INTRODUCTION

TO QUANTUM MECHANICS

PRINCIPLES

1ST LECTURE
FROM THE COURSE
QUANTUM PHYSICS OF LOW DIMENSIONAL STRUCTURES

QPLDS

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CONTENTS

FUNDAMENTAL QUANTUM QUANTITIES

1) A physical <u>state</u> (PS) of a quantum system,

2) A physical <u>quantity</u> (PQ) or an observable - to be eventually measured somehow.

POSTULATES OF QUANTUM MECHANICS

1) For the every PS there exists a vector of state, sometimes represented by the wave-function Ψ,
2) For every PQ there exists a linear operator $\hat{PQ}$ (this works in the Hilbert space (HS) – HS is a complete, unitary space equipped with the complex scalar product, which can be expressed by $\int \Psi^* \Psi dV$),
3) If a measurement of PQ gives a single result, then *f*(PQ), where *f* is a function of PQ, also gives a single results (sometimes complex PQ's are derived from direct measurements of some others PQ's and this approach is completely clear-cut),
4) Quantum aspect of classical quantities can be achieved by their replacement by appropriate operators followed by the replacement of the classical Poisson bracket by the commutation relation:

$$(A,B) = \sum_k \left(\frac{\partial A}{\partial x_k} \frac{\partial B}{\partial p_k} - \frac{\partial A}{\partial p_k} \frac{\partial B}{\partial x_k} \right) \rightarrow [A_i, B_j] = i\hbar \delta_{ij}$$

5) The averaged, and thus measurable, value of PQ can be calculated from the minimized value of the $\int \Psi^* \hat{PQ} \Psi dV$ expression,
6) and from 5. results the existence of the equation of state (ES)

$$\boxed{\hat{PQ}\Psi = C\Psi}$$

and possible (averaged) *C*=<*PQ*> values of the measured PQ.

THE PROOF OF THE POSTULATE No 6

1) $\int \Psi^* \hat{PQ} \Psi dV = \lambda = const.,\qquad \int \Psi^* \Psi dV = 1$

2) we look for minimum of $\int \Psi^* \hat{PQ} \Psi dV$, thus for the minimum-valued Ψ function,

3) $\int \Psi^* \hat{PQ} \Psi dV = \lambda = 1 \cdot \lambda = \lambda \int \Psi^* \Psi dV \;\Rightarrow \int \Psi^* \hat{PQ} \Psi dV - \lambda \int \Psi^* \Psi dV = 0$

4) If Ψ is minimized, then there exists $\Psi' = \Psi + \delta\Psi$, $\delta\Psi' = \delta\Psi$ and

$$\int \Psi'^* \hat{PQ} \Psi' dV - \lambda \int \Psi'^* \Psi' dV \neq 0, \qquad \int \Psi'^* \Psi' dV \neq 1 \text{, but}$$

$$\delta\left[\int \Psi'^* \hat{PQ} \Psi' dV - \lambda \int \Psi'^* \Psi' dV\right] = 0$$

5) $\int \delta\Psi'^* \hat{PQ} \Psi' dV + \int \Psi'^* \delta(\hat{PQ} \Psi') dV - \lambda \int \delta\Psi'^* \Psi' dV - \lambda \int \Psi'^* \delta\Psi' dV = 0$

- second integral: $\int \Psi'^* \delta(\hat{PQ} \Psi') dV = \int \Psi'^* \hat{PQ}\, \delta(\Psi') dV = \int (\hat{PQ} \Psi')^* \delta\Psi' dV$

because: a) the variation doesn't influence operator

b) the $\hat{PQ}$ is a hermitian operator ($\int u^* \hat{PQ}\, w dV = \int (\hat{PQ} u)^* w dV$)

6) $\int \delta\Psi'^* \hat{PQ} \Psi' dV + \int (\hat{PQ} \Psi')^* \delta\Psi' dV - \lambda \int \delta\Psi'^* \Psi' dV - \lambda \int \Psi'^* \delta\Psi' dV = 0$

7) next, 1st term is combined with the 3rd, and 2nd with the 4th:

$$\int \delta\Psi'^{*}(\hat{PQ}\,\Psi' - \lambda\Psi')dV + \int(\hat{PQ}^{+}\,\Psi'^{*} - \lambda\Psi'^{*})\delta\Psi'\,dV = 0$$

and $\begin{matrix}(\hat{PQ}\,\Psi' - \lambda\Psi') = 0 \\ (\hat{PQ}^{+}\,\Psi'^{*} - \lambda\Psi'^{*}) = 0\end{matrix}$, thus $\boxed{\hat{PQ}\,\Psi' = \lambda\Psi'}$, we are quite close to the final

8) the helpful extra derivation. Let's use $\Psi' = \Psi + \delta\Psi$, thus

$$\hat{PQ}(\Psi + \delta\Psi) = \lambda(\Psi + \delta\Psi)$$

$$\hat{PQ}(\Psi) + \hat{PQ}(\delta\Psi) = \lambda\Psi + \lambda(\delta\Psi)$$

$$\hat{PQ}(\Psi) - \lambda\Psi = \lambda(\delta\Psi) - \hat{PQ}(\delta\Psi)$$

9)Thus, <u>right hand side</u> of the above: $\lambda(\delta\Psi) - \hat{PQ}(\delta\Psi)$ should equals

$$\lambda(\delta\Psi) - \hat{PQ}(\delta\Psi) = \lambda(\delta\Psi) - \delta(\hat{PQ}\,\Psi) = \left| \begin{matrix} \delta(\lambda\Psi) = \underbrace{(\delta\lambda)}_{=0}\Psi + \lambda\delta\Psi = \\ = \lambda\delta\Psi \end{matrix} \right| =$$

$$= \delta(\lambda\Psi) - \delta(\hat{PQ}\,\Psi) = \delta(\lambda\Psi - \hat{PQ}\,\Psi) = -\delta(\hat{PQ}\,\Psi - \lambda\Psi)$$

However

$$\boxed{L = -\delta L \Leftrightarrow L = 0}$$

$$\hat{P}Q\Psi = \lambda\Psi$$

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

PURE PS AND MIXED PS

PURE

$| \ >= \lambda_1 |1> + \lambda_2 |2>$, all the elements in the formula are from the Hilbert space, in other words the vectors represent the PS (physical state vector); the components $|1>, |2>$ and the superposition $| \ >$.

Again; the mentioned state-vectors $| \ >$ exist in reality, are REALLY POSSIBLE IN PHYSICAL REALITY

$$\psi = \lambda_1\varphi_1 + \lambda_2\varphi_2$$

$$\psi^* = \lambda_1\varphi_1^* + \lambda_2\varphi_2^*$$

$$< \ | = \lambda_1 <1| + \lambda_2 <2|$$

$$\sqrt{\int \psi^*\psi \, dV} = 1$$

$$|< \ | \ >| = 1$$

however $\psi e^{-i\alpha}$ determined with the restricted accuracy due to the $e^{-i\alpha}$ phase factor,

MIXED

In the mixed state <u>not EVERYTHING</u> is REALLY possible!?

WE GET PROBLEM

I MEAN

WE HAVE TO WAIT…

before <u>EVERYTHING</u> the STATISTICAL OPERATOR of the PURE STATE has to be defined

A STATISTICAL OPERATOR

Question: what we measure in quantum mechanics?

Let assume: we have the observable O and the state-vector $| ps >$, thus $< O >_{ps} = < ps | O | ps >$ is the measured, averaged value of the O observable being represented by the vector of state $| ps >$.

Next,

$$| ps > = \sum_i | i >< i | ps > = | 1 >< 1 | ps > + | 2 >< 2 | ps > = | 1 > \lambda_1 + | 2 > \lambda_2 ,$$

because

$$| ps > = \lambda_1 | 1 > + \lambda_2 | 2 >$$

$$<1|ps>=\lambda_1\underbrace{<1|1>}_{=1}+\lambda_2\underbrace{<1|2>}_{=0}\Rightarrow <1|ps>=\lambda_1$$, etc,

$$<ps|=\sum_k <ps|k><k|=<ps|1><1|+<ps|2><2|=\lambda_1<1|+\lambda_2<2|$$

$$\begin{aligned}<O>_{ps}&=\sum_k\sum_i <ps|k><k|O|i><i|ps>=\\&=\sum_k\sum_i <k|O|i><ps|k><i|ps>=\\&=\sum_k\sum_i <k|O|i><i|ps><ps|k>\end{aligned}$$

Let’s check again the double-sum term:

$$\left[<ps|1><1|+<ps|2><2|\right]O\left[|1><1|ps>+|2><2|ps>\right]=$$

$$<ps|1><1|O|1><1|ps>+<ps|1><1|O|2><2|ps>+$$

$$+<ps|2><2|O|1><1|ps>+<ps|2><2|O|2><2|ps>=$$

$$=<1|O|1><1|ps><ps|1>+\overbrace{<1|O|2>}^{=0}<2|ps><ps|1>+$$

$$+\overbrace{<2|O|1>}^{=0}<1|ps><ps|2>+<2|O|2><2|ps><ps|2>=$$

$$=<1|O|ps><ps|1>+<2|O|ps><ps|2>=$$
$$=\sum_{k}<k|O|SO_{ps}|k>=Tr(O\,SO_{ps})=<O>_{ps},$$

where $SO_{ps}=|ps><ps|$
is the STATISTICAL OPERATOR OF THE PURE STATE BUILT FROM THE STATE VECTOR $|ps>$,

Remarks:
a) $SO_{ps}=|ps><ps|$ is used in calculation of the average value of the observable $<O>_{ps}$,
b) the $<O>_{ps}$ is calculated completely precisely, with no $e^{-i\alpha}$ phase factor like in the method using wave-function formalism $<O>_{ps}=<ps|O|ps>$.

COME BACK

TO

MIXED STATES…

MIXED

A mixed state is composed from pure states and this can be expressed using statistical operators language as follows

$$SO_{mx} = \sum_k p_k SO_{sp(k)}$$

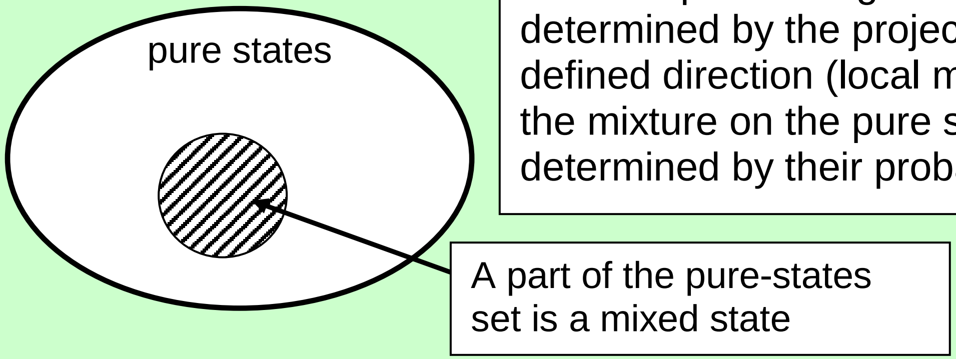
$$SO_{mx} = \sum_k p_k \,|\, ps_k >< ps_k \,|$$

$$< O >_{mx} = \sum_k p_k < O >_{sp(k)}$$

$$< O >_{mx} = \sum_k p_k Tr(O\, SO_{sp(k)}) = Tr(O \sum_k p_k SO_{sp(k)}) = Tr(O\, SO_{mx})$$

$$< O >_{mx} = Tr(O\, SO_{mx})$$

the mixed state: created after tunneling of the two spins through a barrier and determined by the projection onto the well-defined direction (local magnetic field), but the mixture on the pure states is determined by their probabilities



A PICTURE OF THE TIME EVOLUTION – the first probe
(THE EVOLUTION TO BETTER KNOWLEDGE DUE TO THE KNOWLEDGE EVOLUTION J)

The evolution operator

$$G(t,t_0)$$

$$|t> \overset{def}{=} G(t,t_0)|t_0> \quad \text{and} \quad G^+(t,t_0)|t>=|t_0>$$

↑These are very general formulas↑

The aim is to show how are dependent on time:

a) a vector of a physical state (PS),
b) a statistical operator (SO),
c) an observable (O).

SCHRÖDINGER

The existence of the equation of state (ES) was proved as the extension of the postulate 6.
In the SCHRÖDINGER picture the ES has the following form

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}|t>=H|t>$$

THE STARTING POINT IS <u>THE TIME EVOLUTION</u> OF THE STATE VECTOR $|t>$

- after substitution of $|t>=G(t,t_0)|t_0>$ into the ES:

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}G(t,t_0)=HG(t,t_0),\ \ G(t_0,t_0)=I$$

- from that results the solution for $G(t,t_0)$:

$$G(t,t_0)=e^{-iH(t-t_0)/\hbar}$$

$$G^{+}(t,t_0)=e^{iH(t-t_0)/\hbar}=G^{-1}(t,t_0)$$

$$G(t,t_0)G^{-1}(t,t_0)=I$$

- the SO operator time-behavior:

for the pure state:

$$SO_{sp}(t) = |t><t| = G(t,t_0)|t_0><t_0|G^+(t,t_0) = G(t,t_0)SO_{sp}(t_0)G^+(t,t_0)$$

$$\boxed{SO_{sp}(t) = G(t,t_0)SO_{sp}(t_0)G^+(t,t_0)}$$

for the mixed state:

$$SO_{mx}(t) = \sum_k p_k |t,k><t,k| = \sum_k p_k G(t,t_0)|t_0,k><t_0,k|G^+(t,t_0) =$$

$$= G(t,t_0)\sum_k p_k |t_0,k><t_0,k|G^+(t,t_0) = G(t,t_0)\sum_k p_k SO_{sp}(t_0)G^+(t,t_0)$$

$$\boxed{SO_{mx}(t) = G(t,t_0)SO_{mx}(t_0)G^+(t,t_0)}$$

Thus, after differentation of the above for $SO_{mx}(t)$

$$-\frac{\hbar}{i}\frac{\partial SO_{mx}(t)}{\partial t} = -\frac{\hbar}{i}\frac{\partial G}{\partial t}SO_{mx}(t_0)G^+ - \frac{\hbar}{i}GSO_{mx}(t_0)\frac{\partial G^+}{\partial t} = H\,G\,SO_{mx}(t_0)G^+ - G\,SO_{mx}(t_0)G^+H$$

then

$$\boxed{-\frac{\hbar}{i}\frac{\partial SO_{mx}(t)}{\partial t} = [H, SO_{mx}(t)]}, \text{ and } \boxed{\frac{\partial H}{\partial t} \equiv 0}$$

SCHRÖDINGER summarizes:

the *PS* evolves in time $$|t> = G(t,t_0)\,|t_0>$$

the *SO* evolves in time $$-\frac{\hbar}{i}\frac{\partial SO_{mx}(t)}{\partial t} = \left[H, SO_{mx}(t)\right]$$

and the *O* does not evolves in time $$\frac{\partial O}{\partial t} \equiv 0$$

A PICTURE OF THE TIME EVOLUTION – the second probe
THE STATISTICAL OPERATOR EVOLUTION – some derivations

1) $< O >_{mx} = Tr(O\, SO_{mx})$

2) $SO_{mx}(t) = G(t,t_0) SO_{mx}(t_0) G^{+}(t,t_0)$

3) (2)→(1):

$$< O >_{mx} = Tr[O\, SO_{mx}(t)] = Tr[O\, G(t,t_0) SO_{mx}(t_0) G^{+}(t,t_0)]$$

HEISENBERG

Something new; a transformation of the observable *O* into the Heisenberg picture O_H:

$$O_H \overset{def}{=} G^{+}(t,t_0)\, O\, G(t,t_0)$$

From this results, for any arbitrary observable *O*, that

$O = O_H(t_0)$, especially $H = H_H(t_0)$ as $G^{+}(t_0,t_0) = G(t_0,t_0) = 1$.

<u>and again, something new</u>; a transformation of the state vector $|t>$ into the Heisenberg picture $|t>_H$

$$|t>_H \overset{def}{=} G^+ |t>$$

There is a <u>subtle difference</u> between the Heisenberg-like behavior for the statistical operator (*SO)* and the state-vector $|t>$ "at the beginning", for t_0, namely

$$|t>_H = |t_0> \ \underline{\text{and}}\ O_H(t_0) = O$$

what reads: only at the beginning the Schrödinger state vector equals the Heisenberg state-vector, <u>and</u>, only at the beginning the Heisenberg observable equals the observable from the Schrödinger point of view.

HOWEVER, from the above results that, in the Heisenberg picture:
- a) a state vector doesn't evolve in time,
- b) a statistical operator doesn't evolve in time,
- c) an observable evolves in time.

Ad. a - $|t>_H=|t_0>$?!

$$|t>_H = G^+G\,|t_0>=|t_0>$$, here you are.

Ad. b - $SO_H(t)$?!

$$SO_H(t)=G^+SO_{mx}(t)G=G^+GSO_{mx}(t_0)G^+G=SO_{mx}(t_0)$$, that's it.

Ad. c - $O_H(t)$?!

well...

As we know $O_H \overset{def}{=} G^+(t,t_0)\,O\,G(t,t_0)=G^+O\,G$,

then, after differentation of the above and taking advantage from

$G=e^{-iH(t-t_0)/\hbar}$

we have

$$-\frac{\hbar}{i}\frac{\partial O_H(t)}{\partial t}=-\frac{\hbar}{i}\frac{\partial G^+}{\partial t}OG^+-\frac{\hbar}{i}G^+O\frac{\partial G}{\partial t}=G^+OGH-HG^+O\,G=O_H H-HO_H$$

thus

$$\boxed{-\frac{\hbar}{i}\frac{\partial O_H(t)}{\partial t}=\left[O_H(t),H\right]}$$

now HEISENBERG summarizes:

the PS_H doesn't evolve in time $$\frac{\partial |t>_H}{\partial t} \equiv 0$$

the SO_H doesn't evolve in time $$\frac{\partial |SO>_H}{\partial t} \equiv 0$$

and the O_H evolves in time $$-\frac{\hbar}{i}\frac{\partial O_H(t)}{\partial t} = [O_H(t), H]$$

A PICTURE OF THE TIME EVOLUTION – the third probe

TOMONAGA

THE STARTING POINT IS THE SPLIT OF THE HAMILTONIAN INTO THE 2 PIECES;

a) that of the free particles or free physical fields,
b) that of the interaction between the above.

$$\boxed{H = H^{(0)} + H^{(1)}}$$

The free evolution operator

$$G_0 = e^{-iH^{(0)}(t-t_0)/\hbar}$$

The evolution of the state vector

$$\boxed{|\,t>_T \overset{def}{=} G_0^+\,|\,t>}$$

while $|\,t_0>_T = |\,t_0>$.

Thus

$$\frac{\partial\,|\,t>_T}{\partial t} = -\frac{\hbar}{i}\,G_0^+ H^{(1)} G\,|\,t>_T\,,$$

or

$$\boxed{-\frac{\hbar}{i}\frac{\partial\,|\,t>_T}{\partial t} = H_1\,|\,t>_T},$$

where $H_1 = G_0^+ H^{(1)} G_0$

The modified evolution operator of Tomonaga G_T

$| t >_T = G_0^+ | t >= G_0^+ G | t_0 >= G_0^+ G | t_0 >_T = G_T | t_0 >_T$,

$$\boxed{G_T \overset{def}{=} G_0^+ G = e^{-iH^{(1)}(t-t_0)/\hbar}}$$

After substitution of $| t >_T = G_T | t_0 >_H$ into the Tomonaga evolution equation $-\frac{\hbar}{i}\frac{\partial | t >_T}{\partial t} = H_1 | t >_T$ we have

$$-\frac{\hbar}{i}\frac{\partial SO_T(t)}{\partial t} = -\frac{\hbar}{i}\frac{\partial G_0^+}{\partial t} SO\, G_0 - \frac{\hbar}{i} G_0^+ \frac{\partial SO}{\partial t} G_0 - \frac{\hbar}{i} G_0^+\, SO \frac{\partial G_0}{\partial t}$$

and finally,

$$\boxed{-\frac{\hbar}{i}\frac{\partial SO_T(t)}{\partial t} = \left[H_1(t), SO_T(t)\right]}$$

and

$$\boxed{-\frac{\hbar}{i}\frac{\partial O_T(t)}{\partial t} = \left[O_T(t_0), H^{(0)}\right]}$$

now TOMONAGA summarizes:

the PS_T evolves in time
$$-\frac{\hbar}{i}\frac{\partial |t>_T}{\partial t} = H_1 |t>_T$$

the SO_T evolves in time
$$-\frac{\hbar}{i}\frac{\partial SO_T(t)}{\partial t} = \left[H_1(t), SO_T(t)\right]$$

and the O_T evolves in time
$$-\frac{\hbar}{i}\frac{\partial O_T(t)}{\partial t} = \left[O_T(t_0), H^{(0)}\right]$$

EVERYBODY SUMMARIZE ABOUT THE EVOLUTION

Picture	**PS**	**SO**	**O**
Schrödinger	yes	yes	no
Heisenberg	no	no	yes
Tomonaga	yes	yes	yes

HOWEVER

$$< O >_{mx} = < O >_H = < O >_T$$

What is accessible in experimental reality is the same