1.3. Schrödinger-, Heisenberg- and interaction picture

a) The only quantum question

In classical mechanics one can ask about all properties of a particle (position, momentum, energy, angular momentum, ...)
In quantum mechanics one can ask about probabilities.
Essentially there is only one question:

Consider a physical system at time t_1 which is prepared such that an observable $\hat{A}$ has the value a, i.e. the physical system is given by the eigen vector $|a, t_1\rangle$ such that

$$\hat{A}(t_1)|a, t_1\rangle = a|a, t_1\rangle \quad \text{with the hermitian operator } \hat{A}$$

Then what is the probability P that one observes at a later time t_2 the value b for an observable $\hat{B}$?

Answer: If $|a, t_1\rangle$ is normalized, i.e. $\langle a, t_1|a, t_1\rangle = 1$, and for an also normalized eigen bra state of $\hat{B}$ with eigen value b, i.e.

$$\langle b, t_2|\hat{B}(t_2) = b\langle b, t_2| \quad , \quad \langle b, t_2|b, t_2\rangle = 1,$$

the probability P is given by

$$P = |\langle b, t_2|a, t_1\rangle|^2$$

The quantity $\langle b, t_2|a, t_1\rangle$ is called "probability amplitude".

b) generalizations

① for non-normalized states

$$P = \frac{|\langle b, t_2 | a, t_1 \rangle|^2}{\langle b, t_2 | b, t_2 \rangle \ \langle a, t_1 | a, t_1 \rangle}$$

② general pure initial state

system at time t_1 may be specified by $|\psi, t_1\rangle$

$\leadsto$ expand in eigen states of $\hat{A}(t_1)$

$$|\psi, t_1\rangle = \sum_i c_i(t_1)\, |a_i, t_1\rangle$$

with $\hat{A}(t_1)|a_i, t_1\rangle = a_i |a_i, t_1\rangle$

and (for simplicity) with all states normalized:

$$\langle a_i, t_1 | a_j, t_1 \rangle = \delta_{ij} \text{ for all } i, j$$

$$\langle \psi, t_1 | \psi, t_1 \rangle = 1 \quad \Rightarrow \sum_i |c_i|^2 = 1$$

$\Rightarrow$ probability to measure b at time t_2 for observable $\hat{B}(t_2)$:

$$P = |\langle b, t_2 | \psi, t_1 \rangle|^2$$

with normalized eigen state, $\langle b, t_2 | b, t_2 \rangle = 1$

$$\Rightarrow P = \langle b, t_2 | \Big(\sum_{ij} c_i c_j^* \, |a_i, t_1\rangle \langle a_j, t_1| \Big) | b, t_2 \rangle$$

example: (set initial time $t_1 = 0$) probability amplitude to find particle at time t at position x (for pure state)

$$\psi(x, t) = \langle x, t | \psi \rangle$$

③ mixed initial state

Suppose system is initially prepared such that one measures the value a_i with probability p_i for observable $\hat{A}$, $\sum_i p_i = 1$

$$\Rightarrow \mathcal{P} = \sum_i p_i \left| \langle b_r, t_2 | a_i, t_1 \rangle \right|^2$$

$$= \langle b_r, t_2 | \left(\sum_i p_i | a_i, t_1 \rangle \langle a_i, t_1 | \right) | b_r, t_2 \rangle$$

④ general mixed initial state

$$\hat{\varrho}(t_1) = \sum_{ij} d_{ij} | a_i, t_1 \rangle \langle a_j, t_1 |$$

with $\hat{\varrho}^+ = \hat{\varrho}$, i.e. $d_{ij}^* = d_{ji}$, and $\operatorname{tr} \hat{\varrho} = \sum_i d_{ii} = 1$

$$\mathcal{P} = \langle b_r, t_2 | \hat{\varrho}(t_1) | b_r, t_2 \rangle$$

one gets back case ② for $d_{ij} = c_i c_j^*$

and case ③ for $d_{ij} = p_i \delta_{ij}$

c) Heisenberg picture

In the following for convenience we start the clock at the time at which we prepare our system, i.e. $t_1 = 0$, and we ask for the probability $\mathcal{P}$ at time $t (= t_2)$

For a pure initial state $|\psi\rangle$ we have

$$\mathcal{P} = |\langle b, t|\psi\rangle|^2$$

By construction the arbitrary observable $\hat{B}(t)$ depends on t whereas $|\psi\rangle$ does not. This is the Heisenberg picture.

One might decompose $|\psi\rangle$ at $t=0$ in terms of the eigen states of $\hat{B}(t=0)$:

$$|\psi\rangle = \sum_i \langle b_i, t=0|\psi\rangle \, |b_i, t=0\rangle$$

Remark: If we do not know $\langle b_i, t=0|\psi\rangle$ directly, but instead e.g. the spatial decomposition $\langle \vec{r}, t=0|\psi\rangle$, then one can calculate

$$\langle b_i, t=0|\psi\rangle = \int d^3r \, \langle b_i, t=0|\vec{r}, t=0\rangle \underbrace{\langle \vec{r}, t=0|\psi\rangle}_{\psi(\vec{r}, t=0)}$$

$$\langle b, t|\psi\rangle = \sum_i \underbrace{\langle b, t|b_i, t=0\rangle}_{\substack{\text{dynamical} \\ \text{information}}} \underbrace{\langle b_i, t=0|\psi\rangle}_{\text{initialization}}$$

How to get from 0 to t?

Ask first how to get from t to $t+dt$:

We have seen that the momentum operator yields spatial translations: $e^{-i dx \hat{p}/\hbar}|x\rangle = |x+dx\rangle$

On the other hand, we know from mechanics that the momentum is related to translations in space like the Hamiltonian is related to translations in time (up to a subtle sign difference)

$$\Rightarrow e^{+i\, dt\, \hat{H}/\hbar}|b_i, t\rangle = |b_i, t+dt\rangle \quad \text{with Hamiltonian } \hat{H}$$

$$\Rightarrow |b_i, t\rangle + i\frac{1}{\hbar} dt\, \hat{H}|b_i, t\rangle = |b_i, t+dt\rangle$$

$$\Rightarrow -i\hbar\frac{d}{dt}|b_i, t\rangle = \hat{H}|b_i, t\rangle \qquad (*)$$

On the other hand, we can define an operator which takes $|b_i, t\rangle$ to $|b_i, t'\rangle$:

$|b_i, t'\rangle = \hat{U}(t', t)|b_i, t\rangle$, time-translation operator $\hat{U}$

(that $\hat{U}$ is independent of $\hat{B}$ is basically a consequence of $(*)$)

properties of $\hat{U}$:

① $\hat{U}(t, 0)$ satisfies $-i\hbar\frac{d}{dt}\hat{U}(t, 0) = \hat{H}\hat{U}(t, 0)$ (from $(*)$)

② $\hat{U}(t, t) = \mathbb{1}$

③ since $|b_i, t\rangle$ is normalized for every $t \Rightarrow \hat{U}^\dagger(t', t)\hat{U}(t', t) = \mathbb{1}$

$\Rightarrow \hat{U}$ is unitary matrix

④ $\hat{U}(t, t')\hat{U}(t', t'') = \hat{U}(t, t'') \underset{②}{\Rightarrow} U^{-1}(t, t') = U(t', t)$

Remark: The $\hat{U}$s form a group

In general $\hat{H}$ can depend on time. In this case on has the differential equation

$$-i\hbar \frac{d}{dt} \hat{U}(t,0) = \hat{H}(t)\, \hat{U}(t,0) \qquad (*)$$

If $\hat{H}$ does not depend on t (closed system) a solution of $(*)$ which satisfies the boundary condition $\hat{U}(0,0) = \mathbb{1}$ is given by

$$\hat{U}(t,0) = \exp(i\hat{H}t/\hbar)$$

(We will see later how to get $\hat{U}$ for time-dependent $\hat{H}$.)

General strategy how to determine the dynamical information $\langle b_f, t | b_i, t=0 \rangle$:

1. for given $\hat{H}(t)$ determine (in whatever way) $\hat{U}(t,0)$ from $(*)$
2. $\langle b_f, t | b_i, t=0 \rangle = \langle b_f, t=0 | \hat{U}^+(t,0) | b_i, t=0 \rangle$

On can also apply $\hat{U}$ to $\hat{B}(t)$ instead of to its eigen vectors

$$\hat{B}(t) = \hat{U}(t,0)\, \hat{B}(0)\, \hat{U}(0,t) = \hat{U}(t,0)\, \hat{B}(0)\, \hat{U}^+(t,0)$$

$\hat{B}(t)$ satisfies Heisenberg's equation of motion

$$\begin{aligned} i\hbar \frac{d}{dt} \hat{B}(t) &= \left[i\hbar \frac{d}{dt} \hat{U}(t,0)\right] \hat{B}(0)\, \hat{U}^+(t,0) + \hat{U}(t,0)\, \hat{B}(0)\, i\hbar \frac{d}{dt} \hat{U}^+(t,0) \\ &= -\hat{H}(t)\, \hat{U}(t,0)\, \hat{B}(0)\, \hat{U}^+(t,0) + \hat{U}(t,0)\, \hat{B}(0)\, U^+(t,0)\, \hat{H}(t) \\ &= [\hat{B}(t), \hat{H}(t)] \end{aligned}$$

$$\Rightarrow \boxed{\frac{d}{dt} \hat{B}(t) = \frac{i}{\hbar} [\hat{H}(t), \hat{B}(t)]}$$

d) Schrödinger picture

So far we worked in the Heisenberg picture where the observables (and their eigen vectors) depend on time while the physical state vector $|\psi\rangle$ does not.
With the help of $\mathcal{U}(t,0)$ one can shift the time dependence from the operators to the state vector $|\psi\rangle$:
For arbitrary vectors $|f,t\rangle$ and operators $\hat{O}(t)$ (in the Heisenberg picture) we apply the unitary operation

$$|f,t\rangle \longrightarrow |f,t\rangle_S = \hat{\mathcal{U}}(0,t)\,|f,t\rangle$$

$$\hat{O}(t) \longrightarrow \hat{O}_S(t) = \hat{\mathcal{U}}(0,t)\,\hat{O}(t)\,\hat{\mathcal{U}}(t,0)$$

For observables $\hat{B}(t)$ like position, momentum, ... one finds

$$\hat{B}_S = \hat{\mathcal{U}}(0,t)\,\hat{B}(t)\,\hat{\mathcal{U}}(t,0) =$$

$$= \hat{\mathcal{U}}(0,t)\,\hat{\mathcal{U}}(t,0)\,\hat{B}(0)\,\hat{\mathcal{U}}(0,t)\,\hat{\mathcal{U}}(t,0)$$

$$= \underbrace{\hat{\mathcal{U}}(0,0)}_{=\mathbb{1}}\,\hat{B}(0)\,\hat{\mathcal{U}}(0,0) = \hat{B}(0)$$

$\Rightarrow \hat{B}_S$ is time independent

The same is true for the eigen vectors $|b_i\rangle_S$ of $\hat{B}_S$ (recall that the b_i do not change under unitary transformations)

For $|\psi,t\rangle_S$ one gets:

$$\boxed{i\hbar \frac{d}{dt}|\psi,t\rangle_S} = i\hbar \frac{d}{dt}\,\hat{\mathcal{U}}(0,t)\,\underset{\substack{\uparrow \\ \text{time indep.}}}{|\psi\rangle} = \hat{\mathcal{U}}(0,t)\,\hat{H}(t)\,|\psi\rangle$$

$$= \underbrace{\hat{\mathcal{U}}(0,t)\,\hat{H}(t)\,\hat{\mathcal{U}}(t,0)}_{=H_S}\,\underbrace{\hat{\mathcal{U}}(0,t)\,|\psi\rangle}_{|\psi,t\rangle_S} = \boxed{\hat{H}_S\,|\psi,t\rangle_S}$$ Schrödinger equation

Remarks:

- Recall that scalar products do not change under unitary transformations

$$\Rightarrow \langle \varphi | O | \varphi' \rangle = {}_S\langle \varphi | O_S | \varphi' \rangle_S$$

Heisenberg picture   Schrödinger picture

- The same is true for the commutator of position and momentum

$$[x_S, p_S] = i\hbar = [x(t), p(t)]$$

Note that $[x(t), p(t')] \neq i\hbar$ in general

not t!

c) interaction (Dirac) picture

Typically the operator valued differential equation for the time-translation operator

$$-i\hbar \frac{d}{dt} \hat{\mathcal{U}}(t,0) = \hat{H}(t)\, \hat{\mathcal{U}}(t,0)$$

is hard to solve.

Consider the following case:

$$\hat{H}(t) = \hat{H}_0 + \lambda \hat{H}_{int}(t)$$

where $\hat{H}_0$ is independent of time with known eigen states and $\lambda H_{int}(t)$ is small (i.e. all matrix elements are small, formally: λ small)

$\rightsquigarrow$ try to find perturbative solution of problem, i.e. approximate solution in powers of λ

define $\hat{U}_D(t) = e^{-i\hat{H}_0 t/\hbar}\,\hat{U}(t,0)$

$\Rightarrow \quad \hat{U}(t,0) = e^{i\hat{H}_0 t/\hbar}\,\hat{U}_D(t)$

$\Rightarrow$ have to determine $\hat{U}_D$; it satisfies

$$-i\hbar\frac{d}{dt}\hat{U}_D(t) = -\hat{H}_0\,\hat{U}_D(t) - i\hbar\, e^{-i\hat{H}_0 t/\hbar}\frac{d}{dt}\hat{U}(t,0)$$

$$= -\hat{H}_0\,\hat{U}_D(t) + e^{-i\hat{H}_0 t/\hbar}\,\hat{H}(t)\,e^{i\hat{H}_0 t/\hbar}\,\hat{U}_D(t)$$

$$= -\hat{H}_0\,\hat{U}_D(t) + e^{-i\hat{H}_0 t/\hbar}\big(\hat{H}_0 + \lambda\hat{H}_{int}(t)\big)e^{i\hat{H}_0 t/\hbar}\,\hat{U}_D(t)$$

$$= \lambda\,\underbrace{e^{-i\hat{H}_0 t/\hbar}\,\hat{H}_{int}(t)\,e^{i\hat{H}_0 t/\hbar}}_{=:\,\hat{H}_D(t)}\,\hat{U}_D(t)$$

$$\Rightarrow -i\hbar\frac{d}{dt}\hat{U}_D(t) = \underset{\substack{\uparrow \\ \text{small!}}}{\lambda}\,\hat{H}_D(t)\,\hat{U}_D(t) \qquad (*)$$

The unitary operator $e^{-i\hat{H}_0 t/\hbar}$ transforms from the Heisenberg to the interaction picture; e.g. for an eigenstate of $\hat{B}(t)$:

$$|b,t\rangle = \hat{U}(t,0)\,|b,t=0\rangle = e^{i\hat{H}_0 t/\hbar}\,\hat{U}_D(t)\,|b,t=0\rangle$$

$$\Rightarrow \underset{\substack{\uparrow \\ \text{interaction picture}}}{|b,t\rangle_D} := e^{-i\hat{H}_0 t/\hbar}\,|b,t\rangle = \hat{U}_D(t)\,|b,t=0\rangle$$

How to solve $(*)$?

① interested in accuracy of order λ, i.e. neglect λ^2 terms

claim: $\hat{U}_D(t) \approx \exp\left(+i\lambda\int_0^t dt'\,\hat{H}_D(t')/\hbar\right) \approx \mathbb{1} + i\lambda\int_0^t dt'\,\hat{H}_D(t')/\hbar$

proof: calculate left and right hand side of (*):

l.h.s.

$$-i\hbar \frac{d}{dt} \hat{U}_D(t) = -i\hbar \frac{d}{dt}\left(\mathbb{1} + i\lambda \int_0^t dt' \hat{H}_D(t')/\hbar\right) + O(\lambda^2)$$

$$= \lambda \hat{H}_D(t) + O(\lambda^2)$$

r.h.s.

$$\lambda \hat{H}_D(t)\, \hat{U}_D(t) = \lambda \hat{H}_D(t) + O(\lambda^2) \qquad \checkmark$$

② interested in accuracy of order λ^2

$$\rightsquigarrow \hat{U}_D(t) \approx \mathbb{1} + i\lambda \int_0^t dt' \hat{H}_D(t')/\hbar - \lambda^2 \int_0^t dt' \int_0^{t'} dt'' \hat{H}_D(t') \hat{H}_D(t'')/\hbar^2$$

$$-i\hbar \frac{d}{dt} \hat{U}_D(t) \approx \lambda \hat{H}_D(t) + i\frac{1}{\hbar}\lambda^2 \int_0^t dt'' \hat{H}_D(t) \hat{H}_D(t'')$$

$$= \lambda \hat{H}_D(t) \left(\mathbb{1} + i\lambda \int_0^t dt' \hat{H}_D(t')/\hbar\right)$$

$$\approx \lambda \hat{H}_D(t)\, \hat{U}_D(t)$$

③ λ^3 accuracy

$$\hat{U}_D \approx \mathbb{1} + \frac{i\lambda}{\hbar} \int_0^t dt' \hat{H}_D(t') + \left(\frac{i\lambda}{\hbar}\right)^2 \int_0^t dt' \int_0^{t'} dt'' \hat{H}_D(t') \hat{H}_D(t'')$$

$$+ \left(\frac{i\lambda}{\hbar}\right)^3 \int_0^t dt' \int_0^{t'} dt'' \int_0^{t''} dt''' \hat{H}_D(t') \hat{H}_D(t'') \hat{H}_D(t''')$$

$\vdots$

note: the $\hat{H}_D$s are ordered such that the larger time argument is to the left

$\rightsquigarrow$ introduce formal time-ordering operator T by

$$T[A(t)\,B(t')] = \begin{cases} A(t)\,B(t') & \text{for } t > t' \\ B(t')\,A(t) & \text{for } t < t' \end{cases} = \Theta(t-t')A(t)B(t') + \Theta(t'-t)B(t')A(t)$$

$$\Rightarrow \frac{1}{2}\int_0^t dt' \int_0^{t \leftarrow \text{not } t'!} dt''\, T\left[\hat{H}_D(t')\hat{H}_D(t'')\right]$$

$$= \frac{1}{2}\int_0^t dt' \int_0^t dt'' \Big[\Theta(t'-t'')\hat{H}_D(t')\hat{H}_D(t'') + \Theta(t''-t')\hat{H}_D(t'')\hat{H}_D(t')\Big]$$

$$= \frac{1}{2}\int_0^t dt' \int_0^{t'} dt''\, \hat{H}_D(t')\hat{H}_D(t'') + \frac{1}{2}\int_0^t dt'' \int_0^{t''} dt'\, H_D(t'')H_D(t')$$

$$= \int_0^t dt' \int_0^{t'} dt''\, \hat{H}_D(t')\hat{H}_D(t'')$$

with the unit-step function $\Theta(z) = \begin{cases} 0 & \text{for } z<0 \\ 1 & \text{for } z>0 \end{cases}$

same way: $\frac{1}{3!}\int_0^t dt' \int_0^t dt'' \int_0^t dt'''\, T\left[\hat{H}_D(t')\hat{H}_D(t'')\hat{H}_D(t''')\right]$

$$= \int_0^t dt' \int_0^{t'} dt'' \int_0^{t''} dt'''\, H_D(t')H_D(t'')H_D(t''')$$

$\Rightarrow$ formal solution for $\hat{U}_D(t)$:

$$\hat{U}_D(t) = T\exp\left(\frac{-i}{\hbar}\int_0^t dt'\, \hat{H}_D(t')\right)$$

in practice: evaluate expression by expanding to desired order in λ