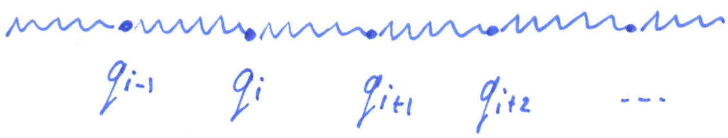
24.11.

Fermi–Pasta–Ulam problem

We start with a chain of massive points connected by springs:

k – the force constant from Hooke's law;

α – the nonlinear spring constant;



Let's write the Newton's law of motion in terms of the generalized coordinates $q_i(t)$ as a deviation from the equilibrium point:

$$m\ddot{q}_i = k[q_{i+1} + q_{i-1} - 2q_i] + \alpha[(q_{i+1}-q_i)^2 - (q_i - q_{i-1})^2] \qquad (1)$$

Than we will assume our chain is infinite and change notations $q_i(t) \to q(x,t)$. For shifted coordinates we use: $q_{i+1}(t) \to e^{\partial_x} q(x,t)$

$$q_{i-1}(t) \to e^{-\partial_x} q(x,t).$$

Indeed, if $\partial_x = \frac{d}{dx}$, $\partial_x^2 = \frac{d^2}{dx^2}$, ..., $\partial_x^n = \frac{d^n}{dx^n}$, that $e^{a\partial_x}$ is the shift operator.

$x \in \mathbb{R}$ and
$q_i(t) = q(x,t)$ if $x = i$
where $i \in \mathbb{N}$

Expanding the exponent in Taylor series as $e^{a\partial_x} = \sum_{n=0}^{\infty} \frac{1}{n!} a^n \partial_x^n$, we arrive at the action of S.O. on arbitrary function $f(x)$:

$$e^{a\partial_x} f(x) = \sum_n \frac{1}{n!} a^n f^{(n)}(x) \equiv f(x+a).$$

$$\boxed{\bullet\ \text{Problem 1: } \underline{\text{calculate } \sqrt{\partial_x}\, x^m}}$$

So, in terms of new notations, Eq.(1) becomes

$$m\partial_t^2 q(x,t) = k(e^{\partial_x} + e^{-\partial_x} - 2)\, q(x,t) + \alpha\left[(e^{\partial_x}-1)\, q(x,t)\right]^2 - \alpha\left[(1-e^{-\partial_x})\, q(x,t)\right]^2$$

or else

$$m\partial_t^2 q(x,t) = 4k\, sh^2\!\left(\frac{\partial_x}{2}\right) q(x,t) + \alpha\left[2e^{\frac{\partial_x}{2}} sh\!\left(\frac{\partial_x}{2}\right) q(x,t)\right]^2 - \alpha\left[2e^{-\frac{\partial_x}{2}} sh\!\left(\frac{\partial_x}{2}\right) q(x,t)\right]^2.$$

Now we should come back and make physical aproximations to solve this equation. We will assume, that our weights are very close each to other and function $q(x,t)$ changes slowly $(\partial_x q(x,t) \ll q(x,t))$. So, we can use Taylor's expantion for sh:

$$sh\!\left(\frac{\partial_x}{2}\right) = \frac{\partial_x}{2} + \frac{1}{3!}\left(\frac{\partial_x}{2}\right)^3 + \ldots = \frac{\partial_x}{2}\left(1 + \frac{\partial_x^2}{24} + \ldots\right).$$

I) At first let's consider the liniar equation ($\alpha = 0$).

$$m\partial_t^2 q(x,t) = 4k\, sh^2\left(\frac{\partial_x}{2}\right) q(x,t)$$

$$m\partial_t^2 q(x,t) = k\partial_x^2\left(1 + \frac{\partial_x^2}{12} + \ldots\right) q(x,t).$$

We keep only quadratic term of spatial derivative and get wave equation $\partial_t^2 q(x,t) = \frac{k}{m}\partial_x^2 q(x,t)$.

This equation was solved by J. d'Alambert and shortly noted with help of d'Alambertian:

$\Box q(x,t) \equiv 0$, $\Box = \nabla^2 - \frac{1}{c^2}\frac{d^2}{dt^2}$. [Note that for 1D space $\nabla^2 = \partial_x^2$]

The solution of such wave equation is arbitrary function

$$q(x,t) = g(x-ct) + f(x+ct),$$

where c is nothing else but phase velocity. $c = \frac{k}{m}$

- Check it!
- Calucate asymptotic at $\alpha \to 0$ of

$$\sum_{n=0}^{\infty} n e^{-\alpha n^2}$$

Next Monday we shall take into account non-linear terms and obtain famous KdV equation! That is how solitons comes into our mechanical problem.