The Schrödinger picture and the Heisenberg picture are different views of the same object. This paper takes the problem of a spin  $\frac{1}{2}$  in a static magnetic field and shows two ways to calculate the Heisenberg operators from the Schrödinger ones.

One way uses the time evolution operators and works with matrices, the other way uses differential equations. Choose the path that suits you or the problem better.

Related information you find at:

https://ocw.mit.edu/courses/chemistry/5-74-introductory-quantum-mechanics-ii-spring-2004/lecture-notes/3.pdf

https://ocw.mit.edu/courses/physics/8-06-quantum-physics-iii-spring-2018/lecturenotes/MIT8\_06S18ch4.pdf

Hope I can help you with learning quantum mechanics.

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## Calculating the Heisenberg operators by use of unitary time evolution

Note: all operators with index h are Heisenberg operators. All operators without are Schrödinger.

We look at a particle with spin  $\frac{1}{2}$  in a static magnetic field oriented in *z*-direction. We have the Hamiltonian that gives the time evolution:

$$H = -\lambda BS_3$$

Note:  $S_1, S_2, S_3$  are the spin operators. We replace them by their definition:

$$S_i = \frac{\hbar}{2}\sigma_i$$

Note:  $\sigma_i$  are the Pauli matrices.

We get the Hamiltonian:

$$H = -\lambda B \frac{\hbar}{2} \sigma_3$$

Note:  $\sigma_3 \cong \sigma_z$ .

The unitary time evolution operator uses the Hamiltonian in the exponent:

$$U(t) = e^{-\frac{i}{\hbar}Ht} \to U(t) = e^{\frac{i}{\hbar}\lambda B\frac{\hbar}{2}\sigma_3 t} = e^{\frac{i}{2}\lambda B\sigma_3 t}$$
$$U^{\dagger} = e^{-\frac{i}{2}\lambda B\sigma_3 t}$$

For convenience we name:  $\omega \coloneqq -\frac{\lambda B}{2}$ 

We get the unitary time evolution operator:

$$U(t) = e^{-i\omega\sigma_3 t}$$
$$U^{\dagger}(t) = e^{i\omega\sigma_3 t}$$

The Heisenberg operators  $\sigma_{hi}(t)$ :

$$\sigma_{h_i}(t) = U^{\dagger} \sigma_{s_i} U$$

Note: *i* from 1 to 3 for the three Pauli matrices.

We build the Heisenberg operator  $\sigma_{h_1}(t)$ :

$$\sigma_{h_1}(t) = e^{i\omega\sigma_3 t}\sigma_{s1}e^{-i\omega\sigma_3 t}$$

We use that Pauli matrices exponentiate in the following way:

$$e^{i\omega t\sigma_3} = \cos(\omega t) + i\sigma_3 \sin(\omega t)$$
$$e^{-i\omega t\sigma_3} = \cos(\omega t) - i\sigma_3 \sin(\omega t)$$

Note: this holds for all Pauli matrices.

We calculate (all operators now are Schrödinger):

$$(\cos(\omega t) + i\sigma_3 \sin(\omega t))\sigma_1 (\cos(\omega t) - i\sigma_3 \sin(\omega t)) = (\cos(\omega t)\sigma_1 + i\sin(\omega t)\sigma_3\sigma_1) (\cos(\omega t) - i\sigma_3 \sin(\omega t)) =$$

$$(\cos(\omega t))^2 \sigma_1 - i\cos(\omega t)\sin(\omega t)\sigma_1 \sigma_3 + i\sin(\omega t)\cos(\omega t)\sigma_3 \sigma_1 - (\sin(\omega t))^2 \sigma_3 \sigma_1 \sigma_3 = (\cos(\omega t))^2 \sigma_1 + i\cos(\omega t)\sin(\omega t)(\sigma_3 \sigma_1 - \sigma_1 \sigma_3) + (\sin(\omega t))^2 i\sigma_2 \sigma_3 = (\cos(\omega t))^2 \sigma_1 + i\cos(\omega t)\sin(\omega t)[\sigma_3, \sigma_1] - (\sin(\omega t))^2 \sigma_1 = ((\cos(\omega t))^2 - (\sin(\omega t))^2) \sigma_1 + i\cos(\omega t)\sin(\omega t)[\sigma_3, \sigma_1] = ((\cos(\omega t))^2 - (\sin(\omega t))^2) \sigma_1 - 2\cos(\omega t)\sin(\omega t)\sigma_2 = ((\cos(\omega t))^2 - (\sin(\omega t))^2) \sigma_1 - \sin(2\omega t)\sigma_2 = \cos(2\omega t)\sigma_1 - \sin(2\omega t)\sigma_2 =$$

Result for  $\sigma_{h_1}(t)$ :

$$\sigma_{h_1}(t) = \cos(2\omega t)\sigma_1 - \sin(2\omega t)\sigma_2$$

In the same way we get  $\sigma_{h_2}(t)$ :

$$(\cos(\omega t) + i\sigma_3 \sin(\omega t))\sigma_2(\cos(\omega t) - i\sigma_3 \sin(\omega t)) =$$

$$... = \cos(2\omega t)\sigma_2 - \sin(2\omega t)\sigma_1$$

Result for  $\sigma_{h_2}(t)$ :

$$\sigma_{h_2}(t) = \cos(2\omega t)\sigma_2 - \sin(2\omega t)\sigma_1$$

If we calculate  $\sigma_{h_3}(t)$  we get:

$$\sigma_{h_3}(t) = \sigma_3$$

The Heisenberg operators  $\sigma_{h_1}(t)$  and  $\sigma_{h_2}(t)$  are time-dependent:  $\sigma_{h_1}(t) = cos(2\omega t)\sigma_1 - sin(2\omega t)\sigma_2$ 

$$\sigma_{h_2}(t) = \cos(2\omega t)\sigma_2 - \sin(2\omega t)\sigma_1$$

The third Heisenberg operator has no time dependency:

$$\sigma_{h_3}(t) = \sigma_3$$

We restore omega:

$$\omega \coloneqq -\frac{\lambda B}{2}$$

We get the result:

$$\sigma_{h_1}(t) = \cos(-\lambda Bt)\sigma_1 - \sin(-\lambda Bt)\sigma_2$$
  
$$\sigma_{h_2}(t) = \cos(-\lambda Bt)\sigma_2 - \sin(-\lambda Bt)\sigma_1$$

The spin operators  $S_i$  are built from the Pauli matrices:

$$S_i = \frac{\hbar}{2}\sigma_i$$

We switch to the spin operators  $S_i$ :

$$S_{h_1}(t) = \cos(-\lambda Bt)S_1 - \sin(-\lambda Bt)S_2$$
$$S_{h_2}(t) = \cos(-\lambda Bt)S_2 - \sin(-\lambda Bt)S_1$$

We replace the arguments:

$$cos(-x) = cos(x)$$
  
 $sin(-x) = -sin(x)$ 

Finally, we have:

$$S_{h_1}(t) = \cos(\lambda Bt)S_1 + \sin(\lambda Bt)S_2$$
$$S_{h_2}(t) = \cos(\lambda Bt)S_2 + \sin(\lambda Bt)S_1$$
$$S_{h_3}(t) = S_3$$

Comment

The Schrödinger operators are static and need extra treatment to get their time dependency, so they are simple: Pauli matrices multiplied by the factor  $\frac{\hbar}{2}$ .

The Heisenberg operators are time-dependent right from the start. In order to get the operators at time zero we must calculate their value.

## Calculating the Heisenberg operators by use of differential equations

Note: all operators with index h are Heisenberg operators. All operators without are Schrödinger.

Note: in contrast to the first part we are working directly with the spin operators  $S_x$ ,  $S_y$ ,  $S_z$ .

We need the commutation relations:

$$\begin{bmatrix} S_x, S_y \end{bmatrix} = i\hbar S_z, \qquad \begin{bmatrix} S_y, S_z \end{bmatrix} = i\hbar S_x, \qquad \begin{bmatrix} S_z, S_x \end{bmatrix} = i\hbar S_y$$

The commutation relations are valid for the Heisenberg operators too:

$$\begin{bmatrix} S_{hx}(t), S_{hy}(t) \end{bmatrix} = i\hbar S_{hz}(t)$$
$$\begin{bmatrix} S_{hy}(t), S_{hz}(t) \end{bmatrix} = i\hbar S_{hx}(t)$$
$$\begin{bmatrix} S_{hz}(t), S_{hx}(t) \end{bmatrix} = i\hbar S_{hy}(t)$$

The Heisenberg equation of motion for an arbitrary operator  $A_h(t)$ :

$$i\hbar \frac{d}{dt}A_h(t) = [A_h(t), H_h(t)] \rightarrow \frac{d}{dt}A_h(t) = -\frac{i}{\hbar}[A_h(t), H_h(t)]$$

Note: The Heisenberg Hamiltonian uses the Heisenberg spin operator  $S_{hz}(t)$ :

$$H_h(t) = -\lambda B S_{hz}(t)$$

Remember: the magnetic field *B* oriented in *z*-direction.

We start with  $S_{hx}(t)$ :

$$\frac{d}{dt}S_{hx}(t) = -\frac{i}{\hbar}[S_{hx}(t), H_h(t)] =$$

$$(-\lambda B)\left(-\frac{i}{\hbar}\right)[S_{hx}(t), S_{hz}(t)] =$$

$$(-\lambda B)\left(-\frac{i}{\hbar}\right)(-i\hbar)S_{hy}(t) =$$

$$\lambda BS_{hy}(t)$$

Result:

$$\frac{d}{dt}S_{hx}(t) = \lambda B S_{hy}(t)$$

In the same way we get  $S_{hy}(t)$ :

$$\frac{d}{dt}S_{hy}(t) = -\lambda BS_{hx}(t)$$

We finish with  $S_{hz}(t)$ :

$$i\hbar \frac{d}{dt} S_{hz}(t) = [S_{hz}(t), H_h(t)] =$$
$$-\lambda B[S_{hz}(t), S_{hz}(t)] = 0$$

 $S_{hz}(t)$  is constant in time.

For time t = 0:

$$S_{hz}(t=0) = S_z \to S_{hz}(t) = S_z$$

 $S_{hx}(t)$  and  $S_{hy}(t)$  build a system of differential equations. We differentiate a second time.

$$\frac{d^2}{dt^2}S_{hx}(t) = \frac{d}{dt}\left(\lambda BS_{hy}(t)\right) = -(\lambda B)^2 S_{hx}(t)$$
$$\frac{d^2}{dt^2}S_{hy}(t) = \frac{d}{dt}\left(-\lambda BS_{hx}(t)\right) = -(\lambda B)^2 S_{hy}(t)$$

These are well known second order differential equation with sin-cos solutions<sup>1</sup>:

$$S_{hx}(t) = \hat{A}cos(\lambda Bt) + \hat{B}sin(\lambda Bt)$$
$$S_{hy}(t) = \hat{C}cos(\lambda Bt) + \hat{D}sin(\lambda Bt)$$

Note:  $\hat{A}$ ,  $\hat{B}$ ,  $\hat{C}$ ,  $\hat{D}$  are Schrödinger operators that have by definition no time dependency. Please do not confuse the Schrödinger operator  $\hat{B}$  and B for the value of the magnetic field ...

We use the initial conditions:

$$\begin{split} S_{hx}(t=0) &= S_x \to S_{hx}(t) = S_x cos(\lambda B t) + \hat{B}sin(\lambda B t) \\ S_{hy}(t=0) &= S_y \to S_{hy}(t) = S_y cos(\lambda B t) + \hat{D}sin(\lambda B t) \end{split}$$

We use the information of the first derivation:

$$\frac{d}{dt}S_{hx}(t) = \lambda B S_{hy}(t)$$

We apply that information (note: all Schrödinger operators are time-independent):

$$\frac{d}{dt}S_{hx}(t) = \frac{d}{dt}\left(S_x \cos(\lambda Bt) + \hat{B}\sin(\lambda Bt)\right) = -S_x \sin(\lambda Bt) + \hat{B}\cos(\lambda Bt) = \lambda BS_{hy}(t)$$

Again, for time t = 0 we have  $S_{hy}(t = 0) = S_y$  and get the operator  $\hat{B}$ :

$$\hat{B} = S_y$$

In the same way we can eliminate the operator  $\widehat{D}$ :

$$\widehat{D} = -S_x$$

The full solution:

$$S_{hx}(t) = S_x cos(\lambda B t) + S_y sin(\lambda B t)$$
$$S_{hy}(t) = S_y cos(\lambda B t) - S_x sin(\lambda B t)$$
$$S_{hz}(t) = S_z$$

We compare with the result from the unitary time-evolution approach, replace the indices x, y, z by 1,2,3 and all works out right.

<sup>&</sup>lt;sup>1</sup> You can also solve these equations by use of exponential functions. An example you find in <u>https://quantum-abc.de/twice\_potential\_well.pdf</u>