1 Heisenberg’s Intuition

Before arriving at his now famous matrix mechanics, Heisenberg first needed to find relevant classical equations and then modify them to work at quantum levels. In doing this, Heisenberg used Bohr’s Correspondence principle as his guide. In particular, it was known that
\[ w_{mn} = E_m - E_n \] (1)
where \( w \) is the frequency of an emitted photon and \( E_m - E_n \) is the difference in energy levels. This was a simple statement of conservation of energy. Also of great importance to Heisenberg was the Rydberg-Ritz Combination Principle, which can be written as
\[ w_{mn} = w_{mk} + w_{kn}. \] (2)

Heisenberg began with the classical representation of periodic motion, a Fourier series, the squaring of which yields
\[ X(t)^2 = \sum_a \sum_b x_a x_b e^{i w_n (a+b)t}. \] (3)

Now, let \( a + b = B \) and let \( Y_B = \sum_a x_a x_{B-a} \). Then equation 3 will read
\[ X(t)^2 = \sum_B Y_B e^{i w_n B t}. \] (4)

At this point, Heisenberg needed to adapt this classical equation of motion as he could no longer assume that the frequencies added in the same way as in classical mechanics. Hence, he modified the equation to fit with the Rydberg-Ritz Combination Principle and obtained
\[ Y_{n,n-B} = \sum_a x_{n,n-a} x_{n-a,n-B} \] (5)
which is matrix multiplication. However, Heisenberg did not recognize this immediately and it was actually Born who noticed that Heisenberg’s equation was really that of a matrix.
2 Commutator of Position and Momentum

From equation (5), it was clear to Heisenberg that the equations for the position and momentum operators are

\[ X(t) = x_{mn}e^{i\omega_{mn}t}n, m \geq 0 \]  

(6)

and

\[ P(t) = p_{mn}e^{i\omega_{mn}t}n, m \geq 0. \]  

(7)

Note that these are matrices as they have values for all \( m, n > 0 \). Differentiating these equations gives

\[ \frac{d}{dt}X(t) = i\omega_{mn}x_{mn}e^{i\omega_{mn}t} = \frac{i}{\hbar}(E_m - E_n)x_{mn}e^{i\omega_{mn}t} = \frac{i}{\hbar}(E_m - E_n)X(t) \]  

(8)

and

\[ \frac{d}{dt}P(t) = i\omega_{mn}p_{mn}e^{i\omega_{mn}t} = \frac{i}{\hbar}(E_m - E_n)p_{mn}e^{i\omega_{mn}t} = \frac{i}{\hbar}(E_m - E_n)P(t). \]  

(9)

Now, note that if we have a diagonal matrix given by

\[
E = \begin{bmatrix}
E_1 & 0 & 0 & 0 & 0 & \cdots \\
0 & E_2 & 0 & 0 & 0 & \cdots \\
0 & 0 & E_3 & 0 & 0 & \cdots \\
0 & 0 & 0 & E_4 & 0 & \cdots \\
0 & 0 & 0 & 0 & E_5 & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots 
\end{bmatrix}
\]

and any matrix for \( X(t) \)

\[
X(t) = \begin{bmatrix}
y_{1,1} & y_{1,2} & y_{1,3} & y_{1,4} & y_{1,5} & \cdots \\
y_{2,1} & y_{2,2} & y_{2,3} & y_{2,4} & y_{2,5} & \cdots \\
y_{3,1} & y_{3,2} & y_{3,3} & y_{3,4} & y_{3,5} & \cdots \\
y_{4,1} & y_{4,2} & y_{4,3} & y_{4,4} & y_{4,5} & \cdots \\
y_{5,1} & y_{5,2} & y_{5,3} & y_{5,4} & y_{5,5} & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots 
\end{bmatrix}
\]

where \( y_{m,n} = x_{mn}e^{i\omega_{mn}t} \), then 

\[-[X(t), E] = \]

\[
\begin{bmatrix}
0 & (E_1 - E_2)y_{1,2} & (E_1 - E_3)y_{1,3} & (E_1 - E_4)y_{1,4} & (E_1 - E_5)y_{1,5} & \cdots \\
(E_2 - E_1)y_{2,1} & 0 & (E_2 - E_3)y_{2,3} & (E_2 - E_4)y_{2,4} & (E_2 - E_5)y_{2,5} & \cdots \\
(E_3 - E_1)y_{3,1} & (E_3 - E_2)y_{3,2} & 0 & (E_3 - E_4)y_{3,4} & (E_3 - E_5)y_{3,5} & \cdots \\
(E_4 - E_1)y_{4,1} & (E_4 - E_2)y_{4,2} & (E_4 - E_3)y_{4,3} & 0 & (E_4 - E_5)y_{4,5} & \cdots \\
(E_5 - E_1)y_{5,1} & (E_5 - E_2)y_{5,2} & (E_5 - E_3)y_{5,3} & (E_5 - E_4)y_{5,4} & 0 & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots 
\end{bmatrix}
\]
which is exactly the same as equation (8). Thus, we have
\[
\frac{d}{dt} X(t) = -\frac{i}{\hbar} [X(t), E] \tag{10}
\]
and
\[
\frac{d}{dt} P(t) = -\frac{i}{\hbar} [P(t), E]. \tag{11}
\]
Next, Heisenberg realized that
\[
E = H(X(t), P(t)) \tag{12}
\]
in which case equation (10) and equation (11) can be written as
\[
\frac{d}{dt} X(t) = -\frac{i}{\hbar} [X(t), H(X(t), P(t))] \tag{13}
\]
and
\[
\frac{d}{dt} P(t) = -\frac{i}{\hbar} [P(t), H(X(t), P(t))] \tag{14}
\]
respectively. Heisenberg postulated that \( \frac{d}{dt} P(t) = f(X(t)) \) held in quantum mechanics where \( f(X(t)) \) is the force. Then, given the Hamiltonian \( H = \frac{P(t)^2}{2} + \frac{k}{m} X(t) \), \( f(X(t)) = -1 \) and
\[
-1 = -\frac{i}{\hbar} [P(t), \frac{P(t)^2}{2} + X(t)] = -\frac{i}{\hbar} ([P(t), X(t)] + [P(t), \frac{P(t)^2}{2}]) \tag{15}
\]
\[
[P(t), \frac{P(t)^2}{2}] = [P(t), P(t)]\frac{P(t)}{2} + P(t)[P(t), \frac{P(t)}{2}] = 0. \tag{16}
\]
Thus
\[
\hbar = [X(t), P(t)] \tag{17}
\]
This equation shows that in quantum mechanics, position and momentum do not commute and this result leads to the Heisenberg uncertainty principle\(^2\).

3 The Simple Harmonic Oscillator

In general, it is rather difficult to solve for the operator of an observable. So, we will look at a simple case, namely, the simple harmonic oscillator. From before, we know that the observables \( Q \) and \( P \) can be written in the form of matrices. Rewriting \( X \) as \( Q \), we have
\[
[Q, P] = QP - PQ = i\hbar I. \tag{18}
\]
Now, if we let \( w = \sqrt{\frac{k}{m}} \), then we can write the Hamiltonian as
\[
H = \frac{P^2}{2m} + \frac{mw^2Q^2}{2}. \tag{19}
\]
Now, let the operators $a$ and $a^\dagger$ be given by:

$$a = \sqrt{\frac{1}{2\hbar}}(\sqrt{mw}Q + \frac{i}{\sqrt{mw}}P)$$  \hspace{1cm} (20)$$

$$a^\dagger = \sqrt{\frac{1}{2\hbar}}(\sqrt{mw}Q - \frac{i}{\sqrt{mw}}P)$$  \hspace{1cm} (21)$$

where $a^\dagger$ is the adjoint of $a^2$. Note that

$$aa^\dagger = \frac{1}{2\hbar}(mwQ^2 + \frac{1}{mw}P^2 + \frac{QP - PQ}{i}) = \frac{1}{2}(\frac{mw}{\hbar}Q^2 + \frac{1}{mw}P^2 + I)$$  \hspace{1cm} (22)$$

and

$$a^\dagger a = \frac{1}{2\hbar}(mwQ^2 + \frac{1}{mw}P^2 + \frac{PQ - PQ}{i}) = \frac{1}{2}(\frac{mw}{\hbar}Q^2 + \frac{1}{mw}P^2 - I)$$  \hspace{1cm} (23)$$

Solving for $H$, we find that

$$H = \frac{wh}{2}(a^\dagger a + \frac{I}{2})$$  \hspace{1cm} (26)$$

and

$$H = \frac{wh}{2}(aa^\dagger - \frac{I}{2})$$.  \hspace{1cm} (27)$$

Now, notice that the commutator of $a$ and $a^\dagger$ is

$$[a, a^\dagger] = I. \hspace{1cm} (28)$$

Using this, the two commutation relations are shown below.

$$[H, a] = [wha^\dagger + \frac{I}{2}, a] = [wha^\dagger, a] = [wha, a]a^\dagger + a[wha^\dagger, a] = -wha$$  \hspace{1cm} (29)$$

$$[H, a^\dagger] = [wha^\dagger + \frac{I}{2}, a^\dagger] = [wha^\dagger, a^\dagger] = [wha, a^\dagger]a^\dagger + a[wha^\dagger, a^\dagger] = wha^\dagger$$  \hspace{1cm} (30)$$

Now, we wish to find the eigenvectors of $H$, which can be written as

$$Hv = \lambda v.$$  \hspace{1cm} (31)$$

If we right multiply equation (29) by $v$, we obtain

$$Hav - aHv = -whav.$$  \hspace{1cm} (32)$$
But $Hv = \lambda v$, so we have

$$Hav = a\lambda v - whav = (a\lambda - wha)v = (\lambda - wh)av.$$  \hfill (33)

Therefore, for any eigenvalue $\lambda$ of $H$, $\lambda - wh$ is also an eigenvalue. Doing the same to equation (30), we obtain

$$Ha^tv = (\lambda + wh)a^tv.$$  \hfill (34)

Now, to see that the Hamiltonian is positive, note that for $v$, an eigenvector,

$$<v, Hv> = \bar{\lambda} <v, v>$$  \hfill (35)

$$<v, Hv> = wh(a^tv + \frac{I}{2})v = wh <v, a^tv> + \frac{wh}{2} <v, v> = wh <av, av> + \frac{wh}{2} <v, v> \geq 0. $$  \hfill (36)

This implies that lambda is real because the right hand side of the equation is real and

$$\lambda <v, v> \geq 0$$

implies that lambda is nonnegative. From this, we can deduce that there exists a $v_0$ such that $av_0 = 0$. If this were not true, then we could continually find lower values using equation (33). Then, we find

$$Hv_0 = wh(a^tv_0 + \frac{v_0}{2}) = \frac{wh}{2}v_0.$$  \hfill (37)

Therefore, the minimum eigenvalue of the Hamiltonian is $\frac{wh}{2}$. By applying equation (34), we find that $\frac{wh}{2} + wh$ is also an eigenvalue. Proceeding inductively, the Hamiltonian takes the form

$$H = wh(n + \frac{1}{2})n \in \mathbb{N}$$  \hfill (38)

or

$$H = \frac{wh}{2}$$

$$\begin{bmatrix}
1 & 0 & 0 & 0 & 0 & \cdots \\
0 & 3 & 0 & 0 & 0 & \cdots \\
0 & 0 & 5 & 0 & 0 & \cdots \\
0 & 0 & 0 & 7 & 0 & \cdots \\
0 & 0 & 0 & 0 & 9 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \cdots & \ddots \\
\end{bmatrix}.$$
References


