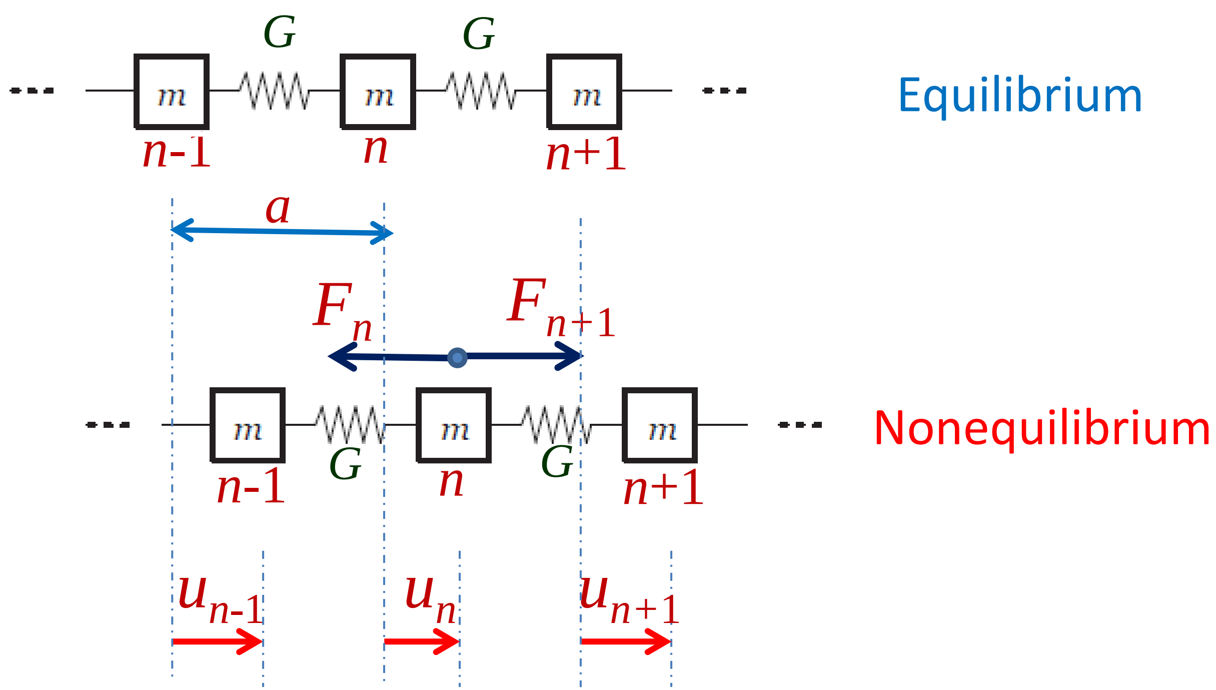
Lattices and discrete wave equation

From discrete to continuum

Figures and numerical simulations - Courtesy: G. Theocharis

Lattice dynamics - equations of motion

- **Lattice dynamics**, and particularly **wave propagation in lattices**, appear in studies of crystalline solids, molecular chains in chemistry and biology, photonic and photonic crystals, etc.



- **Newton's 2nd law:** $$m\ddot{u}_n = -F_n + F_{n+1}$$

Force that particle ***i*-1** exerts on particle ***i***

Linear discrete wave equation

Newton's 2nd law: $m\ddot{u}_n = -F_n + F_{n+1}$

Hook's law: $F_n = G(u_n - u_{n-1})$

linear response

$\Rightarrow$ $m\ddot{u}_n = G(u_{n+1} - 2u_n + u_{n-1})$

Discrete wave equation

A system of **N coupled ODEs**

The dynamics of particle ***n*** depends on the dynamics of ***n*-1** and ***n*+1**

Deriving the dispersion relation

Plane waves: $u_n(t) = u_0 \exp[i(kna - \omega t)]$, $na \equiv x_n$

Position of particle n distance from the origin

$$\left.\begin{aligned} \ddot{u}_n &= -\omega^2 u_0 \exp[i(kna - \omega t)] \\ u_n &= u_0 \exp[i(kna - \omega t)] \\ u_{n\pm1} &= u_0 \exp[i(k(n\pm1)a - \omega t)] \end{aligned}\right\} \Rightarrow -m\omega^2 u_n = G\left(e^{ika} - 2 + e^{ika}\right)u_n$$

Use the identities:

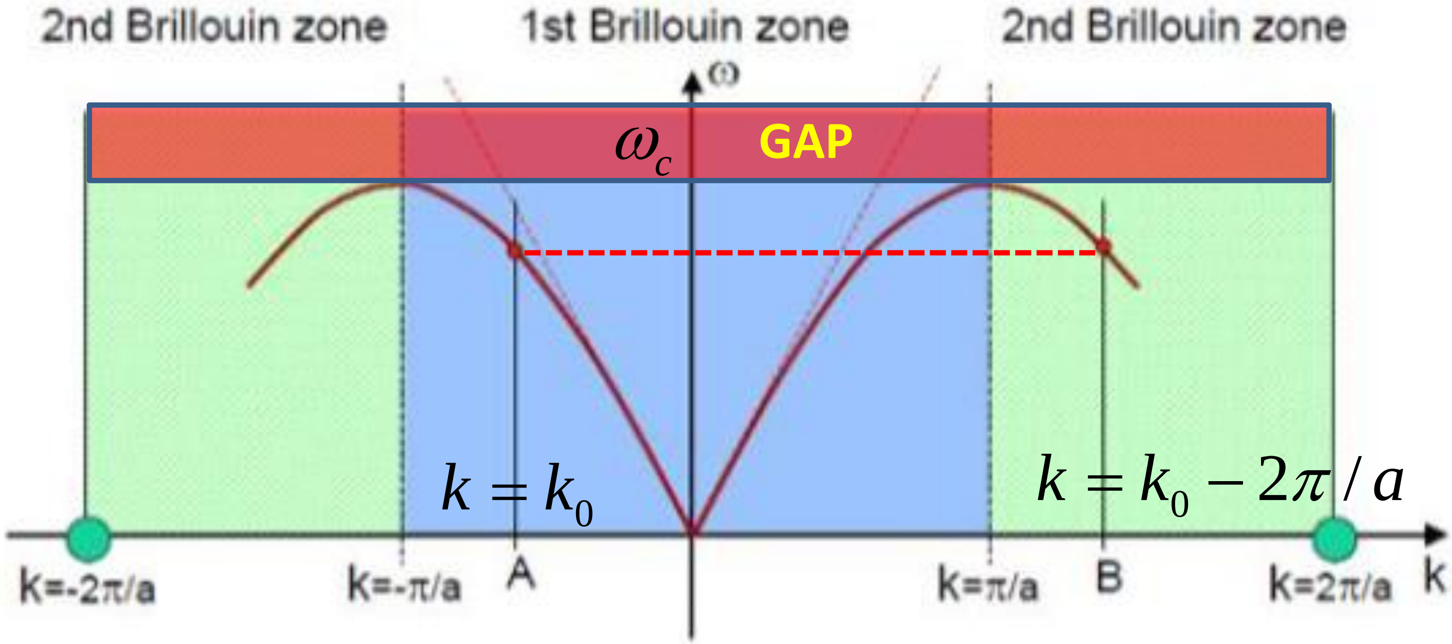
$$2\cos(ka) = e^{ika} + e^{ika}$$

$$1 - \cos(ka) = 2\sin^2(ka/2)$$

and derive the ***dispersion relation***

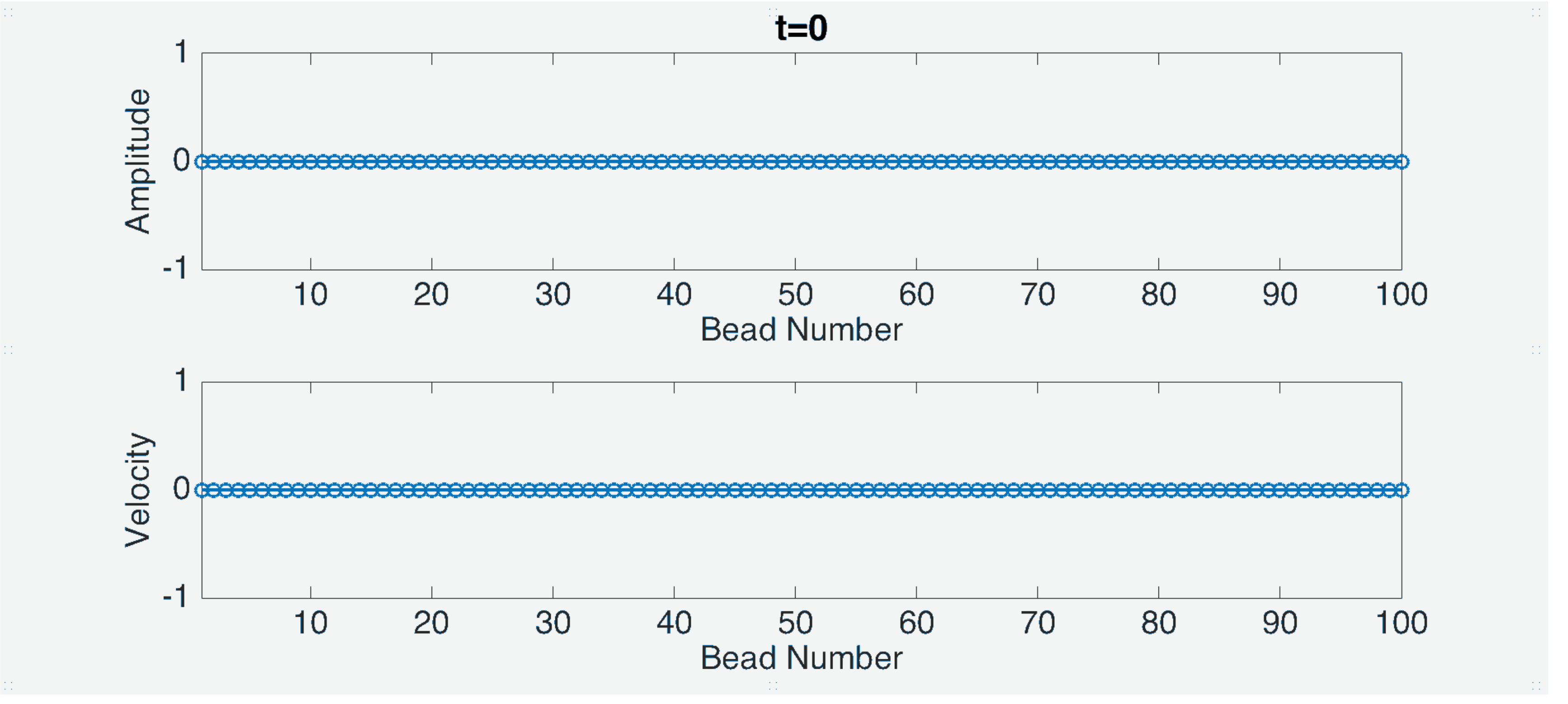
Dispersion relation

$$\omega(k) = 2\sqrt{\frac{G}{m}}\left|\sin\left(\frac{ka}{2}\right)\right|$$



- $0 \le \omega \le \omega_c = 2\sqrt{G/m}$ **For $\omega > \omega_c$ there is no propagation**
- **$\omega = \omega(k)$ is periodic: $\omega(k) = \omega(k+\Gamma)$, $\Gamma = 2\pi/a$**
- **$\omega = \omega(k)$ needs only to be represented for:** $-\pi / a \le k \le \pi / a$

Plane waves for $\omega < \omega_c$



Lattice dynamics: solution of N coupled ODEs

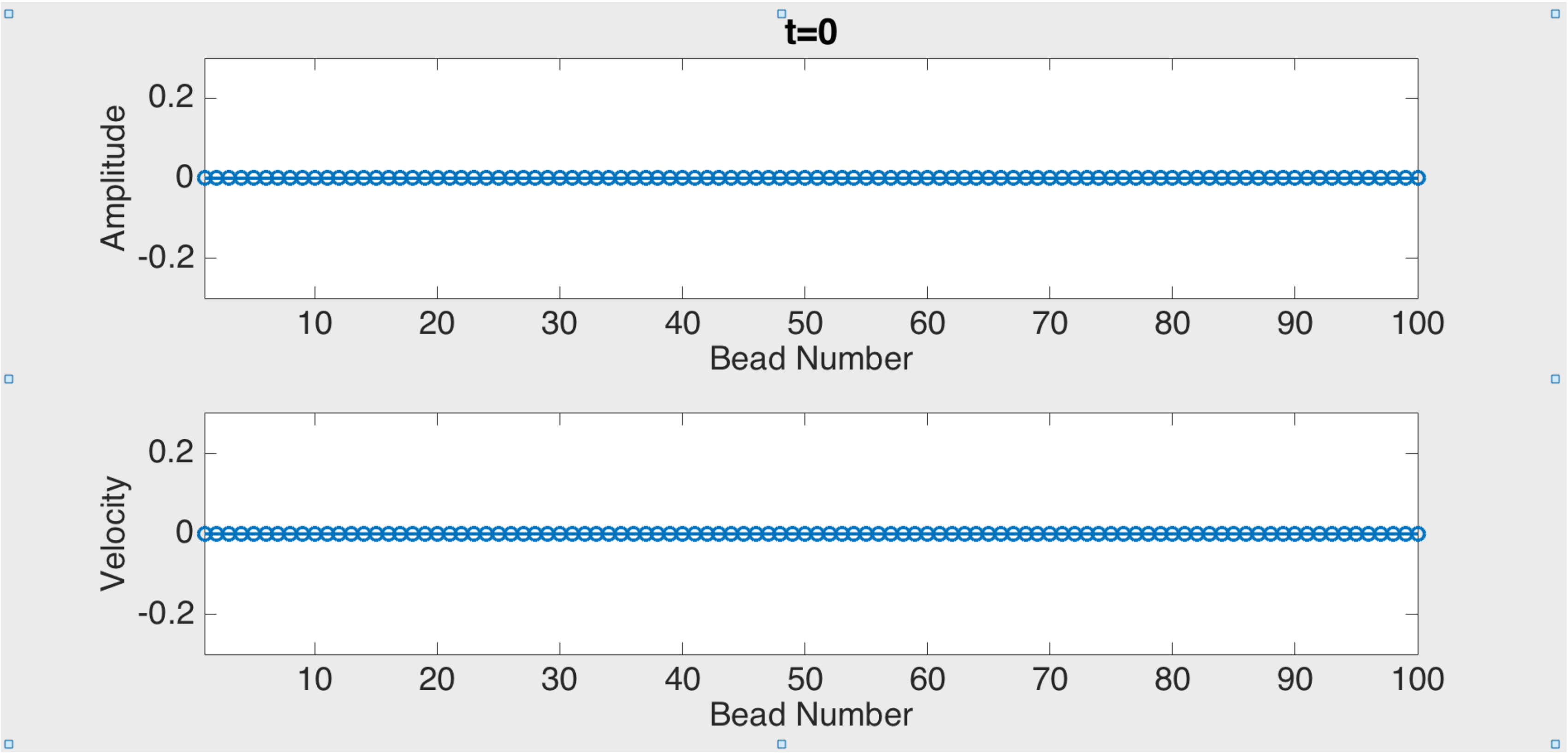
$$\begin{cases} m\ddot{u}_1 = G(u_2 - 2u_1 + u_0) \\ m\ddot{u}_2 = G(u_3 - 2u_2 + u_1) \\ \vdots \\ m\ddot{u}_N = G(u_{N+1} - 2u_N + u_{N-1}) \end{cases}$$

Boundary conditions

$u_0(t) = u_0 \cos(\omega t)$ **Driver**

$u_{N+1}(t) = 0$ **"Hard wall"**

Evanescent waves for $\omega > \omega_c$



When $\omega > \omega_c$ the dispersion relation becomes: $\sin^2\left(\frac{ka}{2}\right) = \frac{\omega^2}{\omega_c^2} > 1$

i.e., ***k*** becomes **purely imaginary** $\rightarrow$ ***evanescent waves***

The continuous limit

We consider the **continuous limit** of the **discrete wave equation**:

$$m\ddot{u}_n = G(u_{n+1} - 2u_n + u_{n-1})$$

valid for solutions with a ***width >> lattice spacing*** ***a***

Imagine that $x_n = na$ is a continuous variable,
with ***n large*** and ***a small***, i.e., $x_n = na \rightarrow x$

We can then expand the solution in a **Taylor series**, around ***x***, as:

$$u_{n\pm1}(t) = u(n(a\pm1),t) = u(x\pm a,t)$$

$$\approx u(x,t) \pm u_x(x,t)a + \frac{1}{2}u_{xx}(x,t)a^2 \pm \frac{1}{6}u_{xxx}(x,t)a^3 + \frac{1}{24}u_{xxxx}(x,t)a^4 + O(a^5)$$

Substituting this expansion into the discrete wave equation, and keeping O(a^4) terms the following wave equation is obtained:

$$u_{tt} - c^2\left(u_{xx} + \frac{a^2}{12}u_{xxxx}\right) = 0,$$

$c^2 = Ga^2/m$ **speed of sound**

Effective wave equations

It is convenient to introduce the following **dimensionless variables**:

$$x \mapsto \frac{1}{L}x, \quad t \mapsto \frac{c_0}{L}t$$

where L is a characteristic **spatial scale,** e.g., the system's length, or the typical wavelength/width of the initial data

Then, the wave equation $u_{tt} - c^2\left(u_{xx} + \frac{a^2}{12}u_{xxxx}\right) = 0$ becomes:

$$u_{tt} - u_{xx} - \delta\, u_{xxxx} = 0, \qquad \delta = \frac{1}{12}\left(\frac{a}{L}\right)^2$$

- **Two interesting cases:**

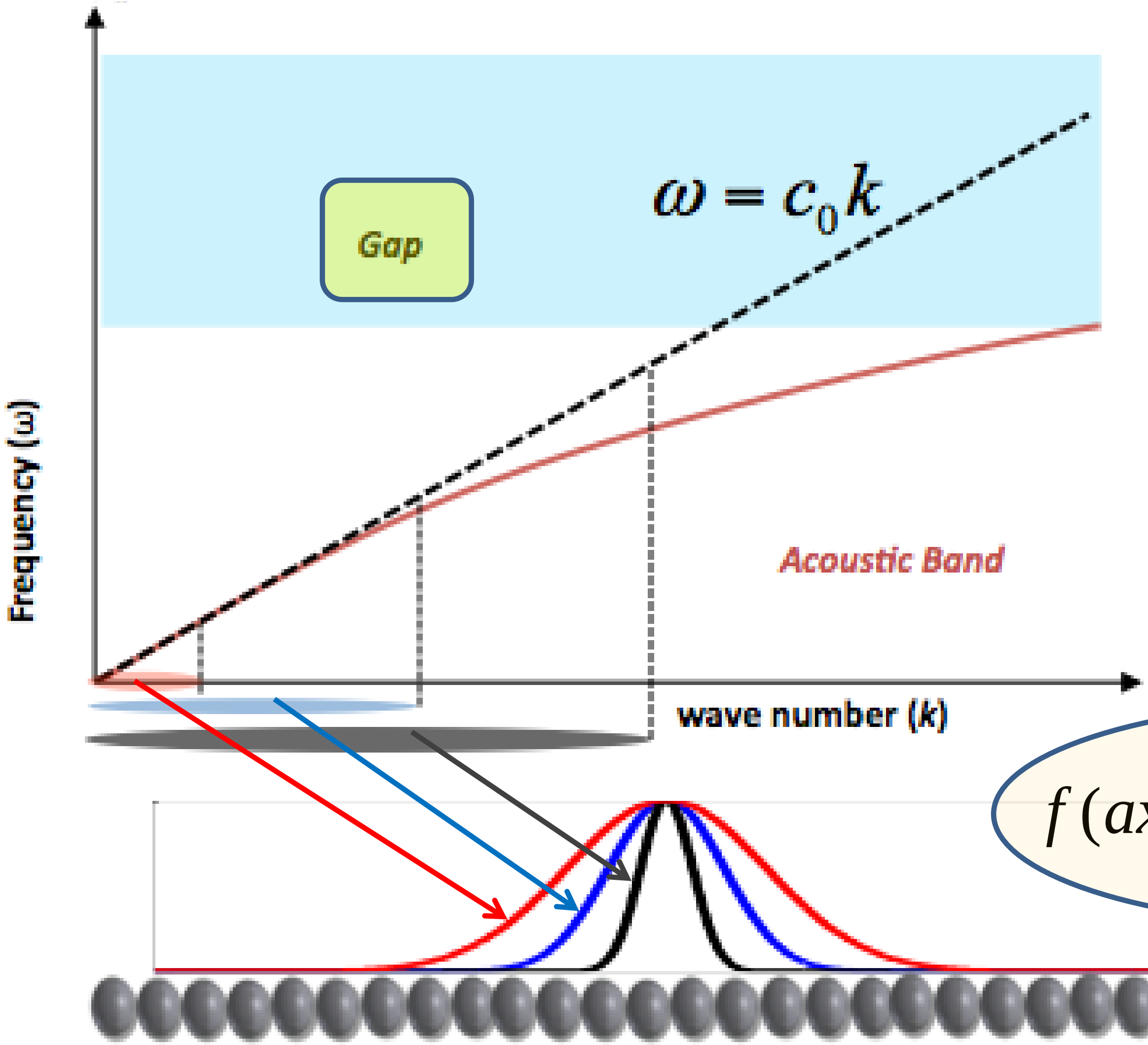
➢ When $\boldsymbol{\delta \to 0}$ the wave equation reduces to: $u_{tt} - u_{xx} = 0$

2nd-order wave equation – dispersionless: $\omega^2(k) = k^2$

➢ When $\boldsymbol{\delta \ll 1}$ the wave equation is of the form of a **linearized Boussinesq equation – dispersive:** $\omega^2(k) = k^2 - \delta\, k^4$

Scenarios for discreteness-induced dispersion

- Broad pulses – very small wavenumbers → dispersionless wave equation
- Intermediate pulses – small wavenumbers → small dispersion
- Short pulses – relatively large wavenumbers k → strong dispersion



Recall:

$$f(ax) \leftrightarrow \frac{1}{a}\hat{f}\left(\frac{x}{a}\right), \; a > 0$$

Broad pulse – negligible dispersion

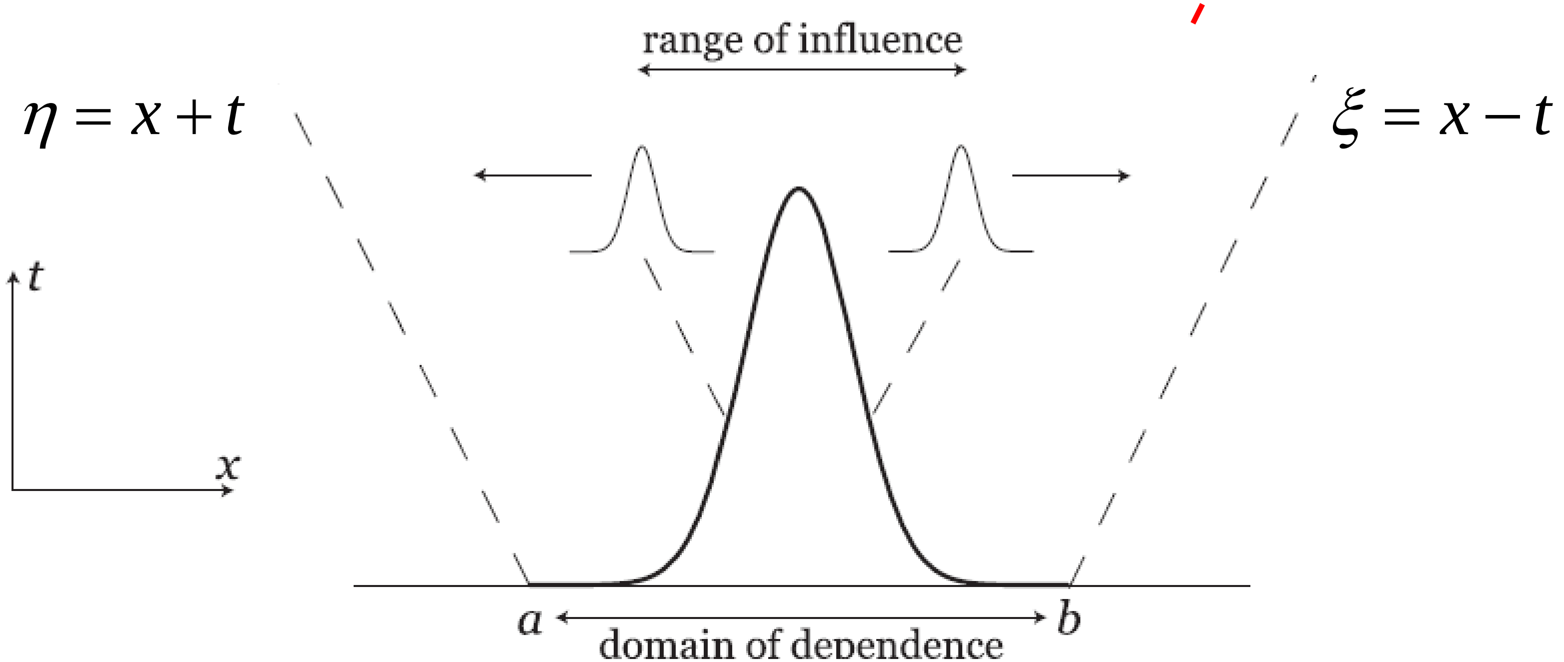
- $\delta \to 0$. The Cauchy problem for the **2nd-order wave equation**:

$$u_{tt} - u_{xx} = 0$$

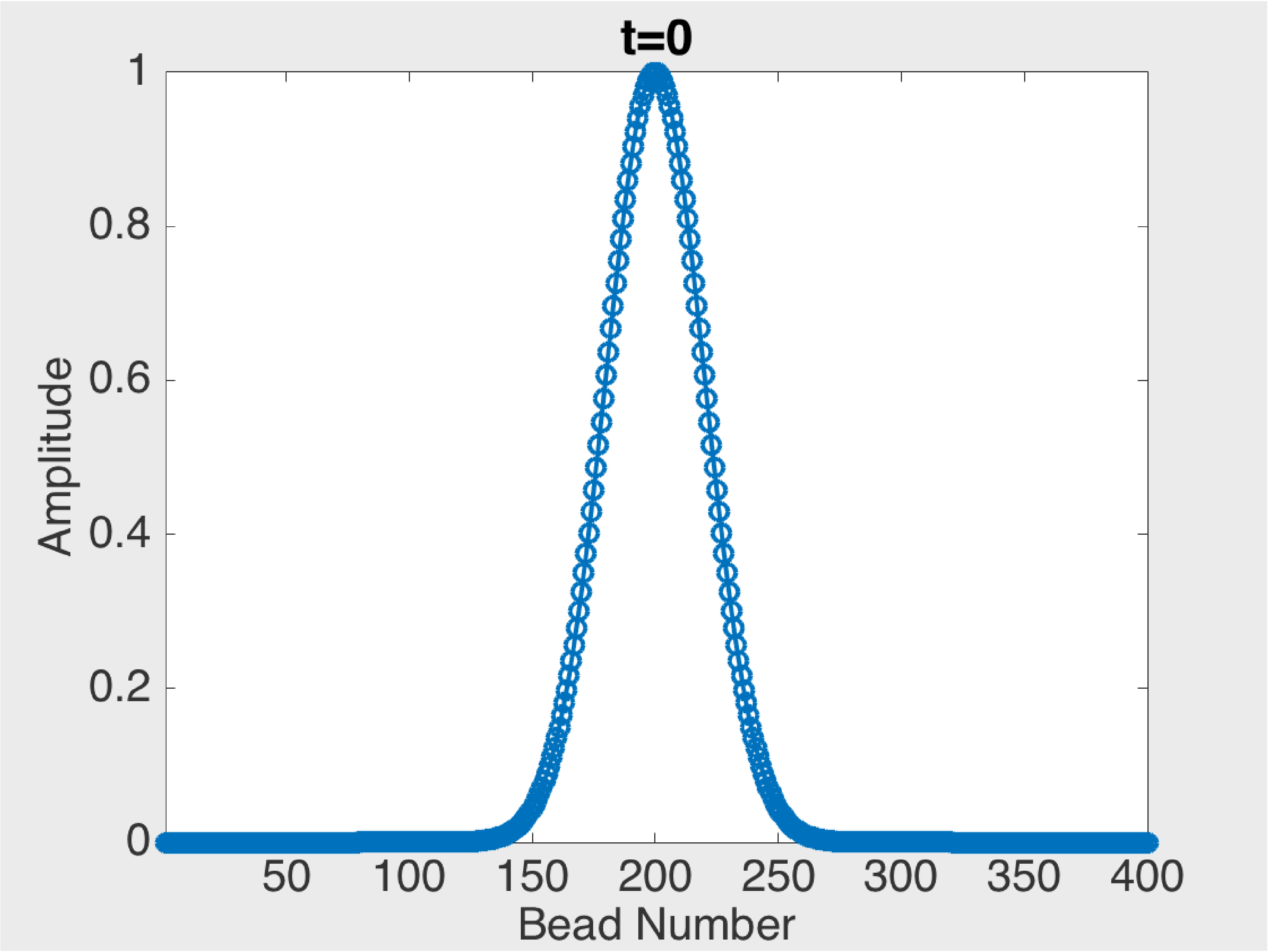
$$u(x,0) = f(x), \;\; u_t(x,0) = g(x)$$

possesses the **D' Alembert solution**:

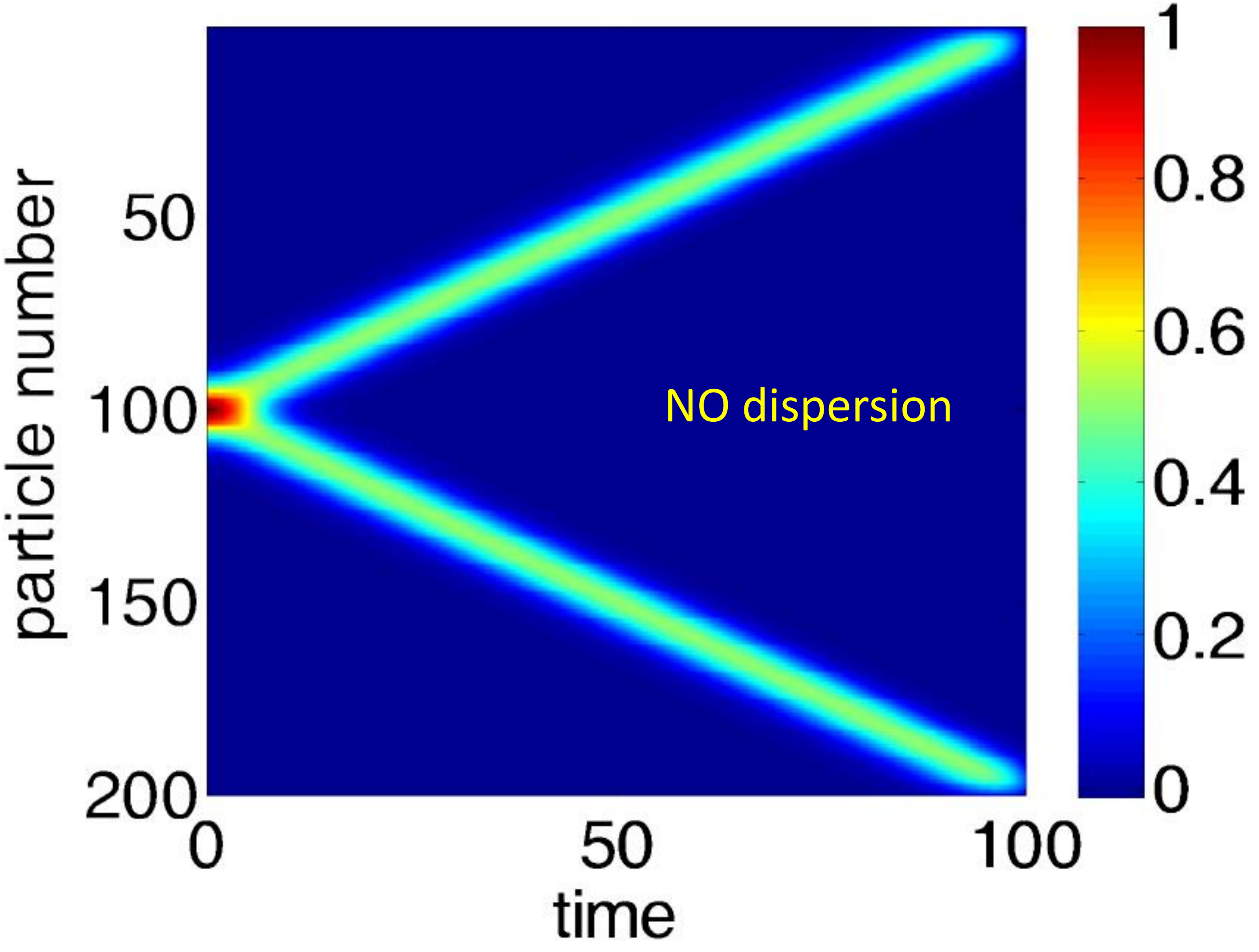
$$u(x,t) = \frac{1}{2}\left[f(x-t) + f(x+t)\right] + \frac{1}{2}\int_{x-t}^{x+t} g(s)ds$$



Broad pulse – evolution



Broad pulse – evolution (contour plot)



Intermediate pulse – small dispersion

- $\delta << 1$ To find the solution of the **linearized Boussinesq** equation:

$$u_{tt} - u_{xx} - \delta u_{xxxx} = 0$$

we use the Fourier transform method:

$$\left.\begin{aligned} &\hat{u}_{tt} + (k^2 - \delta k^4)\hat{u} = 0 \\ &\omega^2(k) = k^2 - \delta k^4 \end{aligned}\right\} \Rightarrow \hat{u}(k,t) = f(k)e^{-i\omega(k)t} + g(k)e^{+i\omega(k)t}$$

$$\Rightarrow u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\left[f(k)e^{i[kx-\omega(k)t]} + g(k)e^{i[kx+i\omega(k)t]}\right]dk$$

wave moving to the **right** — wave moving to the **left**

***f*(*k*)** and ***g*(*k*)**: **Fourier amplitudes** determined by the initial conditions

We are interested in **approximating** the expression for the **right-going wave**: $u(x,t) \propto \int_{-\infty}^{+\infty} f(k)e^{i[kx-\omega(k)t]}dk$

Intermediate pulse – asymptotic behavior

Right-going wave: $u(x,t)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} f(k)e^{i[kx-\omega(k)t]}dk$

Dispersion relation: $\omega(k)=k(1-\delta k^2)^{1/2}\approx k\left(1-\frac{\delta}{2}k^2\right)=k-\frac{\delta}{2}k^3$

$$u(x,t)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} f(k)e^{i[k(x-t)+\frac{\delta}{2}k^3t]}dk$$

We are interested in **the limit of long waves** with ***k* → 0,** hence

we can Taylor expand f(k) around ***k* = 0**: $f(k)\approx f(0)+f'(k)\big|_{k=0}k+\ldots$

$$u(x,t)\approx\frac{1}{2\pi}f(0)\int_{-\infty}^{+\infty} e^{i[k(x-t)+\frac{1}{2}\delta k^3t]}dk$$

The integral is reminiscent of the definition of the **Airy function:**

$$\mathrm{Ai}(z)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\exp\left[i\left(sz+\frac{1}{3}s^3\right)\right]ds=\frac{1}{\pi}\int_0^{+\infty}\cos\left[i\left(sz+\frac{1}{3}s^3\right)\right]ds$$

Solution in terms of the Airy function

Comparing:

$$u(x,t) \approx \frac{1}{2\pi} f(0)\int_{-\infty}^{+\infty} \exp\left\{ i\left[k(x-t) + \frac{\delta}{2}k^3 t \right] \right\} dk$$

$$\mathrm{Ai}(z) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \exp\left[i\left(sz + \frac{1}{3}s^3 \right) \right] ds$$

we define:

$$\frac{1}{2}\delta k^3 t = \frac{1}{3}s^3 \Rightarrow s^3 = \frac{3}{2}\delta k^3 t \Rightarrow k = \sqrt[3]{\frac{2}{3\delta t}}\, s$$

and finally obtain:

$$u(x,t) \approx \frac{1}{2\pi}\frac{f(0)}{\sqrt[3]{(3/2)\delta t}} \int_{-\infty}^{+\infty} \exp\left\{ i\left[\sqrt[3]{\frac{2}{3\delta t}}(x-t)s + \frac{1}{3}s^3 \right] \right\} ds \Rightarrow$$

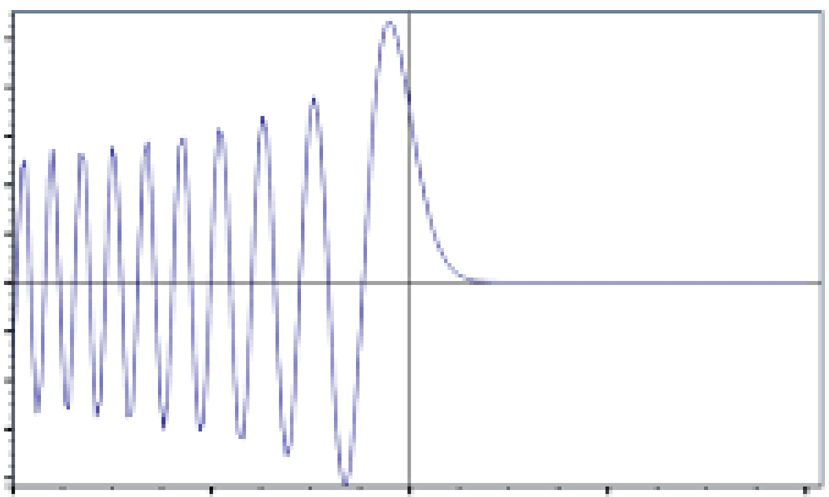
Right-going wave:

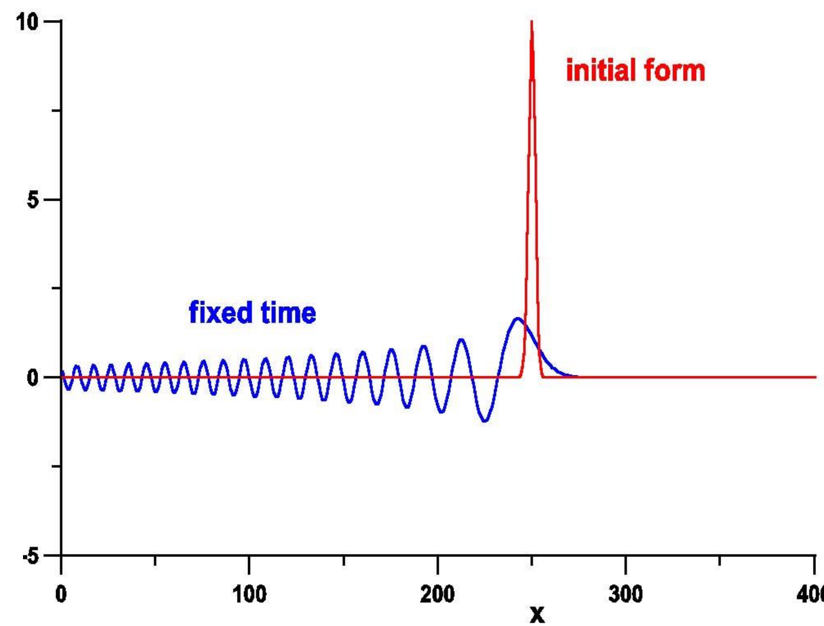
$$u(x,t) \approx \frac{f(0)}{\sqrt[3]{(3/2)\delta t}} \mathrm{Ai}\left(\frac{x\text{-}t}{\sqrt[3]{(3/2)\delta t}} \right)$$

Airy function - Behavior of the solution

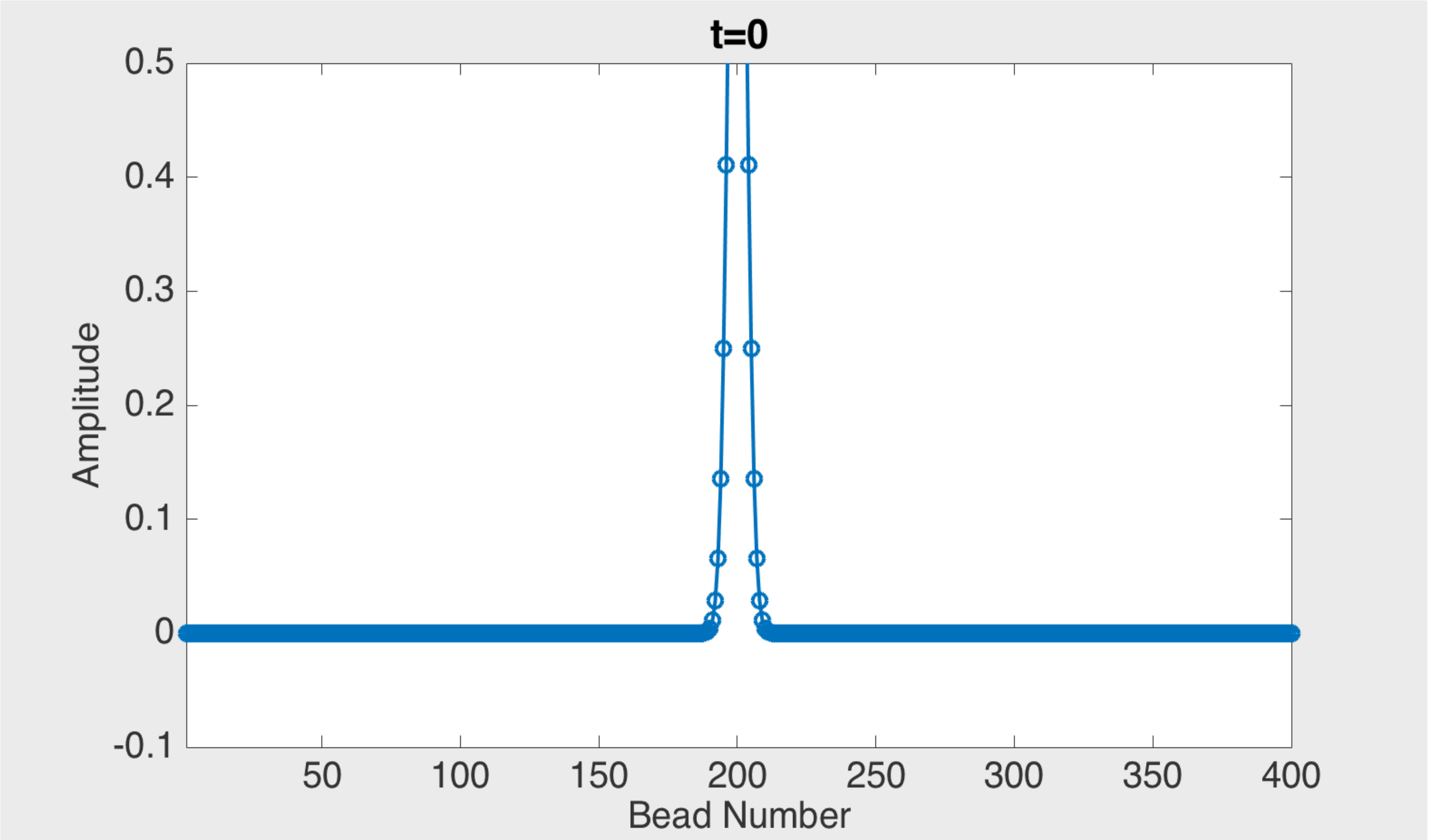
$$\mathrm{Ai}(z) \approx \begin{cases} \dfrac{1}{2\sqrt{\pi}} z^{-1/4} \exp\left(-\dfrac{2}{3} z^{3/2}\right), & z \to +\infty \\ \dfrac{1}{\sqrt{\pi}} |z|^{-1/4} \sin\left(\dfrac{2}{3}|z|^{3/2} + \dfrac{1}{4}\pi\right), & z \to -\infty \end{cases}$$

Hence: $u(x,t)$ **decays exponentially** **ahead of** $x = t$
and **becomes oscillatory** **behind** $x = t$

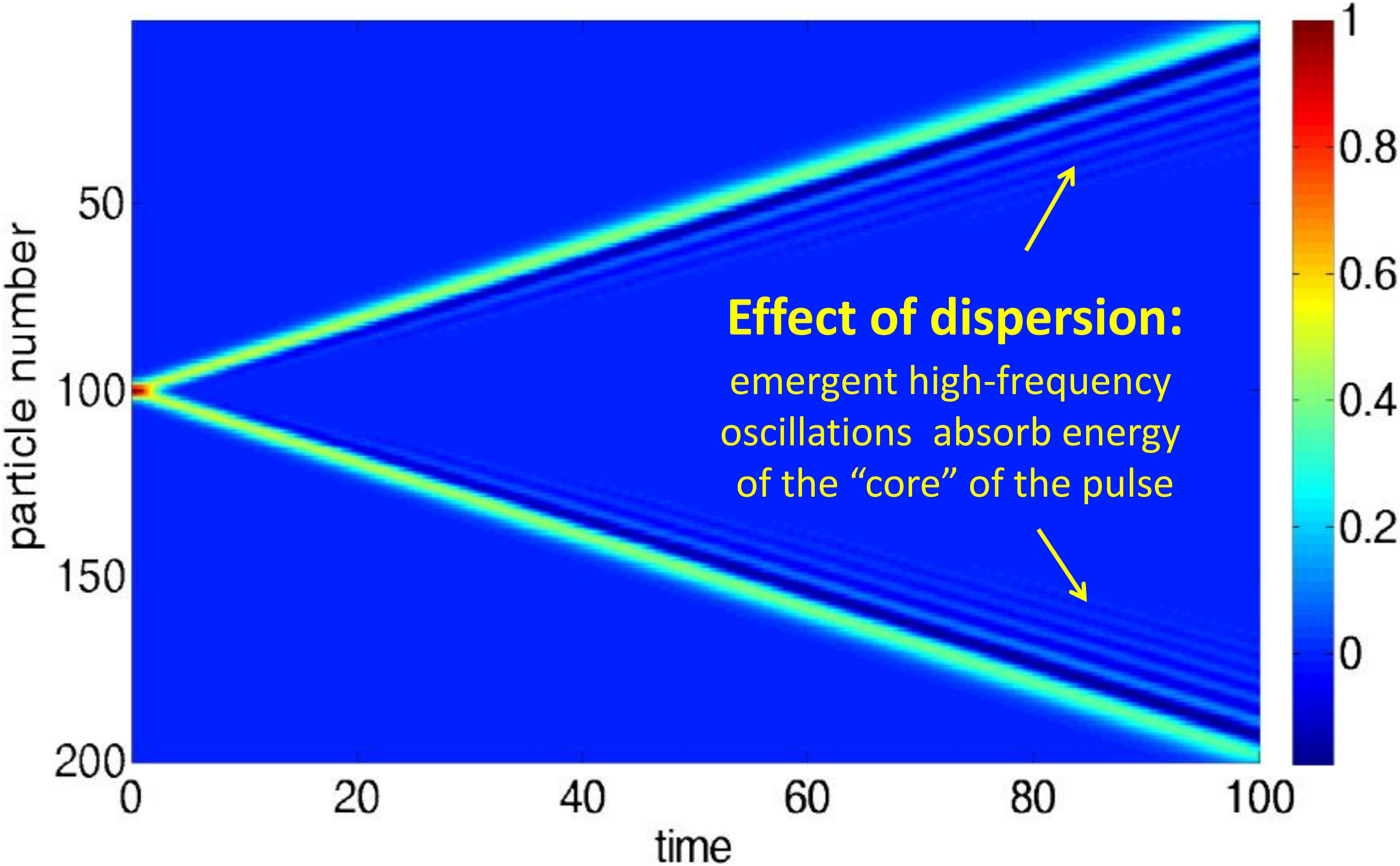




Intermediate pulse – evolution



Intermediate pulse – evolution (contour plot)



Short pulse – evolution