Primer on Vectors and Matrices

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Contents

Introduction

This guide covers the linear algebra you'll need for quantum mechanics. We'll keep things practical and focus on understanding rather than rigorous proofs.

1 Vectors

A vector is just an ordered list of numbers. In QM, vectors often represent quantum states.

1.1 Column Vectors

We usually write vectors as columns:

$$\underline{v} = \begin{pmatrix} 2 \\ -1 \\ 3 \end{pmatrix}$$

1.2 Row Vectors

Sometimes we write them as rows (we'll see why soon):

$$\underline{w}^T = \begin{pmatrix} 1 & 4 & -2 \end{pmatrix}$$

1.3 Vector elements

The element of a vector is denoted

$$[\underline{v}]_n = v_n$$

for example:

$$\underline{v} = \begin{pmatrix} 2 \\ -i \\ 3+2i \end{pmatrix} \implies [\underline{v}]_1 = 2, [\underline{v}]_2 = -i, [\underline{v}]_3 = 3+2i$$

1.4 Vector Addition and Scalar Multiplication

We add vectors element by element. We multiply vectors by scalars by multiplying each element by the scalar.

$$\begin{pmatrix} 2 \\ -1 \end{pmatrix} + \begin{pmatrix} 3 \\ 5 \end{pmatrix} = \begin{pmatrix} 5 \\ 4 \end{pmatrix} \qquad 3\begin{pmatrix} 2 \\ -1 \end{pmatrix} = \begin{pmatrix} 6 \\ -3 \end{pmatrix}$$

1.5 Dot Product

The inner product of two vectors gives a scalar:

$$\underline{v} \cdot \underline{w} = \sum_{n=1}^{N} v_n w_m$$

$$\underline{v} \cdot \underline{w} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \cdot \begin{pmatrix} 4 \\ -1 \\ 2 \end{pmatrix} = 1(4) + 2(-1) + 3(2) = 8$$

1.6 Inner product

The inner product, $\langle \underline{v} | \underline{w} \rangle$, is subtly different to the dot product. The first vector is complex conjugated, then the dot-product is taken

$$\langle \underline{v} | \underline{w} \rangle = \underline{v}^* \cdot \underline{w}$$

Notice that if the vectors only contain real numbers, then the dot product and inner product are the same, but for vectors of complex numbers they are different, e.g.

$$\underline{v} \cdot \underline{w} = \begin{pmatrix} i \\ 2 \end{pmatrix} \cdot \begin{pmatrix} 2 \\ 3 \end{pmatrix} = 2i + 6$$

but

$$\langle \underline{v} | \underline{w} \rangle = \underline{v}^* \cdot \underline{w} = \begin{pmatrix} i \\ 2 \end{pmatrix}^* \cdot \begin{pmatrix} 2 \\ 3 \end{pmatrix} = -2i + 6$$

2 Matrices

Matrices are rectangular arrays of numbers.

2.1 Basic Matrix

$$\underline{\underline{A}} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix}$$

This is a 2×3 matrix (2 rows, 3 columns).

2.2 Square Matrices

Most operators in QM are square matrices:

$$\underline{\underline{H}} = \begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix}$$

2.3 Matrix elements

$[\underline{\underline{A}}]_{ij} \equiv A_{ij}$ denotes the number in the row i column j of the matrix $\underline{\underline{A}}$.

3 Matrix-Vector Multiplication

When a matrix acts on a vector, it transforms it into another vector.

Example:

$$\begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} = \begin{pmatrix} 2(1) + 1(2) \\ 1(1) + 3(2) \end{pmatrix} = \begin{pmatrix} 4 \\ 7 \end{pmatrix}$$

The rule: element $[\underline{\underline{A}}]_{ij}$ of the matrix multiplies element j of the vector, then sum over j.

This is equivalent to taking the dot product of row i of the matrix with the vector to make the ith row of the new vector

$$\begin{pmatrix} \underline{r}_1^T \\ \underline{r}_2^T \end{pmatrix} \underline{v} = \begin{pmatrix} \underline{r}_1 \cdot \underline{v} \\ \underline{r}_2 \cdot \underline{v} \end{pmatrix}$$

In terms of matrix/vector elements, the element of the vector $\underline{\underline{A}}\underline{v}$ is

$$[\underline{\underline{A}}\underline{v}]_i = \sum_j [\underline{\underline{A}}]_{ij} [\underline{v}]_j.$$

Matrices multiplying vectors represent linear transformations of vectors e.g. skews, rotations, inversions, reflections etc.

4 Matrix Multiplication

Multiply matrices by taking rows of the first times columns of the second:

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \begin{pmatrix} 5 & 6 \\ 7 & 8 \end{pmatrix} = \begin{pmatrix} 1(5) + 2(7) & 1(6) + 2(8) \\ 3(5) + 4(7) & 3(6) + 4(8) \end{pmatrix} = \begin{pmatrix} 19 & 22 \\ 43 & 50 \end{pmatrix}$$

Note: Matrix multiplication is **not** commutative. Usually $\underline{\underline{AB}} \neq \underline{\underline{BA}}$ (although there are special cases where $\underline{\underline{AB}} = \underline{\underline{BA}}$).

Matrix multiplication is equivalent to taking the dot product of row i of the left matrix with column j of the right matrix to make the entry in the ith row and jth column of the new vector

$$\begin{pmatrix} \underline{r}_1^T \\ \underline{r}_2^T \end{pmatrix} \begin{pmatrix} \underline{c}_1 & \underline{c}_2 & \underline{c}_3 \end{pmatrix} = \begin{pmatrix} \underline{r}_1 \cdot \underline{c}_1 & \underline{r}_1 \cdot \underline{c}_2 & \underline{r}_1 \cdot \underline{c}_3 \\ \underline{r}_2 \cdot \underline{c}_1 & \underline{r}_2 \cdot \underline{c}_2 & \underline{r}_2 \cdot \underline{c}_3 \end{pmatrix}$$

In terms of matrix/vector elements, the element of the vector $\underline{\underline{A}}\underline{v}$ is

$$[\underline{\underline{A}}\ \underline{\underline{B}}]_{ij} = \sum_k [\underline{\underline{A}}]_{ik} [\underline{\underline{B}}]_{kj}.$$

5 Identity matrix

The identity matrix is square and has ones on its diagonal e.g. for a 3×3 matrix

$$\underline{\underline{1}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

For any matrix

$$\underline{\underline{A}} = \underline{\underline{1}}\ \underline{\underline{A}} = \underline{\underline{A}}\ \underline{\underline{1}}.$$

6 Transpose

The transpose flips rows and columns. Notation: $\underline{\underline{A}}^T$

$$\underline{\underline{A}} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix} \quad \Rightarrow \quad \underline{\underline{A}}^T = \begin{pmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{pmatrix}$$

and in terms of matrix elements $[\underline{\underline{A}}^T]_{ij} = [\underline{\underline{A}}]_{ji}$.

For a column vector:

$$\underline{v} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \quad \Rightarrow \quad \underline{v}^T = \begin{pmatrix} 1 & 2 & 3 \end{pmatrix}$$

This is why we used $\underline{v}^T$ to denote a row vector above.

7 Conjugate Transpose (Hermitian Conjugate)

For complex matrices, we need the conjugate transpose (also called Hermitian conjugate or adjoint). Notation: $\underline{\underline{A}}^\dagger$ or $\underline{\underline{A}}^*$

Take the transpose **and** take the complex conjugate of each element.

Example:

$$\underline{\underline{A}} = \begin{pmatrix} 1+i & 2 \\ 3 & 4-2i \end{pmatrix} \quad \Rightarrow \quad \underline{\underline{A}}^\dagger = \begin{pmatrix} 1-i & 3 \\ 2 & 4+2i \end{pmatrix}$$

Hermitian matrices: If $\underline{\underline{A}} = \underline{\underline{A}}^\dagger$, the matrix is Hermitian. These are crucial in quantum mechanics because observables are represented by Hermitian operators.

8 Determinants

The determinant tells us if a matrix is invertible and has geometric meaning (volume scaling).

8.1 2×2 Determinant

$$\det \begin{pmatrix} a & b \\ c & d \end{pmatrix} = ad - bc$$

Example:

$$\det \begin{pmatrix} 3 & 1 \\ 2 & 4 \end{pmatrix} = 3(4) - 1(2) = 10$$

8.2 3×3 Determinant

Use cofactor expansion along the first row:

$$\det \begin{pmatrix} a & b & c \\ d & e & f \\ g & h & i \end{pmatrix} = a \det \begin{pmatrix} e & f \\ h & i \end{pmatrix} - b \det \begin{pmatrix} d & f \\ g & i \end{pmatrix} + c \det \begin{pmatrix} d & e \\ g & h \end{pmatrix}$$

Example:

$$\det\begin{pmatrix}1 & 2 & 3\\ 0 & 1 & 4\\ 5 & 6 & 0\end{pmatrix} = 1\det\begin{pmatrix}1 & 4\\ 6 & 0\end{pmatrix} - 2\det\begin{pmatrix}0 & 4\\ 5 & 0\end{pmatrix} + 3\det\begin{pmatrix}0 & 1\\ 5 & 6\end{pmatrix}$$
$$= 1(0-24) - 2(0-20) + 3(0-5) = -24 + 40 - 15 = 1$$

Determinants have several important properties:

- $\det(\underline{\underline{AB}}) = \det(\underline{\underline{A}})\det(\underline{\underline{B}})$ (determinant of product is product of determinants)
- $\det(\underline{\underline{A}}^T) = \det(\underline{\underline{A}})$ (transpose doesn't change determinant)
- $\det(\underline{\underline{A}}^{-1}) = \frac{1}{\det(\underline{\underline{A}})}$ (if inverse exists)
- $\det(c\underline{\underline{A}}) = c^n \det(\underline{\underline{A}})$ for $n \times n$ matrix (scaling by scalar)
- $\det(\underline{\underline{1}}) = 1$ (identity matrix has determinant 1)
- If $\det(\underline{\underline{A}}) = 0$, the matrix is singular (not invertible)
- Swapping two rows (or columns) changes the sign of the determinant
- If two rows (or columns) are identical, $\det(\underline{\underline{A}}) = 0$
- A multiple of a row can be added to another row without changing the determinant. The same goes for columns.

9 Matrix Inverse

The inverse $\underline{\underline{A}}^{-1}$ satisfies $\underline{\underline{AA}}^{-1} = \underline{\underline{A}}^{-1}\underline{\underline{A}} = \underline{\underline{I}}$ (identity matrix).

A matrix has an inverse only if $\det(\underline{\underline{A}}) \neq 0$.

9.1 2×2 Inverse Formula

$$\underline{\underline{A}} = \begin{pmatrix}a & b\\ c & d\end{pmatrix} \quad\Rightarrow\quad \underline{\underline{A}}^{-1} = \frac{1}{ad-bc}\begin{pmatrix}d & -b\\ -c & a\end{pmatrix}$$

Example:

$$\underline{\underline{A}} = \begin{pmatrix}3 & 1\\ 2 & 4\end{pmatrix} \quad\Rightarrow\quad \underline{\underline{A}}^{-1} = \frac{1}{10}\begin{pmatrix}4 & -1\\ -2 & 3\end{pmatrix} = \begin{pmatrix}0.4 & -0.1\\ -0.2 & 0.3\end{pmatrix}$$

Check:

$$\underline{\underline{AA}}^{-1} = \begin{pmatrix}3 & 1\\ 2 & 4\end{pmatrix}\begin{pmatrix}0.4 & -0.1\\ -0.2 & 0.3\end{pmatrix} = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} \checkmark$$

For general $n \times n$ matrices, the inverse can be computed using:

$$\underline{\underline{A}}^{-1} = \frac{1}{\det(\underline{\underline{A}})}\text{adj}(\underline{\underline{A}})$$

where $\text{adj}(\underline{\underline{A}})$ is the adjugate matrix - the transpose of the cofactor matrix. For larger matrices, this is usually computed numerically rather than by hand.

Example for 3×3 matrix:

Let $\underline{\underline{A}} = \begin{pmatrix} 1 & 2 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{pmatrix}$

First, find the cofactor matrix. The cofactor C_{ij} is $(-1)^{i+j}$ times the determinant of the 2×2 matrix obtained by deleting row i and column j:

$$C_{11} = (+1)\det\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} = 1, \quad C_{12} = (-1)\det\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} = 1, \quad C_{13} = (+1)\det\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = -1$$
$$C_{21} = (-1)\det\begin{pmatrix} 2 & 0 \\ 0 & 1 \end{pmatrix} = -2, \quad C_{22} = (+1)\det\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} = 1, \quad C_{23} = (-1)\det\begin{pmatrix} 1 & 2 \\ 1 & 0 \end{pmatrix} = 2$$
$$C_{31} = (+1)\det\begin{pmatrix} 2 & 0 \\ 1 & 1 \end{pmatrix} = 2, \quad C_{32} = (-1)\det\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = -1, \quad C_{33} = (+1)\det\begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix} = 1$$

The cofactor matrix is: $\begin{pmatrix} 1 & 1 & -1 \\ -2 & 1 & 2 \\ 2 & -1 & 1 \end{pmatrix}$

The adjugate is the transpose of the cofactor matrix:

$$\text{adj}(\underline{\underline{A}}) = \begin{pmatrix} 1 & -2 & 2 \\ 1 & 1 & -1 \\ -1 & 2 & 1 \end{pmatrix}$$

Since $\det(\underline{\underline{A}}) = 2$, we have:

$$\underline{\underline{A}}^{-1} = \frac{1}{2}\begin{pmatrix} 1 & -2 & 2 \\ 1 & 1 & -1 \\ -1 & 2 & 1 \end{pmatrix}$$

9.2 General Properties

The inverse has several useful properties:

- $(\underline{\underline{A}}^{-1})^{-1} = \underline{\underline{A}}$ (inverse of inverse gives back original)
- $(\underline{\underline{AB}})^{-1} = \underline{\underline{B}}^{-1}\underline{\underline{A}}^{-1}$ (inverse of product reverses order)
- $(\underline{\underline{A}}^{T})^{-1} = (\underline{\underline{A}}^{-1})^{T}$ (transpose and inverse commute)
- $(\underline{\underline{A}}^{\dagger})^{-1} = (\underline{\underline{A}}^{-1})^{\dagger}$ (conjugate transpose and inverse commute)
- $\det(\underline{\underline{A}}^{-1}) = \frac{1}{\det(\underline{\underline{A}})}$

10 Eigenvalues and Eigenvectors

This is likely the most important topic for quantum mechanics.

An eigenvector $\underline{v}$ of matrix $\underline{\underline{A}}$ is a vector that only gets scaled (not rotated) when $\underline{\underline{A}}$ acts on it:

$$\underline{\underline{A}}\underline{v} = \lambda\underline{v}$$

where λ is the eigenvalue (the scaling factor). In this equation both $\underline{v}$ and λ are unknowns.

This has a trivial solution of $\underline{v} = \underline{0}$ (the vector that just contains zeros) and λ = anything. We're normally only interested in the non-trivial solutions, when $\underline{v} \neq \underline{0}$, which we call the **eigenvectors**. For each eigenvector, the corresponding solution for λ is called the **eigenvalue**.

We can rearrange the equation above to

$$(\underline{\underline{A}} - \underline{\underline{1}}\lambda)\underline{v} = \underline{0}$$

so when the solution for $\underline{v}$ is not zero, the matrix $(\underline{\underline{A}} - \underline{\underline{1}}\lambda)$ must not be non-invertible. From the above, we see that the solution is non-invertible if and only if its determinant is zero $\det\left(\underline{\underline{A}} - \underline{\underline{1}}\lambda\right) = 0$, this is called the **characteristic equation**. (This is because the matrix inverse $(\underline{\underline{A}} - \underline{\underline{1}}\lambda) = \mathrm{adj}(\underline{\underline{A}})/\det\left(\underline{\underline{A}} - \underline{\underline{1}}\lambda\right)$.)

10.1 Finding Eigenvalues

Let's see this in an example. To find the eigenvalues we solve the characteristic equation:

$$\det\left(\underline{\underline{A}} - \lambda\underline{\underline{I}}\right) = 0$$

Example: Find eigenvalues of $\underline{\underline{A}} = \begin{pmatrix} 4 & 1 \\ 2 & 3 \end{pmatrix}$

$$\det\begin{pmatrix} 4-\lambda & 1 \\ 2 & 3-\lambda \end{pmatrix} = 0$$
$$(4-\lambda)(3-\lambda) - 2 = 0$$
$$12 - 7\lambda + \lambda^2 - 2 = 0$$
$$\lambda^2 - 7\lambda + 10 = 0$$
$$(\lambda - 5)(\lambda - 2) = 0$$

So $\lambda_1 = 5$ and $\lambda_2 = 2$.

10.2 Finding Eigenvectors

For each eigenvalue, solve $(\underline{\underline{A}} - \lambda\underline{\underline{I}})\underline{v} = \underline{0}$.

For $\lambda_1 = 5$:

$$\begin{pmatrix} -1 & 1 \\ 2 & -2 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

This gives $-v_1 + v_2 = 0$, so $v_2 = v_1$. We can choose $\underline{v}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

For $\lambda_2 = 2$:

$$\begin{pmatrix} 2 & 1 \\ 2 & 1 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

This gives $2v_1 + v_2 = 0$, so $v_2 = -2v_1$. We can choose $\underline{v}_2 = \begin{pmatrix} 1 \\ -2 \end{pmatrix}$.

10.3 Matrix diagonalisation

First we note that if $\underline{v}$ is an eigenvector, then any (non-zero) scalar multiple of $\underline{v}$ is an eigenvector. If we have a set of linearly-independent eigenvectors (which is often, but not always the case), we can choose them to be normalised so $\|\underline{v}_n\| = 1$. We can put these together into a matrix

$$\underline{\underline{V}} = (\underline{v}_1 \ \underline{v}_2 \ \cdots \ \underline{v}_N)$$

If we multiply this matrix by $\underline{\underline{A}}$ we find

$$\begin{aligned} \underline{\underline{A}}\,\underline{\underline{V}} &= (\underline{\underline{A}}\,\underline{v}_1 \ \underline{\underline{A}}\,\underline{v}_2 \ \cdots \ \underline{\underline{A}}\,\underline{v}_N) \\ &= (\lambda_1\underline{v}_1 \ \lambda_2\underline{v}_2 \ \cdots \ \lambda_N\underline{v}_N) \end{aligned}$$

The last line can also be written as

$$(\underline{v}_1 \ \underline{v}_2 \ \cdots \ \underline{v}_N)\begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_N \end{pmatrix} = \underline{\underline{V}}\,\underline{\underline{D}}$$

So we can write $\underline{\underline{A}}\,\underline{\underline{V}}$ as

$$\underline{\underline{A}}\,\underline{\underline{V}} = \underline{\underline{V}}\,\underline{\underline{D}}$$

If the eigenvectors are all linearly independent we can write $\underline{\underline{A}}$ as

$$\underline{\underline{A}} = \underline{\underline{V}}\,\underline{\underline{D}}\,\underline{\underline{V}}^{-1}$$

Alternatively we can write

$$\underline{\underline{D}} = \underline{\underline{V}}^{-1}\,\underline{\underline{A}}\,\underline{\underline{V}}$$

and we say we have **diagonalised** $\underline{\underline{A}}$.

10.4 Why This Matters in QM

In quantum mechanics:

- Observable properties (energy, momentum, etc.) are eigenvalues
- Quantum states that have definite values are eigenvectors
- The Schrödinger equation $\underline{\underline{H}}\psi = E\psi$ is an eigenvalue problem!

When you measure an observable, you always get one of its eigenvalues, and the system collapses into the corresponding eigenvector.

Quick Reference

- Inner product: $\langle \underline{v} | \underline{w} \rangle = v_1^* w_1 + v_2^* w_2 + \cdots$
- Matrix-vector: $[\underline{\underline{A}}\underline{v}]_i = \sum_j [\underline{\underline{A}}]_{ij} v_j$
- Transpose: $[\underline{\underline{A}}^T]_{ij} = [\underline{\underline{A}}]_{ji}$
- Conjugate transpose: $[\underline{\underline{A}}^\dagger]_{ij} = [\underline{\underline{A}}]_{ji}^*$

- Hermitian: $\underline{\underline{A}} = \underline{\underline{A}}^{\dagger}$
- Determinant tells if invertible: $\det\left(\underline{\underline{A}}\right) \neq 0$
- Eigenvalue equation: $\underline{\underline{A}}\underline{v} = \lambda\underline{v}$
- Find eigenvalues: $\det\left(\underline{\underline{A}} - \lambda\underline{\underline{I}}\right) = 0$