

# Computing the Discretised Schrödinger Equation

## Part 2

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## 1 Derivative approximations

### 1.1 Some preliminaries

Let us define the vector  $\vec{S}_i = \begin{pmatrix} a_i \\ b_i \end{pmatrix}$

Therefore the overall matrix of points  $S$  will be:

$$S = \begin{pmatrix} a_0 & \dots & a_n \\ b_0 & \dots & b_n \end{pmatrix}$$

Define:  $\vec{F}(\vec{S}) = \frac{\partial \vec{S}}{\partial \tau}$

We can see that:

$$\frac{\partial}{\partial t} \begin{pmatrix} a_i \\ b_i \end{pmatrix} \approx \underbrace{\begin{pmatrix} b_i - (b_{i+1} + b_{i-1}) \\ a_{i+1} + a_{i-1} - a_i \end{pmatrix}}_{\vec{F}}$$

This is all the definitions we need for the derivative approximations.

### 1.2 Method 1: 2nd Order Approximation

This method produces errors on the order of  $\mathcal{O}(d\tau^3)$

We begin by starting with an initial point on the line,  $\vec{S}_0$ . We must first approximate a half step by the following method: