The Equations of Motion of Systems of Particles

1 System of Coupled Anharmonic Oscillators

Our potential U describes a system of n coupled anharmonic oscillators,

$$U(x_1, \ldots, x_n) = \sum_{i=1}^{n-1} \frac{\kappa}{2}(x_{i+1} - x_i)^2 + \sum_{i,j=1}^{n} \frac{\lambda}{4}(x_i - x_j)^4.$$

The equations of motion of a system of n particles are given by

$$m_i \ddot{x}_i = -\partial_i U(x_1, \ldots, x_n),$$

so

$$\begin{aligned}
m_i \ddot{x}_i =& - \partial_i \sum_{j=1}^{n-1} \frac{\kappa}{2}(x_{j+1} - x_j)^2 - \partial_i \sum_{j,k=1}^{n} \frac{\lambda}{4}(x_k - x_j)^4 \\
=& - \kappa \sum_{j=1}^{n-1}(x_{j+1} - x_j)(\delta_{i,j+1} - \delta_{ij}) - \lambda \sum_{j,k=1}^{n} (x_k - x_j)^3(\delta_{ik} - \delta_{ij}) \\
=& - \kappa \sum_{j=1}^{n-1} \delta_{i,j+1}(x_{j+1} - x_j) + \kappa \sum_{j=1}^{n} \delta_{ij}(x_{j+1} - x_j) \\
& - \lambda \sum_{j,k=1}^{n} \delta_{ik}(x_k - x_j)^3 + \lambda \sum_{j,k=1}^{n} \delta_{ij}(x_k - x_j)^3 \\
=& - \kappa(x_i - x_{i-1}) \sum_{j=1}^{n-1} \delta_{i,j+1} + \kappa(x_{i+1} - x_i) \sum_{j=1}^{n-1} \delta_{ij} \\
& - \lambda \sum_{j=1}^{n}(x_i - x_j)^3 + \lambda \sum_{k=1}^{n}(x_k - x_i)^3 \\
=& - \kappa(x_i - x_{i-1}) \sum_{j=1}^{n-1} \delta_{i,j+1} + \kappa(x_{i+1} - x_i) \sum_{j=1}^{n-1} \delta_{ij} \\
& - \lambda \sum_{j=1}^{n}(x_i - x_j)^3 - \lambda \sum_{k=1}^{n}(x_i - x_k)^3
\end{aligned}$$

$$= -\kappa(x_i - x_{i-1})\sum_{j=1}^{n-1}\delta_{i,j+1} + \kappa(x_{i+1} - x_i)\sum_{j=1}^{n-1}\delta_{ij} - 2\sum_{j=1}^{n}\lambda(x_i - x_j)^3.$$

Note that

$$\sum_{j=1}^{n-1}\delta_{i,j+1} = \left\{\begin{array}{ll} 1 & \text{if } i \neq 1 \\ 0 & \text{otherwise} \end{array}\right\} = 1 - \delta_{i1}$$

and similarly for the sum over j of δ_{ij},

$$\sum_{j=1}^{n-1}\delta_{ij} = \left\{\begin{array}{ll} 1 & \text{if } i \neq n \\ 0 & \text{otherwise} \end{array}\right\} = 1 - \delta_{in}.$$

Then

$$\begin{aligned} m_i\ddot{x}_i =& -\kappa(x_i - x_{i-1})(1 - \delta_{i1}) + \kappa(x_{i+1} - x_i)(1 - \delta_{in}) - 2\sum_{j=1}^{n}\lambda(x_i - x_j)^3 \\ =& -\kappa(x_i - x_{i-1}) + \kappa(x_{i+1} - x_i) + \kappa\delta_{i1}(x_i - x_{i-1}) - \kappa\delta_{in}(x_{i+1} - x_i) \\ & - 2\sum_{j=1}^{n}\lambda(x_i - x_j)^3 \\ =& -\kappa(2x_i - x_{i-1} - x_{i+1}) + \kappa\delta_{i1}x_1 + \kappa\delta_{in}x_n - 2\sum_{j=1}^{n}\lambda(x_i - x_j)^3, \end{aligned}$$

where $x_0 = x_{n+1} = 0$ by assumption.

2 x^4 with a Hyperbolic Term

I think this question should possibly be $U = \sum \kappa\cosh(x_{i+1} - x_i) + \sum \frac{\lambda}{4}x_i^4$.

Our potential is

$$U(x_1, \ldots, x_n) = \sum_{i=1}^{n-1}\cosh\Big(\kappa(x_{i+1} - x_i)\Big) + \sum_{i=1}^{n}\frac{\lambda}{4}x_i^4.$$

The equations of motion of a system of n particles are given by

$$m_i\ddot{x}_i = -\partial_i U(x_1, \ldots, x_n),$$

so

$$\begin{aligned} m_i\ddot{x}_i =& -\partial_i\sum_{j=1}^{n-1}\cosh\Big(\kappa(x_{j+1} - x_j)\Big) - \partial_i\sum_{j=1}^{n}\frac{\lambda}{4}x_j^4 \\ =& -\sum_{j=1}^{n-1}\sinh\Big(\kappa(x_{j+1} - x_j)\Big)\kappa(\delta_{i,j+1} - \delta_{ij}) - \sum_{j=1}^{n}\lambda x_j^3\delta_{ij} \\ =& -\kappa\sum_{j=1}^{n-1}\delta_{i,j+1}\sinh\Big(\kappa(x_{j+1} - x_j)\Big) + \kappa\sum_{j=1}^{n-1}\delta_{ij}\sinh\Big(\kappa(x_{j+1} - x_j)\Big) - \lambda x_i^3 \end{aligned}$$

$$
\begin{aligned}
&= -\kappa \sinh\Big(\kappa(x_i - x_{i-1})\Big) \sum_{j=1}^{n-1} \delta_{i,j+1} + \kappa \sinh\Big(\kappa(x_{i+1} - x_i)\Big) \sum_{j=1}^{n-1} \delta_{ij} - \lambda x_i^3 \\
&= -\kappa \sinh\Big(\kappa(x_i - x_{i-1})\Big)(1 - \delta_{i1}) + \kappa \sinh\Big(\kappa(x_{i+1} - x_i)\Big)(1 - \delta_{in}) - \lambda x_i^3 \\
&= -\kappa \sinh\Big(\kappa(x_i - x_{i-1})\Big) + \kappa \sinh\Big(\kappa(x_{i+1} - x_i)\Big) \\
&\quad + \kappa\delta_{i1} \sinh\Big(\kappa(x_i - x_{i-1})\Big) - \kappa\delta_{in} \sinh\Big(\kappa(x_{i+1} - x_i)\Big) - \lambda x_i^3 \\
&= -\kappa \left(\sinh\Big(\kappa(x_i - x_{i-1})\Big) + \sinh\Big(\kappa(x_i - x_{i+1})\Big)\right) \\
&\quad + \kappa\delta_{i1} \sinh(\kappa x_1) + \kappa\delta_{in} \sinh(\kappa x_n) - \lambda x_i^3
\end{aligned}
$$

since sinh is odd, where we of course assume $x_0 = x_{n+1} = 0$.

3 The Toda Potential

The (non-periodic) Toda potential U is

$$
U(x_1, \dots, x_n) = \sum_{i=1}^{n-1} \exp\Big(\alpha(x_{i+1} - x_i)\Big).
$$

The equations of motion of a system of n particles are given by

$$
m_i \ddot{x}_i = -\partial_i U(x_1, \dots, x_n),
$$

so

$$
\begin{aligned}
m_i \ddot{x}_i &= -\partial_i \sum_{j=1}^{n-1} \exp\Big(\alpha(x_{j+1} - x_j)\Big) \\
&= -\sum_{j=1}^{n-1} \partial_i \left(e^{\alpha x_{j+1}} \cdot e^{-\alpha x_j}\right) \\
&= -\sum_{j=1}^{n-1} \left(e^{\alpha x_{j+1}} \partial_i e^{-\alpha x_j} + e^{-\alpha x_j} \partial_i e^{\alpha x_{j+1}}\right) \\
&= -\sum_{j=1}^{n-1} \left(-\alpha\delta_{ij} e^{\alpha x_{j+1}} e^{-\alpha x_j} + \alpha\delta_{i,j+1} e^{-\alpha x_j} e^{\alpha x_{j+1}}\right) \\
&= -\sum_{j=1}^{n-1} \alpha\delta_{i,j+1} e^{\alpha(x_{j+1} - x_j)} + \sum_{j=1}^{n-1} \alpha\delta_{ij} e^{\alpha(x_{j+1} - x_j)} \\
&= -\alpha e^{\alpha(x_i - x_{i-1})} \sum_{j=1}^{n-1} \delta_{i,j+1} + \alpha e^{\alpha(x_{i+1} - x_i)} \sum_{j=1}^{n-1} \delta_{ij} \\
&= -\alpha e^{\alpha(x_i - x_{i-1})}(1 - \delta_{i1}) + \alpha e^{\alpha(x_{i+1} - x_i)}(1 - \delta_{in}) \\
&= -\alpha e^{\alpha(x_i - x_{i-1})} + \alpha e^{\alpha(x_{i+1} - x_i)} + \alpha\delta_{i1} e^{\alpha(x_i - x_{i-1})} - \alpha\delta_{in} e^{\alpha(x_{i+1} - x_i)} \\
&= -\alpha e^{\alpha(x_i - x_{i-1})} + \alpha e^{\alpha(x_{i+1} - x_i)} + \alpha\delta_{i1} e^{\alpha x_1} - \alpha\delta_{in} e^{-\alpha x_n}.
\end{aligned}
$$

Again, we have to assume that $x_0 = x_{n+1} = 0$.