PHYC 3640 Quantum Physics I: Tutorial 1
Complex Numbers, Operators, and Eigenvalues

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What is the imaginary number?

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The accepted definition of the imaginary number, i, is

$$\mathrm{i}^2 = -1$$

Isn't that pedantic?

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

$$
\begin{aligned}
\sqrt{-1} &= \sqrt{-1} && \\
\sqrt{-1} &= \sqrt{\frac{1}{-1}} && \text{Flip the negative to the denominator} \\
\sqrt{-1} &= \frac{\sqrt{1}}{\sqrt{-1}} && \text{Distribute the square root} \\
\sqrt{\mathrm{i}^2} &= \frac{\sqrt{1}}{\sqrt{\mathrm{i}^2}} && \text{Definition of } \mathrm{i} \\
\mathrm{i} &= \frac{1}{\mathrm{i}} && \sqrt{\mathrm{i}^2} = \mathrm{i} \\
\mathrm{i}^2 &= 1 && \text{Multiply both sides with } \mathrm{i} \\
-1 &= 1 &&
\end{aligned}
$$

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: $1 + 2\mathrm{i},\ \pi - \mathrm{ie},\ 2\mathrm{e}^{1.2\mathrm{i}} \in \mathbb{C}$

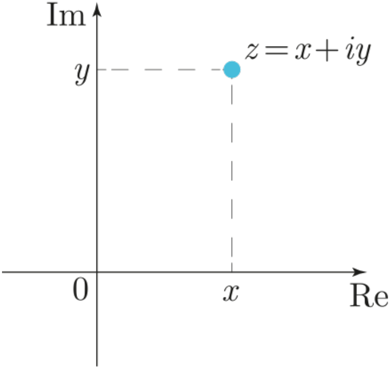
Sometimes you will see i written as j in the context of engineering.

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

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

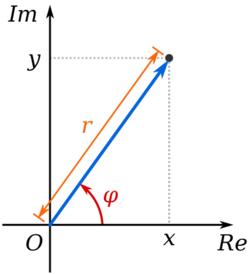
where $x = \mathrm{Re}(z)$ and $y = \mathrm{Im}(z)$. We can then plot this:



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

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

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

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

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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<u>Solutions</u>

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.

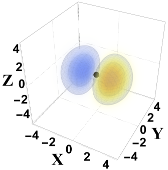
$$Y_{1,0} = \frac{1}{2}\sqrt{\frac{3}{\pi}}\cos(\theta) \qquad Y_{1,-1} = \mathrm{e}^{-\mathrm{i}\phi}\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin(\theta) \qquad Y_{1,+1} = -\mathrm{e}^{\mathrm{i}\phi}\frac{1}{2}\sqrt{\frac{3}{2\pi}}\sin(\theta)$$

$Y_{1,0}$ 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 $\mathbb{R}^3$.

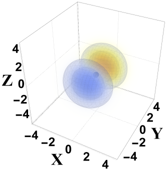
Derive real-valued expressions for the $2p_x$ and $2p_y$ orbitals in terms of $Y_{1,\pm1}$.

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

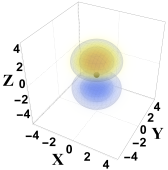
$$Y_{2p_y} = \qquad\qquad = \frac{1}{2}\sqrt{\frac{3}{\pi}}\sin(\theta)\sin(\phi)$$



(a) $2p_x$



(b) $2p_y$



(c) $2p_z$

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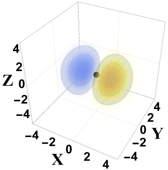
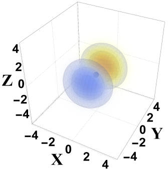
Derive real-valued expressions for the $2p_x$ and $2p_y$ orbitals in terms of $Y_{1,\pm1}$.

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

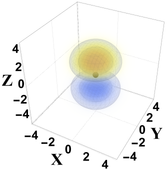
$$Y_{2p_y} = \frac{\mathrm{i}}{\sqrt{2}}\left(Y_{1,-1} + Y_{1,+1}\right) = \frac{1}{2}\sqrt{\frac{3}{\pi}}\sin(\theta)\sin(\phi)$$



(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 (Matrix Style)

The "eigen" in "eigenvalues" and "eigenvectors" comes from German, and it means "proper". These are special numbers and vectors for the system you're studying that are invariant to linear transformations. Basically, they don't bend, rotate, grow, shrink, etc...

Here's a cool Stack-Exchange article on them
https://math.stackexchange.com/questions/300145/what-exactly-are-eigen-things

Quantized systems are normally modelled with matrices. A square matrix $\mathbf{A}$ have eigenvalues λ_i and eigenvectors $\mathbf{x}_i$ that can be found with diagonalization.

$$\mathbf{A}\mathbf{x}_i = \lambda_i \mathbf{x}_i$$

Reminder: What a Determinant Is

$$\det(\mathbf{A}) = |\mathbf{A}| = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc$$

$$\begin{bmatrix} 1 & -2 & 3 \\ 2 & 0 & 3 \\ 1 & 5 & 4 \end{bmatrix} = \begin{bmatrix} \boxed{1} & -2 & 3 \\ 2 & 0 & 3 \\ 1 & 5 & 4 \end{bmatrix} - \begin{bmatrix} 1 & \boxed{-2} & 3 \\ 2 & 0 & 3 \\ 1 & 5 & 4 \end{bmatrix} + \begin{bmatrix} 1 & -2 & \boxed{3} \\ 2 & 0 & 3 \\ 1 & 5 & 4 \end{bmatrix}$$

$$= \boxed{1} \times \begin{vmatrix} 0 & 3 \\ 5 & 4 \end{vmatrix} - \boxed{-2} \times \begin{vmatrix} 2 & 3 \\ 1 & 4 \end{vmatrix} + \boxed{3} \times \begin{vmatrix} 2 & 0 \\ 1 & 5 \end{vmatrix}$$

$$= 1 \times (0 - 15) + 2 \times (8 - 3) + 3 \times (10 - 0)$$

$$= 1(-15) + 2(5) + 3(10)$$

$$= -15 + 10 + 30$$

$$= 25$$

Matrix Eigenvalue Example

Let's work through an example. Take

$$\mathbf{A} = \begin{bmatrix} 2 & 0 & 0 \\ 1 & 2 & -1 \\ 1 & 3 & -2 \end{bmatrix}$$

The eigenvalues can be found by solving for λ in the following equation

$$\det(\mathbf{A} - \lambda \mathbf{I})$$

where $\mathbf{I}$ is the identity matrix

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Matrix Eigenvalue Example

Thus

$$\begin{vmatrix} 2-\lambda & 0 & 0 \\ 1 & 2-\lambda & -1 \\ 1 & 3 & -2-\lambda \end{vmatrix} = 0$$

Taking the determinant yields

$$\begin{aligned} (2-\lambda)\begin{vmatrix} 2-\lambda & -1 \\ 3 & -2-\lambda \end{vmatrix} - 0\begin{vmatrix} \cdots \end{vmatrix} + 0\begin{vmatrix} \cdots \end{vmatrix} &= 0 \\ (2-\lambda)\Big[(2-\lambda)(-2-\lambda) - (-1)(3)\Big] &= 0 \\ \lambda^3 - 2\lambda^2 - \lambda + 2 &= 0 \\ (\lambda-2)(\lambda-1)(\lambda+1) &= 0 \end{aligned}$$

So the eigenvalues are $\{\lambda_1,\, \lambda_2,\, \lambda_3\} = \{2,\, 1,\, -1\}$

Matrix Eigenvalue Example

To find the eigenvectors, we solve the following

$$(\mathbf{A} - \lambda_i \mathbf{I})\, \mathbf{x}_i = 0$$

Consider $\lambda_1 = 2$, we can write the above as an augmented matrix and row reduce it to find the eigenvector

$$\left[\begin{array}{ccc|c} 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 \\ 1 & 3 & -4 & 0 \end{array}\right] = \left[\begin{array}{ccc|c} 1 & 0 & -1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{array}\right]$$

The first line indicates $x - z = 0$, and the second indicates $y - z = 0$. z is an independent variable so let's set it to 1 for convenience. Solving the above two equations gives

$$\mathbf{x}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

Selecting $\lambda_2 = 1$ and $\lambda_3 = -1$ yield eigenvectors of $\mathbf{x}_2 = [0 \;\; 1 \;\; 1]^{\mathrm{T}}$ and $\mathbf{x}_3 = [0 \;\; 1 \;\; 3]^{\mathrm{T}}$ respectively.

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

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

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

Problems

1) Find the Eigenvalues and Eigenvectors of $\mathbf{A} = \begin{bmatrix} 0 & 1 \\ -2 & -3 \end{bmatrix}$.

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 an eigenfunction of* $\psi(x) = A\mathrm{e}^{ik(x-a)}$

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* $y = c_1 \cos\left(\sqrt{\lambda} x\right) + c_2 \sin\left(\sqrt{\lambda} x\right)$

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Solution

Questions?

Want My Slides?

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

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