VIII.

IV. Schrödinger Equation

V. Wave Equation

VIII. 4. Schrödinger Equation

We study the Schrödinger equation over an interval $[0, L]$ with a linear potential term:

$$i\,\partial_t u(x,t) = \partial_{xx}^2 u(x,t) - \underbrace{a\,u(x,t)}_{\substack{\text{potential term} \\ a \geqslant 0}} + f(x,t).$$

We impose Dirichlet boundary conditions,

$$u(0,t) = 0, \qquad u(L,t) = 0, \qquad t > 0,$$

and initial values at $t = 0$:

$$u(x,0) = u_0(x), \qquad 0 \leq x \leq L.$$

<u>Physical meaning</u>: Linearized model for the movement of a particle in a box. The particle cannot exit the box, and at all times $t>0$, the function $|u(x,t)|^2$ is the probability density function of observing the particle at position x.

One can show that the integral

$$\int_0^L |u(x,t)|^2 \text{ remains constant.}$$

<u>Solution strategy</u>:

- We write $u(x,t)$ as Fourier sine series with time-dependent coefficients
- We solve ordinary differential equations in the coefficients
- We put everything back together

We begin with Fourier sine series

$$u(x,t) = \sum_{n=1}^{\infty} b_n(t) \sin\left(\frac{\pi n}{L} x\right)$$

$$u_0(x) = \sum_{n=1}^{\infty} b_n^0 \cdot \sin\left(\frac{\pi n}{L} x\right)$$

$$f(x,t) = \sum_{n=1}^{\infty} \beta_n(t) \sin\left(\frac{\pi n}{L} x\right)$$

We write the derivatives as Fourier sine series

$$\partial_{xx}^2 u(x,t) = \sum_{n=1}^{\infty} b_n(t) (-1) \left(\frac{\pi n}{L}\right)^2 \sin\left(\frac{\pi n}{L} x\right)$$

$$i \partial_t u(x,t) = \sum_{n=1}^{\infty} i\, b_n'(t) \sin\left(\frac{\pi n}{L} x\right)$$

Together, we find

$$\sum_{n=1}^{\infty} i\, b_n'(t) \sin\left(\frac{\pi n}{L} x\right) = \sum_{n=1}^{\infty} \left[(-1)\left(\frac{\pi n}{L}\right)^2 b_n(t) - a b_n(t) + \beta_n(t) \right] \sin\left(\frac{\pi n}{L} x\right)$$

Correspondingly,

$$i\, b_n'(t) = (-1)\left(\frac{\pi n}{L}\right)^2 b_n(t) - a b_n(t) + \beta_n(t)$$

$$= -\left(\left(\frac{\pi n}{L}\right)^2 + a \right) b_n(t) + \beta_n(t)$$

$$b_n'(t) = \frac{-1}{i} \left(\left(\frac{\pi n}{L}\right)^2 + a \right) b_n(t) + \frac{1}{i} \beta_n(t)$$

For the solution, we take the Laplace transform,

$$z B_n(z) - b_n(0) = \frac{-1}{i} \left(\left(\frac{\pi n}{L}\right)^2 + a \right) B_n(z) + \frac{1}{i} \mathcal{L}\left[\beta_n(t) \right]$$

For simplicity, we assume that $f(x,t)$ does not depend on t, i.e., "constant in time", and hence $\beta_n(t)$ will be constant.

$$z\, B_n(z) - b_n(0) = \frac{-1}{i}\left(\left(\frac{\pi n}{L}\right)^2 + a\right) B_n(z) + \frac{1}{i}\,\frac{\beta_n}{z}$$

We isolate $B_n(z)$

$$B_n(z) = \frac{b_n^0}{z - i\left(\frac{\pi^2 n^2}{L^2} + a\right)} - i\beta_n \cdot \frac{1}{z} \cdot \frac{1}{z - i\left(\frac{\pi^2 n^2}{L^2} + a\right)}$$

From here, we find

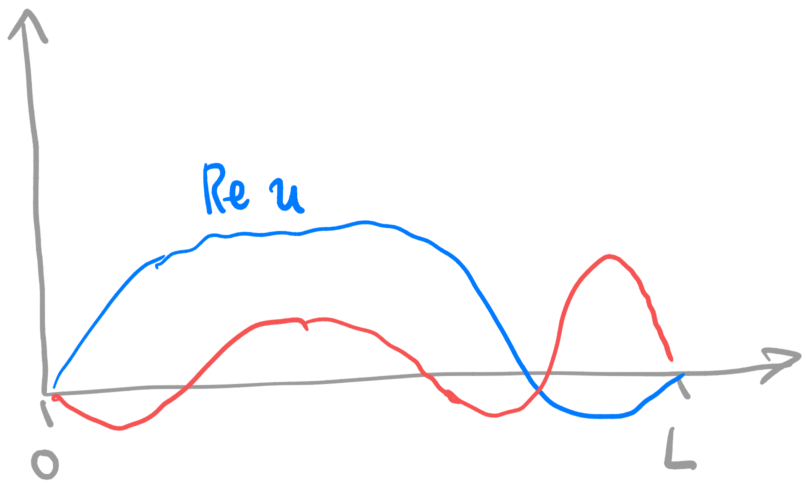
$$b_n(t) = b_n^0\, e^{i\left(\frac{\pi^2 n^2}{L^2} + a\right)t} - i\beta_n \int_0^t e^{i\left(\frac{\pi^2 n^2}{L^2} + a\right)(t-s)}\, ds$$

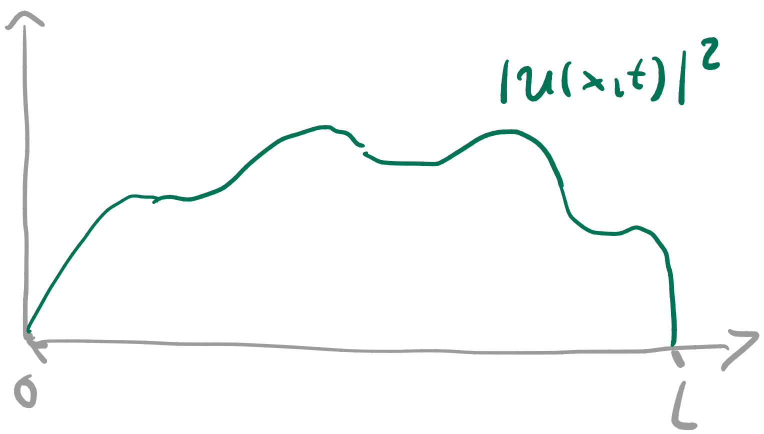
The complete solution is

$$u(x,t) = \sum_{n=1}^{\infty} b_n(t) \sin\left(\frac{\pi n}{L} x\right)$$

Further remarks: The function $u(x,t)$ describes the probability density of observing a particle at position x.

$$|u(x,t)|^2 = |\operatorname{Re} u(x,t)|^2 + |\operatorname{Im} u(x,t)|^2$$





The integral of $|u(x,t)|^2$ remains constant. Hence,

$$\int_0^L |u_0(x)|^2 = 1 \qquad \Longrightarrow \qquad \int_0^L |u(x,t)|^2 = 1$$

To see this,

$$\partial_t |u(x,t)|^2 = \partial_t \left(u(x,t)\ \bar{u}(x,t) \right)$$

$$= \partial_t u(x,t) \cdot \bar{u}(x,t) + u(x,t) \cdot \partial_t \bar{u}(x,t)$$

$$= \left(-i\,\partial_{xx} u + i a u\right) \cdot \bar{u} + u \cdot \left(i\,\partial_{xx}\bar{u} - i a \bar{u} \right)$$

$$= -i\,\partial_{xx} u \cdot \bar{u} + \cancel{i a u \bar{u}} + i u \cdot \partial_{xx}\bar{u} - \cancel{i a u \bar{u}}$$

$$= -i \left[\partial_{xx} u \cdot \bar{u} - u \cdot \partial_{xx} \bar{u} \right]$$

$$= -i \Big[\partial_{xx} u \cdot \bar{u} \underbrace{+ \partial_x u \cdot \partial_x \bar{u} - \partial_x u \cdot \partial_x \bar{u}}_{\text{"addition of zero"}} - u\, \partial_{xx} \bar{u} \Big]$$

$$= -i\left[\partial_x(\partial_x u\cdot\bar{u}) - \partial_x(u\cdot\partial_x\bar{u})\right]$$

This is used as follows:

$$\partial_t \int_0^L |u(x,t)|^2\,dx = \int_0^L \partial_t |u(x,t)|^2\,dx$$

$$= \int_0^L -i\left(\partial_x(\partial_x u\cdot\bar{u}) - \partial_x(u\cdot\partial_x\bar{u})\right)dx$$

$$= -i\int_0^L \partial_x(\partial_x u\cdot\bar{u}) - \partial_x(u\cdot\partial_x\bar{u})\,)\,dx$$

Using fundamental theorem of calculus

$$\partial_t\int_0^L |u(x,t)|^2\,dx = -i\left[\partial_x u(L)\cdot\bar{u}(L) - \partial_x u(0)\bar{u}(0) - u(L)\partial_x\bar{u}(L) + u(0)\partial_x\bar{u}(0)\right]$$

$$= 0$$ ← because boundary conditions $u(0) = u(L) = 0$, $\bar{u}(0) = \bar{u}(L) = 0$

VIII. 5 Wave Equation

We consider the wave equation over the interval $[0, L]$.
The unknown function $u(x,t)$ satisfies

$$\partial_{tt}^2 u(x,t) = \underset{\substack{\uparrow \\ \text{material} \\ \text{parameter}}}{c^2} \partial_{xx}^2 u(x,t) + \underset{\substack{\uparrow \\ \text{external force}}}{f(x,t)} \qquad \begin{matrix} 0 < x < L \\ t > 0 \end{matrix}$$

Boundary conditions (Dirichlet, again)

$$u(0,t) = 0, \qquad u(L,t) = 0$$

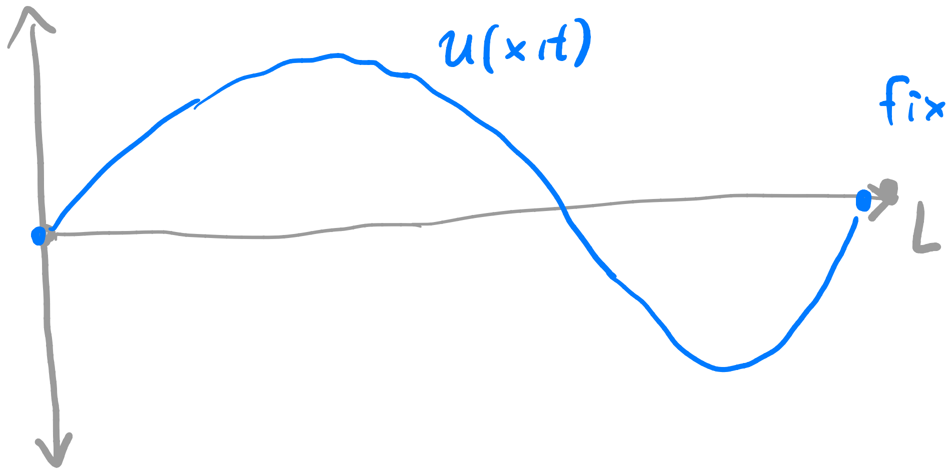
Initial conditions:

$$u(x,0) = u_0(x), \qquad \partial_t u(x,0) = V_0(x)$$

initial values for u and $\partial_t u$

Physics interpretation

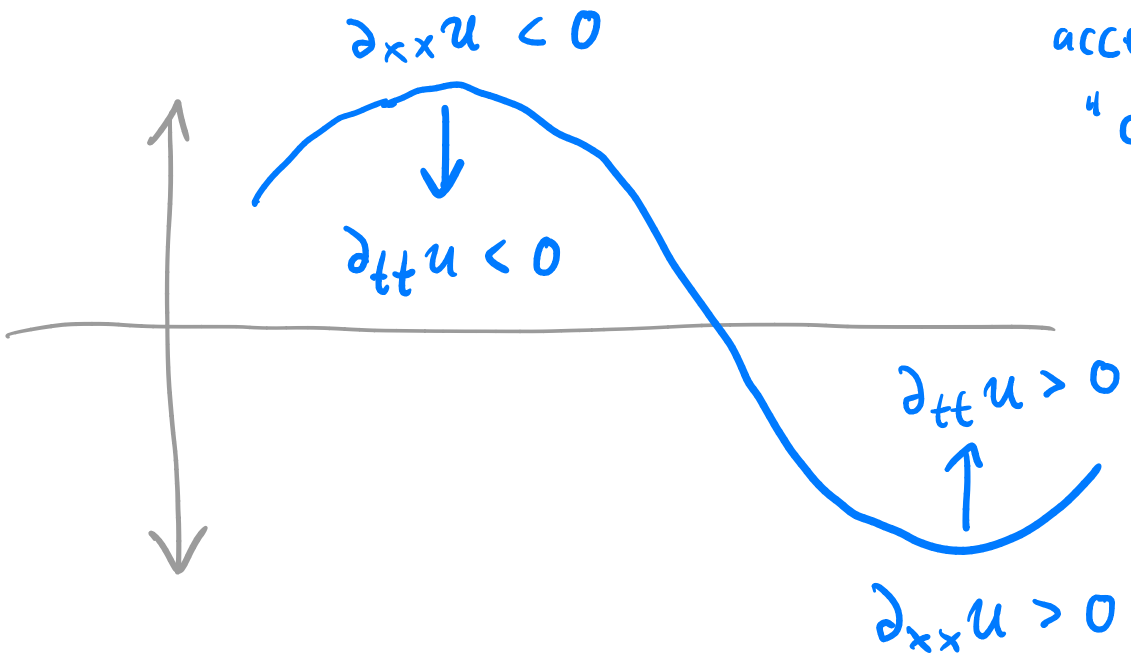
$u(x,t)$ = excitation of an elastic string



fixed at left / right endpoints

u_0 = initial position

v_0 = initial vertical velocity



accelleration depends on the "curvature" of the elastic string

Applications:

vibrations, guitar strings, optics, simplified relativity

We solve this differential equation over $[0, L]$ using Fourier series (extension to odd $2L$-periodic function, take Fourier series)

$$u(x,t) = \sum_{n=1}^{\infty} b_n(t) \sin\left(\frac{\pi n}{L} x\right)$$

$$u_0(x) = \sum_{n=1}^{\infty} b_n^0 \sin\left(\frac{\pi n}{L} x\right)$$

$$v_0(x) = \sum_{n=1}^{\infty} v_n^0 \sin\left(\frac{\pi n}{L} x\right)$$

$$f(x,t) = \sum_{n=1}^{\infty} f_n(t) \sin\left(\frac{\pi n}{L} x\right)$$

Differential equation

$$\partial_t u(x,t) = \sum_{n=1}^{\infty} b_n'(t) \sin\left(\frac{\pi n}{L} x\right)$$

$$\partial_{tt}^2 u(x,t) = \sum_{n=1}^{\infty} b_n''(t) \sin\left(\frac{\pi n}{L} x\right)$$

$$\partial_{xx}^2 u(x,t) = \sum_{n=1}^{\infty} b_n(t) (-1) \left(\frac{\pi n}{L}\right)^2 \sin\left(\frac{\pi n}{L} x\right)$$

Now

$$\partial_{tt}^2 u(x,t) = c^2 \partial_{xx} u(x,t) + f(x,t)$$

$$\sum_{n=1}^{\infty} b_n''(t) \sin\left(\frac{\pi n}{L} x\right) = \sum_{n=1}^{\infty} \left[c^2 (-1) \left(\frac{\pi n}{L}\right)^2 b_n(t) + f_n(t)\right] \sin\left(\frac{\pi n}{L} x\right)$$

Hence, for each $n = 1, 2, \dots$

$$b_n''(t) = c^2 (-1)\left(\frac{\pi n}{L}\right)^2 b_n(t) + f_n(t)$$

initial values :

$$b_n(0) = b_n^0 \quad \longleftarrow \quad \sum_{n=1}^{\infty} b_n(0) \sin\left(\frac{\pi n}{L} x\right) = \sum_{n=1}^{\infty} b_n^0 \sin\left(\frac{\pi n}{L} x\right)$$

$$b_n'(0) = v_n^0 \quad \longleftarrow \quad \sum_{n=1}^{\infty} b_n'(0) \sin\left(\frac{\pi n}{L} x\right) = \sum_{n=1}^{\infty} v_n^0 \sin\left(\frac{\pi n}{L} x\right)$$

We solve this Cauchy problem via the Laplace transform. First,

$$z^2 B_n(z) - z\, b_n(0) - b_n'(0) = c^2 (-1) \left(\frac{\pi n}{L}\right)^2 B_n(z) + F_n(z)$$

Isolating $B_n(z)$,

$$\left[z^2 + c^2 \left(\frac{\pi n}{L}\right)^2\right] B_n(z) = F_n(z) + z\, b_n(0) + b_n'(0)$$

$$B_n(z) = F_n(z) \frac{1}{z^2 + c^2\left(\frac{\pi n}{L}\right)^2} + b_n(0) \frac{z}{z^2 + c^2\left(\frac{\pi n}{L}\right)^2} + b_n'(0) \frac{1}{z^2 + c^2\left(\frac{\pi n}{L}\right)^2}$$

$$= F_n(z) \frac{1}{z^2 + c^2\left(\frac{\pi n}{L}\right)^2} + b_n^0 \frac{z}{z^2 + c^2\left(\frac{\pi n}{L}\right)^2} + v_n^0 \frac{1}{z^2 + c^2\left(\frac{\pi n}{L}\right)^2}$$

We recall Laplace transforms ...

$$\sin(\omega t) \rightsquigarrow \frac{\omega}{z^2+\omega^2} \qquad \cos(\omega t) \rightsquigarrow \frac{z}{z^2+\omega^2}$$

We rewrite

$$B_n(z) = F_n(z)\frac{1}{z^2+c^2\left(\frac{\pi n}{L}\right)^2} + b_n^0 \frac{z}{z^2+c^2\left(\frac{\pi n}{L}\right)^2} + v_n^0 \frac{1}{z^2+c^2\left(\frac{\pi n}{L}\right)^2}$$

$$= F_n(z)\frac{1}{c\frac{\pi n}{L}}\cdot\frac{c\frac{\pi n}{L}}{z^2+c^2\left(\frac{\pi n}{L}\right)^2} + b_n^0 \frac{z}{z^2+c^2\left(\frac{\pi n}{L}\right)^2} + \frac{v_n^0}{c\frac{\pi n}{L}}\cdot\frac{c\frac{\pi n}{L}}{z^2+c^2\left(\frac{\pi n}{L}\right)^2}$$

Therefore,

$$b_n(t) = \frac{1}{c\frac{\pi n}{L}}\int_0^t f(s)\sin\left[c\frac{\pi n}{L}(t-s)\right]ds + b_n^0\cos\left(c\frac{\pi n}{L}t\right) + \frac{v_n^0}{c\frac{\pi n}{L}}\sin\left(c\frac{\pi n}{L}t\right)$$

solves the Cauchy problem.

Check differential equation and initial values

$$\partial_{tt}^2 \left[b_n^\circ \cos\left(c \tfrac{\pi n}{L} t\right) \right] = -c^2 \left(\tfrac{\pi n}{L}\right)^2 b_n^\circ \cos\left(c \tfrac{\pi n}{L} t\right)$$

$$\partial_{tt}^2 \left[\frac{v_n^\circ}{c \frac{\pi n}{L}} \sin\left(c \tfrac{\pi n}{L} t\right) \right] = -c^2 \left(\tfrac{\pi n}{L}\right)^2 \frac{v_n^\circ}{c \frac{\pi n}{L}} \sin\left(c \tfrac{\pi n}{L} t\right)$$

$$\partial_t \int_0^t f(s) \sin\left(c \tfrac{\pi n}{L} [t-s]\right) ds = f(t) \sin(0) + \int_0^t f(s)\, \partial_t \sin\left(c \tfrac{\pi n}{L} [t-s]\right) ds$$

$$= c \frac{\pi n}{L} \int_0^t f(s) \cos\left(c \tfrac{\pi n}{L} [t-s]\right) ds$$

"Leibniz integral rule"

$$\Rightarrow \partial_{tt}^2 \int_0^t f(s) \sin\left(c \tfrac{\pi n}{L} [t-s]\right)$$

$$= c \frac{\pi n}{L} f(t) \cos(0) + c \frac{\pi n}{L} \int_0^t f(s)\, (-1)\, c \frac{\pi n}{L} \sin\left(c \tfrac{\pi n}{L} [t-s]\right) ds$$

$$= c \frac{\pi n}{L} f(t) + (-1)\, c^2 \left(\tfrac{\pi n}{L}\right)^2 \int_0^t f(s) \sin\left(c \tfrac{\pi n}{L} [t-s]\right) ds$$

In summary,

$$\partial_{tt}^2 b_n = \frac{\cancel{c\frac{\pi n}{L}}}{\cancel{c\frac{\pi n}{L}}} f(t) + (-1)\, c^2 \left(\frac{\pi n}{L}\right)^2 b_n(t)$$

initial values :

$$b_n(t) = \frac{1}{c\frac{\pi n}{L}} \int_0^t f(s) \sin\left[c\frac{\pi n}{L}(t-s)\right] ds + b_n^0 \cos\left(c\frac{\pi n}{L} t\right) + \frac{v_n^0}{c\frac{\pi n}{L}} \sin\left(c\frac{\pi n}{L} t\right)$$

$$b_n(0) = \underbrace{\frac{1}{c\frac{\pi n}{L}} \int_0^0 f(s) \sin\left[c\frac{\pi n}{L}(0-s)\right] ds}_{=0} + b_n^0 \underbrace{\cos\left(c\frac{\pi n}{L} 0\right)}_{\cdot 1} + \frac{v_n^0}{c\frac{\pi n}{L}} \underbrace{\sin\left(c\frac{\pi n}{L} 0\right)}_{=0}$$

$$b_n'(0) = \underbrace{\int_0^0 f(s) \cos\left[c\frac{\pi n}{L}(0-s)\right] ds}_{=0} + b_n^0\, c\frac{\pi n}{L} \underbrace{(-\sin)\left(c\frac{\pi n}{L} 0\right)}_{=0} + v_n^0 \underbrace{\cos\left(c\frac{\pi n}{L} 0\right)}_{=1}$$

Coming back to the wave equation ...

The solution

$$u(x,t) = \sum_{n=1}^{\infty} b_n(t) \sin\left(\frac{\pi n}{L} x \right)$$

satisfies the wave equation with Dirichlet boundary conditions and the desired initial values.