Chapter 29 Time evolution of system

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Schrödinger picture
Heisenberg picture
Dirac picture

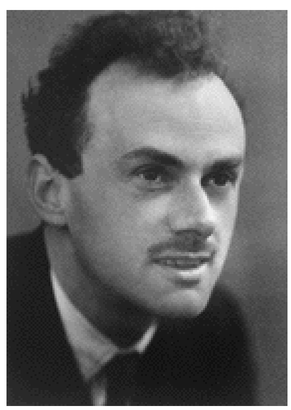
Erwin Rudolf Josef Alexander Schrödinger (12 August 1887– 4 January 1961) was an Austrian theoretical physicist who was one of the fathers of quantum mechanics, and is famed for a number of important contributions to physics, especially the Schrödinger equation, for which he received the Nobel Prize in Physics in 1933. In 1935, after extensive correspondence with personal friend Albert Einstein, he proposed the Schrödinger's cat thought experiment.

http://en.wikipedia.org/wiki/Erwin_Schr%C3%B6dinger

Werner Heisenberg (5 December 1901– 1 February 1976) was a German theoretical physicist who made foundational contributions to quantum mechanics and is best known for asserting the uncertainty principle of quantum theory. In addition, he made important contributions to nuclear physics, quantum field theory, and particle physics. Heisenberg, along with Max Born and Pascual Jordan, set forth the matrix formulation of quantum mechanics in 1925. Heisenberg was awarded the 1932 Nobel Prize in Physics for the creation of quantum mechanics, and its application especially to the discovery of the allotropic forms of hydrogen.

http://en.wikipedia.org/wiki/Werner_Heisenberg

Paul Adrien Maurice Dirac (8 August 1902 – 20 October 1984) was a British theoretical physicist. Dirac made fundamental contributions to the early development of both quantum mechanics and quantum electrodynamics. He held the Lucasian Chair of Mathematics at the University of Cambridge and spent the last fourteen years of his life at Florida State University. Among other discoveries, he formulated the Dirac equation, which describes the behavior of fermions. This led to a prediction of the existence of antimatter. Dirac shared the Nobel Prize in physics for 1933 with Erwin Schrödinger, "for the discovery of new productive forms of atomic theory."



http://en.wikipedia.org/wiki/Paul_Dirac

29.1 Time evolution operator

We define the Unitary operator as

$$\left|\psi(t)\right\rangle = \hat{U}(t,t_0)\left|\psi(t_0)\right\rangle$$

$$\langle\psi(t)| = \langle\psi(t_0)|\hat{U}^+(t,t_0)$$

Normalization

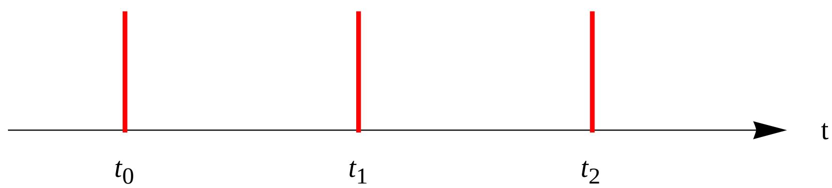
$$\langle\psi(t)|\psi(t)\rangle = \langle\psi(t_0)|\psi(t_0)\rangle = 1$$

Then

$$\langle\psi(t_0)|\hat{U}^+(t,t_0)\hat{U}(t,t_0)|\psi(t_0)\rangle = \langle\psi(t_0)|\psi(t_0)\rangle$$

or

$$\hat{U}^+(t,t_0)\hat{U}(t,t_0) = \hat{1} \text{ (Unitary operator)}$$



We note that

$$|\psi(t_2)\rangle = \hat{U}(t_2,t_1)|\psi(t_1)\rangle = \hat{U}(t_2,t_1)\hat{U}(t_1,t_0)|\psi(t_0)\rangle$$

This should be

$$\hat{U}(t_2,t_0) = \hat{U}(t_2,t_1)\hat{U}(t_1,t_0)$$

29.2 Infinitesimal time-evolution operator

We consider the infinitesimal time evolution operator

$$|\psi(t_0+dt)\rangle = \hat{U}(t_0+dt,t_0)|\psi(t_0)\rangle$$

with

$$\lim_{dt\to 0}\hat{U}(t_0+dt,t_0) = \hat{1}$$

We assert that all these requirements are satisfied by

$$\hat{U}(t_0+dt,t_0) = \hat{1} - i\hat{\Omega}dt$$

The dimension of $\hat{\Omega}$ is a frequency or inverse time.

$$\begin{aligned}\hat{U}^+(t_0+dt,t_0)\hat{U}(t_0+dt,t_0) &= (\hat{1}-i\hat{\Omega}dt)^+(\hat{1}-i\hat{\Omega}dt)\\ &= (\hat{1}+i\hat{\Omega}^+dt)(\hat{1}-i\hat{\Omega}dt)\\ &= \hat{1}+i(\hat{\Omega}^+-\hat{\Omega})dt\\ &= \hat{1}\end{aligned}$$

or

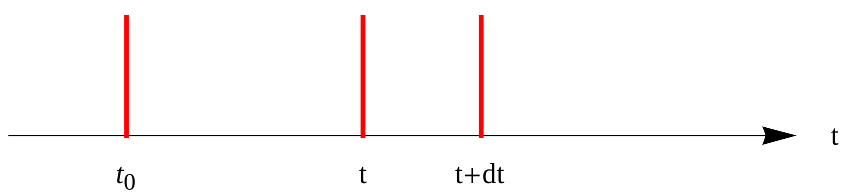
$$\hat{\Omega}^+ = \hat{\Omega} \text{ (Hermitian)}$$

We assume that

$$\hat{\Omega} = \frac{\hat{H}}{\hbar}$$

where $\hat{H}$ is a Hamiltonian.

29.3 Schrödinger equation



$$\hat{U}(t+dt,t_0) = (\hat{1}-i\frac{\hat{H}}{\hbar}dt)\hat{U}(t,t_0)$$

or

$$\hat{U}(t+dt,t_0)-\hat{U}(t,t_0) = -i\frac{\hat{H}}{\hbar}dt\hat{U}(t,t_0)$$

$$\lim_{dt\to 0}\frac{\hat{U}(t+dt,t_0)-\hat{U}(t,t_0)}{dt} = -i\frac{\hat{H}}{\hbar}\hat{U}(t,t_0)$$

or

$$\frac{\partial}{\partial t}\hat{U}(t,t_0) = -i\frac{\hat{H}}{\hbar}\hat{U}(t,t_0)$$

or

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0) = \hat{H}\hat{U}(t,t_0)$$

This is the Schrödinger equation for the time-evolution operator.

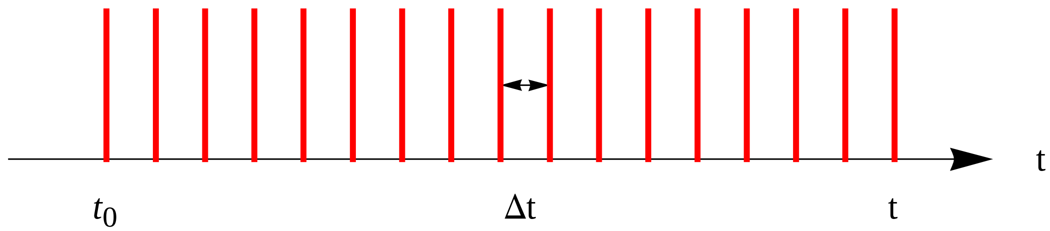
$$i\hbar\frac{\partial}{\partial t}\hat{U}(t,t_0)|\psi(t_0)\rangle = \hat{H}\hat{U}(t,t_0)|\psi(t_0)\rangle$$

or

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$$

29.4 Unitary operator

What is the form of $\hat{U}(t,t_0)$ when $\hat{H}$ is independent of t?



$$\Delta t = \frac{t-t_0}{N}$$

$$\lim_{N\to\infty}[\hat{1} - \frac{i\hat{H}}{\hbar}(\frac{t-t_0}{N})]^N = \exp[-\frac{i\hat{H}}{\hbar}(t-t_0)]$$

or

$$\hat{U}(t,t_0) = \exp[-\frac{i\hat{H}}{\hbar}(t-t_0)]$$

29.5 Ehrenfest's theorem

Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle \qquad \text{or} \qquad \frac{\partial}{\partial t}|\psi(t)\rangle = -\frac{i}{\hbar}\hat{H}|\psi(t)\rangle$$

Taking the Hermitian conjugate of both sides,

$$-i\hbar \frac{\partial}{\partial t}\langle\psi(t)| = \langle\psi(t)|\hat{H}^{+} = \langle\psi(t)|\hat{H}$$

or

$$\frac{\partial}{\partial t}\langle\psi(t)| = \langle\psi(t)|\hat{H}^{+} = \frac{i}{\hbar}\langle\psi(t)|\hat{H}$$

We now consider the time dependence of the average defined by $\langle\psi(t)|\hat{A}|\psi(t)\rangle$

$$\begin{aligned}
\frac{d}{dt}\langle\psi(t)|\hat{A}(t)|\psi(t)\rangle &= (\frac{\partial}{\partial t}\langle\psi(t)|)\hat{A}|\psi(t)\rangle + \langle\psi(t)|\frac{\partial\hat{A}}{\partial t}|\psi(t)\rangle + \langle\psi(t)|\hat{A}(\frac{\partial}{\partial t}|\psi(t)\rangle) \\
&= \frac{i}{\hbar}\langle\psi(t)|\hat{H}\hat{A}|\psi(t)\rangle + \langle\psi(t)|\frac{\partial\hat{A}}{\partial t}|\psi(t)\rangle + \langle\psi(t)|\hat{A}(-\frac{i}{\hbar})|\psi(t)\rangle \\
&= -\frac{i}{\hbar}\langle\psi(t)|[\hat{A},\hat{H}]|\psi(t)\rangle + \langle\psi(t)|\frac{\partial\hat{A}}{\partial t}|\psi(t)\rangle
\end{aligned}$$

or

$$\frac{d}{dt}\langle\psi(t)|\hat{A}|\psi(t)\rangle = -\frac{i}{\hbar}\langle\psi(t)|[\hat{A},\hat{H}]|\psi(t)\rangle + \langle\psi(t)|\frac{\partial\hat{A}}{\partial t}|\psi(t)\rangle$$

29.6 Example Simple harmonics

We consider a particle in a stationary potential.

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

So that we can write

$$\begin{aligned}
\frac{d}{dt}\langle\psi(t)|\hat{x}|\psi(t)\rangle &= -\frac{i}{\hbar}\langle\psi(t)|[\hat{x},\hat{H}]|\psi(t)\rangle \\
&= -\frac{i}{\hbar}\langle\psi(t)|[\hat{x},\frac{\hat{p}^2}{2m}]|\psi(t)\rangle \\
&= -\frac{i}{\hbar}i\hbar\langle\psi(t)|\frac{\hat{p}}{m}]|\psi(t)\rangle
\end{aligned}$$

or

$$\frac{d}{dt}\langle\psi(t)|\hat{x}|\psi(t)\rangle = \langle\psi(t)|\frac{\hat{p}}{m}]|\psi(t)\rangle$$

or

$$\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p\rangle$$

Similarly

$$\begin{aligned}\frac{d}{dt}\langle\psi(t)|\hat{p}|\psi(t)\rangle &= -\frac{i}{\hbar}\langle\psi(t)|[\hat{p},\hat{H}]|\psi(t)\rangle \\ &= -\frac{i}{\hbar}\langle\psi(t)|[\hat{p},V(\hat{x})]|\psi(t)\rangle \\ &= -\frac{i}{\hbar}\frac{\hbar}{i}\langle\psi(t)|\frac{\partial}{\partial\hat{x}}V(\hat{x})]|\psi(t)\rangle\end{aligned}$$

or

$$\frac{d}{dt}\langle\psi(t)|\hat{p}|\psi(t)\rangle = -\langle\psi(t)|\frac{\partial}{\partial\hat{x}}V(\hat{x})]|\psi(t)\rangle$$

or

$$\frac{d}{dt}\langle p\rangle = -\left\langle\frac{dV}{dx}\right\rangle$$

The equations

$$\frac{d}{dt}\langle x\rangle = \frac{1}{m}\langle p\rangle,$$

and

$$\frac{d}{dt}\langle p\rangle = -\left\langle\frac{dV}{dx}\right\rangle$$

express the Ehrenfest's theorem. These forms recall that of classical Hamiltonian-Jacobi equations for a particle.

29.7 Example: Spin precession

We consider the motion of spin S (=1/2) in the presence of an external magnetic field B along the z axis. The magnetic moment of spin is given by

$$\hat{\mu}_z = -\frac{2\mu_B \hat{S}_z}{\hbar} = -\mu_B \hat{\sigma}_z .$$

Then the spin Hamiltonian (Zeeman energy) is described by

$$\hat{H} = -\hat{\mu}_z B = -(-\frac{2\mu_B \hat{S}_z}{\hbar})B = \mu_B \hat{\sigma}_z B$$

Since the Bohr magneton μ_B is given by $\mu_B = \frac{e\hbar}{2mc}$,

$$\mu_B B = \frac{eB\hbar}{2mc} = \frac{\hbar}{2}\frac{eB}{mc} = \frac{\hbar}{2}\omega_0$$

or

$$\omega_0 = \frac{eB}{mc} \qquad \text{(angular frequency of the Larmor precession)}$$

Thus the Hamiltonian can be rewritten as

$$\hat{H} = \frac{\hbar}{2}\omega_0 \hat{\sigma}_z$$

Thus the Schrödinger equation is obtained as

$$|\psi(t)\rangle = \exp[-\frac{i}{\hbar}\hat{H}t]|\psi(t=0)\rangle = \exp[-\frac{i}{2}\omega_0 \hat{\sigma}_z t]|\psi(t=0)\rangle$$

Note that the time evolution operator coincides with the rotation operator

$$\hat{R}_z(\omega_0 t) = \exp[-\frac{i}{2}\omega_0 \hat{\sigma}_z t]$$

We assume that

$$|\psi(t=0)\rangle = |+\rangle_{\mathbf{n}} = \exp[-\frac{i}{2}\hat{\sigma}_z \phi]\exp[-\frac{i}{2}\hat{\sigma}_y \theta]|+\rangle = \begin{pmatrix} e^{-\frac{i\phi}{2}}\cos(\frac{\theta}{2}) \\ e^{\frac{i\phi}{2}}\sin(\frac{\theta}{2}) \end{pmatrix}$$

$$\hat{R}_z(\omega_0 t) = \exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t]$$

The average

$$\langle S_x \rangle_t = \langle \psi(t)|\hat{S}_x|\psi(t)\rangle = \frac{\hbar}{2}{}_{\mathbf{n}}\langle +|\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\sigma_x \exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t]|+\rangle_{\mathbf{n}}$$

$$\langle S_y \rangle_t = \langle \psi(t)|\hat{S}_y|\psi(t)\rangle = \frac{\hbar}{2}{}_{\mathbf{n}}\langle +|\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\sigma_y \exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t]|+\rangle_{\mathbf{n}}$$

$$\langle S_z \rangle_t = \langle \psi(t)|\hat{S}_z|\psi(t)\rangle = \frac{\hbar}{2}{}_{\mathbf{n}}\langle +|\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\sigma_z \exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t]|+\rangle_{\mathbf{n}}$$

Here we have

$$\begin{aligned}\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\sigma_x \exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t] &= \begin{pmatrix} e^{\frac{it\omega_0}{2}} & 0 \\ 0 & e^{-\frac{it\omega_0}{2}} \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} e^{\frac{it\omega_0}{2}} & 0 \\ 0 & e^{-\frac{it\omega_0}{2}} \end{pmatrix} \\ &= \begin{pmatrix} 0 & e^{it\omega_0} \\ e^{-it\omega_0} & 0 \end{pmatrix}\end{aligned}$$

$$\begin{aligned}\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\sigma_y \exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t] &= \begin{pmatrix} e^{\frac{it\omega_0}{2}} & 0 \\ 0 & e^{-\frac{it\omega_0}{2}} \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} e^{\frac{it\omega_0}{2}} & 0 \\ 0 & e^{-\frac{it\omega_0}{2}} \end{pmatrix} \\ &= \begin{pmatrix} 0 & -ie^{it\omega_0} \\ ie^{-it\omega_0} & 0 \end{pmatrix}\end{aligned}$$

$$\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\sigma_z \exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t] = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Thus we have

$$\begin{aligned}\langle S_x \rangle_t &= \frac{\hbar}{2}\sin\theta\cos(\omega_0 t + \phi) \\ &= \frac{\hbar}{2}\sin\theta[\cos(\omega_0 t)\cos\phi - \sin(\omega_0 t)\cos\phi]\end{aligned}$$

$$\langle S_y \rangle_t = \frac{\hbar}{2}\sin\theta[\sin(\omega_0 t)\cos\phi + \cos(\omega_0 t)\sin\phi]$$

$$\langle S_z \rangle_t = \frac{\hbar}{2}\cos\theta$$

At t = 0,

$$\langle S_x \rangle_0 = \frac{\hbar}{2}\sin\theta\cos\phi$$

$$\langle S_y \rangle_0 = \frac{\hbar}{2}\sin\theta\sin\phi$$

$$\langle S_z \rangle_0 = \frac{\hbar}{2}\cos\theta$$

Using this we have

$$\langle S_x \rangle_t = \langle S_x \rangle_0 \cos(\omega_0 t) - \langle S_y \rangle_0 \sin(\omega_0 t)$$

$$\langle S_y \rangle_t = \langle S_x \rangle_0 \sin(\omega_0 t) + \langle S_y \rangle_0 \cos(\omega_0 t)$$

$$\langle S_z \rangle_t = \langle S_z \rangle_0 = \frac{\hbar}{2}\cos\theta$$

$$\langle S_x \rangle_t + i\langle S_y \rangle_t = e^{i\omega_0 t}(\langle S_x \rangle_0 + i\langle S_y \rangle_0)$$

$$\langle S_x \rangle_t = \langle \psi(t)|\hat{S}_x|\psi(t)\rangle = \frac{\hbar}{2}{}_{\mathbf{n}}\langle + |\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\hat{\sigma}_x \exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t]| + \rangle_{\mathbf{n}}$$
$$= \frac{\hbar}{2}{}_n\langle + |\hat{\sigma}_x \cos(\omega_0 t) - \hat{\sigma}_y \sin(\omega_0 t)| + \rangle_{\mathbf{n}}$$

where

$$\langle S_x \rangle_0 = \frac{\hbar}{2}{}_{\mathbf{n}}\langle + |\hat{\sigma}_x| + \rangle_{\mathbf{n}}$$

We also get

$$\langle S_y \rangle_t = \langle \psi(t)|\hat{S}_y|\psi(t)\rangle = \frac{\hbar}{2}{}_{\mathbf{n}}\langle + |\exp[\frac{i}{2}\omega_0\hat{\sigma}_z t]\hat{\sigma}_y \exp[-\frac{i}{2}\omega_0\hat{\sigma}_z t]| + \rangle_{\mathbf{n}}$$
$$= \frac{\hbar}{2}{}_{\mathbf{n}}\langle + |\hat{\sigma}_x \sin(\omega_0 t) + \hat{\sigma}_y \cos(\omega_0 t)| + \rangle_{\mathbf{n}}$$

$$\langle S_y \rangle_0 = \frac{\hbar}{2}{}_{\mathbf{n}}\langle + | \hat{\sigma}_y | + \rangle_{\mathbf{n}}$$

and

$$\begin{aligned}\langle S_z \rangle_t &= \langle \psi(t) | \hat{S}_z | \psi(t) \rangle \\ &= \frac{\hbar}{2}{}_{\mathbf{n}}\langle + | \exp[\frac{i}{2}\omega_0 \hat{\sigma}_z t] \hat{\sigma}_z \exp[-\frac{i}{2}\omega_0 \hat{\sigma}_z t] | + \rangle_{\mathbf{n}} \\ &= \frac{\hbar}{2}{}_{\mathbf{n}}\langle + | \hat{\sigma}_z | + \rangle_{\mathbf{n}} = \langle S_z \rangle_0\end{aligned}$$

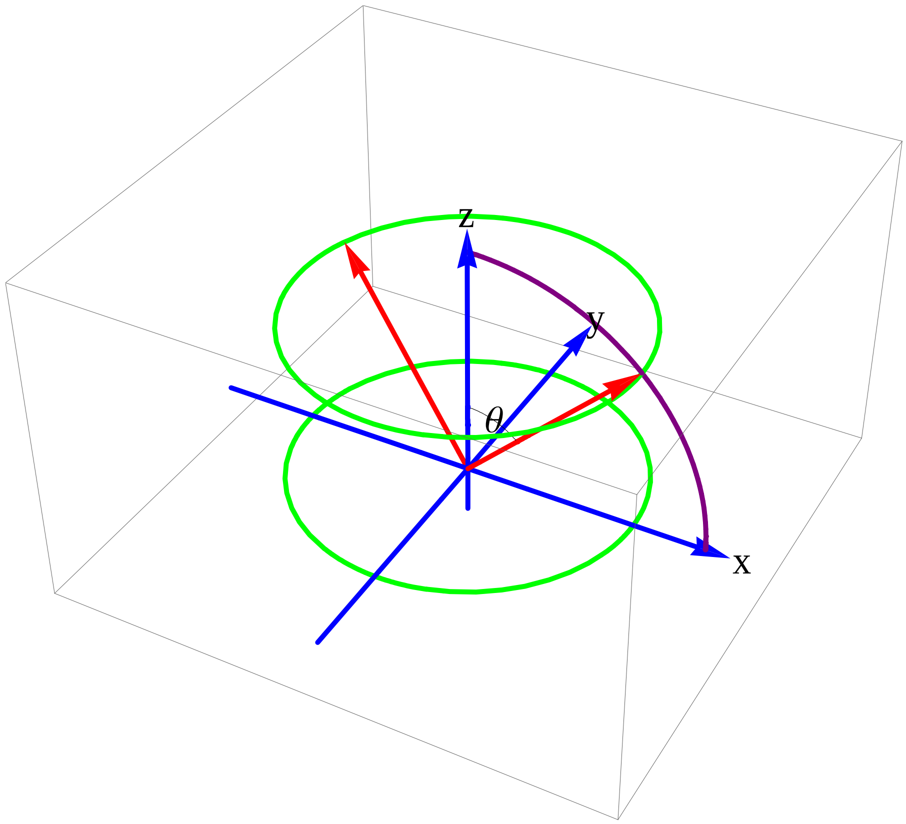
Then

$$\langle S_x \rangle_t = \langle S_x \rangle_0 \cos(\omega_0 t) - \langle S_y \rangle_0 \sin(\omega_0 t)$$

$$\langle S_y \rangle_t = \langle S_x \rangle_0 \sin(\omega_0 t) + \langle S_y \rangle_0 \cos(\omega_0 t)$$

and

$$\langle S_z \rangle_t = \langle S_z \rangle_0$$



29.8 Baker-Hausdorf lemma

In the commutation relations, $[\hat{J}_z, \hat{J}_x] = i\hbar \hat{J}_y$, we put $\hat{J}_z = \frac{\hbar}{2}\hat{\sigma}_z$ and $\hat{J}_x = \frac{\hbar}{2}\hat{\sigma}_x$

Then we have

$$[\frac{\hbar}{2}\hat{\sigma}_z, \frac{\hbar}{2}\hat{\sigma}_x] = i\hbar\frac{\hbar}{2}\hat{\sigma}_y \qquad \text{or} \qquad [\hat{\sigma}_z, \hat{\sigma}_x] = 2i\hat{\sigma}_y .$$

Similarly, we have

$$[\hat{\sigma}_x, \hat{\sigma}_y] = 2i\hat{\sigma}_z , \qquad [\hat{\sigma}_y, \hat{\sigma}_z] = 2i\hat{\sigma}_x$$

We notice the following relations which can be derived from the Baker-Hausdorf lemma:

$$\exp(\hat{A}x)\hat{B}\exp(-\hat{A}x) = \hat{B} + \frac{x}{1!}[\hat{A}, \hat{B}] + \frac{x^2}{2!}[\hat{A},[\hat{A}, \hat{B}]] + \frac{x^3}{3!}[\hat{A},[\hat{A},[\hat{A}, \hat{B}]]] + ...$$

$$\exp[i\frac{\theta}{2}\hat{\sigma}_z]\hat{\sigma}_x \exp[-i\frac{\theta}{2}\hat{\sigma}_z] = \hat{\sigma}_x \cos\theta - \hat{\sigma}_y \sin\theta$$

$$\exp[i\frac{\theta}{2}\hat{\sigma}_z]\hat{\sigma}_y\exp[-i\frac{\theta}{2}\hat{\sigma}_z]=\hat{\sigma}_x\sin\theta+\hat{\sigma}_y\cos\theta$$

((**Proof**))

We note that

$$x=\frac{i\theta}{2},\ \hat{A}=\hat{\sigma}_z, \text{ and } \hat{B}=\hat{\sigma}_x.$$

$$[\hat{A},\hat{B}]=[\hat{\sigma}_z,\hat{\sigma}_x]=2i\hat{\sigma}_y$$

Then we have

$$I=\exp[x\hat{\sigma}_z]\hat{\sigma}_x\exp[-x\hat{\sigma}_z]=\hat{\sigma}_x+\frac{x}{1!}[\hat{\sigma}_z,\hat{\sigma}_x]+\frac{x^2}{2!}[\hat{\sigma}_z,[\hat{\sigma}_z,\hat{\sigma}_x]]+\frac{x^3}{3!}[\hat{\sigma}_z,[\hat{\sigma}_z,[\hat{\sigma}_z,\hat{\sigma}_x]]]$$

$$+\frac{x^4}{4!}[\hat{\sigma}_z,[\hat{\sigma}_z,[\hat{\sigma}_z,[\hat{\sigma}_z,\hat{\sigma}_x]]]]+.....$$

$$I=\hat{\sigma}_x+\frac{1}{1!}\frac{i\theta}{2}2i\hat{\sigma}_y+\frac{1}{2!}\left(\frac{i\theta}{2}\right)^2[\hat{\sigma}_z,2i\hat{\sigma}_y]+\frac{1}{3!}\left(\frac{i\theta}{2}\right)^3[\hat{\sigma}_z,[\hat{\sigma}_z,2i\hat{\sigma}_y]]+\frac{1}{4!}\left(\frac{i\theta}{2}\right)^4[\hat{\sigma}_z,[\hat{\sigma}_z,[\hat{\sigma}_z,2i\hat{\sigma}_y]]]+.$$

or

$$I=\hat{\sigma}_x-\theta\hat{\sigma}_y+i\frac{\theta^2}{2^2}[\hat{\sigma}_y,\hat{\sigma}_z]-\frac{i}{3!}\frac{\theta^3}{2^3}(-2i)[\hat{\sigma}_z,[\hat{\sigma}_y,\hat{\sigma}_z]]+\frac{1}{4!}\frac{\theta^4}{2^4}(-2i)[\hat{\sigma}_z,[\hat{\sigma}_z,[\hat{\sigma}_y,\hat{\sigma}_z]]].....$$
$$=\hat{\sigma}_x-\theta\hat{\sigma}_y+i\frac{\theta^2}{2^2}2i\hat{\sigma}_x-\frac{i}{3!}\frac{\theta^3}{2^3}(-2i)(2i)[\hat{\sigma}_z,\hat{\sigma}_x]+\frac{1}{4!}\frac{\theta^4}{2^4}(-2i)(2i)[\hat{\sigma}_z,[\hat{\sigma}_z,\hat{\sigma}_x]]+...$$

or

$$I=\hat{\sigma}_x-\theta\hat{\sigma}_y-\frac{\theta^2}{2}\hat{\sigma}_x-\frac{i}{3!}\frac{\theta^3}{2^3}(-2i)(2i)^2\hat{\sigma}_y+\frac{1}{4!}\frac{\theta^4}{2^4}(-2i)(2i)(2i)(-2i)\hat{\sigma}_x+...$$
$$=\hat{\sigma}_x-\theta\hat{\sigma}_y-\frac{\theta^2}{2}\hat{\sigma}_x+\frac{\theta^3}{3!}\hat{\sigma}_y+\frac{\theta^4}{4!}\hat{\sigma}_x+...$$
$$==\hat{\sigma}_x(1-\frac{\theta^2}{2}+\frac{\theta^4}{4!}...)-\hat{\sigma}_y(1-\frac{\theta^3}{3!}+...)$$
$$=\hat{\sigma}_x\cos\theta-\hat{\sigma}_y\cos\theta$$

29.10 Schrödinger picture

The Schrödinger equation

$$|\psi(t)\rangle = |\psi_s(t)\rangle$$

$$|\psi_s(t)\rangle = \hat{U}(t,t_0)|\psi_s(t_0)\rangle$$

where $\hat{U}(t,t_0)$ is the time evolution operator;

$$\hat{U}^+(t,t_0) = \hat{U}^{-1}(t,t_0)\,.$$

In the Schrodinger picture, the average of the operator $\hat{A}_s$ in the state $|\psi_s(t)\rangle$ is defined by

$$\langle\psi_s(t)|\hat{A}_s|\psi_s(t)\rangle\,.$$

29.11 Heisenberg picture

The state vector, which is constant, is equal to

$$|\psi_H(t)\rangle = |\psi_s(t_0)\rangle\,.$$

From the definition

$$\langle\psi_H|\hat{A}_H(t)|\psi_H\rangle = \langle\psi_s|\hat{A}_s(t)|\psi_s\rangle\,,$$

or

$$\hat{A}_H(t) = \hat{U}^+(t,t_0)\hat{A}_s(t)\hat{U}(t,t_0)\,.$$

In general, $\hat{A}_H(t)$ depends on time, even if $\hat{A}_s(t)$ does not.

29.12 Heisenberg's equation of motion

The Schrödinger equation can be described in the Schrödinger picture

$$i\hbar\frac{\partial}{\partial t}|\psi_s(t)\rangle = \hat{H}_s(t)|\psi_s(t)\rangle$$

or

$$i\hbar \frac{d}{dt}\hat{U}(t,t_0)|\psi_s(t_0)\rangle = \hat{H}_s(t)\hat{U}(t,t_0)|\psi_s(t_0)\rangle$$

or

$$i\hbar \frac{d}{dt}\hat{U}(t,t_0) = \hat{H}_s(t)\hat{U}(t,t_0)$$

or

$$\frac{d}{dt}\hat{U}(t,t_0) = -\frac{i}{\hbar}\hat{H}_s(t)\hat{U}(t,t_0)$$

and

$$\frac{d}{dt}\hat{U}^+(t,t_0) = \frac{i}{\hbar}\hat{U}^+(t,t_0)\hat{H}_s(t)$$

where $\hat{H}_s^+(t) = \hat{H}_s(t)$. Therefore

$$\begin{aligned}
\frac{d\hat{A}_H(t)}{dt} &= \frac{d\hat{U}^+(t,t_0)}{dt}\hat{A}_s(t)\hat{U}(t,t_0) + \hat{U}^+(t,t_0)\hat{A}_s(t)\frac{d\hat{U}(t,t_0)}{dt} + \hat{U}^+(t,t_0)\frac{d\hat{A}_s(t)}{dt}\hat{U}(t,t_0) \\
&= \frac{i}{\hbar}\hat{U}^+(t,t_0)\hat{H}_s(t)\hat{A}_s(t)\hat{U}(t,t_0) - \hat{U}^+(t,t_0)\hat{A}_s(t)\frac{i}{\hbar}\hat{H}_s(t)\hat{U}(t,t_0) + \hat{U}^+(t,t_0)\frac{d\hat{A}_s(t)}{dt}\hat{U}(t,t_0) \\
&= \frac{i}{\hbar}\hat{U}^+(t,t_0)[\hat{H}_s(t),\hat{A}_s(t)]\hat{U}(t,t_0) + \hat{U}^+(t,t_0)\frac{d\hat{A}_s(t)}{dt}\hat{U}(t,t_0) \\
&= \frac{i}{\hbar}[\hat{H}_H(t),\hat{A}_H(t)] + (\frac{d\hat{A}_s(t)}{dt})_H
\end{aligned}$$

where

$$\hat{H}_H(t) = \hat{U}^+(t,t_0)\hat{H}_s(t)\hat{U}(t,t_0)$$

Finally we obtain the Heisenberg's equation of motion

$$i\hbar\frac{d}{dt}\hat{A}_H(t) = [\hat{A}_H(t),\hat{H}_H(t)] + i\hbar(\frac{d\hat{A}_s(t)}{dt})_H$$

29.13 Simple example

$$\hat{H}_s(t) = \hat{H}, \qquad \hat{A}_s(t) = \hat{A}$$

$t_0 = 0$

$$\hat{U} = e^{-\frac{i}{\hbar}\hat{H}t}$$

$$\hat{A}_H = \hat{U}^+ \hat{A}_s \hat{U} = e^{\frac{i}{\hbar}\hat{H}t} \hat{A}_s e^{-\frac{i}{\hbar}\hat{H}t}$$

$$\hat{H}_H = \hat{H}_s$$

Then we have the Heisenberg's equation of motion:

$$i\hbar \frac{d}{dt}\hat{A}_H = [\hat{A}_H, \hat{H}_H]$$

We get an analogy between the classical equations of motion in the Hamiltonian form and the quantum equations of motion in the Heisenberg's form. $\hat{A}_H$ is called a constant of the motion, when $[\hat{A}_H, \hat{H}_H]$=0 at all times.

$$\begin{aligned}[\hat{A}_H, \hat{H}_H] &= \hat{U}^+ \hat{A}_S \hat{U}\hat{U}^+ \hat{H}_S \hat{U} - \hat{U}^+ \hat{H}_S \hat{U}\hat{U}^+ \hat{A}_S \hat{U} \\ &= \hat{U}^+ [\hat{A}_S, \hat{H}_S] \hat{U}\end{aligned}$$

Therefore $[\hat{A}_H, \hat{H}_H]$ means $[\hat{A}_S, \hat{H}_S] = 0$

29.14 Ehrenfest's theorem: free particle

$$H_S = \frac{1}{2m}\hat{p}_S{}^2 + V(\hat{x}_S),$$

$$H_H = \frac{1}{2m}\hat{p}_H{}^2 + V(\hat{x}_H),$$

$$\begin{aligned}[\hat{x}_H, \hat{p}_H] &= \hat{x}_H \hat{p}_H - \hat{p}_H \hat{x}_H \\ &= \hat{U}^+ \hat{x}\hat{U}\hat{U}^+ \hat{p}\hat{U} - \hat{U}^+ \hat{p}\hat{U}\hat{U}^+ \hat{x}\hat{U} \\ &= \hat{U}^+ [\hat{x}, \hat{p}]\hat{U} = i\hbar \hat{U}^+ \hat{U} = i\hbar \hat{1}\end{aligned}$$

$$\begin{aligned}[\hat{x}_H, \hat{p}_H{}^2] &= \hat{U}^+ [\hat{x}, \hat{p}^2]\hat{U} \\ &= 2i\hbar \hat{U}^+ \hat{p}\hat{U} \\ &= 2i\hbar \hat{p}_H\end{aligned}$$

Heisenberg's equation for the free particles,

$$i\hbar \frac{d}{dt}\hat{x}_H = [\hat{x}_H, \hat{H}_H] = \frac{1}{2m}[\hat{x}_H, \hat{p}_H{}^2] = \frac{1}{2m} i\hbar \frac{\partial}{\partial \hat{p}_H} \hat{p}_H{}^2 = \frac{2}{2m} i\hbar \hat{p}_H ,$$

or

$$\frac{d}{dt}\hat{x}_H = [\hat{x}_H, \hat{H}_H] = \frac{1}{m}\hat{p}_H .$$

Similarly

$$i\hbar \frac{d}{dt}\hat{p}_H = [\hat{p}_H, \hat{H}_H] = \hat{U}^+[\hat{p}, \hat{H}]\hat{U} = \hat{U}^+[\hat{p}, \hat{V}(\hat{x})]\hat{U} = (-i\hbar)\frac{\partial}{\partial \hat{x}_H} V(\hat{x}_H)$$

or

$$\frac{d}{dt}\hat{p}_H = (-)\frac{\partial V(\hat{x}_H)}{\partial \hat{x}_H}$$

We consider a simple harmonics.

$$V(\hat{x}_H) = \frac{1}{2} m\omega^2 \hat{x}_H{}^2$$

$$\frac{d}{dt}\hat{p}_H = -m\omega^2 \hat{x}_H$$

Now consider the linear combination,

$$\frac{d}{dt}(\hat{x}_H + \frac{i}{m\omega}\hat{p}_H) = -i\omega(\hat{x}_H + \frac{i}{m\omega}\hat{p}_H)$$

$$(\hat{x}_H + \frac{i}{m\omega}\hat{p}_H) = \hat{A}_H e^{-i\omega t}$$

or

$$\frac{d}{dt}(\hat{x}_H - \frac{i}{m\omega}\hat{p}_H) = i\omega(\hat{x}_H - \frac{i}{m\omega})$$

$$(\hat{x}_H - \frac{i}{m\omega}\hat{p}_H) = \hat{B}_H e^{i\omega t}$$

where $\hat{A}_H$ and $\hat{B}_H$ are time-independent operators:

$$\hat{A}_H = \hat{x}_H(0) + \frac{i}{m\omega}\hat{p}_H(0)$$

$$\hat{B}_H = \hat{x}_H(0) - \frac{i}{m\omega}\hat{p}_H(0)$$

Note that $\hat{x}_H(0)$ and $\hat{p}_H(0)$ correspond to the operators in the Schrödinger picture. From these equations, we get final results

$$\hat{x}_H = \hat{x}_H(0)\cos\omega t + \frac{1}{m\omega}\hat{p}_H(0)\sin\omega t$$ `

$$\hat{p}_H = \hat{p}_H(0)\cos\omega t - m\omega\hat{x}_H(0)\sin\omega t$$

These look to the same as the classical equation of motion. We see that $\hat{x}_H$ and $\hat{p}_H$ operators oscillate just like their classical analogue.

An advantage of the Heisenberg picture is therefore that it leads to equations which are formally similar to those of classical mechanics.

((Note))

$$i\hbar\frac{d^2}{dt^2}\hat{x}_H = [\frac{d\hat{x}_H}{dt}, \hat{H}_H] = [\frac{\hat{p}_H}{m}, \hat{H}_H] = \frac{1}{m}[\hat{p}_H, \frac{m\omega^2}{2}\hat{x}_H{}^2] = \frac{\omega^2}{2}[\hat{p}_H, \hat{x}_H{}^2] = \frac{\omega^2}{2}\frac{\hbar}{i}2\hat{x}_H$$

or

$$\frac{d^2}{dt^2}\hat{x}_H = -\omega^2\hat{x}_H$$

with the initial condition

$$\frac{d}{dt}\hat{x}_H|_{t=0} = \frac{1}{m}\hat{p}_H(0), \qquad \hat{x}_H|_{t=0} = \hat{x}_H(0)$$

The solution is

$$\hat{x}_H = \hat{C}_1\cos(\omega t) + \hat{C}_2\sin(\omega t)$$

$$\hat{x}_H(0) = \hat{C}_1,$$

$$\frac{d\hat{x}_H}{dt}|_{t=0} = [-\omega\hat{C}_1 \sin(\omega t) + \omega\hat{C}_2 \cos n(\omega t)]_{t=0} = \omega\hat{C}_2 = \frac{\hat{p}_H(0)}{m}$$

Thus we have

$$\hat{C}_2 = \frac{\hat{p}_H(0)}{m\omega}.$$

and

$$\hat{x}_H = \hat{x}_H(0)\cos(\omega t) + \frac{\hat{p}_H(0)}{m\omega}\sin(\omega t)$$

Paul Ehrenfest (January 18, 1880 – September 25, 1933) was an Austrian and Dutch physicist and mathematician, who made major contributions to the field of statistical mechanics and its relations with quantum mechanics, including the theory of phase transition and the Ehrenfest theorem.

http://en.wikipedia.org/wiki/Paul_Ehrenfest

29.15 Analogy with classical mechanics

In the classical mechanics, dynamical variables vary with time according to the Hamilton's equations of motion,

$$\frac{dq_j}{dt} = \frac{\partial H}{\partial p_j},$$

where q_j and p_j are a set of canonical co-ordinate and momentum, and H is the Hamiltonian expressed as a function of them,

$$H = H(q_1, q_2, q_3, ..., q_n, p_1, p_2, p_3, ... p_n)$$

where n is the degree of freedom.

For a given variable $A = v(q_1, q_2, q_3, \ldots, q_n, p_1, p_2, p_3, \ldots p_n)$,

$$\begin{aligned}
\frac{dA}{dt} &= \sum_j \left(\frac{\partial A}{\partial q_j}\frac{dq_j}{dt} + \frac{\partial A}{\partial p_j}\frac{dp_j}{dt} \right) \\
&= \sum_j \left(\frac{\partial A}{\partial q_j}\frac{\partial H}{\partial p_j} - \frac{\partial A}{\partial p_j}\frac{\partial H}{\partial q_j} \right) \\
&= [A, H]_{classical}
\end{aligned}$$

$[\ ]_{classical}$:a classical definition of a Poisson bracket.

29.16 Dirac picture (Interaction picture)

$$\hat{H} = \hat{H}_0 + \hat{V}_s(t)$$

where $\hat{H}_0$ is independent of *t*.

$$|\psi_s(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_0 t}|\psi_I(t)\rangle$$

or

$$|\psi_I(t)\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}|\psi_s(t)\rangle$$

We assume that

$$\langle\psi_I(t)|\hat{A}_I(t)|\psi_I(t)\rangle = \langle\psi_s(t)|\hat{A}_s|\psi_s(t)\rangle$$

For convenience, $\hat{A}_s$ is independent of *t*.

or

$$\langle\psi_s(t)|e^{-\frac{i}{\hbar}\hat{H}_0 t}\hat{A}_I(t)e^{\frac{i}{\hbar}\hat{H}_0 t}|\psi_s(t)\rangle = \langle\psi_s(t)|\hat{A}_s|\psi_s(t)\rangle$$

or

$$e^{-\frac{i}{\hbar}\hat{H}_0 t}\hat{A}_I(t)e^{\frac{i}{\hbar}\hat{H}_0 t} = \hat{A}_s$$

or

$$\hat{A}_I(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{A}_s e^{-\frac{i}{\hbar}\hat{H}_0 t}$$

or

$$\begin{aligned} i\hbar\frac{d}{dt}\hat{A}_I(t) &= i\hbar\frac{i}{\hbar}[\hat{H}_0 e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{A}_s e^{-\frac{i}{\hbar}\hat{H}_0 t} - e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{A}_s e^{-\frac{i}{\hbar}\hat{H}_0 t}\hat{H}_0] \\ &= [\hat{A}_I(t), \hat{H}_0] \end{aligned}$$

Thus every operator behaves as if it would in the Heisenberg representation for a non-interacting system.

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\left|\psi_I(t)\right\rangle &= i\hbar\frac{\partial}{\partial t}e^{\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_s(t)\right\rangle \\ &= -\hat{H}_0 e^{\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_s(t)\right\rangle + e^{\frac{i}{\hbar}\hat{H}_0 t} i\hbar\frac{\partial}{\partial t}\left|\psi_s(t)\right\rangle \end{aligned}$$

Since

$$i\hbar\frac{\partial}{\partial t}\left|\psi_s(t)\right\rangle = [\hat{H}_0 + \hat{V}_s(t)]\left|\psi_s(t)\right\rangle$$

$$i\hbar\frac{\partial}{\partial t}\left|\psi_I(t)\right\rangle = i\hbar\frac{\partial}{\partial t}e^{\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_s(t)\right\rangle = -\hat{H}_0 e^{\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_s(t)\right\rangle + e^{\frac{i}{\hbar}\hat{H}_0 t}[\hat{H}_0 + \hat{V}(t)]\left|\psi_s(t)\right\rangle$$

or

$$i\hbar\frac{\partial}{\partial t}\left|\psi_I(t)\right\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{V}(t)e^{-\frac{i}{\hbar}\hat{H}_0 t}\left|\psi_I(t)\right\rangle = \hat{V}_I(t)\left|\psi_I(t)\right\rangle$$

or

$$i\hbar\frac{\partial}{\partial t}\left|\psi_I(t)\right\rangle = \hat{V}_I(t)\left|\psi_I(t)\right\rangle$$

where

$$\hat{V}_I(t) = ^{\frac{i}{\hbar}\hat{H}_0 t}\hat{V}_s(t)e^{-\frac{i}{\hbar}\hat{H}_0 t} \qquad \text{(Schrödinger-like)}$$

which is a Schrödinger equation with the total $\hat{H}$ replaced by $\hat{V}_I$.

We assume that

$$|\psi_I(t)\rangle = \hat{U}_I(t,t_0)|\psi_I(t_0)\rangle$$

satisfies the equation

$$i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = \hat{V}_I(t)|\psi_I(t)\rangle$$

Then we have the following relation.

$$i\hbar\frac{\partial}{\partial t}\hat{U}_I(t,t_0) = \hat{V}_I(t)\hat{U}_I(t,t_0)$$

with the initial condition

$$\hat{U}_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t}\hat{V}_I(t')\hat{U}_I(t',t_0)dt'$$

We can obtain an approximate solution to this equation [Dyson series].

$$\hat{U}_I(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t}\hat{V}_I(t')[1 - \frac{i}{\hbar}\int_{t_0}^{t'}\hat{V}_I(t'')\hat{U}_I(t'',t_0)dt'']dt'$$

$$= 1 + (-\frac{i}{\hbar})\int_{t_0}^{t}\hat{V}_I(t')dt' + (-\frac{i}{\hbar})^2\int_{t_0}^{t}dt'\int_{t_0}^{t'}dt''\hat{V}_I(t')\hat{V}_I(t'') + ...$$

29.17 Transition probability

Once $\hat{U}_I(t,t_0)$ is given we have

$$|\psi_I(t)\rangle = \hat{U}_I(t,t_0)|\psi_I(t_0)\rangle$$

where

$$|\psi_s(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_0 t}|\psi_I(t)\rangle, \qquad \text{or} \qquad |\psi_I(t)\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}|\psi_s(t)\rangle$$

and

$$\left|\psi_s(t)\right\rangle = \hat{U}(t,t_0)\left|\psi_s(t_0)\right\rangle$$

$$\left|\psi_I(t)\right\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{U}_s(t,t_0)\left|\psi_s(t_0)\right\rangle$$
$$= e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{U}_s(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0}\left|\psi_I(t_0)\right\rangle$$

Then we have

$$\hat{U}_I(t,t_0) = e^{\frac{i}{\hbar}\hat{H}_0 t}\hat{U}_s(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0}$$

Let us now look at the matrix element of $\hat{U}_I(t,t_0)$

$$\hat{H}_0\left|n\right\rangle = E_n\left|n\right\rangle$$

$$\left\langle n\right|\hat{U}_I(t,t_0)\left|m\right\rangle = e^{\frac{i}{\hbar}(E_n t - E_m t_0)}\left\langle n\right|\hat{U}_s(t,t_0)\left|m\right\rangle$$

$$\left|\left\langle n\right|\hat{U}_I(t,t_0)\left|m\right\rangle\right|^2 = \left|\left\langle n\right|\hat{U}_s(t,t_0)\left|m\right\rangle\right|^2$$

((Remark))

When

$$[\hat{H}_0, \hat{A}] \neq 0 \qquad \text{and} \qquad [\hat{H}_0, \hat{B}] \neq 0$$

$$\hat{A}\left|a'\right\rangle = a'\left|a'\right\rangle \qquad \text{and} \qquad \hat{B}\left|b'\right\rangle = b'\left|b'\right\rangle$$

in general,

$$\left|\left\langle b'\right|\hat{U}_I(t,t_0)\left|a'\right\rangle\right|^2 \neq \left|\left\langle b'\right|\hat{U}_s(t,t_0)\left|\left|a'\right\rangle\right\rangle\right|^2$$

Because

$$\langle b'|\hat{U}_I(t,t_0)|a'\rangle = \sum_{n,m} \langle b'|e^{\frac{i}{\hbar}\hat{H}_0 t}|n\rangle\langle n|\hat{U}_s(t,t_0)e^{-\frac{i}{\hbar}\hat{H}_0 t_0}|a'\rangle$$

$$= \sum_{n,m} e^{\frac{i}{\hbar}(E_n t - E_m t_0)}\langle b'|n\rangle\langle n|\hat{U}_s(t,t_0)|m\rangle\langle m|a'\rangle$$

29.18 Application of Schrödinger and Heisenberg pictures

Simple harmonics:

$$\hat{U} = e^{-\frac{i}{\hbar}\hat{H}t}$$

The operator in the Heisenberg picture is defined by

$$\hat{A}_H = \hat{U}^+\hat{A}_s\hat{U} = e^{\frac{i}{\hbar}\hat{H}t}\hat{A}_s e^{-\frac{i}{\hbar}\hat{H}t}$$

where $\hat{H}$ is the Hamiltonian

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

Using the equation of Heisenberg picture, we obtain

$$\hat{x}_H = \hat{x}\cos\omega t + \frac{1}{m\omega}\hat{p}\sin\omega t`$$

and

$$\hat{p}_H = \hat{p}\cos\omega t - m\omega\hat{x}\sin\omega t$$

The matrix of $\hat{x}$ and $\hat{p}$ are given by

$$\hat{x} = \frac{1}{\sqrt{2}\beta}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & \sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix}$$

and

$$\hat{p} = \frac{m\omega_0}{\sqrt{2}i\beta}\begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \\ -\sqrt{1} & 0 & \sqrt{2} & 0 & 0 & \\ 0 & -\sqrt{2} & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & -\sqrt{3} & 0 & \sqrt{4} & \\ 0 & 0 & 0 & -\sqrt{4} & 0 & \\ & & \vdots & & & \end{pmatrix}$$

((**Discussion**))

What are the expectation values $\langle\psi(t)|\hat{x}|\psi(t)\rangle$ and $\langle\psi(t)|\hat{p}|\psi(t)\rangle$?

$$\begin{aligned}\langle\psi(t)|\hat{x}|\psi(t)\rangle &= \langle\psi(0)|\hat{x}_H|\psi(0)\rangle \\ &= \langle\psi(0)|\hat{x}\cos\omega t + \frac{1}{m\omega}\hat{p}\sin\omega t|\psi(0)\rangle \\ &= \langle\psi(0)|\hat{x}|\psi(0)\rangle\cos\omega t + \frac{1}{m\omega}\langle\psi(0)|\hat{p}|\psi(0)\rangle\sin\omega t\end{aligned}$$

$$\begin{aligned}\langle\psi(t)|\hat{p}|\psi(t)\rangle &= \langle\psi(0)|\hat{p}_H|\psi(0)\rangle \\ &= \langle\psi(0)|\hat{p}\cos\omega t - m\omega\hat{x}\sin\omega t|\psi(0)\rangle \\ &= \langle\psi(0)|\hat{p}|\psi(0)\rangle\cos\omega t - m\omega\langle\psi(0)|\hat{x}|\psi(0)\rangle\sin\omega t\end{aligned}$$

Suppose that

(1) $\quad |\psi(0)\rangle = \frac{1}{\sqrt{6}}(|0\rangle + 2|1\rangle + |2\rangle)$

we can calculate the matrix elements $\langle\psi(0)|\hat{x}|\psi(0)\rangle$ and $\langle\psi(0)|\hat{p}|\psi(0)\rangle$ as follows.

$$\begin{aligned}\langle\psi(0)|\hat{x}|\psi(0)\rangle &= \begin{pmatrix}\frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}}\end{pmatrix}\frac{1}{\sqrt{2}\beta}\begin{pmatrix}0 & 1 & 0 \\ 1 & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{6}}\end{pmatrix} \\ &= \frac{1}{\sqrt{2}\beta}\frac{2}{3}(1+\sqrt{2})\end{aligned}$$

$$\langle\psi(0)|\hat{p}|\psi(0)\rangle = \begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{pmatrix} \frac{m\omega_0}{\sqrt{2}\beta i} \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{6}} \\ \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{6}} \end{pmatrix} = 0$$

(2) $$|\psi(0)\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right)$$

$$\langle\psi(0)|\hat{x}|\psi(0)\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \frac{1}{\sqrt{2}\beta} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}\beta}$$

$$\langle\psi(0)|\hat{p}|\psi(0)\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \frac{1}{\sqrt{2}\beta} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = 0$$

$$\langle\psi(t)|\hat{x}|\psi(t)\rangle = \frac{1}{\sqrt{2}\beta}\cos\omega t$$

and

$$\langle\psi(t)|\hat{p}|\psi(t)\rangle = -\frac{m\omega}{\sqrt{2}\beta}\sin\omega t$$

[[**Another method (Schrödinger picture)**]]

$$\begin{aligned} |\psi(t)\rangle &= e^{-i\hat{H}t/\hbar}\frac{1}{\sqrt{2}}\left(|0\rangle + |1\rangle\right) \\ &= \frac{1}{\sqrt{2}}\left(e^{-iE_0 t/\hbar}|0\rangle + e^{-iE_1 t/\hbar}|1\rangle\right) \\ &= \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-iE_0 t/\hbar} \\ e^{-iE_1 t/\hbar} \end{pmatrix} \end{aligned}$$

$$\langle\psi(t)| = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{iE_0 t/\hbar} & {}^{iE_1 t/\hbar} \end{pmatrix}$$

$$\langle\psi(t)|\hat{x}|\psi(t)\rangle = \left(\frac{1}{\sqrt{2}}\right)^2 \frac{1}{\sqrt{2}\beta}\left(e^{iE_0t/\hbar} \quad {}^{iE_1t/\hbar}\right)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} e^{-iE_0t/\hbar} \\ e^{-iE_1t/\hbar} \end{pmatrix}$$

$$= \frac{1}{2}\frac{1}{\sqrt{2}\beta}\left(e^{iE_0t/\hbar} \quad {}^{iE_1t/\hbar}\right)\begin{pmatrix} e^{-iE_1t/\hbar} \\ e^{-iE_0t/\hbar} \end{pmatrix}$$

$$= \frac{1}{2}\frac{1}{\sqrt{2}\beta}(e^{i\omega_0 t} + e^{-i\omega_0 t}) = \frac{1}{\sqrt{2}\beta}\cos\omega_0 t$$
