Integrating the Klein-Gordon on a 2-D Network

A set of Klein-Gordon oscillators each consisting of one degree of freedom (q, p) and coupled to the others on a square lattice network has the Hamiltonian

$$H = \sum_{x,y} \frac{p_{x,y}^2}{2} + \frac{\epsilon_{x,y} q_{x,y}^2}{2} + \frac{|q_{x,y}|^{\sigma+2}}{\sigma+2} - \frac{1}{2W}\left[(q_{x+1,y} - q_{x,y})^2 + (q_{x,y+1} - q_{x,y})^2\right] \tag{1}$$

which is separable into

$$\begin{aligned} H &= T(\vec{p}) + V(\vec{q}) \\ T(\vec{p}) &= \sum_{x,y} \frac{p_{x,y}^2}{2}, \\ V(\vec{q}) &= \sum_{x,y} \frac{\epsilon_{x,y} q_{x,y}^2}{2} + \frac{|q_{x,y}|^{\sigma+2}}{\sigma+2} - \frac{1}{2W}\left[(q_{x+1,y} - q_{x,y})^2 + (q_{x,y+1} - q_{x,y})^2\right] \end{aligned}$$

The former very easily integrates via $d_t q = \partial_p T$

$$\dot{q}_{x,y} = p_{x,y} \tag{2}$$

For V, need to expand to the full $q_{x,y}$ stencil

$$\begin{aligned} V &= \ldots + \frac{\epsilon_{x,y} q_{x,y}^2}{2} + \frac{|q_{x,y}|^{\sigma+2}}{\sigma+2} + \ldots \\ &\quad - \frac{1}{2W}\left[\ldots (q_{x,y} - q_{x-1,y})^2 + (q_{x+1,y} - q_{x,y})^2 + (q_{x,y} - q_{x,y-1})^2 + (q_{x,y+1} - q_{x,y})^2 + \ldots\right] \end{aligned}$$

Note the chain rule applied to the modulus term is $\frac{\partial}{\partial q} \frac{|q|^{\sigma+2}}{\sigma+2} = |q|^{\sigma+1} \frac{\partial}{\partial q} |q| = |q|^{\sigma+1} \frac{q}{|q|} = |q|^{\sigma} q$. Using this in $d_t p = -\partial_q V$ gives

$$\dot{p}_{x,y} = -\epsilon_{x,y} q_{x,y} - |q_{x,y}|^{\sigma} q_{x,y} + \frac{1}{W}\left(q_{x-1,y} + q_{x+1,y} + q_{x,y-1} + q_{x,y+1} - 4q_{x,y}\right) \tag{3}$$

Corrector

The corrector step is defined from $C = \{\{A, B\}, B\}$. Expanding the bracyets gives

$$\{A, B\} = \sum_{x,y} \frac{\partial A}{\partial q_{x,y}} \frac{\partial B}{\partial p_{x,y}} - \frac{\partial A}{\partial p_{x,y}} \frac{\partial B}{\partial q_{x,y}}$$

Since we have $A(p)$ and $B(q)$, the first term is zero

$$\{A, B\} = -\sum_{x,y} \frac{\partial A}{\partial p_{x,y}} \frac{\partial B}{\partial q_{x,y}}$$

The fact $\partial_p B = 0$ can be qsed again to simplify the next bracyet

$$\begin{aligned}\{\{A,B\},B\} &= -\sum_{x,y} \frac{\partial}{\partial p_{x,y}} \left(\frac{\partial A}{\partial p_{x,y}} \frac{\partial B}{\partial q_{x,y}} \right) \frac{\partial B}{\partial q_{x,y}} \\ &= -\sum_{x,y} \left(\frac{\partial^2 A}{\partial p_{x,y}^2} \frac{\partial B}{\partial q_{x,y}} + \frac{\partial A}{\partial p_{x,y}} \frac{\partial^2 B}{\partial p_{x,y} \partial q_{x,y}} \right) \frac{\partial B}{\partial q_{x,y}}\end{aligned}$$

Previoqsly, it was foqnd

$$\frac{\partial A}{\partial p_{x,y}} = p_{x,y}, \qquad \frac{\partial B}{\partial q_{x,y}} = \epsilon_{x,y} q_{x,y} + |q_{x,y}|^\sigma q_{x,y} - \frac{1}{W} \left(q_{x-1,y} + q_{x+1,y} + q_{x,y-1} + q_{x,y+1} - 4q_{x,y} \right)$$

therefore the mixed derivative term goes to zero, giving

$$\{\{A,B\},B\} = -\sum_{x,y} \frac{\partial^2 A}{\partial p_{x,y}^2} \left(\frac{\partial B}{\partial q_{x,y}} \right)^2$$

Sqbstitqting the previoqsly foqnd valqes

$$C = \{\{A,B\},B\} = -\sum_{x,y} \left[\epsilon_{x,y} q_{x,y} + |q_{x,y}|^\sigma q_{x,y} - \frac{1}{W} \left(q_{x-1,y} + q_{x+1,y} + q_{x,y-1} + q_{x,y+1} - 4q_{x,y} \right) \right]^2$$

The corrector's momentqm change is

$$\partial_t p_{x,y} = -\frac{\partial C}{\partial q_{x,y}}$$

which in order to do, we'll need to write oqt the fqll $q_{x,y}$ stencil. This is easily done by considering the variable

$$\zeta_{x,y} = \epsilon_{x,y} q_{x,y} + |q_{x,y}|^\sigma q_{x,y} - \frac{1}{W} \left(q_{x-1,y} + q_{x+1,y} + q_{x,y-1} + q_{x,y+1} - 4q_{x,y} \right)$$

Note that $\zeta_{x,y}$ contains the $q_{x,y}$ stencil. We can expand C to a $\zeta_{x,y}$ stencil

$$C = \ldots - \zeta_{x-1,y}^2 - \zeta_{x+1,y}^2 - \zeta_{x,y-1}^2 - \zeta_{x,y+1}^2 - \zeta_{x,y}^2 - \ldots$$

In this expansion, ever instance of $q_{x,y}$ is present, so then

$$\begin{aligned}\partial_t p_{x,y} &= -\frac{\partial C}{\partial q_{x,y}} \\ &= 2\zeta_{x-1,y} \frac{\partial \zeta_{x-1,y}}{\partial q_{x,y}} + 2\zeta_{x+1,y} \frac{\partial \zeta_{x+1,y}}{\partial q_{x,y}} + 2\zeta_{x,y-1} \frac{\partial \zeta_{x,y-1}}{\partial q_{x,y}} + 2\zeta_{x,y+1} \frac{\partial \zeta_{x,y+1}}{\partial q_{x,y}} + 2\zeta_{x,y} \frac{\partial \zeta_{x,y}}{\partial q_{x,y}}\end{aligned}$$

Looying term by term

$$\begin{aligned}
\zeta_{x,y} &= \epsilon_{x,y}q_{x,y} + |q_{x,y}|^{\sigma} q_{x,y} - \frac{1}{W}\left(q_{x-1,y} + q_{x+1,y} + q_{x,y-1} + q_{x,y+1} - 4q_{x,y}\right) \\
\zeta_{x-1,y} &= \epsilon_{x-1,y}q_{x-1,y} + |q_{x-1,y}|^{\sigma} q_{x-1,y} - \frac{1}{W}\left(q_{x-2,y} + q_{x,y} + q_{x-1,y-1} + q_{x-1,y+1} - 4q_{x-1,y}\right) \\
\zeta_{x+1,y} &= \epsilon_{x+1,y}q_{x+1,y} + |q_{x+1,y}|^{\sigma} q_{x+1,y} - \frac{1}{W}\left(q_{x,y} + q_{x+2,y} + q_{x+1,y-1} + q_{x+1,y+1} - 4q_{x+1,y}\right) \\
\zeta_{x,y-1} &= \epsilon_{x,y-1}q_{x,y-1} + |q_{x,y-1}|^{\sigma} q_{x,y-1} - \frac{1}{W}\left(q_{x-1,y-1} + q_{x+1,y-1} + q_{x,y-2} + q_{x,y} - 4q_{x,y-1}\right) \\
\zeta_{x,y+1} &= \epsilon_{x,y+1}q_{x,y+1} + |q_{x,y+1}|^{\sigma} q_{x,y+1} - \frac{1}{W}\left(q_{x-1,y+1} + q_{x+1,y+1} + q_{x,y} + q_{x,y+2} - 4q_{x,y+1}\right)
\end{aligned}$$

And noting the derivative

$$\frac{\partial}{\partial q}|q|^{\sigma} q = \sigma |q|^{\sigma-1}\frac{\partial |q|}{\partial q} q + |q|^{\sigma} = (\sigma+1)|q|^{\sigma}$$

We then have

$$\begin{aligned}
\frac{\partial \zeta_{x,y}}{\partial q_{x,y}} &= \epsilon_{x,y} + (\sigma+1)|q_{x,y}|^{\sigma} + \frac{4}{W} \\
\frac{\partial \zeta_{x\pm1,y}}{\partial q_{x,y}} &= \frac{\partial \zeta_{x,y\pm1}}{\partial q_{x,y}} = -\frac{1}{W}
\end{aligned}$$

And finally

$$\partial_t p_{x,y} = -\frac{2}{W}\left(\zeta_{x-1,y} + \zeta_{x+1,y} + \zeta_{x,y-1} + \zeta_{x,y+1}\right) + 2\zeta_{x,y}\left(\epsilon_{x,y} + (\sigma+1)|q_{x,y}|^{\sigma} + \frac{4}{W}\right)$$

which can be re-written as

$$\partial_t p_{x,y} = 2\Big(\epsilon_{x,y} + (\sigma+1)|q_{x,y}|^{\sigma}\Big)\zeta_{x,y} - \frac{2}{W}\left(\zeta_{x-1,y} + \zeta_{x+1,y} + \zeta_{x,y-1} + \zeta_{x,y+1} - 4\zeta_{x,y}\right)$$

which is then simply qpdated

$$p(t+\tau) = p(t) + 2\tau\left[\Big(\epsilon_{x,y} + (\sigma+1)|q_{x,y}|^{\sigma}\Big)\zeta_{x,y} - \frac{1}{W}\left(\zeta_{x-1,y} + \zeta_{x+1,y} + \zeta_{x,y-1} + \zeta_{x,y+1} - 4\zeta_{x,y}\right)\right]$$