DALHOUSIE UNIVERSITY

PHYC 3640 Quantum Physics I: Tutorial 1

Complex Numbers, Operators, and Eigenvalues

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September 15, 2022

What is the imaginary number?

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The accepted definition of the imaginary number, i, is

$$i^2 = -1$$

Isn't that pedantic?

Sure, but math involving negative square roots can lead to contradictions. Consider this example

$$\sqrt{-1} = \sqrt{-1}$$

$$\sqrt{-1} = \sqrt{\frac{1}{-1}} \qquad \text{Flip the negative to the denominator}$$

$$\sqrt{-1} = \frac{\sqrt{1}}{\sqrt{-1}} \qquad \text{Distribute the square root}$$

$$\sqrt{\mathrm{i}^2} = \frac{\sqrt{1}}{\sqrt{\mathrm{i}^2}} \qquad \text{Definition of } \mathrm{i}$$

$$\mathrm{i} = \frac{1}{\mathrm{i}} \qquad \sqrt{\mathrm{i}^2} = \mathrm{i}$$

$$\mathrm{i}^2 = 1 \qquad \text{Multiply both sides with } \mathrm{i}$$

$$-1 = 1$$

which is obviously wrong.

Wikipedia does a better job explaining

Square roots of negative numbers [edit]

Care must be used when working with imaginary numbers that are expressed as the principal values of the square roots of negative numbers:[14]

$$6=\sqrt{36}=\sqrt{(-4)(-9)}\neq\sqrt{-4}\sqrt{-9}=(2i)(3i)=6i^2=-6.$$

That is sometimes written as:

$$-1=i^2=\sqrt{-1}\sqrt{-1}\stackrel{\text{(fallacy)}}{=}\sqrt{(-1)(-1)}=\sqrt{1}=1.$$

The fallacy occurs as the equality $\sqrt{xy}=\sqrt{x}\sqrt{y}$ fails when the variables are not suitably constrained. In that case, the equality fails to hold as the numbers are both negative, which can be demonstrated by:

$$\sqrt{-x}\sqrt{-y}=i\sqrt{x}\,i\sqrt{y}=i^2\sqrt{x}\sqrt{y}=-\sqrt{xy}\neq\sqrt{xy},$$

where both x and y are positive real numbers.

https://en.wikipedia.org/wiki/Imaginary_number

What is a complex number?

A complex number is one which has both a real and an imaginary part. e.g.

$$z = 2 - 3\mathrm{i}\,.$$

The real part can be extracted with the “Real” function

$$\mathrm{Re}(z) = \mathrm{Re}(2 - 3\mathrm{i}) = 2\,,$$

and similarly, the imaginary part can be extracted with the “Imaginary” function

$$\mathrm{Im}(z) = \mathrm{Im}(2 - 3\mathrm{i}) = -3\,.$$

We note that both the Re and Im functions both output real numbers.

A bit of notation

$\mathbb{R}$ is the set of Real Numbers.
Examples: $1,\ -2,\ 7.3,\ {}^{1}/_{2},\ \pi,\ \mathrm{e} \in \mathbb{R}$

$\mathbb{I}$ is the set of Imaginary Numbers.
Examples: $\mathrm{i},\ -2\mathrm{i},\ 7.3\mathrm{i},\ {}^{\mathrm{i}}/_{2} \in \mathbb{I}$

$\mathbb{C}$ is the set of Complex Numbers.
Examples: $1 + 2\mathrm{i},\ \pi - \mathrm{i}\mathrm{e},\ 2\mathrm{e}^{1.2\mathrm{i}} \in \mathbb{C}$

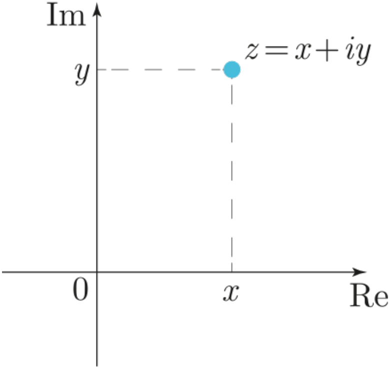
Sometimes you will see i written as j in the context of engineering.

The Complex Plane

Sometimes it's nice to imagine the space of complex numbers as a plane. Let's write the "Cartesian form" of a complex number, z, as

$$z = x + \mathrm{i}y$$

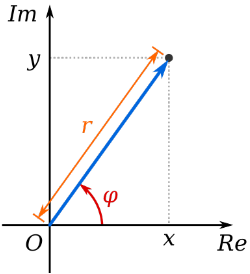
where $x = \mathrm{Re}(z)$ and $y = \mathrm{Im}(z)$. We can then plot this:



https://en.wikipedia.org/wiki/Complex_number

The Complex Plane (Polar)

What if instead we try to represent this point using something like polar coordinates?



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Obviously

$$r = \sqrt{x^2 + y^2}$$

$$\phi = \arctan\left(\frac{y}{x}\right) \qquad \text{(Be careful to choose the correct quadrant!)}$$

There are functions to deal with the quadrant issue. Look up $\arg$ and $\operatorname{atan2}$!

The Complex Plane (Polar)

Using trig, we can write these as

$$z = r\cos(\phi) + \mathrm{i}r\sin(\phi)\,.$$

We remember "Euler's Formula" from calculus, which can be derived using Taylor series

$$\mathrm{e}^{i\phi} = \cos(\phi) + \mathrm{i}\sin(\phi)\,,$$

letting us finally get to the two ways of representing complex numbers

$z = x + \mathrm{i}y$	Cartesian Form
$z = r\mathrm{e}^{\mathrm{i}\phi}$	Polar Form

Complex Conjugates

One last thing. We write the "Complex Conjugate" of $z = x + \mathrm{i}y$ as

$$z^* = x - \mathrm{i}y$$

We now have a *proper* way of getting the magnitude of the complex number. It is called the "Norm".

$$\begin{aligned} \|z\| &= \sqrt{zz^*} \\ &= \sqrt{(x + \mathrm{i}y)(x - \mathrm{i}y)} \\ &= \sqrt{x^2 + \mathrm{i}xy - \mathrm{i}xy - \mathrm{i}^2 y^2} \\ &= \sqrt{x^2 - (-1)y^2} \\ &= \sqrt{x^2 + y^2} \end{aligned}$$

Further, we say the product of a complex number z and its complex conjugate is the "absolute square" of z.

$$|z|^2 = zz^*$$

The result is always a positive real number. This will show up a lot in your quantum mechanics class.

Problems

1) Derive an expression for z^* in the polar form, in terms of r and ϕ.
Hints:
- *Convert from polar to the Cartesian, take the complex conjugate, then convert back.*
- *To derive your new ϕ, try using a geometric argument.*

2) Take linear combinations of z and z^* to derive expressions for $\mathrm{Re}(z)$ and $\mathrm{Im}(z)$.

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Solutions

1) $z^* = r\mathrm{e}^{-\mathrm{i}\phi}$

2) $\mathrm{Re}(z) = \frac{z+z^*}{2}$ and $\mathrm{Im}(z) = \frac{z-z^*}{2\mathrm{i}}$

Problems

3) The spherical harmonic functions are used to describe the quantum mechanical orbitals (You will learn about this later in the course!). Here are three of them.

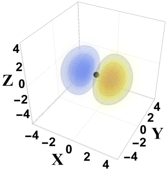
$$Y_{1,0} = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos(\theta) \qquad Y_{1,-1} = \mathrm{e}^{-\mathrm{i}\phi}\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin(\theta) \qquad Y_{1,+1} = -\mathrm{e}^{\mathrm{i}\phi}\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin(\theta)$$

$Y_{1,0}$ is real valued, and is called the $2p_z$ orbital because it is aligned along the z-axis. However, both $Y_{1,-1}$ and $Y_{1,+1}$ are complex and can't be plotted in $\mathbb{R}^3$.

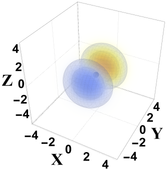
Derive real-valued expressions for the $2p_x$ and $2p_y$ orbitals in terms of $Y_{1,\pm 1}$.

$$Y_{2p_x} = \qquad\qquad = \frac{1}{2}\sqrt{\frac{3}{\pi}}\sin(\theta)\cos(\phi)$$

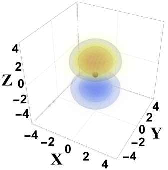
$$Y_{2p_y} = \qquad\qquad = \frac{1}{2}\sqrt{\frac{3}{\pi}}\sin(\theta)\sin(\phi)$$



(a) $2p_x$



(b) $2p_y$



(c) $2p_z$

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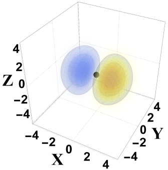
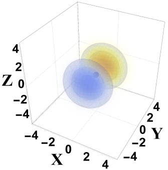
Derive real-valued expressions for the $2p_x$ and $2p_y$ orbitals in terms of $Y_{1,\pm 1}$.

$$Y_{2p_x} = \frac{1}{\sqrt{2}}\left(Y_{1,-1} - Y_{1,+1}\right) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\sin(\theta)\cos(\phi)$$

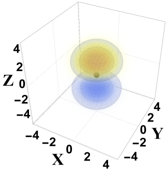
$$Y_{2p_y} = \frac{\mathrm{i}}{\sqrt{2}}\left(Y_{1,-1} + Y_{1,+1}\right) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\sin(\theta)\sin(\phi)$$



(d) $2p_x$



(e) $2p_y$



(f) $2p_z$

Useful Properties

Assume z and w are complex numbers, then:

1. $\mathrm{i} = -1/\mathrm{i}$
2. $\mathrm{i}^3 = -\mathrm{i}$
3. If $z = x + \mathrm{i}y$, then $z^* = x - \mathrm{i}y$
4. If $z = r\mathrm{e}^{\mathrm{i}\phi}$, then $z^* = r\mathrm{e}^{-\mathrm{i}\phi}$
5. $|z|^2 = zz^*$
6. $(z \pm w)^* = z^* \pm w^*$
7. $(z \cdot w)^* = z^* \cdot w^*$
8. $(z/w)^* = z^*/w^*$
9. $\mathrm{Re}(z) = \frac{z+z^*}{2}$
10. $\mathrm{Im}(z) = \frac{z-z^*}{2\mathrm{i}}$

What is an operator?

It's as it sounds, some symbol that indicates an operation. Consider

$$\frac{d}{dx}f(x) = f'(x)$$

in this case, this is the "derivative operator" which operating on the function $f(x)$. It doesn't have to be that simple though, you can define an operator $\hat{D}$ such that

$$\hat{D} = \frac{d^2}{dx^2} + 2\frac{d}{dx} + 7\,,$$

in which case, operating on $f(x)$ would give

$$\hat{D}[f(x)] = f''(x) + 2f'(x) + 7f(x)\,.$$

We could even define an operator to just add 1 to the function it operates on

$$\hat{P}[f(x)] = f(x) + 1\,.$$

so $\hat{P}[x^2] = x^2 + 1$.

Linear Operators

An operator $\hat{O}$ is linear if both of the following are true

$$\hat{O}[f(x) + g(x)] = \hat{O}[f(x)] + \hat{O}[g(x)]$$
$$\hat{O}[zf(x)] = z\hat{O}[f(x)]$$

where z is some complex number.

Example of Linear Operator: $\frac{d}{dx}$
Example of Non-Linear Operator: $\sin(x)$

QUESTION

What are some other linear/non-linear operators?

Eigenvalues (Non-Matrix Style)

We can look at an eigenvalue problem that doesn't use the matrix notation. Consider an operator $\hat{J}$. An eigenvalue equation for this operator would look like

$$J[f(x)] = \lambda f(x)\,,$$

so the challenge is to find an eigenfunction, $f(x)$, and eigenvalue, λ, that satisfy this problem.

Non-Matrix Eigenvalue Example

Let $\hat{J}$ be the "shift operator". This operation would look like

$$\hat{J}[f(x)] = f(x+a)$$

Consider an eigenfunction

$$f(x) = \mathrm{e}^{\ln(c)\frac{x}{a}}$$

then we can show

$$\begin{aligned}
\hat{J}[f(x)] &= f(x+a) \\
&= \mathrm{e}^{\ln(c)\frac{(x+a)}{a}} \\
&= \mathrm{e}^{\ln(c)\left[1+\frac{x}{a}\right]} \\
&= \mathrm{e}^{\ln(c)+\ln(c)\frac{x}{a}} \\
&= \mathrm{e}^{\ln(c)}\mathrm{e}^{\ln(c)\frac{x}{a}} \\
&= c\,f(x)
\end{aligned}$$

thus $f(x) = \mathrm{e}^{\ln(c)\frac{x}{a}}$ is an eigenfunction of $\hat{J}$ with an eigenvalue c.

Problems

1) Create an operator called the "Scale" operator which scales the argument of a function $f(x)$ by some constant a. What are the eigenvectors and eigenvalues for this operator?

2) Let the momentum operator in position space be defined as $\hat{p} = \frac{\hbar}{\mathrm{i}} \frac{d}{dx}$. Find the eigenvalues and eigenvectors of $\hat{p}$.
Hint: *Assume a wave-type eigenfunction for* $\psi(x)$

3) Find the eigenvalues and eigenvectors of the second-order boundary-value equation $y'' + \lambda y = 0$ where $y(0) = y(L) = 0$ assuming there are no negative eigenvalues.
Hint: *Assume* $y = c_1 \cos\left(\sqrt{\lambda} x\right) + c_2 \sin\left(\sqrt{\lambda} x\right)$

Problems

1) Create an operator called the "Scale" operator which scales the argument of a function $f(x)$ by some constant a. What are the eigenvectors and eigenvalues for this operator?
`Solution:` $\hat{K}[f(x)] = f(ax)$, let $f(x) = cx$, then $\hat{K}[f(x)] = c(ax) = af(x)$

2) Let the momentum operator in position space be defined as $\hat{p} = \frac{\hbar}{\mathrm{i}}\frac{d}{dx}$. Find the eigenvalues and eigenvectors of $\hat{p}$.
Hint: *Assume a wave-type eigenfunction for* $\psi(x)$
`Solution:` Let the eigenfunction be in either form

- $\psi(x) = A\mathrm{e}^{ik(x-a)}$
- $\psi(x) = A\cos(k(x-a)) + \mathrm{i}A\sin(k(x-a))$

Then $\hat{p}[\psi(x)] = \hbar k\psi(x)$

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Hint: *Assume* $y = c_1\cos\left(\sqrt{\lambda}x\right) + c_2\sin\left(\sqrt{\lambda}x\right)$
`Solution`

Questions?

Want My Slides?

https://github.com/KyleBryenton/slides-posters

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