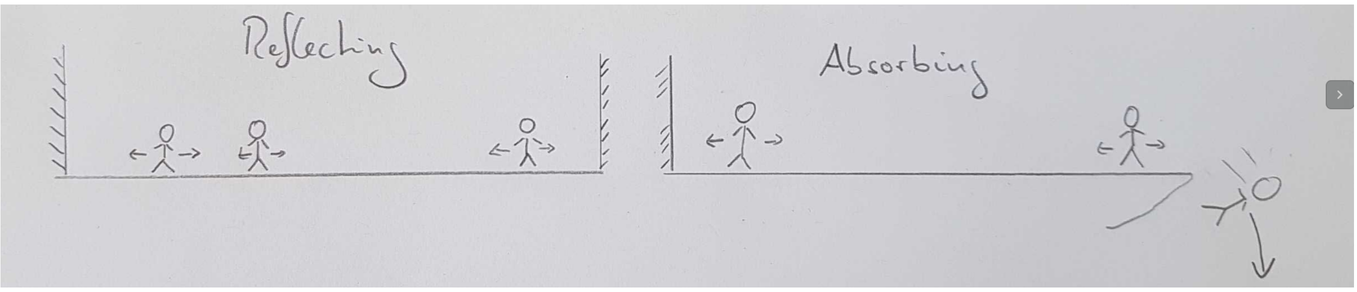
Boundary and initial conditions

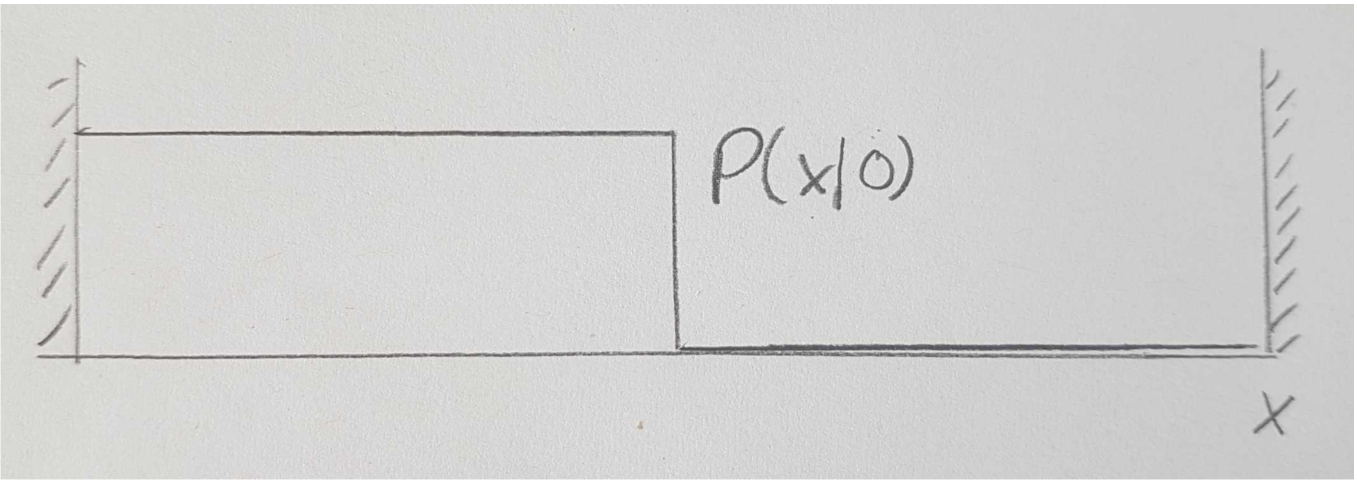
To solve the diffusion equation, you need to specify the distribution $P(x|0)$ in the beginning -- **the initial condition** -- and what happens at the ends of the range your are studying -- **the boundary conditions**.

Boundary conditions for diffusion problems are typically of two forms:

- reflecting: impenetrable wall
- absorbing: everything that passes the boundary is removed



As initial condition, we will consider a case where the left half of our domain is filled and the right half is empty.



Numerical solution

While it is possible to solve the diffusion equation with absorbing or reflecting boundary conditions exactly, we fill focus here on numerical solution:

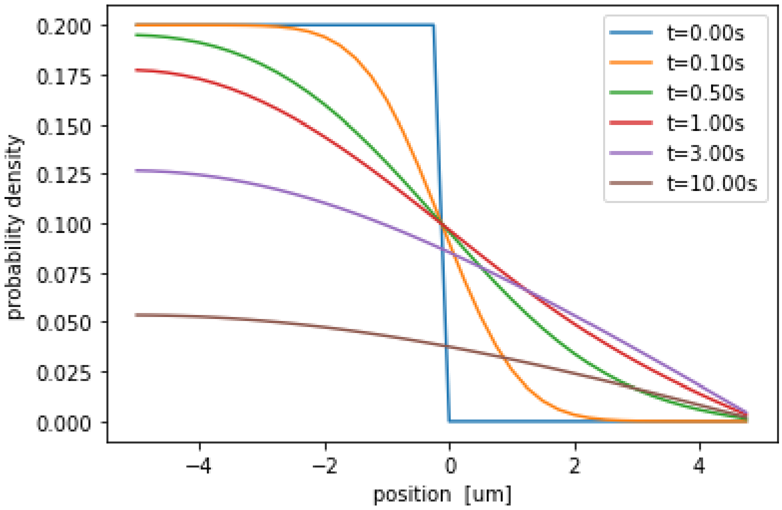
In [32]:

```
import numpy as np
import matplotlib.pyplot as plt

# define the derivative
def dpdt(p, r, l):
    dp = np.zeros_like(p)
    dp[1:-1] += r*(p[:-2] - p[1:-1])  # jump to the right
    dp[1:-1] += l*(p[2:] - p[1:-1]) # jump to the left
    dp[0] += l*p[1] - r*p[0]      # reflecting boundary
    dp[-1] += r*p[-2] - l*p[-1]  # reflecting boundary
    #dp[-1] += r*p[-2] - (r+l)*p[-1]  # absorbing boundary
    return dp

# define parameters and left/right hopping rates
D = 5       # um^2/s
v = 0.0
dx = 0.25    # if dx is too small, numerical solution is unstable
dt = 0.002  # if dt is too large, numerical solution is unstable

r = D/dx**2 + v/dx/2
l = D/dx**2 - v/dx/2
print("left/right rates:", r, l)

# set up the initial condition
xmax = 5    # um
x = np.arange(-xmax,xmax,dx)
p = np.zeros_like(x)
p[x<0] = 1/xmax   # density 1/xmax for x<0, density 0 for x>0

# solve the equation using the forward Euler method
tmax = 1
t=0
for tmax in [0,0.1, 0.5, 1,3, 10]:
    while t<tmax:
        p += dt*dpdt(p, r, l)
        t += dt
    # plot the result
    plt.plot(x,p, label=f"t={t:1.2f}s")

plt.legend()
plt.ylabel('probability density')
plt.xlabel('position  [um]')
```

```
left/right rates: 80.0 80.0
```

Out[32]:

```
Text(0.5, 0, 'position  [um]')
```



Reflecting initial condition

- The initial step function broadens and becomes flat at 1/2 the height.
- Total area under curve is constant.
- Time to spread a distance $x_{max} = 5\mu m$ is about $t = 3$s. This is expected given that $2Dt = 30\mu m^2 \approx x_{max}^2$

Absorbing initial conditions

- At the absorbing initial condition, the probability distribtion goes linearly to 0
- The total amount of probability left gradually decreases.

Dig deeper

- Change `xmax` and explore how the time scale of equilibration changes!
- Explore the steady state behavior of the solution with reflecting boundaries with non-zero v!
- For an absorbing boundary at the right end, plot the amount of probability ($\sum_x p(x|t)$) that is left as a function of time.
- Modify the code such that both boundaries are absorbing.
- Change the initial condition.

In [ ]:

```

```