Quantum Mechanics for Scientists and Engineers

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Unitary and Hermitian operators

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Using unitary operators

Unitary operators to change representations of vectors

Suppose that we have a vector (function) $|f_{old}\rangle$

that is represented

when expressed as an expansion on

the functions $|\psi_n\rangle$

as the mathematical column vector $|f_{old}\rangle = \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{bmatrix}$

These numbers c_1, c_2, c_3, ...

are the projections of $|f_{old}\rangle$

on the orthogonal coordinate axes

in the vector space

labeled with $|\psi_1\rangle$, $|\psi_2\rangle$, $|\psi_3\rangle$ ...

Unitary operators to change representations of vectors

Suppose we want to represent this vector on a new set of orthogonal axes

- which we will label $|\phi_1\rangle$, $|\phi_2\rangle$, $|\phi_3\rangle$ …

Changing the axes

- which is equivalent to changing the basis set of functions
  - does not change the vector we are representing
    - but it does change
      - the column of numbers used to represent the vector

Unitary operators to change representations of vectors

For example, suppose the original vector $|f_{old}\rangle$

was actually the first basis vector in the old basis $|\psi_1\rangle$

Then in this new representation

the elements in the column of numbers

would be the projections of this vector

on the various new coordinate axes

each of which is simply $\langle\phi_m|\psi_1\rangle$

So under this coordinate transformation

or change of basis

$$\begin{bmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{bmatrix} \Rightarrow \begin{bmatrix} \langle\phi_1|\psi_1\rangle \\ \langle\phi_2|\psi_1\rangle \\ \langle\phi_3|\psi_1\rangle \\ \vdots \end{bmatrix}$$

Unitary operators to change representations of vectors

Writing similar transformations for each basis vector $|\psi_n\rangle$

we get the correct transformation

if we define a matrix

$$\hat{U} = \begin{bmatrix} u_{11} & u_{12} & u_{13} & \cdots \\ u_{21} & u_{22} & u_{23} & \cdots \\ u_{31} & u_{32} & u_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

where $u_{ij} = \langle \phi_i | \psi_j \rangle$

and we define our new column of numbers $| f_{new} \rangle$

$$| f_{new} \rangle = \hat{U} | f_{old} \rangle$$

Unitary operators to change representations of vectors

Note incidentally that here

$\left| f_{old} \right\rangle$ and $\left| f_{new} \right\rangle$ are the same vector in the vector space

Only the representation

the coordinate axes

and, consequently

the column of numbers

that have changed

not the vector itself

Unitary operators to change representations of vectors

Now we can prove that $\hat{U}$ is unitary

Writing the matrix multiplication in its sum form

$$\left(\hat{U}^{\dagger}\hat{U}\right)_{ij} = \sum_m u_{mi}^{*} u_{mj} = \sum_m \langle \phi_m | \psi_i \rangle^{*} \langle \phi_m | \psi_j \rangle = \sum_m \langle \psi_i | \phi_m \rangle \langle \phi_m | \psi_j \rangle$$

$$= \langle \psi_i | \left(\sum_m | \phi_m \rangle \langle \phi_m | \right) | \psi_j \rangle = \langle \psi_i | \hat{I} | \psi_j \rangle = \langle \psi_i | \psi_j \rangle = \delta_{ij}$$

so $\hat{U}^{\dagger}\hat{U} = \hat{I}$

hence $\hat{U}$ is unitary

since its Hermitian transpose is therefore its inverse

Unitary operators to change representations of vectors

Hence any change in basis

- can be implemented with a unitary operator

We can also say that

- any such change in representation to a new orthonormal basis
  - is a unitary transform

Note also, incidentally, that

$$\hat{U}\hat{U}^{\dagger} = \left(\hat{U}^{\dagger}\hat{U}\right)^{\dagger} = \hat{I}^{\dagger} = \hat{I}$$

- so the mathematical order of this multiplication makes no difference

Unitary operators to change representations of operators

Consider a number such as $\langle g|\hat{A}|f\rangle$

where vectors $|f\rangle$ and $|g\rangle$ and operator $\hat{A}$ are arbitrary

This result should not depend on the coordinate system

so the result in an "old" coordinate system $\langle g_{old}|\hat{A}_{old}|f_{old}\rangle$

should be the same in a "new" coordinate system

that is, we should have $\langle g_{new}|\hat{A}_{new}|f_{new}\rangle = \langle g_{old}|\hat{A}_{old}|f_{old}\rangle$

Note the subscripts "new" and "old" refer to representations

not the vectors (or operators) themselves

which are not changed by change of representation

Only the numbers that represent them are changed

Unitary operators to change representations of operators

With unitary $\hat{U}$ operator to go from "old" to "new" systems

we can write $\langle g_{new} | \hat{A}_{new} | f_{new} \rangle = \left(| g_{new} \rangle \right)^{\dagger} \hat{A}_{new} | f_{new} \rangle$

$$= \left(\hat{U} | g_{old} \rangle \right)^{\dagger} \hat{A}_{new} \left(\hat{U} | f_{old} \rangle \right) = \langle g_{old} | \hat{U}^{\dagger} \hat{A}_{new} \hat{U} | f_{old} \rangle$$

Since we believe also that $\langle g_{new} | \hat{A}_{new} | f_{new} \rangle = \langle g_{old} | \hat{A}_{old} | f_{old} \rangle$

then we identify $\hat{A}_{old} = \hat{U}^{\dagger} \hat{A}_{new} \hat{U}$

or since $\hat{U} \hat{A}_{old} \hat{U}^{\dagger} = \left(\hat{U} \hat{U}^{\dagger} \right) \hat{A}_{new} \left(\hat{U} \hat{U}^{\dagger} \right) = \hat{A}_{new}$

then $\boxed{\hat{A}_{new} = \hat{U} \hat{A}_{old} \hat{U}^{\dagger}}$

Unitary operators that change the state vector

For example, if the quantum mechanical state $|\psi\rangle$

is expanded on the basis $|\psi_n\rangle$ to give $|\psi\rangle = \sum_n a_n |\psi_n\rangle$

then $\sum_n |a_n|^2 = 1$

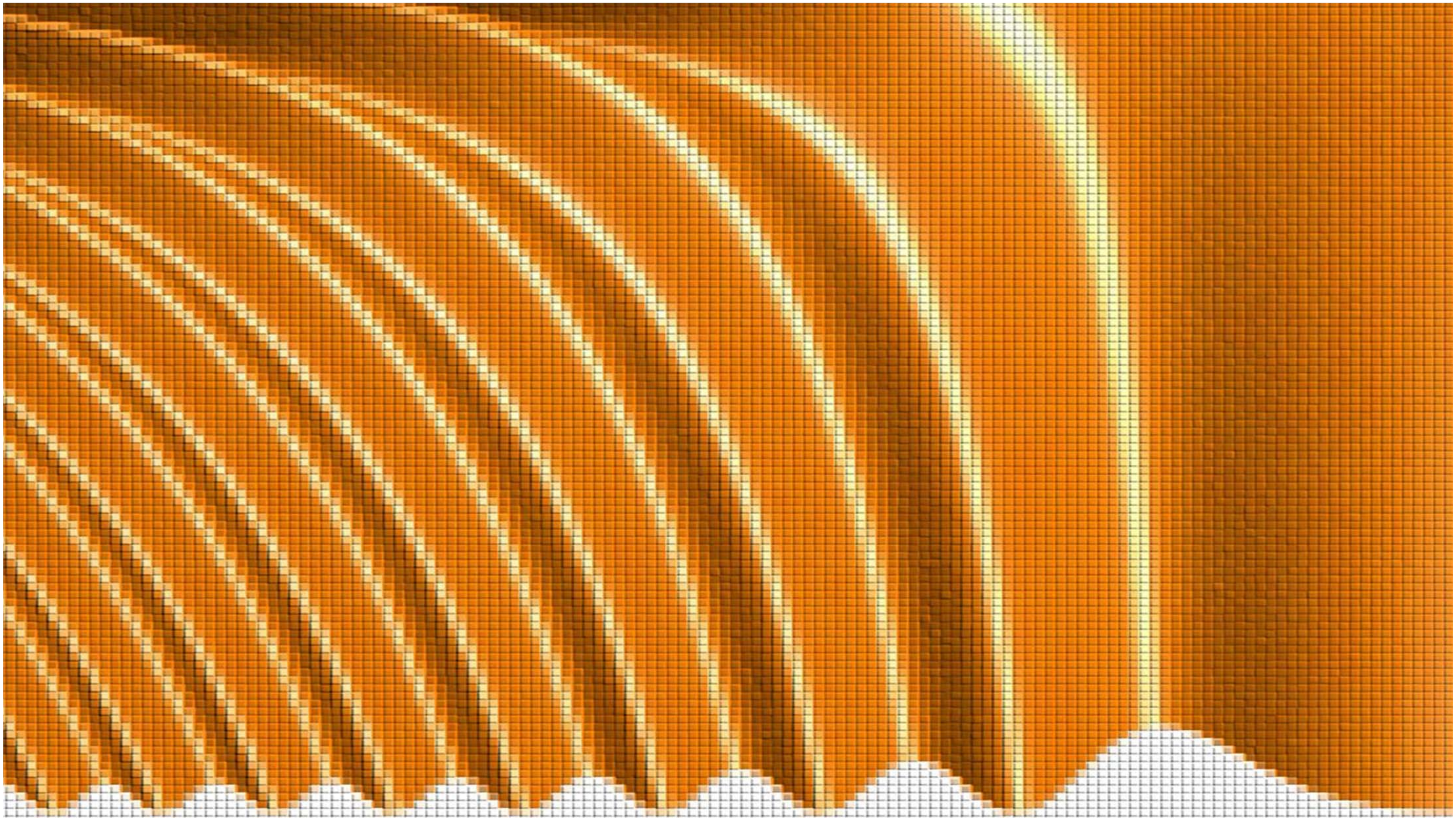
and if the particle is to be conserved

then this sum is retained as the quantum mechanical system evolves in time

But this is just the square of the vector length

Hence a unitary operator, which conserves length

describes changes that conserve the particle



Unitary and Hermitian operators

Hermitian operators

Hermitian operators

A Hermitian operator is equal to its own Hermitian adjoint

$$\boxed{\hat{M}^{\dagger} = \hat{M}}$$

Equivalently it is self-adjoint

Hermitian operators

In matrix terms, with

$$\hat{M} = \begin{bmatrix} M_{11} & M_{12} & M_{13} & \cdots \\ M_{21} & M_{22} & M_{23} & \cdots \\ M_{31} & M_{32} & M_{33} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \quad \text{then} \quad \hat{M}^{\dagger} = \begin{bmatrix} M_{11}^{*} & M_{21}^{*} & M_{31}^{*} & \cdots \\ M_{12}^{*} & M_{22}^{*} & M_{31}^{*} & \cdots \\ M_{13}^{*} & M_{23}^{*} & M_{33}^{*} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

so the Hermiticity implies $M_{ij} = M_{ji}^{*}$ for all i and j

so, also

the diagonal elements of a Hermitian operator must be real

Hermitian operators

To understand Hermiticity in the most general sense

consider

$$\langle g|\hat{M}|f\rangle$$

for arbitrary $|f\rangle$ and $|g\rangle$ and some operator $\hat{M}$

We examine

$$\left(\langle g|\hat{M}|f\rangle\right)^{\dagger}$$

Since this is just a number

a "1 x 1" matrix

it is also true that $\left(\langle g|\hat{M}|f\rangle\right)^{\dagger} \equiv \left(\langle g|\hat{M}|f\rangle\right)^{*}$

Hermitian operators

We can also analyze $\left(\langle g|\hat{M}|f\rangle\right)^{\dagger}$ using the rule $\left(\hat{A}\hat{B}\right)^{\dagger}=\hat{B}^{\dagger}\hat{A}^{\dagger}$ for Hermitian adjoints of products

So $\left(\langle g|\hat{M}|f\rangle\right)^{*}\equiv\left(\langle g|\hat{M}|f\rangle\right)^{\dagger}=\left(\hat{M}|f\rangle\right)^{\dagger}\left(\langle g|\right)^{\dagger}=\left(|f\rangle\right)^{\dagger}\hat{M}^{\dagger}\left(\langle g|\right)^{\dagger}$

$$=\langle f|\hat{M}^{\dagger}|g\rangle$$

Hence, if $\hat{M}$ is Hermitian, with therefore $\hat{M}^{\dagger}=\hat{M}$

then $$\boxed{\left(\langle g|\hat{M}|f\rangle\right)^{*}=\langle f|\hat{M}|g\rangle}$$

even if $|f\rangle$ and $|g\rangle$ are not orthogonal

This is the most general statement of Hermiticity

Hermitian operators

In integral form, for functions $f(x)$ and $g(x)$

the statement $\left(\langle g|\hat{M}|f\rangle\right)^* = \langle f|\hat{M}|g\rangle$ can be written

$$\int g^*(x)\hat{M}f(x)\,dx = \left[\int f^*(x)\hat{M}g(x)\,dx\right]^*$$

We can rewrite the right hand side using $(ab)^* = a^*b^*$

$$\int g^*(x)\hat{M}f(x)\,dx = \int f(x)\left\{\hat{M}g(x)\right\}^*dx$$

and a simple rearrangement leads to

$$\int g^*(x)\hat{M}f(x)\,dx = \int \left\{\hat{M}g(x)\right\}^* f(x)\,dx$$

which is a common statement of Hermiticity in integral form

Bra-ket and integral notations

Note that in the bra-ket notation

the operator can also be considered to operate to the left

$\langle g|\hat{A}$ is just as meaningful a statement as $\hat{A}|f\rangle$

and we can group the bra-ket multiplications as we wish

$$\langle g|\hat{A}|f\rangle \equiv \left(\langle g|\hat{A}\right)|f\rangle \equiv \langle g|\left(\hat{A}|f\rangle\right)$$

Conventional operators in the notation used in integration

such as a differential operator, d/dx

do not have any meaning operating "to the left"

so Hermiticity in this notation is the less elegant form

$$\int g^*(x)\hat{M}f(x)\,dx = \int\left\{\hat{M}g(x)\right\}^* f(x)\,dx$$

Reality of eigenvalues

Suppose $|\psi_n\rangle$ is a normalized eigenvector of the Hermitian operator $\hat{M}$ with eigenvalue μ_n

Then, by definition

$$\hat{M}|\psi_n\rangle = \mu_n|\psi_n\rangle$$

Therefore

$$\langle\psi_n|\hat{M}|\psi_n\rangle = \mu_n\langle\psi_n|\psi_n\rangle = \mu_n$$

But from the Hermiticity of $\hat{M}$ we know

$$\langle\psi_n|\hat{M}|\psi_n\rangle = \left(\langle\psi_n|\hat{M}|\psi_n\rangle\right)^* = \mu_n^*$$

and hence μ_n must be real

Orthogonality of eigenfunctions for different eigenvalues

Trivially $$0 = \langle \psi_m | \hat{M} | \psi_n \rangle - \langle \psi_m | \hat{M} | \psi_n \rangle$$

By associativity $$0 = \left(\langle \psi_m | \hat{M} \right) | \psi_n \rangle - \langle \psi_m | \left(\hat{M} | \psi_n \rangle \right)$$

Using $\left(\hat{A}\hat{B} \right)^\dagger = \hat{B}^\dagger \hat{A}^\dagger$ $$0 = \left(\hat{M}^\dagger | \psi_m \rangle \right)^\dagger | \psi_n \rangle - \langle \psi_m | \left(\hat{M} | \psi_n \rangle \right)$$

Using Hermiticity $\hat{M} = \hat{M}^\dagger$ $$0 = \left(\hat{M} | \psi_m \rangle \right)^\dagger | \psi_n \rangle - \langle \psi_m | \left(\hat{M} | \psi_n \rangle \right)$$

Using $\hat{M} | \psi_n \rangle = \mu_n | \psi_n \rangle$ $$0 = \left(\mu_m | \psi_m \rangle \right)^\dagger | \psi_n \rangle - \langle \psi_m | \mu_n | \psi_n \rangle$$

μ_m and μ_n are real numbers $$0 = \mu_m \left(| \psi_m \rangle \right)^\dagger | \psi_n \rangle - \mu_n \langle \psi_m || \psi_n \rangle$$

Rearranging $$0 = \left(\mu_m - \mu_n \right) \langle \psi_m | \psi_n \rangle$$

But μ_m and μ_n are different, so $0 = \langle \psi_m | \psi_n \rangle$ i.e., orthogonality

Degeneracy

It is quite possible

and common in symmetric problems

to have more than one eigenfunction

associated with a given eigenvalue

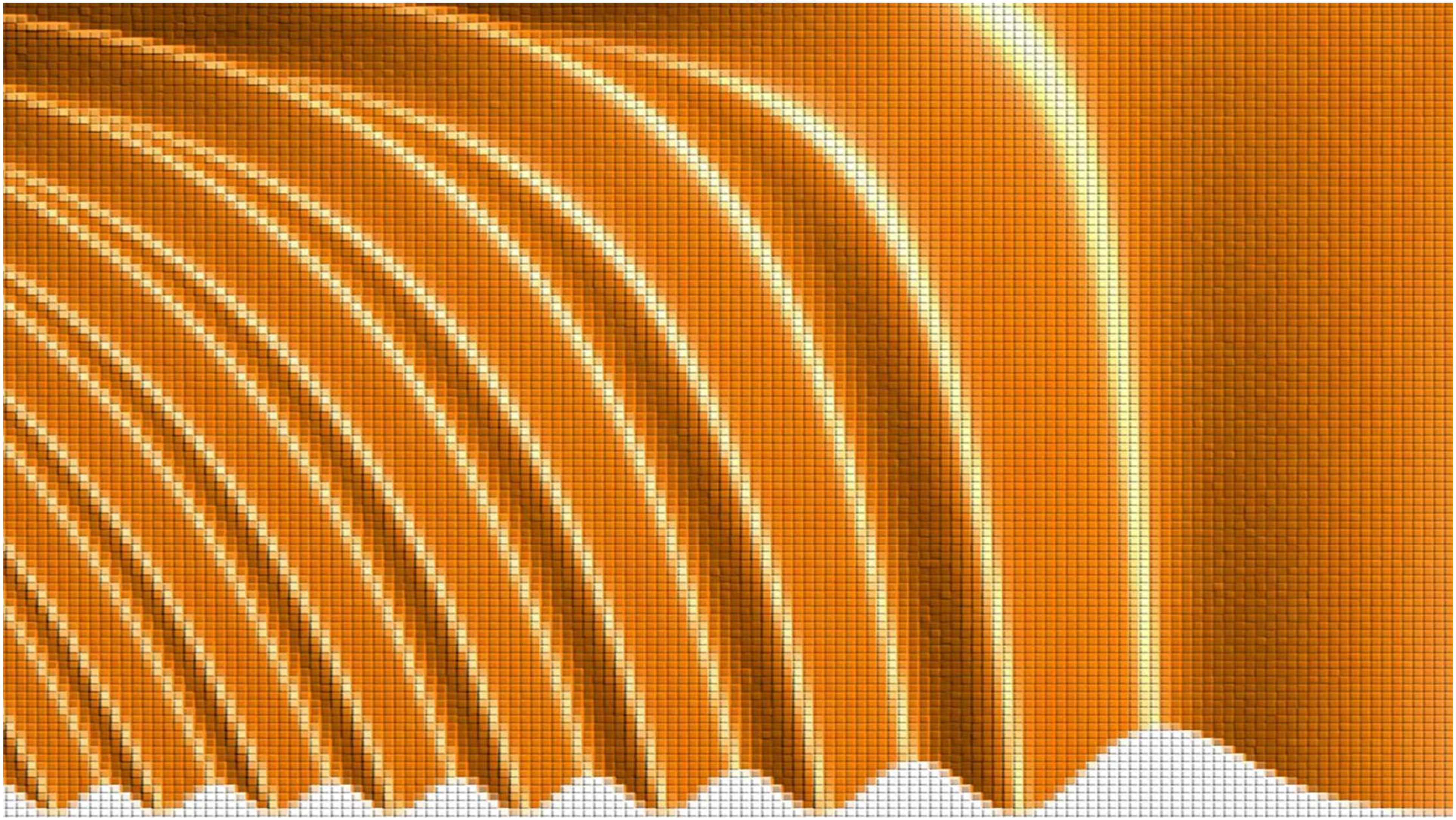
This situation is known as degeneracy

It is provable that

the number of such degenerate solutions

for a given finite eigenvalue

is itself finite



Unitary and Hermitian operators

Matrix form of derivative operators

Matrix form of derivative operators

Returning to our original discussion of functions as vectors

we can postulate a form for the differential operator

$$\frac{d}{dx} \equiv \begin{bmatrix} \ddots & & & & \\ \cdots & -\frac{1}{2\delta x} & 0 & \frac{1}{2\delta x} & 0 & \cdots \\ & \cdots & 0 & -\frac{1}{2\delta x} & 0 & \frac{1}{2\delta x} & \cdots \\ & & & & & \ddots \end{bmatrix}$$

where we presume we can take the limit as $\delta x \to 0$

Matrix form of derivative operators

If we multiply the column vector whose elements are the values of the function then

$$\begin{bmatrix} \ddots & & & & & \\ \cdots & -\frac{1}{2\delta x} & 0 & \frac{1}{2\delta x} & 0 & \cdots \\ \cdots & 0 & -\frac{1}{2\delta x} & 0 & \frac{1}{2\delta x} & \cdots \\ & & & & & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ f(x_i - \delta x) \\ f(x_i) \\ f(x_i + \delta x) \\ f(x_i + 2\delta x) \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ \dfrac{f(x_i + \delta_x) - f(x_i - \delta x)}{2\delta x} \\ \dfrac{f(x_i + 2\delta_x) - f(x_i)}{2\delta x} \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ \left.\dfrac{df}{dx}\right|_{x_i} \\ \left.\dfrac{df}{dx}\right|_{x_i + \delta x} \\ \vdots \end{bmatrix}$$

where we are taking the limit as $\delta x \to 0$

Hence we have a way of representing a derivative as a matrix

Matrix form of derivative operators

Note this matrix is antisymmetric in reflection about the diagonal

and it is not Hermitian

Indeed

somewhat surprisingly

d/dx is not Hermitian

By similar arguments, though

d^2/dx^2 gives a symmetric matrix

and is Hermitian

$$\frac{d}{dx} \equiv \begin{bmatrix} \ddots & & & & & \\ \cdots & -\frac{1}{2\delta x} & 0 & \frac{1}{2\delta x} & 0 & \cdots \\ & \cdots & 0 & -\frac{1}{2\delta x} & 0 & \frac{1}{2\delta x} & \cdots \\ & & & & & \ddots \end{bmatrix}$$

Matrix corresponding to multiplying by a function

We can formally "operate" on the function $f(x)$

by multiplying it by the function $V(x)$

to generate another function $g(x) = V(x) f(x)$

Since $V(x)$ is performing the role of an operator

we can if we wish represent it as a (diagonal) matrix

whose diagonal elements are

the values of the function at each of the different points

If $V(x)$ is real

then its matrix is Hermitian as required for $\hat{H}$