1 Heisenberg Representation

What we have been dealing with so far is called the **Schrödinger** representation. In this representation, operators are constants and all the time dependence is carried by the states. We have

$$|\Psi(t)>= U(t)|\Psi(0)>$$

where

$$U(t) = \exp(-\frac{i}{\hbar}Ht)$$

A matrix element of an operator is then

$$<\Psi(t)|O|\Psi(t)>$$

where O is an operator constructed out of position and momentum operators. To contrast the Schrödinger representation with the Heisenberg representation (to be introduced shortly) we will put a subscript on operators in the Schrödinger representation, so we have X_S, P_S, and O_S. We may then write our matrix element as

$$<\Psi(t)|O_S|\Psi(t)>=<\Psi(0)|U^\dagger(t)O_S U(t)|\Psi(0)>$$

The Heisenberg representation uses time dependent operators and constant in time states. We define the Heisenberg operator by

$$O_H(t) = U^\dagger(t)O_S U(t)$$

The two representations are clearly completely equivalent, and it is a matter of convenience which one is used in a given problem.

Once we have defined Heisenberg operators, we may study their equations of motion and compare to the corresponding classical equations of motion. We will carry through the discussion for a $d = 1$ system where the x coordinate ranges $-\infty$ to $+\infty$. We start with the classical discussion. There is a Lagrangian

$$L = \frac{m}{2}(\frac{dx}{dt})^2 - V(x),$$

with generalized momentum

$$p = \frac{\partial L}{\partial \dot{x}}$$

where $\dot{x} = dx/dt$. From the Lagrangian we construct a *classical* Hamiltonian,

$$H_c = p\dot{x} - L = \frac{p^2}{2m} + V(x)$$

From the classical Hamiltonian, we get classical equations of motion,

$$\dot{x} = \frac{\partial H_c}{\partial p} = \frac{p}{m} \quad \dot{p} = -\frac{\partial H_c}{\partial x} = -\frac{\partial V}{\partial x}$$

Quantizing the system involves introducing operators X_S, and P_S, which satisfy

$$[X_S, P_S] = i\hbar.$$

The quantum Hamiltonian is

$$H = \frac{P_S P_S}{2m} + V(X_S),$$

and the Heisenberg operators

$$X_H(t) = \exp(\frac{i}{\hbar}Ht)X_S \exp(-\frac{i}{\hbar}Ht),$$

and

$$P_H(t) = \exp(\frac{i}{\hbar}Ht)P_S \exp(-\frac{i}{\hbar}Ht).$$

The quantum or Heisenberg equations of motion are

$$\frac{d}{dt}X_H(t) = \frac{i}{\hbar}[H, X_H(t)]$$

and

$$\frac{d}{dt}P_H(t) = \frac{i}{\hbar}[H, P_H(t)].$$

Note that H being constant is the same in Heisenberg and Schrödinger representations,

$$H = \frac{P_S P_S}{2m} + V(X_S) = \frac{P_H P_H}{2m} + V(X_H)$$

Now consider the Heisenberg equation for X_H. We have

$$\frac{d}{dt}X_H(t) = \frac{i}{\hbar}[H, X_H(t)] = \frac{i}{\hbar}U^\dagger(t)[H, X_S]U(t)$$

Now

$$[H, X_S] = [\frac{P_S P_S}{2m} + V(X_S), X_S] = [\frac{P_S P_S}{2m}, X_S] + [V(X_S), X_S]$$

Since every operator commutes with itself,

$$[V(X_S), X_S] = 0,$$

and we are left with

$$[\frac{P_S P_S}{2m}, X_S] = \frac{1}{2m}(P_S P_S X_S - X_S P_S P_S) = \frac{\hbar}{i}\frac{P_S}{m},$$

where we used $[X_S, P_S] = i\hbar$. Putting the pieces together, we have

$$\frac{d}{dt}X_H(t) = \frac{i}{\hbar}U^\dagger(t)\frac{\hbar}{i}\frac{P_S}{m}U(t) = \frac{P_H(t)}{m} \tag{1}$$

which is the same as the classical result for dx/dt.

Now let us get the Heisenberg equation of motion for P_H. We have

$$\frac{d}{dt}P_H(t) = \frac{i}{\hbar}[H, P_H(t)] = \frac{i}{\hbar}U^\dagger[V(X_S), P_S]U,$$

where we used the fact that P_S commutes with itself. To get $[V(X_S), P_S]$, we first take a matrix element and write

$$< x|[V(X_S), P_S]|\Psi >=< x|(V(X_S)P_S - P_S V(X_S))|\Psi >$$

$$= V(x)\frac{\hbar}{i}\partial_x < x|\Psi > - \frac{\hbar}{i}(\partial_x V(x) < x|\Psi >)$$

$$= -\frac{\hbar}{i}(\partial_x V(x)) < x|\Psi >= -\frac{\hbar}{i} < x|\frac{\partial V(X_S)}{\partial X_S}|\Psi >$$

So we have

$$< x|[H, P_S]|\Psi >= -\frac{\hbar}{i} < x|\frac{\partial V(X_S)}{\partial X_S}|\Psi >$$

Since $< x|$ and $|\Psi >$ were arbitrary, we can write the operator equation

$$[H, P_S] = -\frac{\partial V(X_S)}{\partial X_S}$$

Returning to the equation for dP_H/dt, we now have

$$\frac{d}{dt}P_H(t) = -U^\dagger(t)\frac{\partial V(X_S)}{\partial X_S}U(t) = -\frac{\partial V(X_H)}{\partial X_H}, \tag{2}$$

which again is the quantum version of the classical equation for dp/dt. It is generally true in a quantum system that the Heisenberg equations of motion for operators agree with the corresponding classical equations. An important example is Maxwell's equations. These remain true quantum mechanically, with the fields and vector potential now quantum (field) operators.

Application to Harmonic Oscillator In this section, we will look at the Heisenberg equations for a harmonic oscillator. The notation in this section will be $O(t)$ for a Heisenberg operator, and just O for a Schrödinger operator. In terms of the notation of the previous section we have $O_S = O$, and $O_H(t) = O(t)$. Of course we have $O(0) = O$. The Hamiltonian for the oscillator is

$$H = \frac{PP}{2m} + \frac{m\omega_0^2 X^2}{2}, \tag{3}$$

where ω_0 is the natural frequency of the oscillator. The equations of motions for the Heisenberg operators are as follows,

$$\frac{dX(t)}{dt} = \frac{P(t)}{m}, \quad \frac{dP(t)}{dt} = -m\omega_0^2 X(t)$$

As always, the Heisenberg equations for operators are the same as the classical equations of motion. Taking a second time derivative, we have

$$\frac{d^2X(t)}{dt^2} = \frac{1}{m}\frac{dP(t)}{dt} = -\omega_0^2 X(t)$$

This is a differential equation for $X(t)$. We can certainly solve it as a linear combination of $\sin\omega_0 t$ and $\cos\omega_0 t$. We can write

$$X(t) = A\cos\omega_0 t + B\sin\omega_0 t,$$

where A, B are operators which are independent of t. At $t = 0$, we must have $X(0) = X$, so we get that

$$A = X.$$

Also from Eq.(3), we have

$$\frac{dX(t)}{dt}|_{t=0} = \frac{P}{m} = \omega_0 B,$$

so

$$B = \frac{P}{m\omega_0}.$$

We finally have

$$X(t) = X\cos\omega_0 t + \frac{P}{m\omega_0}\sin\omega_0 t. \tag{4}$$

Similar steps lead to

$$P(t) = P\cos\omega_0 t = m\omega_0 X\sin\omega_0 t. \tag{5}$$

Matrix Elements and Energy Levels The expressions for $X(t), P(t)$ look so much like their classical counterparts, it might seem unlikely that they contain information about energy levels and matrix elements. As will be seen, they in fact contain a large amount of such information. Suppose the Hamiltonian has an eigenstate $|n>$ with energy E_n and another eigenstate $|n'>$ with energy $E_{n'}$. Let us write out the matrix element of $X(t)$. We have

$$< n'|X(t)|n >=< n'|\exp(\frac{iHt}{\hbar})X\exp(\frac{-iHt}{\hbar})|n >= \exp(\frac{i(E_{n'} - E_n)t)}{\hbar} < n'|X|n > . \tag{6}$$

This is the matrix element of the left hand side of Eq.(4). Using exponential forms for sin and cos we have for the matrix element of the right hand side,

$$\frac{1}{2}\left(e^{i\omega_0 t}(< n'|X|n > -i < n'|\frac{P}{m\omega_0}|n >) + e^{-i\omega_0 t}(< n'|X|n > +i < n'|\frac{P}{m\omega_0}|n >)\right). \tag{7}$$

Eqs.(6) and (7) must match in detail. Let us start with the case $E_{n'} > E_n$. Then comparing time dependent factors on both sides, the coefficient of $\exp(-i\omega_0 t)$ must vanish, since there is no term of that form in Eq.(6). This gives

$$< n'|X|n > +i < n'|\frac{P}{m\omega_0}|n >= 0. \tag{8}$$

Now matching the coefficient of $\exp(i\omega_0 t$, we also must have

$$\exp(\frac{i(E_{n'} - E_n)t)}{\hbar}) = \exp(i\omega_0 t)$$

This result implies that if $< n'|X|n > \neq 0$, then

$$E_{n'} = E_n + \hbar\omega_0.$$

Let us assume such a state exists. Now apply the same argument to the matrix element

$$< n''|X(t)|n' > .$$

We find again, if $E_{n''} > E_{n'}$ that

$$E_{n''} = E_{n'} + \hbar\omega_0,$$

provided only that $< n''|X|n' > \neq 0$. Using this argument repeatedly, we find a sequence of levels $E_n, E_n + \hbar\omega_0, E_n + 2\hbar\omega_0, \ldots, E_n + l\hbar\omega_0$, with no upper limit on l, provided only that the matrix element of X between a state and the next one higher up is non-vanishing. We will return to the question of which matrix elements of X are non-vanishing later in this section. Before doing that, we explore the case where $E_{n'} < E_n$. Returning to Eqs.(6) and (7), this time the coefficient of $\exp(i\omega_0)t$ must vanish, giving

$$< n'|X|n > -i < n'|\frac{P}{m\omega_0}|n >= 0. \tag{9}$$

The coefficient of $\exp(-i\omega_0 t)$ must match on both sides, so we get

$$E_{n'} = E_n - \hbar\omega_0,$$

so we have found a state with energy one unit of $\hbar\omega_0$ lower, provided that $< n'|X|n > \neq 0$. At first sight it would seem that this process could be repeated indefinitely. However, this would eventually result in the energy eigenvalue going negative. But this is impossible. Consider the expected value of H in a state $|\Psi >$. Writing this out in Hilbert space notation instead of Dirac notation, we have

$$(\Psi, H\Psi) = \frac{1}{2m}(\Psi, PP\Psi) + \frac{1}{2}m\omega_0^2(\Psi, XX\Psi) = \frac{1}{2m}(P\Psi, P\Psi) + \frac{1}{2}m\omega_0^2(X\Psi, X\Psi). \tag{10}$$

Each term on the right side of Eq.(10) is certainly positive, regardless of the particular state. The consequence is that H can have no negative eigenvalues. This means that the argument we have been using cannot generate an infinite sequence of levels below a given one, but it is allowed to generated an infinite sequence above a given one. The consequence is that there must be a lowest state, which we denote as $|0 >$. It is then natural to designate the sequence of levels upward from $|0 >$ as $|n >$, where

$$E_n = E_0 + n\hbar\omega_0,$$

where n is any positive integer.

Finally, let us explore the question of which matrix elements of X and P are non-vanishing. We start with the lowest state, $|0>$. By the discussion just given, both X and P, acting on $|0>$, must lead to a state of higher energy. Let us take matrix elements between $|0>$ and $|1>$. This puts us in the case covered by Eq.(8) so we have

$$< 1(|X + i\frac{P}{m\omega_0})|0 >= 0. \tag{11}$$

This relates matrix elements of X and P. To get a more powerful result, we consider matrix elements between $|0>$ and $|n>$ for $n > 1$. It is easy to see that all such matrix elements of X and P must vanish, since the matrix elements $< n|X(t)|0 >$ and $< n|P(t)|0 >$ have time dependence $\exp(in\omega_0)t)$. But from Eqs.(4) and (5), the only allowed frequency for the matrix element of a state higher in energy is ω_0. (This result holds more generally, namely the matrix elements of X and P are only non-vanishing between a state and the next one up or down in energy.) Now consider the expression

$$(X + i\frac{P}{m\omega_0})|0 >$$

From Eq.(11) it has no matrix element to $|1>$, and since the matrix elements of both X and P vanish for any higher state, we have that

$$(X + i\frac{P}{m\omega_0})|0 >= 0 \tag{12}$$

We can apply any operator to Eq.(12) and still get a vanishing result, so we also have

$$(X - i\frac{P}{m\omega_0})(X + i\frac{P}{m\omega_0})|0 >= 0 \tag{13}$$

Multiplying this out we get

$$\left\{XX + \frac{PP}{(m\omega_0)^2} + \frac{i}{m\omega_0}[X, P]\right\}|0 >= 0 \tag{14}$$

Supplying a factor $m\omega_0^2/2$ and using $[X, P] = i\hbar$, we finally have

$$(H - \frac{\hbar\omega_0}{2})|0 >= 0 \tag{15}$$

or

$$E_0 = \frac{\hbar\omega_0}{2}$$

To summarize, we have found the entire sequence of energy levels of the harmonic oscillator. It is also easy to show that X and P only have matrix elements between $|n>$ and $|n \pm 1>$, except for $n = 0$, where the only non vanishing matrix elements are to $|1>$. A little more work of the same sort done above will deliver the actual values of these matrix elements. This exercise shows that Heisenberg methods can be quite powerful in certain cases.