QUANTUM DYNAMICS

The quantum theories of an isolated system have been explicity determined.. In fact, a further task must be accomplished: it must be established how "the system changes in time", in other word the law of time evolution.

In a quantum theory time evolution must be described by making use of the quantum basic concepts, observables and quantum states.

Let us begin by considering a quantum state $\rho \in \mathcal{S}(\mathcal{H})$. The density operator ρ represents an expectation value identified with a selection procedure that selects single specimens of the physical system for which the expectation value of every observable A is $Tr(\rho A)$. Now, let the physical conditions be such that the specimen selected at time 0 continues to exist for the future time, so that the measurement of A can be performed at time $t > 0$. Since $Tr(\rho A)$ is the expectation value of the measurements performed at $t=0$, it cannot be stated apriori that the expectation value of the measurements at t, $Ev_t(A)$, coincides with $Ev(A) = Tr(\rho A)$

therefore another density operator ρ_t such that
$$Ev_t(A) = Tr(\rho_t A).$$

So, a bijective mapping $S_{(t_0,t_1)} : \mathcal{S}(\mathcal{H}) \to \mathcal{S}(\mathcal{H})$ must exists such that if ρ is the quantum state representing the expectation value of the measurements performed at time t_0, then $S_{(t_0,t_1)}[\rho]$ represents the expectation value of the measurements performed waiting a time $t_1 - t_0$.

However, the delay $t_1 - t_0$ can be equivalently thought as a part of the measurement procedure: once the specimen is selected at time t_0 in the quantum state ρ, given the measurement procedure of $\mathcal{A}$, we introduce a new observable $\mathcal{A}_{t_1}$ that consists in performing the measurement procedure of $\mathcal{A}$, but with a delay $t_1 - t_0$ which is a part of the procedure of $\mathcal{A}_{t_1}$. So, if A_{t_1} is the self-adjoint operator representing $\mathcal{A}_{t_1}$,
$$Ev_{t_1}(A) = Tr(S_{(t_0,t_1)}[\rho] A) = Tr(\rho A_{t_1}).$$

Therefore, another mapping $R_{(t_0,t_1)} : \mathcal{R}(\mathcal{H}) \to \mathcal{R}(\mathcal{H})$ must exists such that
$$Tr(S_{(t_0,t_1)}[\rho] A) = Tr(\rho R_{(t_0,t_1)}[A]).$$

Conceptual consistency entails that also $\mathcal{R}_{(t_0,t_1)}$ must be bijective; this property enables us to define
$$S^{(1)} = S_{(t_0,t_1)}, \quad S^{(2)} = R^{-1}_{(t_0,t_1)}.$$
Now, given any $A \in \mathcal{R}(\mathcal{H})$, $A = R^{-1}_{(t_0,t_1)}[B]$; then
$$Tr(\rho B) = Tr(\rho R_{(t_0,t_1)}[A]) = Tr(S^{(1)}[\rho] A)$$
$$= Tr(S^{(1)}[\rho] S^{(2)}[A]).$$
Therefore, the pair $(S^{(1)}, S^{(2)})$ defined above is a quantum symmetry transformation. By making use of Wigner theorem, we imply that a unitary or anti-unitary operator $U_{(t_0,t_1)}$ must exist such that
$$S^{(1)}[\rho] = U_{(t_0,t_1)} \rho U^{-1}_{(t_0,t_1)}, \quad S^{(2)}[B] = U_{(t_0,t_1)} B U^{-1}_{(t_0,t_1)},$$
i.e.
$$S_{(t_0,t_1)}[\rho] = U_{(t_0,t_1)} \rho U^{-1}_{(t_0,t_1)}, \quad R_{(t_0,t_1)}[A] = U^{-1}_{(t_0,t_1)} A U_{(t_0,t_1)}.$$

So, in quantum theory, time evolution is ruled over a mapping
$$U : \mathbb{R} \to \mathcal{U}(\mathcal{H}), \quad t \to U_t \equiv U_{(0,t)} \quad \text{such that}$$
$$\rho_t \equiv S_{(0,t)}[\rho] = U_t \rho U_t^{-1}, \quad A_t \equiv R_{(0,t)}[A] = U_t^{-1} A U_t.$$

In general U_t is unitary or antiunitary. Let us consider the case of a quantum theory when all U_t are unitary. We can fix $U_0 = \mathbb{1}$. The operator $B_t U_t^{-1}$, where $B_t = \frac{dU_t}{dt}$, is skew-hermitean:

$$U_{t+\Delta t} = U_t + B_t \Delta t + o(\Delta t),$$

$$U^{-1}_{t+\Delta t} = U^*_{t+\Delta t} = U^*_t + B^*_t \Delta t + o^*(\Delta t), \text{ so}$$

$$\mathbb{1} = U^{-1}_{t+\Delta t} U_{t+\Delta t} = \mathbb{1} + (U_t B^*_t + B_t U_t^{-1})\Delta t + o(\Delta t);$$

therefore $(B_t U_t^{-1})^* = U_t B^*_t = -B_t U_t^{-1}$. The operator $H_t = i B_t U_t^{-1}$ is hermitean $H^*_t = H_t$.

To describe evolution of quantum state the correspondence $t \to \rho_t$ is to be found.

Now $\rho_t = U_t \rho U_t^{-1} = U_t \sum_j \mu_j |\psi^{(j)}\rangle\langle\psi^{(j)}| U_t^{-1}$

$$= \sum_j \mu_j |U_t\psi^{(j)}\rangle\langle U_t\psi^{(j)}| .$$

The $\psi^{(j)}_t = U_t \psi^{(j)}$ are determined by the equation $i\frac{d\psi^{(j)}_t}{dt} = H_t \psi_t^{(t)}$, indeed

$$i\frac{d\psi_t}{dt} = i\frac{d}{dt}(U_t\psi) = iB_t\psi = i B_t U_t^{-1} U_t\psi$$

$$= i(-iH_t)\psi_t = H_t\psi .$$

Exercise. Prove that $\frac{dA_t}{dt} = i[\hat{H}_t, A_t]$, where $\hat{H}_t = U_t^{-1}\hat{A}_t U_t$.

$i\frac{d\psi_t}{dt} = H_t\psi_t$ is Schroedinger equation.

$\frac{dA_t}{dt} = i[\hat{H}_t, A_t]$ is Heisenberg equation.

1. HOMOGENEOUS TIME

According to quantum time evolution, the following relations hold if $t_0 \leq t_1 \leq t_2$

$$S_{(t_0,t_2)} = S_{(t_1,t_2)} S_{(t_0,t_1)} \;, \quad R_{(t_0,t_2)} = R_{(t_1,t_2)} R_{(t_0,t_1)} ,$$

which imply $S_{(t_0,t_2)}[\rho] = U_{(t_0,t_2)} \rho U^{-1}_{(t_0,t_2)} = (U_{(t_1,t_2)} U_{(t_0,t_1)}) \rho (U_{(t_1,t_2)} U_{(t_0,t_1)})^{-1}$.

According to Wigner theorem,

$$U_{(t_1,t_2)} U_{(t_0,t_1)} = \omega_{(t_0,t_1,t_2)} U_{(t_0,t_2)} \;, \quad |\omega_{(t_0,t_1,t_2)}| = 1 \qquad (1)$$

Time is homogeneous if $S_{(t_0,t_0+\Delta t)} = S_{(t_1,t_1+\Delta t)}$, that is to say if it is independent of the time chosen as origin of time. Accordingly, $U_{(t_0,t_0+t)} = \omega(t_0) U_{(0,t)}$.

Therefore equation (1) implies

$$U_{t_1} U_{t_2} = e^{i\alpha(t_1,t_2)} U_{t_1+t_2} . \qquad (2)$$

A first consequence of time homogeneïty is that U_t is unitary: put $t_1 = t_2 = \frac{t}{2}$ in (2).
Another consequence is that, by (2), a $\phi(t) \in \mathbb{C}$, with $|\phi(t)| = 1$, exists such that $V_t = \phi(t) U_t$ satisfies $S_t[\rho] = V_t \rho V_t^{-1}$, $V_t = e^{-iHt}$, where H is a self-adjoint operator, called Hamiltonian operator. The Schrodinger and Heisenberg equations takes a simpler form:

$$i \frac{d\psi_t}{dt} = H \psi_t \;, \quad \frac{dA_t}{dt} = i[H, A_t] .$$

Time is homogeneous for an isolated system, but it can be homogeneous also if other transformations are not symmetries.

2. QUANTUM DYNAMICS OF AN ISOLATED SYSTEM

From a group theoretical point of view, time evolution from time t to time $t+a_0$ is identifiable with the transformation of spatial vectors at time t, identified by $\begin{bmatrix} t \\ x \\ y \\ z \\ 1 \end{bmatrix}$, into $\begin{bmatrix} t+a_0 \\ x \\ y \\ z \\ 1 \end{bmatrix}$.

Therefore, this transformation can be realized through the matrix $\begin{bmatrix} 1 & 0 & 0 & 0 & a_0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \equiv \hat{h}_0(a_0)$, indeed

$$\hat{h}_0(a_0) \begin{bmatrix} t \\ x \\ y \\ z \\ 1 \end{bmatrix} = \begin{bmatrix} t+a_0 \\ x \\ y \\ z \\ 1 \end{bmatrix}.$$

Hence, the transformation is a time translation.

To describe also time translations, the transformation group $\hat{\mathcal{G}}$ must be extended to the group $\hat{\mathcal{G}}_0$ generated by $\hat{\mathcal{G}}$ and the sub-group $\hat{H}_0 = \{\hat{h}_0(s) \mid s \in \mathbb{R}\}$ of time translations: $\hat{\mathcal{G}}_0 = \mathcal{G}(\hat{H}_0, \hat{\mathcal{G}})$.

Any element $\hat{g} \in \hat{\mathcal{G}}_0$ can be factorized as

$$\hat{g} = \hat{h}_0(x_0)\hat{h}_1(x_1)\hat{h}_2(x_2)\cdots\hat{h}_9(x_9).$$

Since for an isolated time is always homogeneous, the trasformation g can be realized on observables as $S_g[A] = U_g A U_g^{-1}$, where

$U_g = e^{iP_0x_0} e^{-iP_xx_1} \cdots e^{iG_zx_9}$. P_0 is the self-adjoint generator of $U_t = e^{iHt}$, i.e. $P_0 = H$.

For an isolated system we can find the commutation relation of P_0 with the other generators by following the method used to find relations (12)

Let us begin with $[J_j, P_0]$. The product $\hat{h}_0(s)\hat{h}_6(s)\hat{h}_0(-s)\hat{h}_6(-s)$ can be easily computed since $\hat{h}_0(x)\hat{h}_6(y)=\hat{h}_6(y)\hat{h}_0(s)$, so that $\hat{h}_0(s)\hat{h}_6(s)\hat{h}_0(-s)\hat{h}_6(-s)=\mathbb{1}$, therefore $[P_0, A_6]=i\alpha_z$.

Analogously we find

$$[J_x, P_0]=i\alpha_x, \; [J_y, P_0]=i\alpha_y, \text{ besides } [J_z, P_0]=i\alpha_z.$$

Now, $[J_x, P_0]=-i\left[[J_y,J_z], P_0\right]=i\left[[J_z,P_0],J_y\right]+i\left[[P_0,J_y],J_z\right]=\mathbb{O}$.

Since $\hat{h}_0(x)\hat{h}_j(y)=\hat{h}_j(y)\hat{h}_0(x)$, for $j=x,y,z$, we have $[P_j, P_0]=i\beta_j$.

Now $[P_x, P_0]=-i[[J_y,P_z],P_0]=i\left[[P_z,P_0],J_y\right]+i\left[[P_0,J_y],P_z\right]=\mathbb{O}$

Hence $[P_j, P_0]=\mathbb{O}$, $[J_j,P_0]=\mathbb{O}$ hold.

For the product $\hat{h}_0(s)\hat{h}_z(s)\hat{h}_0(-s)\hat{h}_z(-s)$ we find

$$\begin{bmatrix} 1 & & & & s \\ & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix}\begin{bmatrix} 1 & & & & \\ s & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix}\begin{bmatrix} 1 & & & & -s \\ & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix}\begin{bmatrix} 1 & & & & \\ -s & 1 & & & \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix}=\begin{bmatrix} 1 & & & & \\ & 1 & & & -s^2 \\ & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix}=\mathbb{1}+(-1)\hat{a}_1 s^2.$$

Therefore, according to prop. 3.3 in TQ.5,

$$[G_x, P_0]=-i(\alpha_1+A_1)=i(\alpha_x+P_x);$$

analogously we find $[G_y,P_0]=i(\alpha_y+P_y)$, $[G_z,P_0]=i(\alpha_z+P_z)$

Now, $[G_x, P_0] = -i[[J_y, G_z], P_0]$

$$= i[[G_z, P_0], J_y] + i[[P_0, J_y], G_z]$$

$$= i[i(\alpha_z + P_z), J_y] = -[P_z, J_y]$$

$$= i P_x ,$$

i.e. $\alpha_x = 0$, so that $[G_x, P_0] = i P_x$.

Analogously we find

$$[G_y, P_0] = i P_y , \quad [G_z, P_0] = i P_z .$$

The comutation relation derived are

a) $[P_j, P_0] = [J_j, P_0] = 0$, b) $[G_j, P_0] = i P_j$. (3)

2.1 COMPLETENESS OF MULTIPLICATION OPERATOR

In order to explicitly identify P_0 in the quantum theory of an isolated system, we shall make use of the "completeness" of the multiplication operators in $L_2(\mathbb{R}^3)$.

In the Hilbert space $L_2(\mathbb{R}^3)$ the following statement holds:

Let A be a self-adjoint operator.
If $[A, F_j] = 0 \quad \forall j$, then $A = f(\vec{F})$, i.e. A is an operator function of $\vec{F}$, so that

$$(A\psi)(\vec{x}) = f(\vec{x})\, \psi(\vec{x}) .$$

We shall sketch a proof for $L_2(\mathbb{R})$:

Let $D \subseteq D_A \cap D_F$ be a domain such that $\bar{D} = \mathcal{H}$, and let $\psi_0 \in D_A \cap D_F$ be a fixed vector such that $\varphi = \frac{\psi}{\psi_0} \in D_A \cap D_F$, $\forall \psi \in D$.

Define $\varphi_0 = A\psi_0$; φ_0 is fixed, independent of ψ.

The operator B^ψ, $(B^\psi \phi)(x) = \varphi(x)\phi(x)$ is a function of F: $B^\psi = \varphi(F)$; therefore

$$[B^\psi, A] = [B^\psi, F] = 0.$$

Now, $A\psi = A\left(\frac{\psi}{\psi_0}\psi_0\right) = A(B^\psi \psi_0) = B^\psi A \psi_0$

$$= B^\psi \varphi_0;$$

hence $(A\psi)(x) = (B^\psi \varphi_0)(x) = \varphi(x)\varphi_0(x)$

$$= \frac{\varphi_0(x)}{\psi_0(x)}\psi(x) = f(x)\psi(x)$$

where $f(x) = \frac{\varphi_0(x)}{\psi_0(x)}$; thus $A = f(F)$.

The proof can be extended to $L_2(\mathbb{R}^3)$:
[if $[A, F_j] = 0$, $\forall j$, then $A = f(\vec{F})$.] (4)

This property of $\vec{F}$ is called "completeness".

2.2. EXPLICIT IDENTIFICATION OF $H=P_0$

The commutation relations (3) are implied by the structural properties of $\mathcal{G}_0$ in the quantum theory of an isolated system.
By making use of them, the hamiltonian operator $H=P_0$ can be explicitly determined, at least in the simplest theory of an isolated system.

If the inducing representation $L: SO(3) \to \mathcal{U}(\mathcal{H}_0)$ is the trivial one, i.e. $\mathcal{H}_0 = \mathbb{C}$ and $L_R = 1 \; \forall R$, the Hilbert space of the quantum theory of an isolated system is
$\mathcal{H} = L_2(\mathbb{R}^3)$; moreover
$$P_j = -i\frac{\partial}{\partial x_j}, \quad J_j = -i\left(x_k\frac{\partial}{\partial x_l} - x_l\frac{\partial}{\partial x_k}\right), \; j,k,l \text{ in cyclic order}, \; G_j = \mu F_j.$$

According to (3.b), $[G_j, P_0] = iP_j$;
now, the operator $H_0 = \frac{P_x^2+P_y^2+P_z^2}{2\mu} \equiv \frac{P^2}{2\mu}$ satisfies
$$[G_j, H_0] = \mu\left[F_j, \frac{P^2}{2\mu}\right] = \mu i\frac{\partial}{\partial P_j}\left(\frac{P^2}{2\mu}\right) = iP_j = [G_j, P_0],$$
by Lemma 3.1 in TQ.4. Hence
$$[F_j, P_0 - H_0] = 0, \quad \forall j.$$
Completeness of $\vec{F}$ implies that
$$P_0 - H_0 = \phi(\vec{F}).$$

However, also $[P_j, P_0] = 0$ holds by (3.a);

therefore $\left[P_j, \phi(\vec{F})\right] = \left[P_j, P_0\right] - \left[P_j, \frac{P^2}{2\mu}\right] = 0$.

So, $\left(\left[P_j, \phi(\vec{F})\right]\psi\right)(\vec{x}) = 0 =$

$$= \left(P_j\, \phi(\vec{F})\psi\right)(\vec{x}) - \left(\phi(\vec{F})\, P_j\psi\right)(\vec{x})$$

$$= -i\frac{\partial}{\partial x_j}\left[\phi(\vec{x})\, \psi(\vec{x})\right] - \left(i\phi(x)\right)\frac{\partial \psi}{\partial x_j}(\vec{x})$$

$$= -i\,\frac{\partial \phi}{\partial x_j}(\vec{x})\psi(\vec{x}) - i\,\phi(\vec{x})\frac{\partial \psi}{\partial x_j}(\vec{x}) + i\,\phi(\vec{x})\frac{\partial \psi}{\partial x_j}(\vec{x})$$

$$= -i\,\frac{\partial \phi}{\partial x_j}(\vec{x})\; \psi(\vec{x}) = 0 \quad , \quad \forall j \; .$$

Then $\phi(\vec{x}) = \text{constant}$, i.e., $\phi(\vec{F}) = E_0$.

Thus

$$\boxed{P_0 = \frac{P^2}{2\mu} + E_0}$$