QM(2017) Lecture Notes
VI.2 Heisenberg Matrix Mechanics*

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§1 Harmonic Oscillator

Operator algebra for harmonic oscillator

The classical Hamiltonian for harmonic oscillator in one dimension is

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2 \tag{1}$$

The corresponding operator $\hat{H}$ is obtained by replacing the position and momentum x, p by the operators $\hat{x}, \hat{p}$ satisfying canonical commutation relation $[\hat{x}, \hat{p}] = i\hbar$. Note that we will not use any explicit representation of the operators. The commutation relation is sufficient to obtain all the answers.

We introduce operators $N, a, a^\dagger$ by

$$a = \frac{1}{\sqrt{2m\omega\hbar}}(\hat{p} - im\omega\hat{x}), \tag{2}$$

$$a^\dagger = \frac{1}{\sqrt{2m\omega\hbar}}(\hat{p} + im\omega\hat{x}), \tag{3}$$

$$N = a^\dagger a. \tag{4}$$

It is easy to see that these operators satisfy the following identities:

$$[a, a^\dagger] = 1, \qquad [N, a] = -a, \qquad [N, a^\dagger] = a^\dagger, \tag{5}$$

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 = (N + 1/2)\hbar\omega. \tag{6}$$

The last expression in (Eq.(6)) is obtained by expressing the operators $\hat{x}, \hat{p}$ appearing in $\hat{x}^2, \hat{p}^2$ in terms of $a, a^\dagger$, expanding the squares, *maintaining the order of operators carefully* and using the relations (Eq.(5)).

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Eigenvalues of N are non negative

Let ν be an eigenvalue and $|\psi\rangle$ be the corresponding normalized eigenvector:

$$N|\psi\rangle = \nu|\psi\rangle. \tag{7}$$

Taking scalar product[1] with $|\psi\rangle$, we see that $\langle\psi|N|\psi\rangle = \nu$ is positive because

$$\langle\psi|N|\psi\rangle = \langle\psi|a^\dagger a|\psi\rangle = (a\psi, a\psi) = \|a\psi\|^2 \geq 0. \tag{8}$$

The operator a lowers the eigenvalues of N

Let ν be an eigenvalue of N and $|\psi\rangle$ be the corresponding eigenvector as in (Eq.(7)). The operator a act like lowering operator for the eigenvalues of N. The vector $|\phi_1\rangle$, obtained by applying a on $|\psi\rangle$, is an eigenvector of N with eigenvalue $\nu - 1$. To see this consider $N|\phi_1\rangle$

$$\begin{aligned} N|\phi_1\rangle &= Na|\psi\rangle = (aN - a)|\psi\rangle && (9)\\ &= (a\nu - a)|\psi\rangle = (\nu-1)a|\psi\rangle && (10)\\ \therefore N|\phi_1\rangle &= (\nu-1)|\phi_1\rangle. && (11) \end{aligned}$$

Hence $|\phi_1\rangle$, if non zero, is an eigenvector of N with eigenvalue $\nu - 1$. Using this successively, we see that the result $a^n|\psi\rangle$, of applying r powers of a on $|\psi\rangle$ would give an eigenvector of N with eigenvalue $\nu - r$:

$$N\,(\,a^r|\psi\rangle\,) = (\nu - r)\,(\,a^r|\psi\rangle\,). \tag{12}$$

Now there are two possibilities: $a^r|\psi\rangle = 0$ or else if the vector $a^r|\psi\rangle$ is non zero, it is an eigenvector of N with eigenvalue $\nu - r$. since the eigenvalues of N have to be non negative, we must have

$$a^r|\psi\rangle = 0 \text{ for all } r > \nu \tag{13}$$

Taking m to be the maximum integer such that $m < \nu$ we see that

$$a^m|\psi\rangle \neq 0 \quad \text{and} \quad a^{m+1}|\psi\rangle = 0 \tag{14}$$

Using $|0\rangle$ to denote vector obtained from $(a^m|\psi\rangle)$ after normalization, we see that $|0\rangle$ is an eigenvector of N with eigenvalue 0. To see, this consider

$$N|0\rangle = a^\dagger a(a^m|\psi\rangle) = 0 = a^\dagger(a^{m+1}|\psi\rangle) = 0. \tag{15}$$

where (Eq.(14)) has been used in the last step.
To summarize, we have the results that $|0\rangle$ is a normalized eigenvector of N with zero as an eigenvalue and satisfies

$$a|0\rangle = 0. \tag{16}$$

The eigenvalues of N are all non negative integers

We will now show that $(a^\dagger)^r \equiv |\phi_r\rangle$ raises eigenvalue of N by r units. In other words $(a^\dagger)^r|0\rangle$ is an eigenvector of N with eigenvalue r. This proof will be completed by the method of induction.

The give statement is obviously true for $m = 0$. Let us now assume the statement be true for $r = m$, *i.e.* we assume

$$N|\phi_m\rangle = m|\phi_m\rangle. \tag{17}$$

to be true and prove the statement for $r = m + 1$:

$$\begin{aligned} N|\phi_{m+1}\rangle &= N(a^\dagger)^{m+1}|0\rangle = Na^\dagger|\phi_m\rangle \\ &= (a^\dagger N + a^\dagger)|\phi_m\rangle = a^\dagger\,(m+1)|\phi_m\rangle \\ &= (m+1)(a^\dagger|\phi_m\rangle) = (m+1)|\phi_{m+1}\rangle. && (18) \end{aligned}$$

[1] We use (ϕ, χ), as well as Dirac notation $\langle\phi|\chi\rangle$, to denote scalar product of two vectors ϕ, χ.

Therefore, $|\phi_{m+1}\rangle$ is an eigenvector of N with eigenvalue $(m+1)$. To summarize, we have the result that the eigenvalues of N are given by $0, 1, 2, \cdots, m, \cdots$. The corresponding normalised eigenvectors will be denoted by

$$|0\rangle, |1\rangle, |2\rangle, \cdots, |m\rangle, \cdots .$$

These are also eigenvectors of $\hat{H}$, the ket $|n\rangle$ corresponds to the eigenvalue $(n+\frac{1}{2})\hbar\omega$, because

$$\hat{H}|n\rangle = (N+\tfrac{1}{2})\hbar\omega\,|n\rangle = \hbar\omega\left(N|n\rangle + \tfrac{1}{2}|n\rangle\right) = (n+\tfrac{1}{2})\hbar\omega|n\rangle. \tag{19}$$

The third postulate of quantum mechanics tells us that the allowed energies coincide with the eigenvalues of the Hamiltonian. Hence the desired energy levels of of the harmonic oscillator are

$$\boxed{E_n = (n+\tfrac{1}{2})\hbar\omega.} \tag{20}$$

Properties of eigenvectors

Let $|n\rangle$ be the normalised eigenvector of N with eigenvalue n. Action of $a^\dagger$ on $|n\rangle$ gives a vector proportional to $|n+1\rangle$ and we write

$$a^\dagger|n\rangle = c_n|n+1\rangle. \tag{21}$$

The constant c_n can be found by taking the inner product of vector in Eq.(21) with itself. This leads to

$$\langle n|aa^\dagger|n\rangle = |c_n|^2\langle n+1|n+1\rangle = |c_n|^2. \tag{22}$$

The left hand side of Eq.(22) is seen to be $(n+1)$ by computing

$$\begin{aligned} aa^\dagger|n\rangle &= (a^\dagger a+1)|n\rangle, \qquad (\because [a,a^\dagger]=1) \\ &= (N+1)|n\rangle = (n+1)|n\rangle \qquad (23) \\ \therefore \quad \langle n|aa^\dagger|n\rangle &= n+1 \qquad (24) \end{aligned}$$

which when used in Eq.(22) gives $(n+1) = |c_n|^2$ and hence the result

$$\boxed{a^\dagger|n\rangle = \sqrt{(n+1)}|n+1\rangle}. \tag{25}$$

In a similar fashion (verify!) we get

$$\boxed{a|n\rangle = \sqrt{(n-1)}|n-1\rangle}. \tag{26}$$

Recursive use of Eq.(24) leads to the result that all states $|n\rangle$ can be obtained by applying powers of $a^\dagger$ on $|0\rangle$:

$$|n\rangle = \frac{1}{\sqrt{n}}a^\dagger|n-1\rangle = \frac{1}{\sqrt{n(n-1)}}(a^\dagger)^2|n-2\rangle = \cdots = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle. \tag{27}$$

Questions

[1] Writing order of operators carefully, verify Eq.(6).

[2] Use method mathematical induction to show that

$$[x, p^n] = i\hbar n p^{n-1}, \qquad [p, x^n] = -i\hbar n p^{n-1}; \tag{28}$$
$$[N, a^r] = -ra^r, \qquad [N, (a^\dagger)^r] = r(a^\dagger)^r. \tag{29}$$

[3] Use the results in Eq.(29) to show that $(a^\dagger)^r$ raises the eigenvalue of N by r and a^r lowers the eigenvalue by r. (Eq.(12)).

[4] Check carefully if you have followed steps in Eq.(8).

[5] Prove that if eigenvalues of a hermitian operator are positive, its expectation value in every state is positive.

[6] Define eigenvalue and eigenvector of an operator carefully.

[7] Can zero be an eigenvalue? Can null vector be an eigenvector of an operator?

[8] One can always find a large r so that Eq.(13) holds. Is a corresponding statement true for $(a^\dagger)^r$? WHY??

[9] The lowest energy state of harmonic oscillator has non zero energy. This is related to uncertainty relation. The details are given in every text book and must be most frequently asked question in interviews. So if you do not know already this fact, learn from a text book of your choice.

[10] Make a flow chart for this derivation of energy levels of harmonic oscillator.

[11] Remember that c_n in Eq.(22) is a complex number whose absolute value is determined to be $\sqrt{(n+1)}$ and the phase is undetermined. The phase has been taken to be zero and c_n is fixed as real positive constant. Does this matter? WHY?

The issue of fixing phases will be discussed when it is important to address it, otherwise the phase will be taken to be zero.

[12] Simplify $\langle 0|a$, $\langle 0|a^\dagger$, $\langle n|(a)^m$, $\langle n|(a^\dagger)^m$, and find vectors dual to them.

§2 Angular Momentum Eignevalues and Eigenvectors

The operator $\vec{J}^2 = J_x^2 + J_y^2 + J_z^2$ is seen to commute with each of the three angular momentum operator components J_x, J_y, J_z

$$[\vec{J}^2, J_x] = 0, \quad [\vec{J}^2, J_y] = 0, \quad [\vec{J}^2, J_z] = 0, \tag{30}$$

Some useful relations are

$$\begin{aligned} \vec{J}^2 &= \frac{1}{2}(J_+J_- + J_-J_+) + J_z^2, & (31)\\ J_+J_- &= J^2 - J_z^2 + \hbar J_z, & (32)\\ J_-J_+ &= J^2 - J_z^2 - \hbar J_z. & (33) \end{aligned}$$

Details of proofs of the above relations Eq.(30)-(31) are left as an exercise for the reader.

It is seen from Eq.(30) that J^2 commutes with every component of angular momentum. As different components of angular momentum do not commute, J^2 and and any one (not all three) component of $\vec{J}$ can be measured simultaneously and will have complete set of simultaneous orthonormal eigenvectors. Every one chooses to work with J^2, J_z, so do we for our present purposes. However, it should be clear that the results obtained below will apply to every component $\hat{n}\cdot\vec{J}$ where $\hat{n}$ is an arbitrary unit vector. Let us, therefore, assume that $|\psi\rangle$ is an eigenvector of j^2 and J_z with eigenvalues $\lambda\hbar^2$ and $\mu\hbar$ respectively:

$$J^2|\psi\rangle = \lambda\hbar^2|\psi\rangle \qquad J_z|\psi\rangle = \mu\hbar|\psi\rangle. \tag{34}$$

It is to noted that $\hbar$ has dimension of angular momentum, and hence λ and μ will be dimensionless numbers. Our aim is get restrictions on λ, μ and find their permissible values. The results so obtained will apply to any set of operators satisfying the same commutation relations as the components of $\vec{J}$.

Step-I: Use positivity of J_+J_- and J_-J_+ to get bounds on μ

The relation $J_+ = J_-^\dagger$ implies that

$$\begin{aligned}\langle\psi|J_+J_-|\psi\rangle &= (\psi, J_+J_-\psi) = (\psi, (J_-)^\dagger J_-\psi)\\ &= (J_-\psi, J_-\psi) = \|J_-\psi\| \geq 0.\end{aligned} \tag{35}$$

It therefore follows that the operators J_+J_- and J_-J_+ are positive operators in the sense that their expectation values are positive.

$$\langle\psi|J_+J_-|\psi\rangle \geq 0, \qquad \langle\psi|J_-J_+|\psi\rangle \geq 0 \tag{36}$$

Using Eq.(31) in (36) we get

$$\langle\psi|\vec{J}^2 - J_z^2 + \hbar J_z|\psi\rangle \geq 0. \tag{37}$$

Remembering that ψ is a simultaneous eigenvector of J^2 and J_z, Eq.(37) gives

$$\langle\psi|J^2 - J_z^2 + \hbar J_z|\psi\rangle \geq 0 \Rightarrow \lambda - \mu^2 + \mu \geq 0. \tag{38}$$

Similarly, starting with $(\psi, J_-J_+\psi) \geq 0$, we will get

$$\lambda - \mu^2 - \mu \geq 0. \tag{39}$$

The two equations ((38)) and ((39)) give $\mu^2 \leq \lambda$, thus absolute value of J_z is bounded. This result corresponds to the fact that the length of projection of a vector is always less than the length of the vector.

Step-II: J_+ is a raising operator for J_z

The action of J_+ on $|\psi\rangle$ gives a vector $|\phi_1\rangle$ which is also a simultaneous eigenvector of J^2 and J_z with eigenvalues $\lambda\hbar^2$ and $(\mu+1)\hbar$ respectively, *i.e.*,

$$J^2|\phi_1\rangle = \lambda\hbar^2|\phi_1\rangle, \tag{40}$$

and

$$J_z|\phi_1\rangle = (\mu+1)\hbar|\phi_1\rangle. \tag{41}$$

Proof:

$$\begin{aligned}J^2\phi_1 &= J^2(J_+|\psi\rangle)\\ &= (J^2J_+|\psi\rangle \qquad (\because J^2J_+ = J + J^2)\\ &= J_+J^2|\psi\rangle\\ &= J_+(\lambda\hbar^2)|\psi\rangle\end{aligned} \tag{42}$$

Hence

$$J^2|\phi_1\rangle = \lambda\hbar^2 J + |\psi\rangle = \lambda\hbar^2|\phi_1\rangle. \tag{43}$$

Also

$$\begin{aligned}J_z|\phi_1\rangle &= J_z(J_+|\psi\rangle)\\ &= (J_+J_z + \hbar J_+)|\psi\rangle \qquad (\because (J_zJ_+ - J_+J_z) = \hbar J_z)\\ &= (J_+\mu\hbar + \hbar J_+)|\psi\rangle\\ &= (\mu+1)\hbar|\psi\rangle = (\mu+1)\hbar|\phi_1\rangle \therefore \quad J_z|\phi_1\rangle = (\mu+1)\hbar|\phi_1\rangle\end{aligned} \tag{44}$$

Similarly, the states $|\phi_2\rangle = J_+|\phi_1\rangle, |\phi_3\rangle = J_+|\phi_2\rangle \cdots$ obtained by repeated action of J_+ on $|\psi\rangle$, are eigenvectors of J^2 and J_z as given in the table below.

States	Eigenvalue of J^2	Eigenvalue of J_z
$\|\phi_1\rangle = J_+\|\psi\rangle$	$\lambda\hbar^2$	$(\mu+1)\hbar$
$\|\phi_2\rangle = J_+\|\phi_1\rangle = (J_+)^2\|\psi\rangle$	$\lambda\hbar^2$	$(\mu+2)\hbar$
$\|\phi_3\rangle = J_+\|\phi_2\rangle = (J_+)^3\|\psi\rangle$	$\lambda\hbar^2$	$(\mu+3)\hbar$
$\cdots$	$\cdots$	$\cdots$

Step-III: J_- is lowering operator for J_z

In a manner similar to the Step-II above,the commutation relation

$$J_z J_- - J_- J_z = -hbar J_z \tag{45}$$

can be used to show that the states $|\chi_1\rangle, |\chi_2\rangle, |\chi_3\rangle, \cdots$, obtained by repeated application of J_- on $|\psi\rangle$ are also eigenvectors of J^2 and J_z with eigenvalues as given in table below.

States	Eigenvalue of J^2	Eigenvalue of J_z
$|\chi_1\rangle = J_-|\psi\rangle$	$\lambda\hbar^2$	$(\mu+1)\hbar$
$|\chi_2\rangle = J_-|\chi_1\rangle = (J_-)^2|\psi\rangle$	$\lambda\hbar^2$	$(\mu+2)\hbar$
$|\chi_3\rangle = J_-|\chi_2\rangle = (J_-)^3|\psi\rangle$	$\lambda\hbar^2$	$(\mu+3)\hbar$
$\cdots$	$\cdots$	$\cdots$

Thus, if $\mu\hbar$ is an eigenvalue of J_z, $(mu \pm 1)\hbar, (\mu \pm 2)\hbar, (\mu \pm 3)\hbar \cdots$ are all eigenvalues of J_z as application of J_+ (or J_-) gives a non zero vector.

Step-IV: The difference between the maximum and minimum values of μ is an integer

We have seen that the eigenvalues λ and μ satisfy

$$\mu^2 \leq \lambda. \tag{46}$$

This relation shows that for a fixed λ , the eigenvalue $\mu\hbar$ of J_z cannot increase or decrease indefinitely. Thus for a given value of λ, there is a maximum eigenvalue and there is a minimum eigenvalue of J_z.

Let μ_1 be the minimum eigenvalue of J_z for a given λ and $|\chi\rangle$ be the corresponding eigenvector:

$$J^2|\chi\rangle = \lambda\hbar^2|\chi\rangle, \qquad J_z|\chi\rangle = \mu\hbar|\chi\rangle. \tag{47}$$

Then the action of J_- on $|\chi\rangle$ must give null vector, otherwise $J_-|\chi\rangle$ will be an eigenvector of J_z with eigenvalue $(\mu-1)\hbar$. Hence $J_-|\chi\rangle = 0$. Thus its norm must be zero giving

$$\langle\chi|J_+J_-|\chi\rangle = 0 \Rightarrow \langle\chi|J^2 - J_z^2 + \hbar J_z|\chi\rangle \Rightarrow \lambda\hbar^2 - \mu_1^2\hbar^2 + \mu_1\hbar^2 = 0. \tag{48}$$

Hence we have the relation

$$\lambda - \mu_1^2 + \mu_1 = 0 \tag{49}$$

In a similar fashion, repeated application of $J+$ on $|\chi\rangle$ will generate eigenvectors of J_z with eigenvalues $(\mu_1+1)\hbar, (\mu_1+2)\hbar, (\mu_1+3)\hbar, \cdots$. Let $\mu_2\hbar$ be the maximum allowed eigenvalue, then $\mu_2 = \mu_1 + N$ for some integer N. Let $|\phi\rangle$ be the corresponding eigenvector of J_z. Then $J_+|\phi\rangle = 0$. Taking the norm of $J_+|\phi\rangle$, we get

$$\langle\phi|J_-J_+|\phi\rangle = 0, \text{ or, } \langle\phi|J^2 - J_z^2 - \hbar J_z|\phi\rangle = 0. \tag{50}$$

or

$$\lambda\hbar^2 - \mu_2^2\hbar^2 - \mu_2\hbar^2 = 0. \tag{51}$$

Therefore, we have

$$\lambda - \mu_2^2 - \mu_2 = 0. \tag{52}$$

Subtracting the two equations (47) and (52) we get

$$\begin{aligned} \mu_2^2 + \mu_2 - \mu_1^2 + \mu_1 &= 0 \\ \text{or } (\mu_2 - \mu_1)(\mu_2 + \mu_1) + (\mu_2 - \mu_1) &= 0, \\ \text{or } (\mu_2 + \mu_1)(\mu_2 - \mu_1 + 1) &= 0 \end{aligned} \tag{53}$$

Therefore, we have

$$\mu_2 = -\mu_1 \quad \text{or} \quad \mu_2 = \mu_1 - 1. \tag{54}$$

Since $\mu_2 = \mu_1 - 1 \Longrightarrow \mu_2 < \mu_1$ which contradicts our earlier assumption that μ_2 is the maximum and μ_1 is the minimum allowed eigenvalue of J_z, hence we must have

$$\mu_2 = -\mu_1. \tag{55}$$

This equation, when used with $\mu_2 - \mu_1 = N$, implies that

$$\mu_2 = -\mu_1 = \frac{N}{2} \quad \lambda = \frac{N}{2}\left(\frac{N}{2} + 1\right). \tag{56}$$

Next we change the notation and call $\frac{N}{2} = j$ and state our final result as follows. The eigenvalue of J^2 are $j(j+1)\hbar^2$ with allowed values $j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \cdots$. For a fixed value of j the eigenvalues of J_z are between $-j\hbar, j\hbar$ in steps of 1. The simultaneous, normalised eigenvectors of J^2 and J_z will be denoted by $|j,m\rangle$. Here $m\hbar$ denotes the eigenvalue of J_z and can take $(2j+1)$ values $-j, -j+1, \cdots, j$.

Summary

1. It is customary to denote the it normalised, simultaneous eigenvectors of J^2 and J_z by $|j,m\rangle$ so that

$$J^2|j,m\rangle = j(j+1)\hbar^2|k,m\rangle \tag{57}$$
$$J_z|j,m\rangle = m\hbar|j,m\rangle \tag{58}$$

   and $m = j, j-1, \cdots, -j$.

2. The operators $J_\pm$ acting on $|j,m\rangle$ give a ket vector *proportional* to $|j, m\pm 1\rangle$. The proportionality constant can be worked out using (32) and (33). So, writing

$$J_+|j,m\rangle = C|j,m+1\rangle \tag{59}$$

   and taking scalar product of this equation with the dual $\langle j,m|J_-$ we get

$$\langle j,m+1|J_-J_+|j,m+1\rangle = |C|^2\langle j,m+1|j,m+1\rangle \tag{60}$$

   Using the relation ((32)) in the left hand side, and the fact that $|j,m\rangle$ and $|j,m+1\rangle$ are normalised, we get

$$|C|^2 = j(j+1)\hbar^2 - m^2\hbar^2 - m\hbar^2 \Rightarrow C = \sqrt{j(j+1) - m(m+1)}\hbar. \tag{61}$$

   This result and similar steps for $J_-|j,m\rangle$ give

$$\boxed{J_\pm|jm\rangle = \sqrt{j(j+1) - m(m\pm 1)}\,\hbar\,|j,m\pm 1\rangle}. \tag{62}$$

3. The operators J_+ and J_- annihilate the states with highest and lowest J_z values, respectively, because J_z value cannot be increased beyond j nor can it be decreased below $-j$. Therefore

$$J_+|j,j\rangle = 0, \qquad J_-|j,-j\rangle = 0. \tag{63}$$

4. In the above we have worked with J^2 and J_z, however the results remain true for component of $\vec{J}$ along any direction. In fact one can find simultaneous eigenvectors of J^2 and *any one* component $J_n = \hat{n}.\vec{J}$, along a fixed direction given by unit vector $\hat{n}$. For a given j the eigenvalues of J_n will be the same $-j, -j+1, \cdots, j$, in steps of one.

5. The above results are applicable to operators satisfying angular momentum commutation relations except that the half integral values are ruled out for the orbital angular momentum, because of additional requirement of single valuedness of the wave function.

6. A crucial technique in the derivation of the eigenvalues of angular momentum has been use of positivity for operators of the form $X^\dagger X$ and raising and lowering action of $J_\pm$. These techniques are very general and appear in many other applications involving the use of commutator algebra.

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Created : June 2017
Printed : August 3, 2017 KApoor

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