, we could express guess wave function as a combination of them:

$$\psi = \sum_n c_n \psi_n \quad (102)$$

And the real eigenfunctions should observe:

$$\hat{H}\psi_n = E_n\psi_n \quad (103)$$

Then for the guess value of the guess wave functions:

$$\begin{aligned}
 \langle \hat{H} \rangle &= \langle \psi | \hat{H} | \psi \rangle = \left\langle \sum_m c_m \psi_m | \hat{H} \right| \sum_n c_n \psi_n \rangle = \left\langle \sum_m c_m \psi_m | \hat{H} \sum_n c_n \psi_n \right\rangle \\
 &= \left\langle \sum_m c_m \psi_m | \sum_n c_n \hat{H} \psi_n \right\rangle = \left\langle \sum_m c_m \psi_m | \sum_n c_n E_n \psi_n \right\rangle = \sum_m c_m^* \langle \psi_m | \sum_n c_n E_n \psi_n \rangle \\
 &= \sum_m \sum_n (c_m^* c_n E_n) \langle \psi_m | \psi_n \rangle = \sum_m \sum_n (c_m^* c_n E_n) \delta_{mn} = \sum_n (c_n^* c_n) E_n = \sum_n |c_n|^2 E_n
 \end{aligned} \tag{104}$$

And we know that:

$$1 = \langle \psi | \psi \rangle = \left\langle \sum_m c_m \psi_m | \sum_n c_n \psi_n \right\rangle = \sum_m \sum_n c_m^* c_n \langle \psi_m | \psi_n \rangle = \sum_n |c_n|^2 \tag{105}$$

Namely the result of (104) is a weighted average of all the eigenvalues. And we know the ground state is the eigenstate with the lowest eigenvalue, so we could draw the conclusion:

$$E_{gs} \leq \langle \hat{H} \rangle \tag{106}$$

The relationship between variational method and huge matrix method It is in the next pdf page. The main idea is, variational method used the 3rd point of approximation: truncation.

Variational Method in view of Matrix:

$$\begin{pmatrix} H_{11} - ES_{11} & H_{12} - ES_{12} & \dots & H_{1n} - ES_{1n} \\ H_{21} - ES_{21} & H_{22} - ES_{22} & \dots & H_{2n} - ES_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ H_{n1} - ES_{n1} & H_{n2} - ES_{n2} & \dots & H_{nn} - ES_{nn} \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \vdots \\ C_n \end{pmatrix} = 0$$

\Downarrow non-trivial Solution

$$\begin{vmatrix} H_{11} - ES_{11} & H_{12} - ES_{12} & \dots & H_{1n} - ES_{1n} \\ H_{21} - ES_{21} & H_{22} - ES_{22} & \dots & H_{2n} - ES_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ H_{n1} - ES_{n1} & H_{n2} - ES_{n2} & \dots & H_{nn} - ES_{nn} \end{vmatrix} = 0$$

$J(E) = 0$ with $J(E)$ having E^n as the highest power

n roots for E and lowest one is best estimate for E_{gs}

For Variational Method, usually we Add truncation



3rd point in "Huge matrix Simplification"

!

Example of variational method: 1D harmonic oscillator Here I choose two different trial functions to carry out this method.

For the first one, I just chose the solution of 1D harmonic oscillator, so the final result is equal to the actual ground state energy $\frac{\hbar}{2}$. It is not the usual case of variational method, but could prove the effectiveness of variational method: that is, if we choose the correct form, it at least could help us to determine the best parameters.

For the second one, we just chose a trial function which is not the solution. So the result is $\frac{\hbar\omega}{2} \cdot \sqrt{2}$, namely $\sqrt{2} - 1 \simeq 0.414$ times higher than the actual ground state energy. This result observed our conclusion (101).

Example of Variational Method: 1D Harmonic Oscillator

Problem Description: Find the ground state energy by variational method for 1D harmonic oscillator, whose Hamiltonian is $\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2$

Process of Solving: Select Gaussian function $\psi(x) = A e^{-bx^2}$ as the trial function, b is the variational parameter, while A is Normalization factor Constant.

So firstly, A is also certain for a given "b":

$$1 = |A|^2 \int_{-\infty}^{+\infty} e^{-2bx^2} dx = |A|^2 \sqrt{\frac{\pi}{2b}}$$

$$\begin{aligned} A_1 &\leftrightarrow b_1 \\ A_2 &\leftrightarrow b_2 \\ &\vdots \\ A_n &\leftrightarrow b_n \end{aligned}$$

$$\text{The relation between } A \text{ and } b \text{ is: } A = \left(\frac{2b}{\pi} \right)^{\frac{1}{4}}$$

Then Secondly, since we know the wave function and the operator, we could calculate the expectation value.

$$\begin{aligned} \langle \hat{H} \rangle &= \int (A e^{-bx^2})^\dagger \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 \right) (A e^{-bx^2}) dx \\ &= \int (A e^{-bx^2})^\dagger \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) (A e^{-bx^2}) dx + \int (A e^{-bx^2})^\dagger \left(\frac{1}{2} m\omega^2 x^2 \right) (A e^{-bx^2}) dx \\ &= -\frac{\hbar^2}{2m} |A|^2 \int_{-\infty}^{+\infty} e^{-bx^2} \frac{d^2}{dx^2} (e^{-bx^2}) dx + \frac{1}{2} m\omega^2 |A|^2 \int_{-\infty}^{+\infty} e^{-2bx^2} x^2 dx \end{aligned}$$

$$\text{For the first term: } \int_{-\infty}^{+\infty} e^{-bx^2} \frac{d^2}{dx^2} (e^{-bx^2}) dx = \int_{-\infty}^{+\infty} e^{-bx^2} \frac{d}{dx} [e^{-bx^2} \cdot (-2bx)] dx$$

$$= \int_{-\infty}^{+\infty} e^{-bx^2} [e^{-bx^2} (-2bx) (-2bx) + e^{-bx^2} (2b^2)] dx$$

$$= \int_{-\infty}^{+\infty} [e^{-2bx^2} (4b^2 x^2) - 2b e^{-2bx^2}] dx$$

$$= 4b^2 \int_{-\infty}^{+\infty} e^{-2bx^2} \cdot x^2 dx - 2b \int_{-\infty}^{+\infty} e^{-2bx^2} dx$$

$$\text{We could use the Gaussian Integral: } \int_{-\infty}^{+\infty} e^{-\frac{1}{2} \alpha' x^2 + b' x} dx = \sqrt{\frac{2\pi}{\alpha'}} \exp\left(\frac{b'^2}{2\alpha'}\right)$$

$$\int_{-\infty}^{\infty} x^2 e^{-\frac{1}{2} \alpha'' x^2} dx = \frac{1}{\alpha''} \sqrt{\frac{2\pi}{\alpha''}}$$

$$\alpha'' = 4b$$

$$= 4b^2 \cdot \frac{1}{\alpha''} \sqrt{\frac{2\pi}{\alpha''}} = \frac{4b^2}{4b} \sqrt{\frac{2\pi}{4b}} = b \sqrt{\frac{\pi}{2b}} = \sqrt{\frac{b\pi}{2}}$$

$$b' = 0 \quad \alpha' = 4b$$

$$= -2b \sqrt{\frac{2\pi}{4b}} = -2b \sqrt{\frac{\pi}{2b}} = -\sqrt{2b\pi}$$

$$\begin{aligned} \text{The first term} &= -\frac{\hbar^2}{2m} |A|^2 \left(\sqrt{\frac{b\pi}{2}} - \sqrt{2b\pi} \right) = -\frac{\hbar^2}{2m} \sqrt{\frac{b\pi}{\pi}} \left(\sqrt{\frac{b\pi}{2}} - \sqrt{2b\pi} \right) \\ &= -\frac{\hbar^2}{2m} \sqrt{\frac{2b}{\pi}} \left(\sqrt{\frac{b\pi}{2}} - 2\sqrt{\frac{b\pi}{2}} \right) \\ &= -\frac{\hbar^2}{2m} \sqrt{\frac{2b}{\pi}} \left(-\sqrt{\frac{b\pi}{2}} \right) \\ &= \frac{\hbar^2}{2m} \left(\sqrt{\frac{2b}{\pi}} \sqrt{\frac{b\pi}{2}} \right) \\ &= \frac{b\hbar^2}{2m} \end{aligned}$$

$$\text{For the second term: } \frac{1}{2} m \omega^2 |A|^2 \underbrace{\int_{-\infty}^{\infty} e^{-2bx^2} x^2 dx}_{\text{use:}}$$

use:

$$\int_{-\infty}^{\infty} x^2 e^{-\frac{1}{2} \alpha'' x^2} dx = \frac{1}{\alpha''} \sqrt{\frac{2\pi}{\alpha''}} \quad \text{Here } \alpha'' = 4b$$

$$\begin{aligned} \therefore &= \frac{1}{2} m \omega^2 |A|^2 \frac{1}{4b} \sqrt{\frac{2\pi}{4b}} = \frac{1}{2} m \omega^2 \left(\frac{2b}{\pi} \right)^{\frac{1}{2}} \frac{1}{4b} \sqrt{\frac{\pi}{2b}} \\ &= \frac{1}{2} m \omega^2 \sqrt{\frac{2b}{\pi}} \sqrt{\frac{\pi}{2b}} \cdot \frac{1}{4b} \\ &= \frac{m \omega^2}{8b} \end{aligned}$$

$$\text{So the total is: } \langle H \rangle = \frac{\hbar^2 b}{2m} + \frac{m \omega^2}{8b}$$

We could symbolize it $\langle H \rangle_b$, indicating b is its parameter

$$\frac{\partial \langle H \rangle_b}{\partial b} = \frac{\hbar^2}{2m} - \frac{m \omega^2}{8b^2} = 0 \Rightarrow b = \frac{m \omega}{2\hbar}$$

$$\langle H \rangle \left(b = \frac{m \omega}{2\hbar} \right) = \frac{\hbar^2}{2m} \frac{m \omega}{2\hbar} + \frac{m \omega^2}{8} \frac{2\hbar}{m \omega} = \frac{w\hbar}{4} + \frac{w\hbar}{4} = \frac{1}{2} w\hbar$$

Process of Solving ②:

Choose $\psi(x) = \frac{\beta}{\alpha^2 + x^2}$

$$\int |\psi|^2 dx = 1 = \int_{-\infty}^{\infty} \frac{\beta^2}{(\alpha^2 + x^2)^2} dx = \frac{\pi \beta^2}{2\alpha^3} \Rightarrow \beta = \sqrt{\frac{2\alpha^3}{\pi}}$$

$$\begin{aligned} \langle T \rangle &= \int_{-\infty}^{\infty} \left(\frac{\beta}{\alpha^2 + x^2} \right) \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \left(\frac{\beta}{\alpha^2 + x^2} \right) \right) dx \\ &= -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \frac{\beta^2}{\alpha^2 + x^2} \frac{d}{dx} \left[-\frac{2x}{(\alpha^2 + x^2)^2} \right] dx \\ &= +\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \frac{\beta^2}{\alpha^2 + x^2} \left[2 \frac{1}{(\alpha^2 + x^2)^2} - 2 \frac{2x}{(\alpha^2 + x^2)^3} \right] dx \\ &= \frac{\hbar^2 \beta^2}{m} \int_{-\infty}^{\infty} \frac{1}{\alpha^2 + x^2} \left[\frac{1}{(\alpha^2 + x^2)^2} - \frac{2x}{(\alpha^2 + x^2)^3} \right] dx \\ &= \frac{\hbar^2 \beta^2}{m} \int_{-\infty}^{\infty} \left[\frac{1}{(\alpha^2 + x^2)^3} - \frac{2x}{(\alpha^2 + x^2)^4} \right] dx \\ &= \frac{\hbar^2 \beta^2}{m} \int_{-\infty}^{\infty} \frac{-3x^2 + \alpha^2}{(\alpha^2 + x^2)^4} dx \\ &= \frac{\pi \beta^2 \hbar^2}{8m\alpha^5} \end{aligned}$$

$$\begin{aligned} \langle V \rangle &= \int_{-\infty}^{\infty} \frac{\beta}{\alpha^2 + x^2} \frac{1}{2} m \omega^2 x^2 \frac{\beta}{\alpha^2 + x^2} dx \\ &= \int_{-\infty}^{\infty} \frac{1}{2} \frac{m \omega^2 \beta^2 x^2}{(\alpha^2 + x^2)^2} dx \\ &= \frac{\pi m \beta^2 \omega^2}{4\alpha} \end{aligned}$$

$$\langle H \rangle = \langle T \rangle + \langle V \rangle = \frac{\pi \beta^2 \hbar^2}{8m\alpha^5} + \frac{\pi m \beta^2 \omega^2}{4\alpha}$$

// Using the
Normalization result

$$\frac{\hbar^2}{4m\alpha^2} + \frac{\alpha^2 m \omega^2}{2} \text{ then } \frac{\partial \langle H \rangle}{\partial \alpha} = -\frac{2\hbar^2}{4m\alpha^3} + m\alpha \omega^2 \Rightarrow \alpha^2 = \frac{\hbar}{\sqrt{2}m\omega}$$

$$\langle H \rangle (\alpha = \left(\frac{\hbar}{\sqrt{2}m\omega} \right)^{\frac{1}{2}}) = \frac{1}{2} \hbar \omega (\sqrt{2})$$

2.1.3 Time-independent Perturbation Theory

Perturbation theory is often used when we know the exact solution of a famous case(I mean the eigenvalues and eigenfunctions pairs), but the system we are facing's Hamiltonian is a little different from the known one. But still we could make good use of the known system to get an approximation of the real system.

Time-independent Perturbation Theory is composed of degenerate and non-degenerate cases.

In the following several pdf pages, firstly I would give the proof of the time-independent degenerate theory.

The relationship between perturbation theory and huge matrix method and thus the degenerate perturbation theory comes out Then I would try to understand the time-independent degenerate perturbation theory from the view of the huge matrix. The main idea is, perturbation method used the 2nd point of approximation: choose a orthogonal basis(and this basis is just the eigenfunctions of \hat{H}_0).

And during this process, we would get the time-independent degenerate perturbation theory naturally.

Time-independent Non-degenerate Perturbation Theory

it is "prime" not "one"

$$\hat{H} = \hat{H}_0 + \hat{H}' \quad \text{and we know } \hat{H}_0 \Psi_n^{(0)} = E_n^{(0)} \Psi_n^{(0)}$$

\downarrow

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}' , \lambda \text{ helps us to count number: the order of } \lambda \text{ is equal to order of } \hat{H}'$$

Due to the perturbation term

Eigenfunctions and eigenvalues would have their 1, 2 ... to n order correction

$$\left\{ \begin{array}{l} E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots \\ \Psi_n = \Psi_n^{(0)} + \lambda \Psi_n^{(1)} + \lambda^2 \Psi_n^{(2)} + \dots \end{array} \right.$$

Now everything is prepared. We could write $\hat{H} \Psi_n = E_n \Psi_n$:

$$\begin{aligned} \text{LHS} &= \hat{H} \Psi_n = (\hat{H}_0 + \lambda \hat{H}') (\Psi_n^{(0)} + \lambda \Psi_n^{(1)} + \lambda^2 \Psi_n^{(2)} + \dots) \\ &= \hat{H}_0 \Psi_n^{(0)} + \lambda (\hat{H}_0 \Psi_n^{(1)} + \hat{H}' \Psi_n^{(0)}) + \lambda^2 (\hat{H}_0 \Psi_n^{(2)} + \hat{H}' \Psi_n^{(1)}) + \dots \end{aligned}$$

$$\begin{aligned} \text{RHS} &= E_n \Psi_n = (E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots) (\Psi_n^{(0)} + \lambda \Psi_n^{(1)} + \lambda^2 \Psi_n^{(2)} + \dots) \\ &= E_n^{(0)} \Psi_n^{(0)} + \lambda (E_n^{(1)} \Psi_n^{(0)} + E_n^{(0)} \Psi_n^{(1)}) + \lambda^2 (E_n^{(2)} \Psi_n^{(0)} + E_n^{(1)} \Psi_n^{(1)} + E_n^{(0)} \Psi_n^{(2)}) + \dots \end{aligned}$$

The coefficients before every order λ should be the same!

$$\text{So: for } \lambda^0 \text{ terms: } \hat{H}_0 \Psi_n^{(0)} = E_n^{(0)} \Psi_n^{(0)}$$

$$\lambda^1 : \hat{H}_0 \Psi_n^{(1)} + \hat{H}' \Psi_n^{(0)} = E_n^{(1)} \Psi_n^{(0)} + E_n^{(0)} \Psi_n^{(1)}$$

$$\lambda^2 : \hat{H}_0 \Psi_n^{(2)} + \hat{H}' \Psi_n^{(1)} = E_n^{(2)} \Psi_n^{(0)} + E_n^{(1)} \Psi_n^{(1)} + E_n^{(0)} \Psi_n^{(2)}$$

$$\vdots \quad \vdots \quad \vdots$$

The 1st and 2nd Perturbation theories are often used.

① 1st Order:

$$E_n^{(1)} = \int \Psi_n^{*(0)} \hat{H}' \Psi_n^{(0)} d\tau = \langle \Psi_n^{(0)} | \hat{H}' | \Psi_n^{(0)} \rangle$$

$$\Psi_n^{(1)} = \sum_{i \neq n} \frac{\langle \Psi_i^{(0)} | \hat{H}' | \Psi_n^{(0)} \rangle}{E_n^{(0)} - E_i^{(0)}} \Psi_i^{(0)}$$

② 2nd order:

$$E_n^{(2)} = \int \psi_n^{*(0)} \hat{H}^1 \psi_n^{(0)} d\tau = \sum_{\tilde{\nu} \neq n} \frac{\left| \int \psi_{\tilde{\nu}}^{*(0)} \hat{H}^1 \psi_n^{(0)} d\tau \right|^2}{(E_n^{(0)} - E_{\tilde{\nu}}^{(0)})}$$



physical meaning: For a given state "n" Eigenvalues for the states higher than $E_n^{(0)}$ would push (E_n) down
 lower up $\hat{H} = \hat{H}_0 + \hat{H}'$

Proof: $E_n^{(1)} \rightarrow \psi_n^{(1)} \rightarrow E_n^{(2)}$

$$\textcircled{1} E_n^{(1)}: \text{For } \lambda': \hat{H}_0 \psi_n^{(1)} + \hat{H}' \psi_n^{(0)} = E_n^{(1)} \psi_n^{(0)} + E_n^{(0)} \psi_n^{(1)}$$

We know the basis of \hat{H}_0 is orthogonal. So multiply $\psi_n^{*(0)}$ and integrate:

$$\text{LHS: } \int \psi_n^{*(0)} \hat{H}_0 \psi_n^{(1)} d\tau + \int \psi_n^{*(0)} \hat{H}' \psi_n^{(0)} d\tau$$

||

$$\begin{aligned} \int \psi_n^{*(0)} \hat{H}_0^* \psi_n^{(1)} d\tau &= \int (\hat{H}_0 \psi_n^{(0)})^* \psi_n^{(1)} d\tau \\ &= \int (E_n^{(0)} \psi_n^{(0)})^* \psi_n^{(1)} d\tau \\ &= \int E_n^{(0)} \psi_n^{(0)*} \psi_n^{(1)} d\tau \\ &= E_n^{(0)} \int \psi_n^{(0)*} \psi_n^{(1)} d\tau \end{aligned}$$

the same

$$\text{LHS} = \boxed{E_n^{(0)} \int \psi_n^{*(0)} \psi_n^{(1)} d\tau} + \int \psi_n^{*(0)} \hat{H}' \psi_n^{(0)} d\tau$$

$$\text{RHS: } E_n^{(1)} \int \psi_n^{(0)*} \psi_n^{(0)} d\tau + E_n^{(0)} \int \psi_n^{*(0)} \psi_n^{(1)} d\tau$$

$$= E_n^{(1)} + \boxed{E_n^{(0)} \int \psi_n^{*(0)} \psi_n^{(1)} d\tau}$$

$$\text{So } E_n^{(1)} = \int \psi_n^{*(0)} \hat{H}^1 \psi_n^{(0)} d\tau = \langle \psi_n^{(0)} | \hat{H}^1 | \psi_n^{(0)} \rangle$$

Above we make the both sides have terms involving $\psi_n^{(1)}$ to eliminate it.

② But now we know $E_n^{(1)}$ then we could get $\psi_n^{(1)}$:

$$\text{Rewrite } \lambda' \text{ equation: } \underbrace{\hat{H}_0 \psi_n^{(1)}}_{\lambda'} + \hat{H}' \psi_n^{(0)} = E_n^{(1)} \psi_n^{(0)} + E_n^{(0)} \underbrace{\psi_n^{(1)}}_{\lambda'}$$

Still, we could eliminate $\psi_n^{(0)}$ by multiplying $\psi_{\tilde{\nu}}^{*(0)}$ and integrate ($\tilde{\nu} \neq n$):

$$\int \psi_{\tilde{\nu}}^{*(0)} \hat{H}_0 \psi_n^{(1)} d\tau + \int \psi_{\tilde{\nu}}^{*(0)} \hat{H}' \psi_n^{(0)} d\tau = \underbrace{\int \psi_{\tilde{\nu}}^{*(0)} \psi_n^{(0)} d\tau}_{=0} + E_n^{(0)} \int \psi_{\tilde{\nu}}^{*(0)} \psi_n^{(1)} d\tau$$

Then we could use completeness property to transform the question of getting $\psi_n^{(1)}$ to the question of getting a group of Coefficients :

$$\psi_n^{(1)} = \sum_{m \neq n} a_m \psi_m^{(0)} \quad \text{A Question: why } m \neq n?$$

Because for the λ' equation, if $\psi_n^{(1)}$ satisfies then $(\psi_n^{(1)} + d\psi_n^{(0)})$ would also satisfy.

Then the $(\alpha')'$ equation becomes :

$$\sum_{m \neq n} a_m \int \psi_r^{*(0)} \hat{H}_0 \psi_m^{(0)} dr + \int \psi_r^{*(0)} \hat{H}' \psi_n^{(0)} dr = E_n^{(0)} \sum_{m \neq n} a_m \int \psi_r^{*(0)} \psi_m^{(0)} dr$$

$$\sum_{m \neq n} a_m E_m^{(0)} \delta_{im} + \int \psi_r^{*(0)} \hat{H}' \psi_n^{(0)} dr = E_n^{(0)} a_i$$

$$E_r^{(0)} a_i + \int \psi_r^{*(0)} \hat{H}' \psi_n^{(0)} dr = E_n^{(0)} a_i$$

$$a_i = \frac{\int \psi_r^{*(0)} \hat{H}' \psi_n^{(0)} dr}{E_n^{(0)} - E_r^{(0)}} = \frac{\langle \psi_r^{(0)} | \hat{H}' | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_r^{(0)}} \quad (i \neq n)$$

Express in state function form : $\psi_n = \psi_n^{(0)} + \sum_{i \neq n} \frac{\int \psi_r^{*(0)} \hat{H}' \psi_n^{(0)} dr}{E_n^{(0)} - E_i^{(0)}} \psi_r^{(0)}$

$$= \psi_n^{(0)} + \sum_{i \neq n} \frac{\langle \psi_r^{(0)} | \hat{H}' | \psi_n^{(0)} \rangle}{E_n^{(0)} - E_i^{(0)}} \psi_r^{(0)}$$

③ $E_n^{(2)}$

(λ^2) equation : $\underbrace{\hat{H}_0 \psi_n^{(2)}}_{\text{1st order}} + \underbrace{\hat{H}' \psi_n^{(1)}}_{\text{2nd order}} = \underbrace{E_n^{(0)} \psi_n^{(2)}}_{\text{1st order}} + \underbrace{E_n^{(1)} \psi_n^{(1)}}_{\text{2nd order}} + E_n^{(2)} \psi_n^{(0)}$

There are two unknowns, but another thing \Rightarrow Could be cancelled if

We multiply $\psi_n^{*(0)}$ and integrate, so it becomes :

~~$$\int \psi_n^{*(0)} \hat{H}_0 \psi_n^{(2)} dr + \int \psi_n^{*(0)} \hat{H}' \psi_n^{(1)} dr = E_n^{(0)} \int \psi_n^{*(0)} \psi_n^{(2)} dr + E_n^{(1)} \int \psi_n^{*(0)} \psi_n^{(1)} dr + E_n^{(2)} \int \psi_n^{*(0)} \psi_n^{(0)} dr$$~~

use $\psi_n^{(1)}$ result

$$\text{So } E_n^{(2)} = \int \psi_n^{*(0)} \hat{H}' \psi_n^{(1)} dr \stackrel{\text{1st order}}{\underline{\underline{=}}} \sum_{i \neq n} \frac{\left| \int \psi_r^{*(0)} \hat{H}' \psi_n^{(0)} dr \right|^2}{E_n^{(0)} - E_i^{(0)}} \stackrel{\text{2nd order}}{\underline{\underline{=}}}$$

total is 2nd order! Good!

Perturbation Results from Matrix's point of view

We have used the basis of \hat{H}_0 , so $S_{ij} = S_{\tilde{i}\tilde{j}}$, namely the 2nd point simplification. So it reduces to:

$$\begin{pmatrix} H_{11}-E & H_{12}' & H_{13}' & \dots \\ H_{21}' & H_{22}-E & H_{23}' & \dots \\ H_{31}' & H_{32}' & H_{33}-E & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \vdots \end{pmatrix} = 0$$

What 1st order perturbation do in matrix's view:

$$\begin{pmatrix} H_{11}-E & \text{Zero} & & \\ \text{Zero} & H_{22}-E & & \\ & H_{33}-E & \dots & \end{pmatrix} \begin{pmatrix} C_1 \\ C_2 \\ C_3 \\ \vdots \end{pmatrix} = 0$$

2nd order in Matrix's view:

$$\begin{array}{c|c|c} \begin{array}{c} H_{nn}-E - H_{ni}' \\ | \\ H_{in}' - H_{ii}-E \end{array} & \xrightarrow{\text{Read out}} & \begin{array}{c} H_{nn}-E & H_{ni}' \\ H_{in}' & H_{ii}-E \end{array} \end{array} = 0$$

Let's treat a more general case: Call it (*) equation

$$\begin{vmatrix} \varepsilon_A - E & \Delta \\ \Delta^* & \varepsilon_B - E \end{vmatrix} = 0 \Rightarrow E = \frac{\varepsilon_A + \varepsilon_B}{2} \pm \frac{1}{2} \sqrt{(\varepsilon_A - \varepsilon_B)^2 + 4|\Delta|^2}$$

For Non-degenerate theory, we have used $\varepsilon_A - \varepsilon_B \gg |\Delta|$

then $E \approx \begin{cases} \varepsilon_A + \frac{|\Delta|^2}{\varepsilon_A - \varepsilon_B} \\ \varepsilon_B - \frac{|\Delta|^2}{\varepsilon_A - \varepsilon_B} \end{cases}$

Back to the 2nd order perturbation theory's notation:

$$E_n \approx H_{nn} + \frac{|H'_{nn}|^2}{H_{nn} - H_{ii}}$$

Here although we use "H_{nn}" and "H_{ii}", which are same notations as 1st order perturbation theory, but its meaning differ!

Because we usually do 1st order correction first, then do 2nd order correction.

So we could know the 1st order result, which could make the result better

if it is used.

$$\text{So here } H_{nn} = E_n^{(0)} + H'^{nn} \quad H_{ii} = E_i^{(0)} + H'^{ii}$$

$$\begin{aligned} \text{Then the result becomes: } E_n &\approx E_n^{(0)} + H'^{nn} + \frac{|H'_{nn}|^2}{E_n^{(0)} + H'^{nn} - E_i^{(0)} - H'^{ii}} \\ &= E_n^{(0)} + H'^{nn} + \frac{|H'_{nn}|^2 \leftarrow \text{2nd order}}{[E_n^{(0)} - E_i^{(0)}] + [H'^{nn} - H'^{ii}]} \\ &\quad \swarrow \qquad \swarrow \\ &\quad \text{0th order} \qquad \text{1st order} \end{aligned}$$

So we can do a further approximation:

$$E_n \approx E_n^{(0)} + H'^{nn} + \frac{|H'_{nn}|^2}{E_n^{(0)} - E_i^{(0)}}$$

And we should remember that for (*) equation. We have used the approximation $\epsilon_A - \epsilon_B \gg |\Delta|$, but how about other cases?

$$\text{Back to the solution: } E = \frac{\epsilon_A + \epsilon_B}{2} \pm \frac{1}{2} \sqrt{(\epsilon_A - \epsilon_B)^2 + 4|\Delta|^2}$$

if $\epsilon_A = \epsilon_B = \epsilon$ then $E = \begin{cases} \epsilon + |\Delta| \\ \epsilon - |\Delta| \end{cases}$

Back to perturbation theory, it means the two states have same energy, that is "degenerate"!

Degenerate Theory:

still we need to use (0th + 1st) to replace H_{nn} and H_{ii}

$$\left| \begin{array}{cc} H_{nn} - E & H'_{ni} \\ H'_{in} & H_{ii} - E \end{array} \right| = 0 \Rightarrow \left| \begin{array}{cc} \underline{\epsilon_n^{(0)} + H'_{nn} - E} & H'_{ni} \\ H'_{in} & \underline{\epsilon_n^{(0)} + H'_{ii} - E} \end{array} \right| = 0$$

A new thing is: use $\epsilon_i^{(0)} = \epsilon_n^{(0)}$, but their 1st order may differ

(Compared to 2nd order non-degenerate perturbation theory)

The final result is:

$$E \pm = \epsilon_n^{(0)} + \frac{\epsilon_n^{(1)} + \epsilon_i^{(1)}}{2} \pm \frac{1}{2} \sqrt{(\epsilon_n^{(1)} - \epsilon_i^{(1)})^2 + 4|H'_{ni}|^2}$$

Note:

Here we don't use the approximation like what we did to the denominator of 2nd order perturbation result above.

Example of Time-independent Non-degenerate Perturbation Theory Here still, we used 1D harmonic oscillator as an example to show how the Time-independent Perturbation Theory(more precisely, non-degenerate one)works. The problem description could be seen in Figure 16, and the solution is in the following pdf pages.

SQ6 Harmonic Oscillator – an exactly solvable problem treated by 1st and 2nd order perturbation theory

Consider an 1D harmonic oscillator in which the potential energy function is $U(x) = \frac{1}{2}k(1+\epsilon)x^2$, where ϵ is meant to be $\epsilon \ll 1$. Referring to harmonic oscillator quantum physics, **write down** the exact eigenvalues of the problem.

Knowing the exact results, we actually don't need the perturbation theory. However, it will be interesting to see how good (or bad) perturbation theory works.

- (a) The exact eigenvalues can be **expanded** into a power series in ϵ , i.e., considering $\epsilon \ll 1$. **Do it.**
- (b) Now we take the unperturbed problem to be

$$\hat{H}_0 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}kx^2 \quad (4)$$

and the perturbed problem as

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}k(1+\epsilon)x^2 = \hat{H}_0 + \hat{H}' \quad (5)$$

Identify the perturbation term \hat{H}' and **obtain** the 1st order perturbation in the energy for **all states**.

- (c) Next consider only the **ground state**. **Find** the 2nd order perturbation to the ground state energy. Hence, **write down** the ground state energy including 0th, 1st, and 2nd order terms.
- (d) **Compare** the perturbation result with the exact result in part (a) to the same order.
- (e) **(Optional for TA, just for fun)** **How about** the 1st order correction to the ground state wavefunction?

[Remark: This is Problem 6.2 and Problem 6.4(b) in Griffiths' *Introduction to Quantum Mechanics*.]

Figure 16: PHYS3022 SQ6 problem description

SQ 6

(a)

$$\begin{aligned} E_n &= \hbar w(n + \frac{1}{2}) \text{ where } mw^2 = k(1 + \varepsilon) \Rightarrow w = \sqrt{\frac{k(1+\varepsilon)}{m}} \\ &= \hbar (n + \frac{1}{2}) \sqrt{\frac{k(1+\varepsilon)}{m}} \\ &= \hbar w_0 (n + \frac{1}{2}) \sqrt{1+\varepsilon} \end{aligned}$$

$$\begin{aligned} \text{use Taylor's expansion : } E_n &= \hbar w_0 (n + \frac{1}{2}) \sqrt{1+\varepsilon} \\ &= \hbar w_0 (n + \frac{1}{2}) (1 + \frac{1}{2}\varepsilon - \frac{1}{8}\varepsilon^2 + \dots) \end{aligned}$$

(b)

$$\hat{H}' = \hat{H} - \hat{H}_0 = \frac{1}{2}\varepsilon kx^2$$

$$E'_n = \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle = \int \psi_n^{(0)} \hat{H}' \psi_n^{(0)} dx$$

Here ψ_n^0 is the eigenfunctions of the 1D harmonic oscillator problem whose $U(x) = \frac{1}{2}kx^2$, so $\psi_n^0 = \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\frac{1}{2}\xi^2}$, where $m\omega_0^2 = K$, $\xi = \sqrt{\frac{m\omega_0}{K}} x$

$$E'_n = \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{2}} \frac{1}{2^n n!} \int H_n^2(\xi) e^{-\xi^2} \cdot \frac{1}{2}\varepsilon kx^2 dx$$
$$w_0 = \sqrt{\frac{K}{m}}$$

use $x = \sqrt{\frac{\hbar}{m\omega_0}} \xi$

$$\begin{aligned} &= \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{2}} \frac{1}{2^n n!} \cdot \int H_n^2(\xi) e^{-\xi^2} \cdot \frac{1}{2}\varepsilon k \frac{\hbar}{m\omega_0} \xi^2 \cdot \sqrt{\frac{\hbar}{m\omega_0}} d\xi \\ &= \frac{1}{\sqrt{\pi}} \frac{1}{2^n n!} \cdot \frac{1}{2}\varepsilon \cdot \frac{\hbar}{m\omega_0} K \int H_n^2(\xi) e^{-\xi^2} \xi^2 d\xi \\ &= \frac{1}{2^{n+1} n!} \frac{\varepsilon \hbar}{\sqrt{\pi} m\omega_0} \int H_n^2(\xi) e^{-\xi^2} \xi^2 d\xi \\ &= \frac{1}{2^{n+1} n!} \frac{\varepsilon}{\sqrt{\pi}} \omega_0 \hbar \int H_n^2(\xi) e^{-\xi^2} \xi^2 d\xi \end{aligned}$$

Maybe it could be solved, but we can have an easier way!

$$\begin{aligned} E'_n &= \langle \psi_n^0 | \hat{H}' | \psi_n^0 \rangle = \langle \psi_n^0 | \frac{1}{2}\varepsilon kx^2 | \psi_n^0 \rangle \\ &= \langle \psi_n^0 | \varepsilon V(x) | \psi_n^0 \rangle \\ &= \varepsilon \langle \psi_n^0 | V(x) | \psi_n^0 \rangle \\ &= \frac{1}{2}\varepsilon \langle \psi_n^0 | V(x) + \frac{\hat{p}^2}{2m} | \psi_n^0 \rangle \\ &= \frac{1}{2}\varepsilon E_n^0 = \frac{1}{2}\varepsilon (n + \frac{1}{2}) \hbar \omega_0 \end{aligned}$$

(C)

Second order perturbation to the ground state energy :

$$= \sum_{\vec{r} \neq 0} \frac{\left| \int \psi_{\vec{r}}^{*(0)} \hat{H}^1 \psi_0^{(0)} d\tau \right|^2}{E_0^{(0)} - E_{\vec{r}}^{(0)}}$$

We know $E_n^{(0)} = \frac{1}{2} \pi \omega (\frac{1}{2} + n)$; $E_0^{(0)} - E_{\vec{r}}^{(0)} = \frac{1}{2} \pi \omega_0 - \pi \omega_0 (\frac{1}{2} + \vec{r}) = -\vec{r} \pi \omega_0$

for the integral: $\psi_{\vec{r}}^{*(0)} = \left(\frac{m \omega_0}{\pi \hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^i i!}} H_i(\xi) e^{-\frac{1}{2} \xi^2}$

$$\begin{aligned} \psi_0^{(0)} &= \left(\frac{m \omega_0}{\pi \hbar}\right)^{\frac{1}{4}} H_0(\xi) e^{-\frac{1}{2} \xi^2} \\ &= \left(\frac{m \omega_0}{\pi \hbar}\right)^{\frac{1}{4}} e^{-\frac{1}{2} \xi^2} \end{aligned}$$

$$\begin{aligned} \left| \int \psi_{\vec{r}}^{*(0)} \hat{H}^1 \psi_0^{(0)} d\tau \right|^2 &= \left(\frac{m \omega_0}{\pi \hbar} \right) \frac{1}{2^i i!} \left| \int H_i(\xi) e^{-\xi^2} \frac{1}{2} \varepsilon k x^2 dx \right|^2 \\ &= \frac{m \omega_0}{\pi \hbar} \frac{1}{2^i i!} \left| \int H_i(\xi) e^{-\xi^2} \frac{1}{2} \varepsilon k \frac{\pi}{m \omega_0} \xi^2 \sqrt{\frac{\pi}{m \omega_0}} d\xi \right|^2 \\ &\quad \uparrow \\ &\text{using } x = \sqrt{\frac{\pi}{m \omega_0}} \xi \\ &= \frac{1}{\pi} \frac{1}{2^i i!} \frac{1}{4} \varepsilon^2 k \frac{\pi^2}{m^2 \omega_0^2} \left| \int H_i(\xi) e^{-\xi^2} \xi^2 d\xi \right|^2 \\ &= \frac{\pi^2 \varepsilon^2 k}{2^{i+2} i! \pi m^2 \omega_0^2} \left| \int H_i(\xi) e^{-\xi^2} \xi^2 d\xi \right|^2 \end{aligned}$$

$$2\text{-nd order} = \sum_{\vec{r} \neq 0} - \frac{\pi \varepsilon^2 k}{2^{i+2} i! \pi m^2 \omega_0^2} \left| \int H_i(\xi) e^{-\xi^2} \xi^2 d\xi \right|^2$$

$$\text{Ground state energy} = \frac{1}{2} \pi \omega_0 + \frac{1}{2^{n+1} n!} \frac{\varepsilon}{\pi} \frac{\pi k}{m \omega_0} \int H_n^2(\xi) e^{-\xi^2} \xi^2 d\xi$$

$$\text{Substitute } n=0 \quad - \sum_{\vec{r} \neq 0} \frac{\pi \varepsilon^2 k}{2^{i+2} i! \pi m^2 \omega_0^2} \left| \int H_i(\xi) e^{-\xi^2} \xi^2 d\xi \right|^2$$

$$\text{then 1-st : } \frac{1}{2} \frac{\varepsilon}{\pi} \frac{\hbar k}{m w_0} \int_{-\infty}^{\infty} e^{-\xi^2} \xi^2 d\xi$$

$$\text{And we know: } \int_{-\infty}^{\infty} x^2 e^{-\frac{1}{2} \alpha x^2} dx = \frac{1}{\alpha} \sqrt{\frac{2\pi}{\alpha}} \\ \downarrow \\ = 1 \Rightarrow \alpha = 2$$

$$\text{integral} = \frac{1}{2} \pi$$

$$= \frac{1}{2} \frac{\varepsilon}{\pi} \frac{\hbar k}{m w_0} \frac{1}{2} \pi = \frac{1}{4} \varepsilon \frac{\hbar k}{m w_0} \quad m w_0^2 = k \\ = \frac{1}{4} \varepsilon (w_0 \hbar) \quad w_0 = \sqrt{\frac{k}{m}}$$

2-nd: We could do integrated, but we have investigated the property of \hat{a}^+ and \hat{a}^- , which could help us simplify calculation.

$$\hat{H}' = \frac{1}{2} \varepsilon k \hat{x}^2, \quad \hat{x} = \sqrt{\frac{\hbar}{2m w_0}} (\hat{a}^+ + \hat{a}^-), \quad \text{where } \hat{a}^+ \psi_n = \sqrt{n+1} \psi_{n+1} \\ \hat{a}^- \psi_n = \sqrt{n} \psi_{n-1}$$

$$\text{so } \hat{H}' = \frac{1}{2} \varepsilon k \hat{x}^2 = \frac{\hbar \varepsilon w_0}{4} (\hat{a}_+^2 + \hat{a}_+ \hat{a}_- + \hat{a}_- \hat{a}_+ + \hat{a}_-^2)$$

$$E_n^2 = \sum_{l \neq n} \frac{|\langle \psi_l^0 | H' | \psi_n^0 \rangle|^2}{E_l^0 - E_n^0} = \frac{\hbar^2 \varepsilon^2 w_0^2}{16} \sum_{l \neq n} \frac{|\langle \psi_l^0 | \hat{a}_+^2 + \hat{a}_+ \hat{a}_- + \hat{a}_- \hat{a}_+ + \hat{a}_-^2 | \psi_n^0 \rangle|^2}{\hbar w_0 (n-l)}$$

For $\hat{a}^+ \hat{a}^-$ and $\hat{a}^- \hat{a}^+$, they acts on ψ_n^0 would return ψ_n^0 (may with some constants), but $n \neq l \therefore \langle \psi_n^0 | \psi_l^0 \rangle = 0$, so we could neglect these two.

$$E_n^2 = \frac{\hbar^2 \varepsilon^2 w_0^2}{16} \sum_{l \neq n} \frac{|\langle \psi_l^0 | \hat{a}_+^2 + \hat{a}_-^2 | \psi_n^0 \rangle|^2}{\hbar w_0 (n-l)}$$

$$= \frac{\hbar^2 \varepsilon^2 w_0^2}{16} \sum_{l \neq n} \frac{|\langle \psi_l^0 | \hat{a}_+^2 | \psi_n^0 \rangle + \langle \psi_l^0 | \hat{a}_-^2 | \psi_n^0 \rangle|^2}{\hbar w_0 (n-l)}$$

$$= \frac{\hbar^2 \varepsilon^2 w_0^2}{16} \sum_{l \neq n} \frac{|\sqrt{(n+1)(n+2)} S_{l,n+2} + \sqrt{n(n-1)} S_{l,n-2}|^2}{(n-l)}$$

$$= \frac{\hbar^2 \varepsilon^2 w_0^2}{16} \left[-\frac{(n+1)(n+2)}{2} + \frac{n(n-1)}{2} \right] = -\frac{\varepsilon^2 \hbar w_0}{8} (n + \frac{1}{2}) = -\frac{\varepsilon^2}{8} E_n^0$$

So for ground state: $n=0$ $E_0^{(2)} = -\frac{\varepsilon^2 \hbar \omega_0}{16}$

Finally: $E_0 = E_0^{(0)} + E_0^{(1)} + E_0^{(2)} = \frac{1}{2} \hbar \omega_0 + \frac{1}{4} \varepsilon \omega_0 \hbar - \frac{\varepsilon^2 \hbar \omega_0}{16}$

(d) In (a) we have:

$$\begin{aligned}E_n &= \hbar \omega_0 (n + \frac{1}{2}) \sqrt{1+\varepsilon} \\&= \hbar \omega_0 (n + \frac{1}{2}) (1 + \frac{1}{2} \varepsilon - \frac{1}{8} \varepsilon^2 + \dots)\end{aligned}$$

$$\begin{aligned}So \quad E_0 &\approx \hbar \omega_0 \cdot \frac{1}{2} (1 + \frac{1}{2} \varepsilon - \frac{1}{8} \varepsilon^2) \\&= \frac{1}{2} \hbar \omega_0 + \frac{1}{4} \varepsilon \omega_0 \hbar - \frac{\varepsilon^2}{16} \hbar \omega_0\end{aligned}$$

So the Perturbation Theory's result
is equal to Taylor's expansion result!

2.2 Physics Of Atoms

2.3 Atomic Transitions, Light-Matter Interaction And Approximation

References

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Acknowledgement

My mail box becomes filled with Christmas wishes, the university library has placed the decorated Christmas tree. I finally recognized the 2022 fall semester has reached to its end.

Three months have passed quickly. And now I was very happy to write these sentences because I think I have achieved one of my goals at the beginning of this semester, that is, to have a good understanding in Quantum Mechanics.

Now, although I may still have some weaknesses, I think at least I have made much improvement compared to three months ago.

Here, I want to express my thanks to Prof. Hui for his effort during the whole semester, without whom I can not make the current progress. I have learnt a lot from Prof. Hui, besides the many unique understandings in Quantum Mechanics I have not heard before, the most impressive point I would keep in mind forever is **physical sense**.

It is impossible not to have heard this word before, but it is this semester that I finally knew how important physical sense is in physics studies and what it represents in Quantum Mechanics, thus I may be able to understand physics in a more intuitive way even in other physics courses in the future. Prof. Hui has shown me how to understand the result almost every times and he kept asking me what is the physics behind the massive mathematical derivations and calculations for different problems. This precious gain is what I have not expected before this semester's study, and although I may be still not too proficient in physical sense, at least the view of physical sense has been rooted in my brain thus notifying me to pay attention to it in the future study.

Many thanks to Prof. Hui!