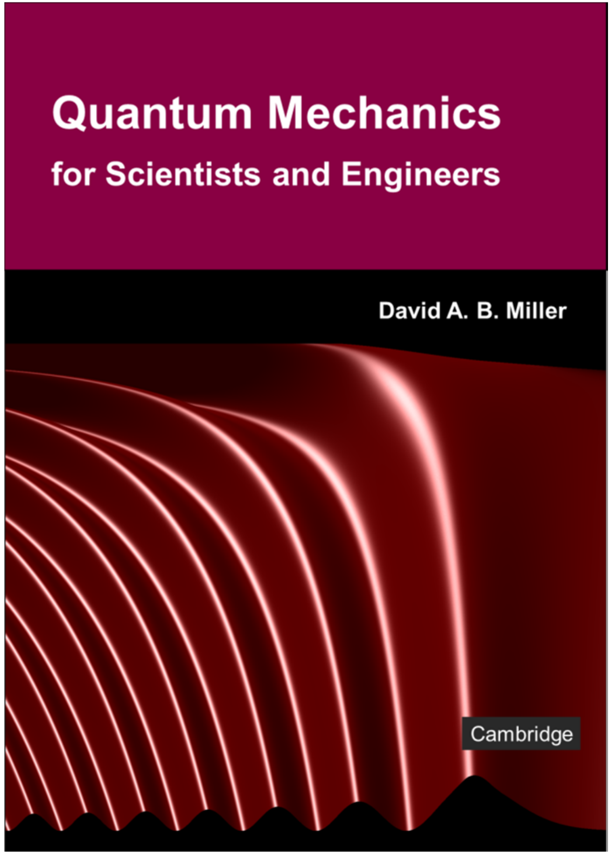
6.2 Unitary and Hermitian operators

Slides: Video 6.2.5 Matrix form of derivative operators

Text reference: Quantum Mechanics for Scientists and Engineers

Section 4.12 – 4.13



Unitary and Hermitian operators

Matrix form of derivative operators

Quantum mechanics for scientists and engineers

David Miller

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 $\hat{H}$