FY2045 Quantum Mechanics I

Fall 2023

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Week 4

Some information

- **Important:** Lecture Monday September 18th is cancelled.
- Office hour Tuesday September 12th and 19th cancelled. I will try to find new times, but feel free to send me an email if you have questions or drop by my office.
- **Mandatory exercise will be posted before Monday September 18th.** More practical information will be posted soon.
- **Reference group meeting today.** Last 10-15 minutes of second lecture for discussion without me present.

Harmonic oscillator

Why the harmonic oscillator again?

"Because an arbitrary smooth potential can usually be approximated as a harmonic potential at the vicinity of a stable equilibrium point, it is one of the most important model systems in quantum mechanics."[1]
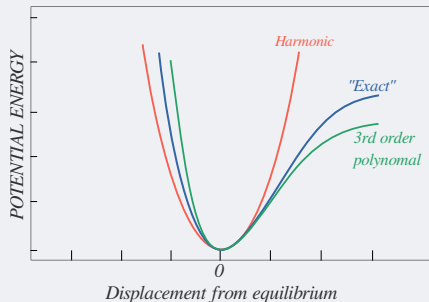
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[1]Wikipedia — Quantum Harmonic Oscillator.

Ladder operators

Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2.$$

Introduce **ladder operators**

$$a = \frac{1}{\sqrt{2\hbar m\omega}}(i\hat{p} + m\omega\hat{q}),$$
$$a^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(-i\hat{p} + m\omega\hat{q}),$$

with $(a)^\dagger = a^\dagger$ — they are not Hermitian.

Commutation relations for a and $a^\dagger$

Since $\hat{q}$ and $\hat{p}$ do not commute
($\hat{q}\hat{p} - \hat{p}\hat{q} = i\hbar$), neither do a and $a^\dagger$:

$$a^\dagger a = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2},$$
$$aa^\dagger = \frac{\hat{H}}{\hbar\omega} + \frac{1}{2},$$

meaning we have

$$[a, a^\dagger] = aa^\dagger - a^\dagger a = 1.$$

Number operator

Define the **number operator** $\hat{N} = a^\dagger a$, and write

$$\hat{H} = \hbar\omega \left(\hat{N} + \frac{1}{2} \right).$$

Eigenvectors of $\hat{N}$ will also be eigenvectors of $\hat{H}$:

$$\hat{N}|n\rangle = n|n\rangle \quad \Rightarrow \quad \hat{H}|n\rangle = \hbar\omega \left(n + \frac{1}{2} \right) |n\rangle \equiv E_n|n\rangle.$$

with orthonormalized eigenvectors $|n\rangle$.

Commutation relations for $\hat{N}$

Commutators of $\hat{N}$ with a and $a^\dagger$:

$$[\hat{N}, a] = -a,$$
$$[\hat{N}, a^\dagger] = a^\dagger.$$
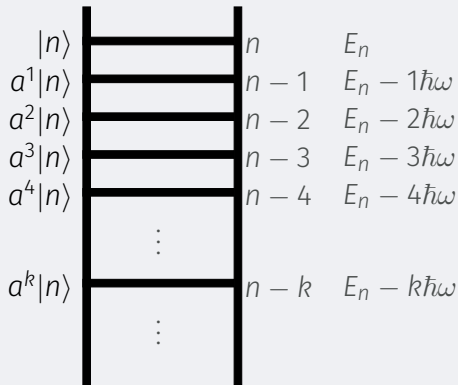
What do the ladder operators do?

$$\hat{H}a|n\rangle = (E_n - \hbar\omega)a|n\rangle.$$

If $a|n\rangle \neq 0$, $a|n\rangle$ is an eigenvector of $\hat{H}$ with eigenvalue $E_n - \hbar\omega$. a is a **lowering** or **annihilation operator**.

Can repeat this argument: If $a^k|n\rangle \neq 0$, $a^k|n\rangle$ is an eigenvector of $\hat{H}$ with eigenvalue $E_n - k\hbar\omega$.

$|n\rangle$		n	E_n
$a^1|n\rangle$		$n-1$	$E_n - 1\hbar\omega$
$a^2|n\rangle$		$n-2$	$E_n - 2\hbar\omega$
$a^3|n\rangle$		$n-3$	$E_n - 3\hbar\omega$
$a^4|n\rangle$		$n-4$	$E_n - 4\hbar\omega$
	$\vdots$		
$a^k|n\rangle$		$n-k$	$E_n - k\hbar\omega$
	$\vdots$		

Energy spectrum

The norm of a vector must be positive:

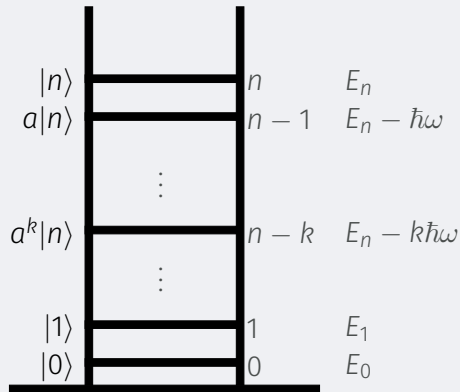$$0 \leq ||a|n\rangle||^2 = \langle n|a^\dagger a|n\rangle = \langle n|\hat{N}|n\rangle = n\langle n|n\rangle = n.$$

We must require

$$a|0\rangle = 0.$$

Hence $|0\rangle$ is the ground state with energy $E_0 = \frac{1}{2}\hbar\omega$, and we get the energy eigenvalues

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \text{ with } n = 0, 1, 2...$$

Eigenstates

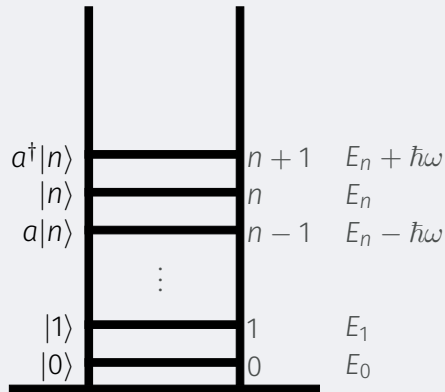$a|n\rangle$ is an eigenstate of $\hat{H}$ with eigenvalue $E_n - \hbar\omega$:

$$a|n\rangle = e^{-i\omega t}\sqrt{n}|n-1\rangle \overset{t=0}{=} \sqrt{n}|n-1\rangle.$$

Similarity, $a^\dagger|n\rangle$ is an eigenstate of $\hat{H}$ with eigenvalue $E_n + \hbar\omega$:

$$a^\dagger|n\rangle = e^{i\omega t}\sqrt{n+1}|n+1\rangle \overset{t=0}{=} \sqrt{n+1}|n+1\rangle.$$

$a^\dagger$ is called a **raising** or **creation operator.** Hence,

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle.$$

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Wavefunctions in position space

The wavefunctions for the *n*'th state in position space is given by $\langle q|n\rangle \propto \langle q|(a^\dagger)^n|0\rangle$. **What is $|0\rangle$?**

We use $a|0\rangle = 0 \rightarrow \langle q|a|0\rangle = 0$, with

$$a = \frac{i\hat{p} + m\omega\hat{q}}{\sqrt{2\hbar m\omega}} = \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dq} + \sqrt{\frac{m\omega}{2\hbar}}q,$$

resulting in a differential equation with solution

$$\langle q|0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega q^2}{2\hbar}}.$$

Excited states

$$\begin{aligned}
\langle q|n\rangle &= \frac{1}{\sqrt{n!}}\langle q|(a^\dagger)^n|0\rangle \\
&= \frac{1}{\sqrt{2^n n!}}\left(x - \frac{d}{dx}\right)^n \langle q|0\rangle \\
&= \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{H_n(x)}{\sqrt{2^n n!}} e^{-x^2/2},
\end{aligned}$$

with $x = \sqrt{m\omega/\hbar}\cdot q$, and H_n the *n*'th Hermite polynomial.

Coherent states

Is it possible to find a state resembling the classical oscillating state?

Yes:

$$a|\alpha\rangle = e^{-i\omega t}\alpha|\alpha\rangle,$$

an eigenstate of the lowering operator!?

$$|\alpha\rangle = c_0 \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle.$$

This results in an oscillating expectation value

$$\langle q\rangle = q_0 \cos(\omega t - \Theta),$$

and an oscillating wavepacket,

$$|\langle q|\alpha\rangle|^2 = \sqrt{\frac{m\omega}{\pi\hbar}} e^{-\frac{m\omega}{\hbar}[q-q_0\cos(\omega t-\Theta)]^2},$$

with constant width. These states are called coherent states.

Quantization of Angular Momentum

Angular momentum operators

Define angular momentum operator **J**
with components J_x, J_y, and J_z —
Hermitian operators with commutation
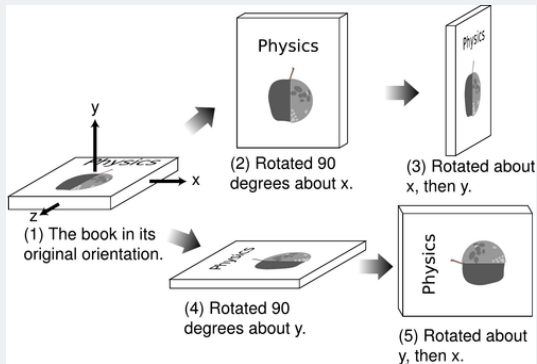relations

$$[J_x, J_y] = i\hbar J_z,$$
$$[J_y, J_z] = i\hbar J_x,$$
$$[J_z, J_x] = i\hbar J_y.$$

Non-commutativity related to
non-commutativity of rotations in 3D.[1]

Picture source: Benjamin Crowell, General Relativity, p. 270.

∅11.2, H8.1-8.2, G4.3

[1]For more on this, see the lecture notes by Prof. Neil, on which today's lecture was based.

Angular momentum operators

Define angular momentum operator $\mathbf{J}$ with components $J_x, J_y,$ and J_z — Hermitian operators with commutation relations

$$[J_x, J_y] = i\hbar J_z,$$
$$[J_y, J_z] = i\hbar J_x,$$
$$[J_z, J_x] = i\hbar J_y.$$

Non-commutativity related to non-commutativity of rotations in 3D.[1]

Also define $\mathbf{J}^2 = J_x^2 + J_y^2 + J_z^2$, which satisfies

$$[\mathbf{J}^2, J_i] = 0, \; i = x, y, z.$$

Since they commute, we can find **simultaneous eigenvectors** of $\mathbf{J}^2$ and e.g. J_z.
Assume orthonormalized eigenvectors $|a, b\rangle$ such that

$$\mathbf{J}^2|a, b\rangle = a|a, b\rangle,$$
$$J_z|a, b\rangle = b|a, b\rangle.$$

Ø11.2, H8.1-8.2, G4.3

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Eigenvalues

Ladder operators

We again define ladder operators

$$J_\pm = J_x \pm iJ_y,$$

with commutation relations

$$[J^2, J_\pm] = 0,$$
$$[J_x, J_\pm] = \pm \hbar J_\pm.$$

$J_\pm |a, b\rangle$ is an eigenvector of both J^2 and J_z with eigenvalue a and $b \pm \hbar$, respectively:

$$J_\pm |a, b\rangle \propto |a, b \pm \hbar\rangle.$$

What are a and b?

Since the norm of a vector must be positive, we must have:

$$a - b(b \pm \hbar) \geq 0.$$

Must have a maximum and minimum eigenvalue of J_z such that

$$J_+ |a, b_{\max}\rangle = 0 \text{ and } J_- |a, b_{\min}\rangle = 0.$$

We find $(n = 0, 1, 2, \dots)$

$$b_{\max} = -b_{\min} = \frac{n\hbar}{2}, \text{ and } a = \frac{\hbar^2}{4} n(n+2).$$

Eigenvalues

In standard notation, we get

$$J^2|j, m\rangle = \hbar^2 j(j+1)|j, m\rangle,$$
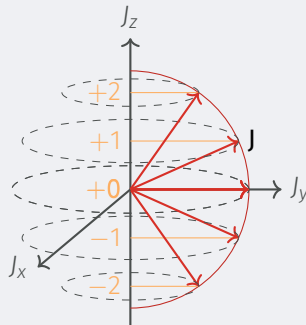$$J_z|j, m\rangle = \hbar m|j, m\rangle,$$

with

$$j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots,$$
$$m = -j, -j+1, \ldots, j-2, j-1, j.$$

Orientation of **J** for different values of m:

Based on figure by Izaak Neutelings