

The Schrödinger equation is a second-order partial differential equation that describes the time evolution of a quantum system, represented by its wave function. It is given by:

$$i\partial_t u(x, t) = \Delta u(x, t) + V(x, t)u(x, t), \quad (1)$$

where Δ is the Laplacian operator, $V(x, t)$ is the potential, and $u(x, t)$ is the wave function. The weak form of the Schrödinger equation is given by:

$$i \int_{\Omega} (\partial_t u) \bar{v} = \int_{\Omega} \nabla u \cdot \nabla \bar{v} + \int_{\Omega} V(x, t)u\bar{v}, \quad (2)$$

where $v := v(x, t)$ is a test function. Discretizing the time domain and approximating the time derivative with finite differences, we get:

$$i \int_{\Omega} \left(\frac{u^{t+dt} - u^t}{dt} \right) \bar{v} = \int_{\Omega} \nabla u^{t+dt} \cdot \nabla \bar{v} + \int_{\Omega} V(x, t)u^t \bar{v} \quad (3)$$

Rearranging, we get:

$$i \int_{\Omega} u^{t+dt} \bar{v} - dt \int_{\Omega} \nabla u^{t+dt} \cdot \nabla \bar{v} = i \int_{\Omega} u^t \bar{v} + dt \int_{\Omega} V(x, t)u^t \bar{v}, \quad (4)$$

which can be solved iteratively using a time-stepping method.