Quantum Mechanics Final Review-Harmonic Oscillator

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1 Notes

1.1 From the Beginning...

We begin our review of the famous harmonic oscillator (which can be found in Chapter 2) by writing down the non-relativistic, time dependent Schrödinger equation.

$$\hat{\boldsymbol{H}} |\Psi(\boldsymbol{r}, t)\rangle = i\hbar \frac{d}{dt} |\Psi(\boldsymbol{r}, t)\rangle \tag{1.1}$$

$$\left(\frac{\boldsymbol{p}^2}{2m} + V(r) \right) |\Psi(\boldsymbol{r}, t)\rangle = i\hbar \frac{d}{dt} |\Psi(\boldsymbol{r}, t)\rangle \tag{1.2}$$

We can solve the time independent version of (1.2) by assuming stationary states, allowing us to use separable solutions for our wave function $\Psi(\boldsymbol{r}, t)$. The derivation of that is outside of the scope of these notes, but one can readily arrive at the time independent Schrödinger equation by following the usual steps of transforming a PDE to an ODE, noting that the time problem is a simple ODE, solving for the time solution, plugging back in, and arriving at the following time independent functional form of the Schrödinger equation

$$\left(\frac{\boldsymbol{p}^2}{2m} + V(r) \right) |\Psi(\boldsymbol{r})\rangle = E |\Psi(\boldsymbol{r})\rangle \tag{1.3}$$

where E is the energy of our eigenstate.

1.2 Solving the TISE

We are now in a position to begin describing properties of the harmonic oscillator. Our Hamiltonian $\hat{\boldsymbol{H}}$ becomes

$$\hat{\boldsymbol{H}} = \frac{\boldsymbol{P}^2}{2m} + \frac{m\omega^2}{2} \hat{\boldsymbol{r}} \tag{1.4}$$

It is important to point out that there are two approaches to solving this, one requiring more effort than the other. The more taxing method would utilize a power series solution, a fair way of solving a second order differential equation (which will require some rearranging and some intermediate quantities to transform (1.3) to a form in which this method does work) which leads to Hermite polynomials. Conversely, one can thank the heavens for Dirac and his solution to this problem. This involves defining two operators

$$\boldsymbol{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{\boldsymbol{x}} + \frac{i}{m\omega}\hat{\boldsymbol{P}}\right) \qquad \boldsymbol{a}^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{\boldsymbol{x}} - \frac{i}{m\omega}\hat{\boldsymbol{P}}\right) \tag{1.5}$$

the **destruction (lowering)** and **creation (raising)** operators, respectively. As one can surmise by the names given, they raise/lower our eigenstates by integer values (as seen in Scott's notes of Ch 2.6). These operators obey the following commutation relations

$$[a, a^{\dagger}] = aa^{\dagger} - a^{\dagger}a \tag{1.6}$$

$$aa^{\dagger} = \frac{m\omega}{2\hbar}\left(\boldsymbol{x}^2 - \frac{i}{m\omega}\hat{\boldsymbol{x}}\hat{\boldsymbol{p}} + \frac{i}{m\omega}\hat{\boldsymbol{p}}\hat{\boldsymbol{x}} + \frac{\hat{\boldsymbol{p}}^2}{m^2\omega^2}\right) \tag{1.7}$$

$$= \boldsymbol{x}^2 + \frac{\hat{\boldsymbol{p}}^2}{m^2\omega^2} - \frac{i}{m\omega}[\hat{\boldsymbol{x}}, \hat{\boldsymbol{p}}] \tag{1.8}$$

$$a^{\dagger}a = \frac{m\omega}{2\hbar}\left(\boldsymbol{x}^2 + \frac{i}{m\omega}\hat{\boldsymbol{x}}\hat{\boldsymbol{p}} - \frac{i}{m\omega}\hat{\boldsymbol{p}}\hat{\boldsymbol{x}} + \frac{\hat{\boldsymbol{p}}^2}{m^2\omega^2}\right) \tag{1.9}$$

$$= \boldsymbol{x}^2 + \frac{\hat{\boldsymbol{p}}^2}{m^2\omega^2} + \frac{i}{m\omega}[\hat{\boldsymbol{x}}, \hat{\boldsymbol{p}}] \tag{1.10}$$

$$[a, a^{\dagger}] = \frac{m\omega}{2\hbar}\left(\boldsymbol{x}^2 + \frac{\hat{\boldsymbol{p}}^2}{m^2\omega^2} - \frac{i}{m\omega}[\hat{\boldsymbol{x}}, \hat{\boldsymbol{p}}] - (\boldsymbol{x}^2 + \frac{\hat{\boldsymbol{p}}^2}{m^2\omega^2} + \frac{i}{m\omega}[\hat{\boldsymbol{x}}, \hat{\boldsymbol{p}}])\right) \tag{1.11}$$

$$= \frac{m\omega}{2\hbar}\left(2\frac{-i}{m\omega}[\hat{\boldsymbol{x}}, \hat{\boldsymbol{p}}]\right) = \frac{(-2i)i\hbar}{2\hbar} = 1 \tag{1.12}$$

$$[a, a^{\dagger}] = 1 \tag{1.13}$$

where we made use of the commutation relation between the position and momentum operator

$$[\hat{\boldsymbol{x}}_i, \hat{\boldsymbol{p}}_j] = i\hbar\delta_{ij}$$

With this commutation relation, our Hamiltonian is readily written as

$$\hat{\boldsymbol{H}} = \left(a^{\dagger}a + \frac{1}{2}\right)\hbar\omega \tag{1.14}$$

where $a^{\dagger}a$ is known as the *Number operator* $\hat{\boldsymbol{N}}$ for the current state.

1.3 Behavior of a and $a^\dagger$

The destruction and creation (1.5) operators have the following behavior when acting on an state together

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle \tag{1.15}$$

$$\hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{1.16}$$

$$\hat{N}\,|n\rangle = a^\dagger a\,|n\rangle = n\,|n\rangle \tag{1.17}$$

$$\tag{1.18}$$

Thus, if we are given some ground state wave function $|\psi(x)\rangle$ (or any wave function) and we are asked to find the n^{th} wave function, one simply just needs to apply the raising/ lowering operators repeatedly until arriving at the n^{th} state. It is important to note that the lowering operator $\hat{a}$ acting on the ground state $|n=0\rangle$ will return zero due to the reality that we can't go to a state below the ground state. Similarly, we can make the same argument for the raising operator $\hat{a}^\dagger$ and the highest energy state for a given system. This yields

$$a\,|n=0\rangle = 0 \qquad\qquad a^\dagger\,|n=M\rangle = 0 \tag{1.19}$$

where M is some integer representing the highest energy level of a given system. Another important feature of this system, after being solved for, is the allowed values of our eigen energies

$$E_n = \left(n+\frac{1}{2}\right) \qquad n = 0, 1, 2, ..., M \tag{1.20}$$

If we have a N dimensional problem, such that our SE has multiple spatial separable solutions, we can write our solution as

$$\Psi(x_1, x_2, ..., x_N) = \psi_1(x_1)\psi_2(x_2)...\psi_N(x_N)$$

where each of these solve their corresponding 1D problem. Each wave function would have their own energy of

$$E_i = \hbar\omega\left(n_i+\frac{1}{2}\right) \tag{1.21}$$

To find the total energy, one would just simply add the energy for every solution ψ of our N dimensional problem which is given by (1.21)

$$E_{Tot} = \sum_i E_i = \sum_i \hbar\omega\left(n_i+\frac{1}{2}\right) \tag{1.22}$$

where n_i represents the principal quantum number for the i^{th} solution (wave function) ψ to our N dimensional problem. If we had a 3 dimensional problem, our total energy would be

$$E_{Tot} = \sum_{i=1}^{3} E_i = \sum_{i=1}^{3} \hbar\omega\left(n_i+\frac{1}{2}\right) = \hbar\omega\left(n_1+n_2+n_3+\frac{3}{2}\right) \tag{1.23}$$

1.4 Degeneracy in H.O. systems

Last but not least, it is important to talk about degeneracy of a state. When looking for degeneracy for a N-dimensional problem consisting of harmonic oscillators, we are really just looking to find the multiplicity of a given energy state having N oscillators available. This sounds reminiscent of " out of N oscillators, how many ways can I arrange them to get the quantum number n". This problem has already been solved by Albert Einsten in 1907 (Einstein Solids) and we can refer to his solution to finding the multiplicity (the degeneracy) of a certain microstate (eigen energy). The degeneracy/multiplicity for a certain energy level is given by

$$\Omega(N, n) = \binom{N + n - 1}{n} = \frac{(N + n - 1)!}{n!(N + n - 1 - n)!} = \frac{(N + n - 1)!}{n!(N - 1)!} \qquad [1.24]$$

Where n is the principal quantum number and N is the number of oscillators.

The way to interpret this is: Given N oscillators in the system, how many ways can I arrange my energy quanta (b/c energy is discretized) among the different N quantum numbers (n_1, n_2,...,n_N) in the system.

We can compare this with the "traditional" method of counting the different combinations for a 3D oscillator system and compare with (1.22).

<u>n = 0</u>

n_x	n_y	n_z
0	0	0

$$\Omega(3, 0) = \frac{(3 + 0 - 1)!}{0!(2 - 1)!} = 1 \qquad [1.25]$$

<u>n = 1</u>

n_x	n_y	n_z
1	0	0
0	1	0
0	0	1

$$\Omega(3, 1) = \frac{(3 + 1 - 1)!}{1!(2 - 1)!} = 3 \qquad [1.26]$$

<u>n = 2</u>

n_x	n_y	n_z
2	0	0
0	2	0
0	0	2
1	1	0
0	1	1
1	0	1

$$\Omega(3,2) = \frac{(3+2-1)!}{2!(2-1)!} = 6 \tag{1.27}$$

One can continue the counting scheme and see that this multiplicity/degeneracy will hold true for a system consisting of N oscillators.

2 Exercises

These two problems seemed to be good and cover some helpful stuff.

2.1 HW Problem 2.8

Calculate $\langle 0|aaa^\dagger aa^\dagger a^\dagger|0\rangle$ and $\langle n|a^\dagger a^\dagger a^\dagger a|m\rangle$.

First let's look at $\langle 0|aaa^\dagger aa^\dagger a^\dagger|0\rangle$:

Using

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{2.1}$$
$$a|n\rangle = \sqrt{n}\,|n-1\rangle \tag{2.2}$$
$$a^\dagger a|n\rangle = n|n\rangle \tag{2.3}$$

$$\begin{aligned}
&\langle 0|aaa^\dagger aa^\dagger a^\dagger|0\rangle \\
&= \langle 0|aaa^\dagger aa^\dagger(1)|1\rangle \\
&= \langle 0|aaa^\dagger a(\sqrt{2})|2\rangle \\
&= \sqrt{2}\,\langle 0|aaa^\dagger(\sqrt{2})|1\rangle \\
&= 2\,\langle 0|aa(\sqrt{2})|2\rangle \\
&= 2\sqrt{2}\,\langle 0|a(\sqrt{2})|1\rangle \\
&= 4\,\langle 0|(1)|0\rangle \\
&= 4\,\langle 0|0\rangle \\
&= 4
\end{aligned}$$

by the orthonormality of the harmonic oscillator eigenstates.

This was done using only the first two relations; the number operator can be used as well to reduce the number of steps slightly.

Next we will look at $\langle n|a^\dagger a^\dagger a^\dagger a|m\rangle$. Using first the number operator, we find

$$\langle n|a^\dagger a^\dagger a^\dagger a|m\rangle$$

$$= \langle n|a^\dagger a^\dagger m|m\rangle$$

Then using the creation (raising) operator, we find

$$= \langle n|a^\dagger m\sqrt{m+1}|m+1\rangle$$

$$= \langle n|m\sqrt{m+1}\sqrt{m+2}|m+2\rangle$$

$$= m\sqrt{m+1}\sqrt{m+2}\delta_{n,m+2}$$

where we again used the orthonormality of harmonic oscillator eigenstates. Thus, if $n = m+2$, it returns $m\sqrt{m+1}\sqrt{m+2}$, otherwise it is zero.

2.2 HW Problem 2.10

Consider a particle of mass m in a harmonic oscillator with spring constant $k = m\omega^2$.
(a) Write the momentum and position operators for a particle of mass m in a harmonic oscillator characterized by frequency ω in terms of the creation and destruction operators.
(b) Calculate $\langle n|x^2|n\rangle$and $\langle n|p^2|n\rangle$. Compare the product of these two matrix elements to the constraint of the uncertainty relation as a function of n.
(c) Show that the expectation value of the potential energy in an energy eigenstate of the harmonic oscillator equals the expectation value of the kinetic energy in that state.

A valuable skill for solving certain types of problems is to write an operator (such as position or momentum) in terms of raising and lowering operators, as is demonstrated here.

(a) Starting from the raising and lowering operators,

$$a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{ip}{m\omega}\right), a = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{ip}{m\omega}\right) \quad [2.4]$$

where here and henceforth x and p are the position and momentum operators. By adding them, we can find x:

$$a^\dagger + a = \sqrt{\frac{m\omega}{2\hbar}}(2x) \quad [2.5]$$

so we find that

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \quad [2.6]$$

Similarly, by subtracting a from $a^\dagger$, we find

$$a^\dagger - a = -\sqrt{\frac{2}{m\omega\hbar}}(ip) \quad [2.7]$$

so that

$$p = i\sqrt{\frac{m\omega\hbar}{2}}(a - a^\dagger) \quad [2.8]$$

(b) squaring x that we found in terms of a and $a^\dagger$,

$$\langle n|x^2|n\rangle = \frac{\hbar}{2m\omega}\langle n|a^\dagger a^\dagger + a^\dagger a + aa^\dagger + aa|n\rangle \tag{2.9}$$

By orthonormality, we can throw out the first and last terms, since application of either the raising operator or the lowering operator twice will leave the state ket in a different state, which is orthogonal to n. Then we have

$$\frac{\hbar}{2m\omega}\langle n|a^\dagger a + aa^\dagger|n\rangle = \frac{\hbar}{2m\omega}(n + n + 1) \tag{2.10}$$

where we used $a^\dagger a\,|n\rangle = n\,|n\rangle$ and $aa^\dagger = a^\dagger a + 1$ from the commutation relation,

$$\therefore \langle n|X^2|n\rangle = \frac{\hbar}{2m\omega}(2n + 1) \tag{2.11}$$

Similarly for $\langle n|p^2|n\rangle$, we have

$$\langle n|p^2|n\rangle = -\frac{\hbar m\omega}{2}\langle n|a^\dagger a^\dagger - a^\dagger a - aa^\dagger + aa|n\rangle = \frac{\hbar m\omega}{2}\langle n|a^\dagger a + aa^\dagger|n\rangle \tag{2.12}$$

so that

$$\langle n|p^2|n\rangle = \frac{\hbar m\omega}{2}(2n + 1) \tag{2.13}$$

Multiplying the expectation values with one another, we arrive at

$$\langle n|x^2|n\rangle\langle n|p^2|n\rangle = \frac{\hbar m\omega}{2}(2n + 1)\frac{\hbar}{2m\omega}(2n + 1) = \frac{\hbar^2}{4}(2n + 1)^2 \tag{2.14}$$

From the uncertainty principle, we know that this must be equal to or greater than $\hbar^2$. We see that this condition is satisfied in all cases, since the harmonic oscillator eigenstates n must be non-negative integers. For the ground state, $n = 0$, and we are right at the uncertainty limit.

(c) The expectation value of the potential energy is

$$\langle n|V|n\rangle = \langle n|\frac{m\omega^2 x^2}{2}|n\rangle = \frac{m\omega^2}{2}(\frac{\hbar}{2m\omega}(2n + 1)) = \frac{\hbar\omega(2n + 1)}{4} \tag{2.15}$$

And the expectation value of the kinetic energy is

$$\langle n|T|n\rangle = \langle n|\frac{p^2}{2m}|n\rangle = \frac{1}{2m}(\frac{\hbar m\omega}{2}(2n + 1)) = \frac{\hbar\omega(2n + 1)}{4} \tag{2.16}$$

Thus we see that $\langle n|T|n\rangle = \langle n|V|n\rangle = \frac{\hbar\omega(n+\frac{1}{2})}{2}$, which is half the total energy.