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FROM THE NEWTON EQUATION TO THE WAVE EQUATION IN SOME SIMPLE CASES

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Abstract. We prove that, in some simple situations at least, the one-dimensional wave equation is the limit as the microscopic scale goes to zero of some time-dependent Newton type equation of motion for atomistic systems. We address both some linear and some nonlinear cases.

1. Introduction.

1.1. Motivation.

We investigate here the macroscopic limit of the time-dependent Newton equation ruling the evolution of a set of particles at the microscopic scale. The equation we find in the limit is, not unexpectedly, a wave-type equation. We perform our study in a simplified context. The setting is one-dimensional. The interaction law between our particles is either quadratic (thus giving rise to linear forces) or nonlinear (with suitable additional conditions). In the latter case, when no particular convexity is assumed, we will only be able to prove results in the linearized context (in a sense made precise below).

To begin with, we need to mention that, formally, the connection between the Newton equation of motion and the wave equation is clear. Consider indeed the Newton equation of motion for N^d particles that have positions $i + X_i(t) \in \mathbb{R}^d$, indexed by $i \in \mathbb{Z}^d \cap [1, N]^d$ and functions of the time t. For simplicity here, i is

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assumed to be the equilibrium position of the atom labelled by i. The equation reads

$$\begin{cases} \dfrac{d^2X_i}{dt^2} = -\displaystyle\sum_{j\neq i} \nabla V(i-j+X_i-X_j), \\ X_i(0)=X_i^0,\ \dfrac{dX_i}{dt}(0)=V_i^0. \end{cases} \tag{1}$$

Assuming that

$$X_i(t) = N\phi\left(\frac{i}{N},\frac{t}{N}\right),$$

and considering a macroscopic time $\tau = t/N$, we rewrite (1) as

$$\frac{1}{N}\frac{\partial^2\phi}{\partial\tau^2}\left(\frac{i}{N},\frac{t}{N}\right) = -\sum_{j\neq i}\nabla V\left[i-j+N\left(\phi\left(\frac{i}{N},\frac{t}{N}\right)-\phi\left(\frac{j}{N},\frac{t}{N}\right)\right)\right].$$

Note that in this formal presentation, we do not concern ourselves with the convergence of the above series, and that we take all particles alike, thus all interaction potentials as being one single "universal" potential V. As $N\to\infty$, we remark

$$N\left(\phi\left(\frac{i}{N},\frac{t}{N}\right)-\phi\left(\frac{j}{N},\frac{t}{N}\right)\right) \approx \nabla\phi\left(\frac{i}{N},\frac{t}{N}\right)\cdot(i-j) - \frac{1}{2N}D^2\phi\left(\frac{i}{N},\frac{t}{N}\right)(i-j,i-j).$$

Since ∇V is odd (due to action-reaction principle),

$$\frac{1}{N}\frac{\partial^2\phi}{\partial\tau^2}\left(\frac{i}{N},\frac{t}{N}\right) \approx \underbrace{\sum_{k\neq 0}\nabla V\left[k+\nabla\phi\left(\frac{i}{N},\frac{t}{N}\right)\cdot k\right]}_{=0} + \frac{1}{2N}\sum_{k\neq 0}\underbrace{D^2V\left[k+\nabla\phi\left(\frac{i}{N},\frac{t}{N}\right)\cdot k\right]D^2\phi\left(\frac{i}{N},\frac{t}{N}\right)(k,k)}_{=\nabla\left[\nabla V\left(k+\nabla\phi\left(\frac{i}{N},\frac{t}{N}\right)k\right)\cdot k\right]}.$$

Hence, assuming that $i/N\to x$, a fixed macroscopic point, we conclude that ϕ satisfies the nonlinear wave equation:

$$\frac{\partial^2\phi}{\partial\tau^2}(x,\tau) - \operatorname{div}\left[D_A E(\nabla\phi)\right] = 0, \tag{2}$$

where

$$E(A) = \frac{1}{2}\sum_{k\in\mathbb{Z}^d\setminus\{0\}} V(k+Ak), \tag{3}$$

for $A\in\mathbb{R}^{d\times d}$.

The question of mathematically proving in some suitable circumstances that the above formal limit holds true has already been investigated by several authors and we in particular wish to cite [2, 5]. We provide here our own view on the subject. The results we obtain are definitely limited. Even proving that an equation of the form (2) is well posed in dimension larger than two is a difficult subject [4]. In the current state of our understanding, we do not know how to significantly extend the results we present here. In our opinion, the mathematical state of the art is thus far from covering the formal derivation we have just recalled above.

1.2. **Summary of our results.** As mentioned above, we restrict ourselves to the one-dimensional setting (see Remark 3 below for a comment on this simplification). Equation (1) then writes

$$\begin{cases} \dfrac{d^2X_i}{dt^2} = -\displaystyle\sum_{j\neq i} V'(i-j+X_i-X_j), \\ X_i(0) = X_i^0, \quad \dfrac{dX_i}{dt}(0) = V_i^0, \end{cases} \tag{4}$$

while (2)-(3) reduces to

$$\begin{cases} \dfrac{\partial^2\phi}{\partial\tau^2}(x,\tau) - \dfrac{\partial}{\partial x}\left[\dfrac{1}{2}\displaystyle\sum_{k\neq 0} V'\left(k + \dfrac{\partial\phi}{\partial x}(x,\tau)k\right)k\right] = 0, \\ \phi(x,0) = \phi^0(x), \quad \dfrac{\partial\phi}{\partial t}(x,0) = \phi^1(x), \end{cases} \tag{5}$$

supplied with the boundary conditions $\phi(0,t) = 0$, and $\phi(1,t) = 0$.

We will devote some of our attention to the simplest possible case of a nearest-neighbour interaction (henceforth abbreviated as *NN* interaction). Equation (4) then becomes

$$\begin{cases} \dfrac{d^2X_i}{dt^2} = V'(1+X_{i+1}-X_i) - V'(1+X_i-X_{i-1}), \\ X_i(0) = X_i^0, \quad \dfrac{dX_i}{dt}(0) = V_i^0, \end{cases} \tag{6}$$

with the convention that $X_0 = 0$, $X_{N+1} = 0$, and (5) reads

$$\begin{cases} \dfrac{\partial^2\phi}{\partial\tau^2}(x,\tau) - \dfrac{\partial}{\partial x}\left[V'\left(1 + \dfrac{\partial\phi}{\partial x}(x,\tau)\right)\right] = 0, \\ \phi(x,0) = \phi^0(x), \quad \dfrac{\partial\phi}{\partial t}(x,0) = \phi^1(x), \\ \phi(0,\tau) = 0, \quad \phi(1,\tau) = 0. \end{cases} \tag{7}$$

The linear wave equation is obtained for the specific interaction potential $V(x) = \frac{1}{2}(x-1)^2$.

For a next-to-nearest-neighbour interaction (henceforth abbreviated as *NNN* interaction), (4) reads

$$\begin{cases} \dfrac{d^2X_i}{dt^2} = -V_1'(1+X_i-X_{i+1}) - V_1'(1+X_i-X_{i-1}) \\ \qquad\qquad -V_2'(2+X_i-X_{i+2}) - V_2'(2+X_i-X_{i-2}), \\ X_i(0) = X_i^0, \quad \dfrac{dX_i}{dt}(0) = V_i^0, \end{cases} \tag{8}$$

with the convention $X_i = 0$ for $i \in \{-1, 0, N+1, N+2\}$. and (5) reads

$$\begin{cases} \dfrac{\partial^2\phi}{\partial\tau^2}(x,\tau) - \dfrac{\partial}{\partial x}\left[V_1'\left(1 + \dfrac{\partial\phi}{\partial x}(x,\tau)\right) + 2V_2'\left(2 + 2\dfrac{\partial\phi}{\partial x}(x,\tau)\right)\right] = 0, \\ \phi(x,0) = \phi^0(x), \quad \dfrac{\partial\phi}{\partial t}(x,0) = \phi^1(x), \\ \phi(0,\tau) = 0, \quad \phi(1,\tau) = 0. \end{cases} \tag{9}$$

Again, the linear wave equation corresponds to the case $V_1(x) = \frac{c_1}{2}(x-1)^2$ and $V_2(x) = \frac{c_2}{2}(x-2)^2$, see (40) below.

We will examine the *linear* case and prove indeed the convergence of the Newton equations (6) and (8) to (7) and (9), respectively, in Subsections 2.1 and 3.1 (convex case) and 3.2 (non convex case) below. In the convex case, the strategy is to use the energy conservation of both systems (the discrete one and the continuous one). Since both the corresponding energies are convex, this implies convergence. For the non convex case, we will provide two different strategies of proof. The first one uses an explicit spectral decomposition of the underlying finite difference operator. The second one is more general, and is based on the fact that energy preservation for the discrete system implies the existence of bounds, which in turn implies compactness in weak topology. This allows to pass to the limit in the equation. Next, strong convergence is proved using energy conservation for the continuous equation.

Not surprisingly, the nonlinear setting is significantly more difficult. If convexity is present in the problem at the microscopic scale, then it is possible to conclude, and the argument is actually simple. A typical case, which will be addressed in Section 2.2, is a convex nearest-neighbour interaction. Indeed, in such a case, up to some technical details, the proof is very similar to the linear case.

Extending the argument to other cases seems not possible. Of course, a trivial situation is when all interactions (nearest neighbour, next-to-nearest-neighbour, etc) are convex. The proof of Section 2.2 may then be straightforwardly extended, (see Subsection 3.3) to cover this situation. A more interesting case is when the energy functional present in the limit equation (2) is convex, but the equation at the microscopic scale does not have interaction potentials that are all convex. Loosely stated, some microscopic interactions disappear in the passage to continuum and therefore need not be assumed convex. Formalizing the argument is however beyond our reach and we are unable to prove convergence of (6) to (7) nor of (8) to (9). In the nonlinear "non-convex" setting, we are only able to prove convergence in a different regime, which we call the *linearized regime.* This is the purpose of Section 3.4. We introduce a parameter $\gamma \in (0,1)$ and modify the Newton equation as follows:

$$\begin{cases} \dfrac{d^2 X_i}{dt^2} = N^\gamma \left[V'\left(1 + \dfrac{X_{i+1} - X_i}{N^\gamma}\right) - V'\left(1 + \dfrac{X_i - X_{i-1}}{N^\gamma}\right)\right], \\ X_i(0) = X_i^0, \quad \dfrac{dX_i}{dt}(0) = V_i^0, \end{cases} \tag{10}$$

in the NN case, with the convention that $X_0 = 0$ and $X_{N+1} = 0$. Then we can prove that the corresponding limit is

$$\begin{cases} \dfrac{\partial^2 \phi}{\partial \tau^2}(x,\tau) - V''(1)\dfrac{\partial^2 \phi}{\partial x^2}(x,\tau) = 0, \\ \phi(x,0) = \phi^0(x), \quad \dfrac{\partial \phi}{\partial t}(x,0) = \phi^1(x), \\ \phi(0,\tau) = 0, \quad \phi(1,\tau) = 0. \end{cases} \tag{11}$$

Similarly, in the NNN case

$$\begin{cases} \dfrac{d^2X_i}{dt^2} = N^\gamma \left[V_1'\left(1+\dfrac{X_{i+1}-X_i}{N^\gamma}\right) - V_1'\left(1+\dfrac{X_i-X_{i-1}}{N^\gamma}\right) \right. \\ \qquad\qquad \left. +V_2'\left(2+\dfrac{X_{i+2}-X_i}{N^\gamma}\right) - V_2'\left(2+\dfrac{X_i-X_{i-2}}{N^\gamma}\right)\right] = 0, \\ X_i(0) = X_i^0, \quad \dfrac{dX_i}{dt}(0) = V_i^0, \end{cases} \tag{12}$$

with the convention $X_i = 0$ for $i \in \{-1, 0, N+1, N+2\}$, we obtain the limit equation:

$$\begin{cases} \dfrac{\partial^2 \phi}{\partial \tau^2}(x,\tau) - (V_1''(1) + 4V_2''(2))\,\dfrac{\partial^2 \phi}{\partial x^2}(x,\tau) = 0, \\ \phi(x,0) = \phi^0(x), \quad \dfrac{\partial \phi}{\partial t}(x,0) = \phi^1(x), \\ \phi(0,\tau) = 0, \quad \phi(1,\tau) = 0. \end{cases} \tag{13}$$

Here, our second strategy of proof developed for the linear (non-convex) case, that is, the one using weak convergence, applies. It is however necessary to slightly adapt it in order to treat the nonlinear terms in the equations, since weak convergence does not allow to pass to the limit in such terms. However, the fact that $\gamma \in (0,1)$ implies that the equation becomes linear in the limit $N \to \infty$, which saves the situation.

Note that V_1 ($= V$ in the NN case) is supposed to be minimum at its equilibrium length, that is, 1, while V_2 is minimum at 2. This is consistent with the assumption made above that the lattice $\mathbb{Z}$ is an equilibrium state of the discrete system.

Also, let us point out that, in the nearest-neighbour case, equations (6) and (7) are left unchanged if we add an affine function to V. Hence, we will assume, when necessary, that $V(1) = V'(1) = 0$. Similarly, in the next-to-nearest neighbour case, we will assume, when necessary, that $V_1(1) = V_1'(1) = 0$ and $V_2(2) = V_2'(2) = 0$.

2. **Nearest-neighbour interaction.**

2.1. **Linear case.**

We begin with the simplest possible case, where interaction is only considered between nearest neighbours and the interaction potential is taken as $V(x) = \frac{1}{2}(x-1)^2$, (hence $V'(x) = x - 1$). Then (6) reads

$$\begin{cases} \dfrac{d^2X_i}{dt^2} = X_{i+1} - 2X_i + X_{i-1}, \\ X_i(0) = X_i^0, \quad \dfrac{dX_i}{dt}(0) = V_i^0, \end{cases} \tag{14}$$

with $X_0 = 0$ and $X_{N+1} = 0$, while (7) reads

$$\begin{cases} \dfrac{\partial^2 \phi}{\partial \tau^2}(x,\tau) - \dfrac{\partial^2 \phi}{\partial x^2}(x,\tau) = 0, \\ \phi(x,0) = \phi^0(x), \quad \dfrac{\partial \phi}{\partial t}(x,0) = \phi^1(x), \\ \phi(0,\tau) = 0, \quad \phi(1,\tau) = 0. \end{cases} \tag{15}$$

We have the following.

Proposition 1. *Let* $(\phi^0, \phi^1) \in \left[H^4(0,1)\right]^2$ *be such that* $\phi^0(0) = 0$ *and* $\phi^0(1) = 0$. *Define, for all* $N \in \mathbb{N}$, *and for all* $1 \leq i \leq N$,

$$X_i^0 = N\phi^0\left(\frac{i}{N}\right), \quad V_i^0 = \phi^1\left(\frac{i}{N}\right). \tag{16}$$

Let $X_i(t)$ *be the unique solution to* (14), *with the convention* $X_0 = 0,\ X_{N+1} = 0$, *and let* $\phi \in L^\infty\left(\mathbb{R}^+, H^1(0,1)\right)$ *be the unique solution of* (15). *Then, we have the convergences*

$$\forall \tau > 0, \quad \sup_{1\leq i\leq N}\left|\frac{1}{N}X_i(N\tau) - \phi\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0, \tag{17}$$

and

$$\forall \tau > 0, \quad \left[\sup_{1\leq i\leq N}\left|\frac{dX_i}{dt}(N\tau) - \frac{\partial\phi}{\partial\tau}\left(\frac{i}{N},\tau\right)\right|\right] \underset{N\to\infty}{\longrightarrow} 0. \tag{18}$$

Proving this Proposition amounts to proving consistency of some natural (centered second order) finite difference scheme for the wave equation. Such a proof can be found in [6] for instance. For consistency, we provide an elementary proof below. But before we get to that, let us briefly explain the bottom line of the proof. For this purpose, we argue somewhat formally and have to introduce some notation. The notation will be useful throughout this article. For a function Φ, we denote by

$$D_\varepsilon\Phi(x) = \varepsilon^{-1}(\Phi(x+\varepsilon/2) - \Phi(x-\varepsilon/2)), \tag{19}$$

where, of course, ε plays the role of $1/N$. This discrete differentiation can be iterated. We for instance have

$$D_\varepsilon^2\Phi = \varepsilon^{-2}(\Phi(x+\varepsilon) - 2\Phi(x) + \Phi(x-\varepsilon)).$$

Using this notation, proving (after renormalization in time) the convergence of the solution to (14) to the solution to (15) basically amounts to proving (if we omit the truncation error terms) that the solution Φ_ε to

$$\frac{\partial^2\Phi_\varepsilon}{\partial t^2} - D_\varepsilon^2\Phi_\varepsilon = 0, \tag{20}$$

with suitable (vanishing) initial and boundary conditions, vanishes with ε. This is an immediate consequence of the fact that Φ_ε satisfies the energy equality

$$\frac{d}{dt}\left(\left\|\frac{\partial}{\partial t}\Phi_\varepsilon\right\|^2 + \|D_\varepsilon\Phi_\varepsilon\|^2\right) = 0. \tag{21}$$

The proof of Proposition 1 actually formalizes the above argument rigorously.

Proof. We start by recalling that in view of [9, Theorem 3.1.2], the solution ϕ to (15) is unique in $C^0(\mathbb{R}^+, H^1(0,1))$, and satisfies

$$\phi \in C^0\left(\mathbb{R}^+, H^4(0,1)\right)$$

Next, we define

$$\delta_i^N(\tau) = \frac{1}{N}X_i(N\tau) - \phi\left(\frac{i}{N},\tau\right),$$

with the convention $\delta_{N+1}^N(\tau) = 0$. Using (14) and (15), we have

$$\frac{d^2\delta_i}{d\tau^2} = N\left(X_{i+1}(N\tau) - 2X_i(N\tau) + X_{i-1}(N\tau)\right) - \frac{\partial^2\phi}{\partial x^2}\left(\frac{i}{N},\tau\right).$$

Hence,

$$\frac{d^2\delta_i}{d\tau^2} - N^2\left(\delta_{i+1} - 2\delta_i + \delta_{i-1}\right)$$
$$= N^2\left[\phi\left(\frac{i-1}{N},\tau\right) - 2\phi\left(\frac{i}{N},\tau\right) + \phi\left(\frac{i+1}{N},\tau\right)\right] - \frac{\partial^2\phi}{\partial x^2}\left(\frac{i}{N},\tau\right) := D_i^N(\tau). \tag{22}$$

Using a Taylor expansion, it is clear that $D_i^N(\tau)$ in (22) satisfies

$$\left|D_i^N(\tau)\right| \leq C\frac{\|\phi(\cdot,\tau)\|_{H^4(\frac{i}{N},\frac{i+1}{N})}}{N^{3/2}},$$

for some universal constant $C > 0$. Hence,

$$\frac{1}{N}\sum_{i=1}^{N} D_i^N(\tau)^2 \leq C\frac{\|\phi\|^2_{H^4(0,1)}}{N^4}. \tag{23}$$

Multiplying equation (22) by $\frac{d\delta_i}{d\tau}$, we obtain

$$\frac{1}{2}\frac{d}{d\tau}\left(\frac{d\delta_i}{d\tau}\right)^2 - N^2\left(\delta_{i+1} - 2\delta_i + \delta_{i-1}\right)\frac{d\delta_i}{d\tau} = D_i^N(\tau)\frac{d\delta_i}{d\tau}.$$

Summing over i, we get, since $\delta_{N+1}(\tau) = \delta_0(\tau) = 0$,

$$\frac{d}{d\tau}\sum_{i=1}^{N}\left(\frac{d\delta_i}{d\tau}\right)^2 + \frac{d}{d\tau}\sum_{i=1}^{N-1} N^2(\delta_{i+1}-\delta_i)^2 + N^2\frac{d}{d\tau}\left(\delta_1^2 + \delta_N^2\right) = 2\sum_{i=1}^{N} D_i^N(\tau)\frac{d\delta_i}{d\tau},$$

that is,

$$\frac{d}{d\tau}\left[\sum_{i=1}^{N}\left(\frac{d\delta_i}{d\tau}\right)^2 + \sum_{i=0}^{N} N^2(\delta_{i+1}-\delta_i)^2\right] = 2\sum_{i=1}^{N} D_i^N(\tau)\frac{d\delta_i}{d\tau}. \tag{24}$$

This estimate is the rigorous formalization of (21). Using the Cauchy-Schwarz inequality, we find, setting $F_N = \frac{1}{N}\sum\left(\frac{d\delta_i}{d\tau}\right)^2$,

$$F_N(\tau) = F_N(\tau) - F_N(0) \leq 2\int_0^\tau\left(\frac{1}{N}\sum_{i=1}^{N} D_i^N(s)^2\right)^{1/2}\sqrt{F_N(s)}ds,$$

where we have used the fact that $\delta_i(0) = 0$ for all i. Hence, applying (23), we infer that

$$F_N(\tau) \leq C\frac{\|\phi\|_{C^0(\mathbb{R}^+,H^4(0,1))}}{N^2}\int_0^\tau\sqrt{F_N(s)}ds,$$

with $C > 0$ independent of N. This clearly implies

$$F_N(\tau) \leq C\frac{\|\phi\|^2_{C^0(\mathbb{R}^+,H^4(0,1))}}{N^4}\tau^2, \tag{25}$$

so

$$\sup_{1\leq i\leq N}\left|\frac{d\delta_i}{d\tau}\right| \leq C\frac{\|\phi\|_{C^0(\mathbb{R}^+,H^4(0,1))}}{N^{3/2}}\tau, \tag{26}$$

which proves (18). Integrating (26) with respect to τ, yields (17). □

Remark 1. Actually, the exact agreement (16) between the discrete and the continuous initial data is not necessary. A condition on the smallness of $X_i^0 - N\phi^0\left(\frac{i}{N}\right)$ (and a similar condition on $V_i^0 - \phi^1\left(\frac{i}{N}\right)$) is sufficient. This remark also holds for Propositions 2, 3, 4, 6 below. The exact formalization of "small" depends on the case under study, and is typically an exponential decay as $N \to \infty$.

Remark 2. It is clear in the above proof that the convergences in Proposition 1 can be made more precise. For instance, we have (26), which gives a rate of convergence for (17) and (18). Further, using (23), (24), and (25), one easily proves that

$$\frac{d}{d\tau}\left[\sum_{i=0}^{N} N^2\left(\delta_{i+1}-\delta_i\right)^2\right] \leq C\frac{\|\phi\|_{C^0(\mathbb{R}^+,H^4(0,1))}}{N}\sqrt{F_N(\tau)} \leq C\frac{\|\phi\|^2_{C^0(\mathbb{R}^+,H^4(0,1))}}{N^3}\tau.$$

Integrating in time, we find

$$\frac{1}{N}\sum_{i=1}^{N}\left[X_{i+1}(N\tau)-X_i(N\tau)-N\left(\phi\left(\frac{i+1}{N},\tau\right)-\phi\left(\frac{i}{N},\tau\right)\right)\right]^2 \leq C\frac{\|\phi\|^2_{C^0(\mathbb{R}^+,H^4(0,1))}}{N^4}\tau^2,$$

hence

$$\forall\tau>0,\quad \sup_{1\leq i\leq N}\left|X_{i+1}(N\tau)-X_i(N\tau)-\frac{\partial\phi}{\partial x}\left(\frac{i}{N},\tau\right)\right| \leq \frac{\|\phi\|_{C^0(\mathbb{R}^+,W^{2,\infty}(0,1))}}{N}+C\frac{\|\phi\|_{C^0(\mathbb{R}^+,H^4(0,1))}}{N^{3/2}}\tau.$$

This may be seen as a convergence of the discrete space derivative of X_i to the space derivative of ϕ.

Remark 3. It is immediately seen in the above proof that we could equally well argue with the potential $V(x)=\frac{1}{2}(\|x\|^2-1)$ (or any second-order polynomial) in dimension $d>1$, where $\|\cdot\|$ denotes the Euclidean norm. This remark also holds true for all our proofs and results of Sections 2.1, 3.1 and 3.2 below. The difficulty is that, in our understanding, no such potential makes physical sense for the problems we study. The d-dimensional ($d>1$) analogue of $V(x)=\frac{1}{2}(x-1)^2$ would be $V(x)=\frac{1}{2}\left(\|x\|-1\right)^2$, a potential which we do not know how to treat. In the one-dimensional setting, it reduces to $\frac{1}{2}(x-1)^2$ since we deal with models for nearest neighbours where we implicitly assume particles are ordered. This is the current intrinsic limitation of our work that forces us to only treat the one-dimensional setting.

2.2. **Nonlinear convex case.** We now consider a general nonlinear, not necessarily quadratic nearest-neighbour interaction V. In order for our limit equation to naturally make sense, we assume V convex. Then, we have

Proposition 2. *Assume that $V\in C^4$, $V'(1)=0$ and that $V''\geq\alpha>0$ for some constant α. Assume that $\phi\in C^0\left([0,T),C^4([0,1])\right)$ is a solution to (7). Let $N\in\mathbb{N}$, and define, for all $1\leq i\leq N$,*

$$X_i^0 = N\phi^0\left(\frac{i}{N}\right),\quad V_i^0=\phi^1\left(\frac{i}{N}\right).$$

Let $X_i(t)$ be the unique solution to (6), with the convention $X_0 = 0,\ X_{N+1} = 0$. Then, we have the convergences

$$\forall \tau \in (0,T), \qquad \sup_{1\le i\le N} \left| \frac{1}{N} X_i(N\tau) - \phi\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0, \tag{27}$$

and

$$\forall \tau \in (0,T), \qquad \sup_{1\le i\le N} \left| \frac{dX_i}{dt}(N\tau) - \frac{\partial \phi}{\partial \tau}\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0. \tag{28}$$

Remark 4. Local existence for (7) is proved for instance in [7, Theorem II, Theorem IV], under the assumption that $\phi^0 \in H^{s+1}$, $\phi^1 \in H^s$, and $V'' \in C^s$, with $s > 3/2$. The solution is then in $C^0([0,T), H^{s+1}(0,1)) \cap C^1([0,T), H^s(0,1))$. If $V \in C^4$, we can apply this with $s = 2$, hence $\phi \in C^0([0,T), H^3(0,1))$ only. This is why the C^4 regularity of the solution needs to be *assumed* in the statement of Proposition 2.

Proof. We define

$$\delta_i^N(\tau) = \frac{1}{N} X_i(N\tau) - \phi\left(\frac{i}{N},\tau\right),$$

ith the convention that $\delta_{N+1}^N(\tau) = \delta_0^N(\tau) = 0$. Using (6) and (7), we have

$$\frac{d^2\delta_i}{d\tau^2} = N\left(V'(1 + X_{i+1}(N\tau) - X_i(N\tau)) - V'(1 + X_i(N\tau) - X_{i-1}(N\tau))\right) - \frac{\partial}{\partial x}\left[V'\left(1 + \frac{\partial \phi}{\partial x}\left(\frac{i}{N},\tau\right)\right)\right]. \tag{29}$$

The main idea of the proof is to introduce the following energy

$$E_i(\tau) = V\left(1 + X_{i+1}(N\tau) - X_i(N\tau)\right) - V\left[1 + N\phi\left(\frac{i+1}{N},\tau\right) - N\phi\left(\frac{i}{N},\tau\right)\right] - NV'\left[1 + N\phi\left(\frac{i+1}{N},\tau\right) - N\phi\left(\frac{i}{N},\tau\right)\right](\delta_{i+1} - \delta_i), \tag{30}$$

where the presence of the last term, the first order derivative, basically allows to proceed *as if* the potential V were quadratic, and therefore reduces the proof, up to technicalities, to the proof performed for the linear case in the previous section. Let us formalize this. Consider its variation in time

$$\begin{aligned}\frac{dE_i}{d\tau} \;=\; & N\Big[V'\left(1 + X_{i+1}(N\tau) - X_i(N\tau)\right) \\ & -V'\left[1 + N\phi\left(\frac{i+1}{N},\tau\right) - N\phi\left(\frac{i}{N},\tau\right)\right]\Big]\frac{d}{d\tau}(\delta_{i+1} - \delta_i) \\ & +N\Big[V'(1 + X_{i+1}(N\tau) - X_i(N\tau)) \\ & -V'\left(1 + N\phi\left(\frac{i+1}{N},\tau\right) - N\phi\left(\frac{i}{N},\tau\right)\right) \\ & -NV''\left(1 + N\phi\left(\frac{i+1}{N},\tau\right) - N\phi\left(\frac{i}{i}N,\tau\right)\right)(\delta_{i+1} - \delta_i)\Big] \\ & \times\left(\frac{\partial \phi}{\partial \tau}\left(\frac{i+1}{N},\tau\right) - \frac{\partial \phi}{\partial \tau}\left(\frac{i}{N},\tau\right)\right)\end{aligned} \tag{31}$$

Multiplying (29) by $\frac{d\delta_i}{d\tau}$ and summing over i, we have

$$\begin{aligned}\frac{d}{d\tau}\left[\frac{1}{2}\sum_{i=0}^{N}\left(\frac{d\delta_i}{d\tau}\right)^2\right] &= N\sum_{i=0}^{N}\Big[V'\left(1+X_{i+1}(N\tau)-X_i(N\tau)\right)- \\ &\quad V'\left(1+X_i(N\tau)-X_{i-1}(N\tau)\right)\Big]\frac{d\delta_i}{d\tau} \\ &\quad -\sum_{i=0}^{N}\frac{\partial}{\partial x}\left[V'\left(1+\frac{\partial\phi}{\partial x}\left(\frac{i}{N},\tau\right)\right)\right]\frac{d\delta_i}{d\tau} \\ &= -N\sum_{i=0}^{N}V'\left(1+X_{i+1}(N\tau)-X_i(N\tau)\right)\frac{d}{d\tau}(\delta_{i+1}-\delta_i) \\ &\quad -\sum_{i=0}^{N}V''\left(1+\frac{\partial\phi}{\partial x}\left(\frac{i}{N},\tau\right)\right)\frac{\partial^2\phi}{\partial x^2}\left(\frac{i}{N},\tau\right)\frac{d\delta_i}{d\tau}\end{aligned}$$

Adding the sum over i of (31) to this equality, we have

$$\begin{aligned}&\frac{d}{d\tau}\sum_{i=0}^{N}\left[\frac{1}{2}\left(\frac{d\delta_i}{d\tau}\right)^2+E_i\right]= \\ &\qquad -N\sum_{i=0}^{N}V'\left(1+N\phi\left(\frac{i+1}{N}\right)-N\phi\left(\frac{i}{N}\right)\right)\frac{d}{d\tau}(\delta_{i+1}-\delta_i) \\ &\qquad +N\sum_{i=0}^{N}\Bigg[V'(1+X_{i+1}-X_i)-V'\left(1+N\phi\left(\frac{i+1}{N}\right)-N\phi\left(\frac{i}{N}\right)\right) \\ &-NV''\left(1+N\phi\left(\frac{i+1}{N}\right)-N\phi\left(\frac{i}{N}\right)\right)(\delta_{i+1}-\delta_i)\Bigg]\left(\frac{\partial\phi}{\partial\tau}\left(\frac{i+1}{N},\tau\right)-\frac{\partial\phi}{\partial\tau}\left(\frac{i}{N}\right)\right) \\ &\qquad\qquad -\sum_{i=0}^{N}V''\left(1+\frac{\partial\phi}{\partial x}\left(\frac{i}{N}\right)\right)\frac{\partial^2\phi}{\partial x^2}\left(\frac{i}{N}\right)\frac{d\delta_i}{d\tau}.\end{aligned}$$

Rearranging the first sum of the right-hand side, we have

$$\begin{aligned}\frac{d}{d\tau}\sum_{i=0}^{N}\left[\frac{1}{2}\left(\frac{d\delta_i}{d\tau}\right)^2+E_i\right] &= -N\sum_{i=0}^{N}\frac{A_i^N}{N^3}\frac{d\delta_i}{d\tau} \\ &+N\sum_{i=0}^{N}\Bigg[V'(1+X_{i+1}-X_i)-V'\left(1+N\phi\left(\frac{i+1}{N}\right)-N\phi\left(\frac{i}{N}\right)\right) \\ &\quad -NV''\left(1+N\phi\left(\frac{i+1}{N}\right)-N\phi\left(\frac{i}{N}\right)\right)(\delta_{i+1}-\delta_i)\Bigg] \\ &\qquad \times\left(\frac{\partial\phi}{\partial\tau}\left(\frac{i+1}{N},\tau\right)-\frac{\partial\phi}{\partial\tau}\left(\frac{i}{N}\right)\right),\end{aligned}\tag{32}$$

with

$$\begin{aligned}\frac{A_i^N}{N^3} &= V'\left[1+N\phi\left(\frac{i+1}{N}\right)-N\phi\left(\frac{i}{N}\right)\right]-V'\left[1+N\phi\left(\frac{i}{N}\right)-N\phi\left(\frac{i-1}{N}\right)\right] \\ &\quad -V''\left(1+\frac{\partial\phi}{\partial x}\left(\frac{i}{N}\right)\right)\frac{\partial^2\phi}{\partial x^2}\left(\frac{i}{N}\right).\end{aligned}$$

We also have, using a Taylor expansion,

$$
\begin{aligned}
&V'\left[1+N\phi\left(\frac{i+1}{N},\tau\right)-N\phi\left(\frac{i}{N},\tau\right)\right]-V'\left[1+N\phi\left(\frac{i}{N},\tau\right)-N\phi\left(\frac{i-1}{N},\tau\right)\right]\\
&\quad=V''\left[1+\frac{\partial\phi}{\partial x}\left(\frac{i}{N},\tau\right)\right]\left(\frac{1}{N}\frac{\partial^2\phi}{\partial x^2}\left(\frac{i}{N},\tau\right)+\frac{1}{12N^3}\frac{\partial^4\phi}{\partial x^4}\left(\frac{i+\theta_i^1}{N},\tau\right)\right)+\\
&\quad\frac{1}{2}V^{(3)}\left[1+\frac{\partial\phi}{\partial x}\left(\frac{i}{N},\tau\right)\right]\left[\frac{1}{3N^3}\frac{\partial^2\phi}{\partial x^2}\left(\frac{i}{N},\tau\right)\frac{\partial^3\phi}{\partial x^3}\left(\frac{i}{N},\tau\right)+\frac{B_i^N(\tau)}{N^4}\right]\\
&\qquad\qquad+\frac{1}{6}V^{(4)}\left[1+\frac{\partial\phi}{\partial x}\left(\frac{i}{N},\tau\right)\right]\frac{C_i^N(\tau)}{N^3},
\end{aligned}
$$

with $\theta_i^1\in(0,1)$, where B_i^N satisfies:

$$\left|B_i^N(\tau)\right|\leq C\|\phi(\cdot,\tau)\|^2_{C^4(0,1)},$$

for some universal constant C, and where C_i^N satisfies

$$\left|C_i^N(\tau)\right|\leq C\|\phi(\cdot,\tau)\|^3_{C^4(0,1)}.$$

Hence,

$$
\begin{aligned}
\left|A_i^N\right|\leq C\Big[&\|V''\|_{L^\infty}\|\phi(\cdot,\tau)\|_{C^4(0,1)}+\|V^{(3)}\|_{L^\infty}\|\phi(\cdot,\tau)\|^2_{C^4(0,1)}\\
&+\|V^{(4)}\|_{L^\infty}\|\phi(\cdot,\tau)\|^3_{C^4(0,1)}\Big]
\end{aligned}
\tag{33}
$$

Next, we use a Taylor expansion of the term in the second sum of the right-hand side of (32), writing it as

$$
\begin{aligned}
&V'(1+X_{i+1}-X_i)-V'\left(1+N\phi\left(\frac{i+1}{N}\right)-N\phi\left(\frac{i}{N}\right)\right)\\
&\qquad-NV''\left(1+N\phi\left(\frac{i+1}{N}\right)-N\phi\left(\frac{i}{N}\right)\right)(\delta_{i+1}-\delta_i)\\
&\quad=V^{(3)}\left(N\phi\left(\frac{i+1}{N}\right)-N\phi\left(\frac{i}{N}\right)+N\theta_i(\delta_{i+1}-\delta_i)\right)N^2\left(\delta_{i+1}-\delta_i\right)^2,
\end{aligned}
\tag{34}
$$

for some $\theta_i\in(0,1)$. As a result, we have

$$
\begin{aligned}
\frac{d}{d\tau}\sum_{i=0}^N\left[\frac{1}{2}\left(\frac{d\delta_i}{d\tau}\right)^2+E_i\right]&=-\frac{1}{N^2}\sum_{i=0}^N A_i^N(\tau)\frac{d\delta_i}{d\tau}\\
&+N\sum_{i=0}^N D_i^N(\tau)N^2(\delta_{i+1}-\delta_i)^2\left(\frac{\partial\phi}{\partial\tau}\left(\frac{i+1}{N},\tau\right)-\frac{\partial\phi}{\partial\tau}\left(\frac{i}{N}\right)\right),
\end{aligned}
\tag{35}
$$

with A_i^N satisfying (33), and, according to (34), D_i^N satisfies

$$|D_i^N(\tau)|\leq\|V^{(3)}\|_{L^\infty}. \tag{36}$$

Hence,

$$
\begin{aligned}
\left|\frac{d}{d\tau}\sum_{i=0}^N\left[\frac{1}{2}\left(\frac{d\delta_i}{d\tau}\right)^2+E_i\right]\right|&\leq\frac{1}{N^2}\sum_{i=0}^N\left|A_i^N(\tau)\right|\left|\frac{d\delta_i}{d\tau}\right|\\
&+\sum_{i=1}^N\left|D_i^N(\tau)\right|N^2(\delta_{i+1}-\delta_i)^2\|\phi\|_{C^2(\mathbb{R}^+\times(0,1))}
\end{aligned}
\tag{37}
$$

We now return to the definition of E_i, that is, (30), and using a Taylor expansion and the fact that $V'' \geq \alpha > 0$, we easily prove

$$E_i(\tau) \geq \frac{\alpha}{2} N^2 \left(\delta_{i+1} - \delta_i\right)^2. \tag{38}$$

This, together with (37), (33) and (36), implies

$$\left| \frac{d}{d\tau} \sum_{i=1}^N \left[\frac{1}{2} \left(\frac{d\delta_i}{d\tau} \right)^2 + E_i \right] \right| \leq \frac{A}{N^{3/2}} \left[\sum_{i=1}^N \frac{1}{2} \left(\frac{d\delta_i}{d\tau} \right)^2 \right]^{1/2} + A' \sum_{i=1}^N E_i, \tag{39}$$

where

$$A \leq C \left[\|V''\|_{L^\infty} \|\phi(\cdot,\tau)\|_{C^4(0,1)} + \|V^{(3)}\|_{L^\infty} \|\phi(\cdot,\tau)\|^2_{C^4(0,1)} \right.$$
$$\left. + \|V^{(4)}\|_{L^\infty} \|\phi(\cdot,\tau)\|^3_{C^4(0,1)} \right],$$

for some universal constant C, and

$$A' \leq \frac{2}{\alpha} \|V^{(3)}\|_{L^\infty} \|\phi\|_{C^2(\mathbb{R}^+ \times (0,1))}.$$

Hence, (39) implies

$$\left| \frac{dF}{d\tau} \right| \leq \frac{A}{N^{3/2}} \sqrt{F} + A'F, \text{ where } F(\tau) = \sum_{i=1}^N \left[\frac{1}{2} \left(\frac{d\delta_i}{d\tau} \right)^2 + E_i \right].$$

This also reads

$$\left| \frac{d\sqrt{F}}{d\tau} \right| \leq \frac{A}{2N^{3/2}} + \frac{A'}{2} \sqrt{F}.$$

Hence, applying Gronwall's Lemma, we have

$$\sqrt{F(\tau)} \leq \frac{A}{A' N^{3/2}} \left(e^{\frac{A'}{2}\tau} - 1 \right).$$

This and (38) imply that

$$\sum_{i=1}^N \left(\frac{d\delta_i}{d\tau} \right)^2 \leq \frac{2A^2}{(A')^2 N^3} \left(e^{\frac{A'}{2}\tau} - 1 \right)^2,$$
$$\sum_{i=1}^N \left(\delta_{i+1} - \delta_i\right)^2 \leq \frac{2A^2}{\alpha (A')^2 N^5} \left(e^{\frac{A'}{2}\tau} - 1 \right)^2.$$

The first line clearly implies (28), while the second one, together with the fact that $\delta_0 = \delta_{N+1} = 0$, implies (27). ☐

We conclude this section by mentioning that, using the tools which we develop in Section 3.2.2, it is possible to study the above problem in the case when V is not convex, but when its graph is contained between two quadratic functions at infinity (see condition (93) below). In such a case, we are not able to prove convergence for system (6), but for system (10) that has a different normalization. We prove that the solution converges to that of (11). This will be formalized in Proposition 7. We postpone this study until Subsection 3.4 below.

3. **Next-to-nearest-neighbour interaction.** We consider in this section the case of a next-to-nearest-neighbour interaction, that is, equations (8) and (9).

3.1. **Linear convex case.** For now, we assume that (8) and (9) are linear, and that both potentials V_1 and V_2 are (quadratic and) convex, that is,

$$V_1(x) = \frac{c_1}{2}(x-1)^2, \quad V_2(x) = \frac{c_2}{2}(x-2)^2, \quad \text{with } c_1 > 0,\ c_2 > 0.$$

Hence, (8) becomes

$$\begin{cases} \dfrac{d^2 X_i}{dt^2} = c_1(X_{i+1} - 2X_i + X_{i-1}) + c_2(X_{i+2} - 2X_i + X_{i-2}), \\ X_i(0) = X_i^0, \quad \dfrac{dX_i}{dt}(0) = V_i^0, \end{cases} \tag{40}$$

and (9) reads

$$\begin{cases} \dfrac{\partial^2 \phi}{\partial \tau^2}(x,\tau) - (c_1 + 4c_2)\dfrac{\partial^2 \phi}{\partial x^2}(x,\tau) = 0, \\ \phi(x,0) = \phi^0(x), \quad \dfrac{\partial \phi}{\partial t}(x,0) = \phi^1(x), \\ \phi(0,\tau) = 0, \quad \phi(1,\tau) = 0. \end{cases} \tag{41}$$

This case is extremely simple and we easily have:

Proposition 3. *Assume $c_1 > 0$ and $c_2 > 0$. Let $N \in \mathbb{N}$, let $(\phi^0, \phi^1) \in \left[H^4(0,1)\right]^2$ be such that $\phi^0(0) = 0$ and $\phi^1(1) = 1$. Define, for all $1 \le i \le N$,*

$$X_i^0 = N\phi^0\left(\frac{i}{N}\right), \quad V_i^0 = \phi^1\left(\frac{i}{N}\right).$$

Let $X_i(t)$ be the unique solution to (40), with the convention $X_i = i$ for $i \in \{-1, 0, N+1, N+2\}$, and let $\phi \in L^\infty\left(\mathbb{R}^+, H^1(0,1)\right)$ be the unique solution of (41). Then, we have the convergences

$$\forall \tau > 0, \quad \sup_{1 \le i \le N} \left| \frac{1}{N} X_i(N\tau) - \phi\left(\frac{i}{N}, \tau\right) \right| \underset{N \to \infty}{\longrightarrow} 0,$$

and

$$\forall \tau \in (0,T), \quad \sup_{1 \le i \le N} \left| \frac{dX_i}{dt}(N\tau) - \frac{\partial \phi}{\partial \tau}\left(\frac{i}{N}, \tau\right) \right| \underset{N \to \infty}{\longrightarrow} 0.$$

Proof. The proof is performed exactly as that of Proposition 1. The only difference is that the centered finite difference

$$Y_{i+1} - 2Y_i + Y_{i-1},$$

is replaced by

$$c_1\left(Y_{i+1} - 2Y_i + Y_{i-1}\right) + c_2\left(Y_{i+2} - 2Y_i + Y_{i-2}\right),$$

where $Y_i = X_i$, or $Y_i = N\phi(i/N)$. The terms in c_1 and c_2 are manipulated separately and because both c_1 and c_2 are positive, the proof easily carries over to this case. □

3.2. **Linear non-convex case.** We investigate in this section the case of a harmonic interaction, that is, (40) and (41), but we drop the assumption ($c_1 > 0$ and $c_2 > 0$). In order for our limit problem (41) to be well posed, we need to assume

$$c_1 + 4c_2 > 0. \tag{42}$$

Hence, c_1 or c_2 may be non-positive, provided they satisfy the constraint (42).

Momentarily returning to our formal model with discrete derivatives (19) allows to immediately understand the interesting situation. Consider the equation

$$\frac{\partial^2 \Phi_\varepsilon}{\partial t^2} - c_1 D_\varepsilon^2 \Phi_\varepsilon - 4\, c_2\, D_{2\varepsilon}^2 \Phi_\varepsilon = 0, \tag{43}$$

which is obviously the formal analogue to (40). Elementary manipulations yields the energy estimate

$$\frac{d}{dt}\left(\left\| \frac{\partial}{\partial t} \Phi_\varepsilon \right\|^2 + c_1 \left\| D_\varepsilon \Phi_\varepsilon \right\|^2 + 4\, c_2 \left\| D_{2\varepsilon} \Phi_\varepsilon \right\|^2 \right) = 0.$$

When both c_1 and c_2 are nonnegative, we immediately observe (and this is of course in agreement with our proof in the previous section 3.1), that this imposes that Φ_ε vanishes in the limit. Let us now argue somewhat differently and use the elementary identity

$$4\, D_\varepsilon^2 \Phi = 4\, D_{2\varepsilon}^2 \Phi - \varepsilon^2\, D_\varepsilon^4 \Phi.$$

We may rewrite our equation (43) in the form

$$\frac{\partial^2 \Phi_\varepsilon}{\partial t^2} - (c_1 + 4c_2) D_\varepsilon^2 \Phi_\varepsilon + c_2 \varepsilon^2 D_\varepsilon^4 \Phi_\varepsilon = 0, \tag{44}$$

and obtain the energy estimate

$$\frac{d}{dt}\left(\left\| \frac{\partial}{\partial t} \Phi_\varepsilon \right\|^2 + (c_1 + 4c_2) \left\| D_\varepsilon \Phi_\varepsilon \right\|^2 - c_2 \varepsilon^2 \left\| D_\varepsilon^2 \Phi_\varepsilon \right\|^2 \right) = 0. \tag{45}$$

We readily observe that if $c_1 + 4c_2 > 0$ *and* $c_2 \leq 0$ we again "formally" obtain convergence. This can be easily formalized rigorously. The only interesting case is thus when $c_1 + 4c_2 > 0$ *and* $c_2 > 0$. This is the purpose of the rest of this section to investigate this case. The strategy of proof consists in cutting the Fourier expansion of the solution at some frequency k_ε, in order to eliminate the negative part of the spectrum of the operator $-(c_1 + 4c_2) D_\varepsilon + c_2 \varepsilon D_\varepsilon^4$. It is immediately seen on this operator that, formally, the value of k_ε should be of order $\sqrt{\frac{c_1+4c_2}{c_2}}\frac{1}{\varepsilon}$ (see (60) and (63) below). Of course, this cut-off asymptotically disappears as $\varepsilon \to 0$.

Remark 5. For interactions at a longer distance, such as NNNN interactions etc, similar conclusions may be obtained.

3.2.1. *A proof using spectral decomposition.* Before stating our result, we recall the definition of Fourier coefficients of a function defined on $(0, 1)$:

Definition 3.1. Let $\phi \in L^1(0, 1)$. Then we define its Fourier coefficient of order $k \in \mathbb{N}^* = \mathbb{N} \setminus \{0\}$, by

$$\widehat{\phi}(k) = \int_0^1 \phi(x) \sin(k\pi x)\, dx.$$

We now state.

Proposition 4. *Assume that* (42) *holds, and that* ϕ *is the solution to* (41)*, with* $\phi^0, \phi^1 \in C^4(0, 1)$*. Assume that the functions* ϕ^0 *and* ϕ^1 *satisfy*

$$\exists C > 0, \quad \exists \theta > 0, \quad s.t. \quad \forall k \in \mathbb{N}^*, \quad \left|\widehat{\phi^0}(k)\right| + \left|\widehat{\phi^1}(k)\right| \leq C e^{-\theta k}. \tag{46}$$

For any $N \in \mathbb{N}$*, define*

$$\forall 0 \leq i \leq N, \quad X_i^0 = N \phi^0\left(\frac{i}{N}\right), \quad V_i^0 = \phi^1\left(\frac{i}{N}\right), \tag{47}$$

and let X_i be the unique solution to (40). Then, we have the convergences

$$\forall \tau > 0, \qquad \sup_{1\leq i\leq N}\left|\frac{1}{N}X_i(N\tau) - \phi\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0, \tag{48}$$

and

$$\forall \tau > 0, \qquad \sup_{1\leq i\leq N}\left|\frac{dX_i}{dt}(N\tau) - \frac{\partial\phi}{\partial\tau}\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0. \tag{49}$$

Remark 6. The assumption (46) implies that the functions ϕ^0 and ϕ are analytic [10]. Indeed, a simple computation then proves that $\left|\frac{d^k\phi^0}{dx^k}(x)\right| \leq C\frac{k!}{\theta^k}$, which shows that the Taylor series of ϕ^0 at any point has a positive convergence radius.

Proof. We are first going to prove the convergence locally in time, that is, we claim that there exists $T^* > 0$ such that

$$\forall \tau \in [0,T^*], \qquad \sup_{1\leq i\leq N}\left|\frac{1}{N}X_i(N\tau) - \phi\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0, \tag{50}$$

and

$$\forall \tau \in [0,T^*], \qquad \sup_{1\leq i\leq N}\left|\frac{dX_i}{dt}(N\tau) - \frac{\partial\phi}{\partial\tau}\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0. \tag{51}$$

As in the preceding proofs, we use the difference

$$\delta_i^N(\tau) = \frac{1}{N}X_i(N\tau) - \phi\left(\frac{i}{N},\tau\right),$$

with the convention that $\delta_{N+1}^N = \delta_{-1}^N = 0$. Then, we have, for $1 \leq i \leq N-1$,

$$\begin{aligned}\frac{d^2\delta_i}{dt^2} &= N^2 c_1\left(\delta_{i+1}+\delta_{i-1}-2\delta_i\right) + N^2 c_2\left(\delta_{i+2}+\delta_{i-2}-2\delta_i\right)\\ &+ c_1\left[N^2\left(\phi\left(\frac{i+1}{N},\tau\right)+\phi\left(\frac{i-1}{N},\tau\right)-2\phi\left(\frac{i}{N},\tau\right)\right) - \frac{\partial^2\phi}{\partial x^2}\left(\frac{i}{N},\tau\right)\right]\\ &+ 4c_2\left[\frac{N^2}{4}\left(\phi\left(\frac{i+2}{N},\tau\right)+\phi\left(\frac{i-2}{N},\tau\right)-2\phi\left(\frac{i}{N},\tau\right)\right) - \frac{\partial^2\phi}{\partial x^2}\left(\frac{i}{N},\tau\right)\right].\end{aligned}$$

Hence, using a Taylor expansion here again, we have

$$\frac{d^2\delta_i}{d\tau^2} = N^2 c_1\left(\delta_{i+1}+\delta_{i-1}-2\delta_i\right) + N^2 c_2\left(\delta_{i+2}+\delta_{i-2}-2\delta_i\right) + \frac{1}{N^2}D_i^N(\tau), \tag{52}$$

where

$$\begin{aligned}D_i^N(\tau) \;=\; & c_1\left(N\int_{i/N}^{(i+1)/N}\frac{(Nx-i)^3}{6}\frac{\partial^4\phi}{\partial x^4}(x,\tau)dx\right.\\ &\left. +N\int_{i/N}^{(i-1)/N}\frac{(Nx-i)^3}{6}\frac{\partial^4\phi}{\partial x^4}(x,\tau)dx\right)\\ &+c_2\left(N\int_{i/N}^{(i+2)/N}\frac{(Nx-i)^3}{6}\frac{\partial^4\phi}{\partial x^4}(x,\tau)dx\right.\\ &\left. +N\int_{i/N}^{(i-2)/N}\frac{(Nx-i)^3}{6}\frac{\partial^4\phi}{\partial x^4}(x,\tau)dx\right).\end{aligned}$$

In particular,

$$\left|D_i^N\right| \leq C\left\|\phi\right\|_{C^0[(0,T),C^4(0,1)]}, \tag{53}$$

for some constant C independent on N and ϕ. Equation (52) may be rewritten in vector form as

$$\begin{aligned} \frac{d^2\delta}{d\tau^2} &= -c_1 N^2 A\delta - c_2 N^2 (4A - A^2)\delta + c_2 N^2 KY + \frac{1}{N^2} D^N, \\ &= -(c_1 + 4c_2) N^2 A\delta + N^2 c_2 A^2 \delta + \frac{1}{N^2} D^N, \end{aligned} \tag{54}$$

where $A \in \mathbb{R}^{(N+1)\times(N+1)}$ is the discretization of the Laplacian by finite differences:

$$A = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{pmatrix}, \quad \text{and} \quad K = \begin{pmatrix} 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & \cdots & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & 0 & 0 \\ 0 & \cdots & \cdots & 0 & 1 \end{pmatrix}.$$

Here, we have used the fact that $K\delta = 0$ due to boundary conditions. We are now going to take advantage of the fact that we know explicitly the eigenvalues and eigenvectors of A, namely,

$$\lambda_k = 4\sin^2\left(\frac{k\pi}{2(N+2)}\right), \tag{55}$$

$$(u_k)_i = \sin\left(\frac{ik\pi}{N+2}\right), \tag{56}$$

for all $1 \leq k \leq N+1$ and $1 \leq i \leq N+1$. Hence, the matrix $-(c_1+4c_2)N^2 A + N^2 c_2 A^2$ appearing in the right-hand side of (54) has N eigenvalues $N^2\mu_k$, with μ_k given by

$$\mu_k = (c_1 + 4c_2)\lambda_k - c_2\lambda_k^2, \tag{57}$$

with the corresponding eigenvectors given by (56). Note that (42) holds, so that:

- if $c_2 \leq 0$, then all μ_k are positive, hence, applying the same strategy as in the proof of Proposition 1, one easily gets

$$\frac{d}{d\tau}\left[\left\|\frac{d\delta}{d\tau}\right\|^2 + (c_1 + 4c_2)(A\delta, \delta) - c_2\left(A^2\delta, \delta\right)\right] = \frac{2}{N^2}\sum_{i=1}^{N-1} D_i^N \frac{d\delta_i}{d\tau},$$

  where $(\cdot,\cdot)$ denotes the canonical scalar product of $\mathbb{R}^N$, and $\|\cdot\|$ the corresponding norm. Hence, using the same arguments as in the proof of Proposition 1, one easily concludes.
- If $c_2 > 0$ and $c_1 \geq 0$, then $\mu_k = c_1\lambda_k + c_2\lambda_k(4 - \lambda_k) \geq c_1\lambda_k > 0$, hence the above strategy applies.
- If $c_2 > 0$ and $c_1 < 0$, then some μ_k are negative and the above strategy does not apply. We therefore concentrate on this case for the rest of the proof.

Note that the first two observations are consistent with our formal considerations before the beginning of the present Subsection 3.2.1.

Setting

$$\alpha_k = (\delta, u_k), \quad \beta_k = \left(D^N, u_k\right), \tag{58}$$

we have

$$\begin{cases} \frac{d^2\alpha_k}{d\tau^2} + N^2\mu_k\alpha_k = \frac{1}{N^2}\beta_k, \\ \alpha_k(0) = \dfrac{d\alpha_k}{d\tau}(0) = 0. \end{cases}$$

This set of equations may be explicitly solved: if $\mu_k > 0$, then

$$\alpha_k(\tau) = -\frac{1}{N\sqrt{\mu_k}} \cos\left(N\sqrt{\mu_k}\tau\right) \int_0^\tau \frac{1}{N^2}\beta_k(s) \sin\left(N\sqrt{\mu_k}s\right) ds + \frac{1}{N\sqrt{\mu_k}} \sin\left(N\sqrt{\mu_k}\tau\right) \int_0^\tau \frac{1}{N^2}\beta_k(s) \cos\left(N\sqrt{\mu_k}s\right) ds,$$

whereas if $\mu_k \leq 0$, then

$$\alpha_k(\tau) = -\frac{1}{N\sqrt{|\mu_k|}} \cosh\left(N\sqrt{|\mu_k|}\tau\right) \int_0^\tau \frac{1}{N^2}\beta_k(s) \sinh\left(N\sqrt{|\mu_k|}s\right) ds + \frac{1}{N\sqrt{|\mu_k|}} \sinh\left(N\sqrt{|\mu_k|}\tau\right) \int_0^\tau \frac{1}{N^2}\beta_k(s) \cosh\left(N\sqrt{|\mu_k|}s\right) ds.$$

Here, we use the convention that, if $\mu_k = 0$, then we replace $\sinh(N\sqrt{|\mu_k|}s)/N\sqrt{|\mu_k|}$ by its limit s as $\mu_k \to 0$. Hence, we have the following estimates:

$$|\alpha_k(\tau)| \leq \begin{cases} \dfrac{1}{N^2}\displaystyle\int_0^\tau |\beta_k(s)|ds & \text{if } \mu_k > 0, \\ \dfrac{1+\tau}{N^2} \cosh^2\left(N\sqrt{|\mu_k|}\tau\right) \displaystyle\int_0^\tau |\beta_k(s)|ds & \text{if } \mu_k \leq 0. \end{cases} \tag{59}$$

Note that $\mu_k \leq 0$ is equivalent to $\lambda_k > (c_1 + 4c_2)/c_2$, which, according to (55), may happen only if

$$k \geq \frac{2}{\pi}\sqrt{\frac{c_1+4c_2}{c_2}}(N+1) := C_0(N+1). \tag{60}$$

We have, using (59),

$$\begin{aligned} \|\delta(\tau)\|^2 &= \sum_{k=1}^N |\alpha_k(\tau)|^2 \\ &\leq \sum_{\mu_k>0} \left(\frac{1}{N^2}\int_0^\tau |\beta_k(s)|ds\right)^2 \\ &\quad + \sum_{\mu_k\leq 0} \left(\frac{1+\tau}{N^2}\cosh^2\left(N\sqrt{|\mu_k|}\tau\right)\int_0^\tau |\beta_k(s)|ds\right)^2 \end{aligned} \tag{61}$$

Then, we point out that Lemma A.2 allows to apply Lemma A.1 to ϕ. Hence,

$$\exists C > 0, \quad \forall s > 0, \quad |\beta_k(s)| \leq C\sqrt{N}k^4 e^{-\theta k}. \tag{62}$$

We collect (53), (58) and (62), and insert them in (61), getting

$$\begin{aligned} \|\delta(\tau)\|^2 &\leq \sum_{\mu_k>0} \frac{\tau^2}{N^4} CN\|\phi\|^2_{C^0[(0,T),C^4(0,1)]} + \sum_{\mu_k\leq 0} C\frac{(1+\tau^2)^2}{N^3}k^8 e^{4N\sqrt{|\mu_k|}\tau - 2\theta k} \\ &\leq C\frac{\tau^2}{N^2}\|\phi\|^2_{C^0[(0,T),C^4(0,1)]} + C\frac{(1+\tau^2)^2}{N^3}\sum_{\mu_k\leq 0} k^8 e^{8N\tau - 2\theta C_0 N} \\ &\leq C\frac{\tau^2}{N^2}\|\phi\|^2_{C^0[(0,T),C^4(0,1)]} + C(1+\tau^2)^2 N^5 \; e^{(4\tau - \theta C_0)2N}, \end{aligned}$$

where the constant C does not depend on N nor on ϕ. Hence, if

$$T^* \leq \frac{\theta C_0}{4} = \frac{\theta}{2\pi}\sqrt{\frac{c_1+4c_2}{c_2}}, \tag{63}$$

this concludes the proof of (50). Then, returning to (59), we see that it implies in fact

$$\forall k \text{ s.t. } 0 \leq k \leq N, \quad |\alpha_k| \leq \begin{cases} C\frac{\tau^2}{N^2}\|\phi\|^2_{C^0[(0,T),C^4(0,1)]} & \text{if } \mu_k > 0, \\ C(1+\tau^2)^2 e^{(4\tau-\theta C_0)N} & \text{if } \mu_k \leq 0. \end{cases}$$

Hence, using the same strategy of energy estimate as in the proof of Proposition 1, one easily proves that

$$\frac{d}{d\tau}\left[\left\|\frac{\partial\delta}{\partial\tau}\right\|^2 + N^2\left((c_1+4c_2)A\delta - c_2A^2\delta,\delta\right)\right] = \frac{1}{N^2}\left(D^N, \frac{\partial\delta}{\partial\tau}\right).$$

Integrating this equation with respect to τ and using the above estimates, together with

$$(c_1+4c_2)A\delta - c_2A^2\delta = \sum_{k=1}^N |\alpha_k|^2\mu_k u_k,$$

shows (51).

We point out that the time T^* depends only on c_1, c_2 and θ, which is the decay rate of the Fourier coefficients of ϕ. Now, in view of Lemma A.2, these quantities are left unchanged by the dynamics. Therefore, we can repeat the above argument, proving (48) and (49). □

Remark 7. The above proof heavily relies on the fact that we have an explicit expression of the eigenvectors of the matrix A. Therefore, such a strategy does not apply to the case where c_1 and c_2 depend on the space variable.

We conclude this section with a remark about the fast decay of the Fourier coefficients. It is necessary in the following sense: it is possible to build initial data for which the convergence of Proposition 4 fails. This is proved in the following lemma:

Lemma 3.2. *Assume that $c_1 = -2$ and $c_2 = 1$, so that $c_1 + 4c_2 > 0$. There exist $\phi^0 \in C^4(0,1)$ and $\phi^1 \in C^4(0,1)$ such that, if $(X_i)_{1\leq i\leq N}$ is the solution to (40), with $\left(X_i^0\right)_{1\leq i\leq N}$ and $\left(V_i^0\right)_{1\leq i\leq N}$ defined by (47), then the convergences (48) and (49) do not hold.*

The proof of this lemma is postponed to Appendix C. Let us however give here the main ideas of this proof. The values chosen for c_1 and c_2 imply that

$$\forall k \geq \frac{N}{2}, \quad \mu_k \leq -\frac{1}{2},$$

where μ_k is defined by (57). Hence, if one defines, as an initial data,

$$\phi^0(x) = \sum_{k\geq 1}\frac{1}{k^6}\sin(k\pi x), \quad \text{and} \quad \phi^1 = 0,$$

then X^0 defined by (47) is equal to

$$X^0 = \sum_{k\geq 1}\frac{1}{k^6}v_k,$$

where v_k is defined by

$$v_k^i = \sin\left(\frac{ik\pi}{N}\right),$$

and is an eigenvector of the operator associated with the eigenvalue μ_k. Hence, the solution X to (40) is explicitly given by:

$$X = \sum_{k\geq 1} \alpha_k(\tau) v_k, \quad \text{where} \quad \alpha_k(\tau) = \begin{cases} \dfrac{1}{k^4}\cos(\sqrt{\mu_k}\tau) & \text{if } \mu_k > 0, \\ \dfrac{1}{k^4}\cosh(\sqrt{-\mu_k}\tau) & \text{if } \mu_k < 0. \end{cases}$$

If the sequence $(v_k)_{k\in\mathbb{N}}$ was an orthonormal basis, the norm of X would easily shown to be equal to

$$\left\|\frac{1}{N}X(N\tau)\right\|^2 = \frac{1}{N^2}\sum_{k\geq 1}|\alpha_k|^2 \geq \frac{1}{N^2}\sum_{k\geq N/2}\frac{1}{k^{12}}\cosh(\sqrt{-\mu_k}t)^2 \geq C\frac{\cosh^2\left(N\tau/\sqrt{2}\right)}{N^{14}}.$$

This contradicts the convergence of X to ϕ for all time $t > 0$, in the sense of Proposition 1. The above argument has a flaw because $(v_k)_{k\in\mathbb{N}}$ is not an orthonormal basis of $\mathbb{R}^N$, and this is why the proof is much more involved (see Appendix C).

3.2.2. *A proof using weak convergence.* In the present section, we study the case of (40) and (41), aiming at proving a result similar to Proposition 4. However, here, we are not going to use any hypothesis of the form (46), nor (and this is much more important methodologically) any explicit spectral decomposition of the discrete operator.

In the following, we identify any vector $X \in \mathbb{R}^N$ with the piecewise constant function on each interval $\left[\frac{i-\frac{1}{2}}{N}, \frac{i+\frac{1}{2}}{N}\right]$, namely

$$f_X(x) = X_i, \quad \forall x \in \left[\frac{i-\frac{1}{2}}{N}, \frac{i+\frac{1}{2}}{N}\right].$$

Therefore, we identify any L^p norm and convergence of X with the corresponding norm and convergence of f_X. For instance,

$$\|X\|_{L^p(0,1)} := \|f_X\|_{L^p(0,1)} = \left(\frac{1}{N}\sum_{i=0}^{N}|X_i|^p\right)^{1/p}, \tag{64}$$

and for the L^2 scalar product,

$$(X, Y) = \frac{1}{N}\sum_{i=0}^{N} X_i Y_i.$$

In addition, we say that X weakly converges in L^p to f if f_X weakly converges to f in L^p:

$$X \underset{N\to\infty}{\rightharpoonup} f \text{ in } L^p \quad \Longleftrightarrow \quad f_X \underset{N\to\infty}{\rightharpoonup} f \text{ in } L^p. \tag{65}$$

It is clear from these definitions that if X is bounded in L^p, then, up to extracting a subsequence, it converges weakly in L^p, if $1 < p < \infty$.

We define the discrete gradient ∇_N by

$$\forall X \in \mathbb{R}^N, \quad (\nabla_N X)_i = N\left(X_{i+1} - X_i\right), \tag{66}$$

where we implicitly assume that if $i \leq 0$ or $i \geq N+1$, then $X_i = 0$. This will be the case for all the vectors we use in the sequel.

We are now in position to state the main result of this section:

Proposition 5. *Assume that* (42) *holds, and that* ϕ *is the solution to* (41), *with* $\phi^0, \phi^1 \in H^1(0,1)$. *Consider the initial conditions* $N\phi^0\left(\frac{i}{N}\right)$ *and* $\phi^1\left(\frac{i}{N}\right)$ *for* (40). *There exists a filtered initial condition (made precise in* (72)-(73) *and* (74)-(75) *below)* X_i^0, V_i^0 *such that*

$$\sup_{1\le i\le N}\left|\frac{1}{N}X_i^0-\phi^0\left(\frac{i}{N}\right)\right|+\left|V_i^0-\phi^1\left(\frac{i}{N}\right)\right|\underset{N\to\infty}{\longrightarrow}0, \tag{67}$$

and, denoting by X_i *the unique solution to* (40) *with initial condition* X_i^0, V_i^0,

$$\forall\tau>0,\qquad \sup_{1\le i\le N}\left|\frac{1}{N}X_i(N\tau)-\phi\left(\frac{i}{N},\tau\right)\right|\underset{N\to\infty}{\longrightarrow}0, \tag{68}$$

and

$$\forall\tau>0,\qquad \sup_{1\le i\le N}\left|\frac{dX_i}{dt}(N\tau)-\frac{\partial\phi}{\partial\tau}\left(\frac{i}{N},\tau\right)\right|\underset{N\to\infty}{\longrightarrow}0. \tag{69}$$

Before we get to the detailed proof of Proposition 5, let us give the bottom line argument. For this purpose, we again use our formal model and discrete differentiation like in (43) or, equivalently and more appropriately for the argument that follows, (44), which we reproduce here for convenience:

$$\frac{\partial^2\Phi_\varepsilon}{\partial t^2}-(c_1+4c_2)D_\varepsilon^2\Phi_\varepsilon+c_2\varepsilon^2D_\varepsilon^4\Phi_\varepsilon=0.$$

We have already mentioned the corresponding formal energy estimate (45):

$$\frac{d}{dt}\left(\left\|\frac{\partial}{\partial t}\Phi_\varepsilon\right\|^2+(c_1+4c_2)\left\|D_\varepsilon\Phi_\varepsilon\right\|^2-c_2\varepsilon^2\left\|D_\varepsilon^2\Phi_\varepsilon\right\|^2\right)=0.$$

The only interesting case, we recall, is the case when $c_1+4c_2>0$ and $c_2>0$. In that case, the above energy estimate does not immediately allow to conclude, since the right-most term is non-positive. The idea is then to further differentiate k times (44) and obtain a similar energy estimate

$$\frac{d}{dt}\left(\left\|D_\varepsilon^k\frac{\partial}{\partial t}\Phi_\varepsilon\right\|^2+(c_1+4c_2)\left\|D_\varepsilon^{k+1}\Phi_\varepsilon\right\|^2-c_2\varepsilon^2\left\|D_\varepsilon^{k+2}\Phi_\varepsilon\right\|^2\right)=0.$$

for each differentiation order k. In order to "eliminate" the non-positive contribution of the last term, we now weight and combine all these estimates so as to obtain

$$\frac{d}{dt}\sum_{k=1}^{+\infty}\delta^{2k}\left(\left\|D_\varepsilon^k\frac{\partial}{\partial t}\Phi_\varepsilon\right\|^2+(c_1+4c_2)\left\|D_\varepsilon^{k+1}\Phi_\varepsilon\right\|^2-c_2\varepsilon^2\left\|D_\varepsilon^{k+2}\Phi_\varepsilon\right\|^2\right)=0.$$

for some parameter δ. This parameter is next adjusted, in function of ε, so as to cancel the series of the two right-most terms by making it a telescopic series. We therefore conclude that some norm of the form

$$\sum_{k=1}^{+\infty}\delta^{2k}\left\|D_\varepsilon^{k+1}\Phi_\varepsilon\right\|^2$$

remains bounded over time. Up to an extraction, we may assume Φ_ε is weakly convergent, and it remains to deduce that the convergence is strong. This will be a consequence of the preservation of the energy by the equation, together with the fact that strong convergence holds at initial time.

The precise value of δ which allows us to carry out the above strategy is given in (84) below. This may be seen as an equivalent to the cut-off in Fourier series at the frequency $N\sqrt{\frac{c_2}{c_1+4c_2}} = \sqrt{\frac{c_2}{c_1+4c_2}}\frac{1}{\varepsilon}$ mentioned in Section 3.2.1.

We may now begin formalizing the above outlined argument.

Proof. First step: choice of the initial condition. In order to choose the initial conditions X^0 and V^0, we first decompose ϕ^0 and ϕ^1 in Fourier series, writing

$$\phi^0(x) = \sum_{p\geq 1} 2\widehat{\phi^0}(p)\sin(\pi p x), \tag{70}$$

$$\phi^1(x) = \sum_{p\geq 1} 2\widehat{\phi^1}(p)\sin(\pi p x), \tag{71}$$

where for any $\psi \in L^1(0,1)$, $\widehat{\psi}$ is given by Definition 3.1.

Then, we define the initial data for the discrete system as the truncation of the Fourier series (70) and (71), that is, we fix $a > 0$ independent of N, which will be made precise later on, and set

$$\frac{1}{N}X_i^0 = \tilde{\phi}_N^0\left(\frac{i}{N}\right), \tag{72}$$

where

$$\tilde{\phi}_N^0(x) = \sum_{1\leq p\leq Na} 2\widehat{\phi^0}(p)\sin(\pi p x), \tag{73}$$

and

$$V_i^0 = \tilde{\phi}_N^1\left(\frac{i}{N}\right), \tag{74}$$

where

$$\tilde{\phi}_N^1(x) = \sum_{1\leq p\leq Na} 2\widehat{\phi^1}(p)\sin(\pi p x). \tag{75}$$

We note that

$$\phi^0(x) - \tilde{\phi}_N^0(x) = \sum_{p\geq Na} 2\widehat{\phi^0}(p)\sin(\pi p x). \tag{76}$$

Since ϕ^0 is in $H_0^1(0,1)$, when symmetrized around the origin and repeated periodically with period 2, it is in $H^1_{\mathrm{loc}}(\mathbb{R})$. Hence, its Fourier coefficients satisfy

$$\sum_{p\geq 0} |p|^2 \left|\widehat{\phi^0}(p)\right|^2 < \infty.$$

Thus, applying Cauchy-Schwarz inequality to (76), we find

$$\left|\phi^0(x) - \tilde{\phi}_N^0(x)\right| \leq \left(\sum_{p\geq Na}\frac{4}{|p|^2}\right)^{1/2}\left(\sum_{p\geq Na}|p|^2\left|\widehat{\phi^0}(p)\right|^2\right)^{1/2} \leq \frac{C}{\sqrt{Na}}.$$

Similarly, one easily shows

$$\left|\phi^1(x) - \tilde{\phi}_N^1(x)\right| \leq \frac{C}{\sqrt{Na}},$$

which proves that (67) holds. In addition, still with the same type of argument, we have

$$\left|\frac{\partial\phi^0}{\partial x} - \frac{\partial\tilde{\phi}^0}{\partial x}\right| \leq \frac{C}{\sqrt{Na}}. \tag{77}$$

Second step: weak convergence.
We define

$$Y_i(\tau) = \frac{1}{N} X_i(N\tau).$$

Using (66), equation (40) reads

$$\frac{d^2 Y_i}{d\tau^2} = N^2 c_1 \left(Y_{i+1} - 2Y_i + Y_{i-1}\right) + N^2 c_2 \left(Y_{i+2} - 2Y_i + Y_{i-2}\right).$$

Defining A as the matrix of the discrete Laplacian with homogeneous boundary conditions, we point out that this also reads

$$\frac{d^2 Y}{d\tau^2} = (c_1 + 4c_2) N^2 AY - \frac{c_2}{N^2} \left(N^2 A\right)^2 Y - c_2 N^2 KY, \tag{78}$$

where

$$A = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{pmatrix}, \quad \text{and} \quad K = \begin{pmatrix} 1 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & \cdots & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & \cdots & 0 & 0 \\ 0 & \cdots & \cdots & 0 & 1 \end{pmatrix}.$$

Since that $Y_0 = Y_N = 0$, the last term of (78) vanishes:

$$\frac{d^2 Y}{d\tau^2} = (c_1 + 4c_2) N^2 AY - \frac{c_2}{N^2} \left(N^2 A\right)^2 Y.$$

Next, we note that, since this equation is linear with constant coefficients, we can apply the operator $N^2 A$, finding

$$\forall k \geq 0, \quad \frac{d^2}{d\tau^2} \left[(N^2A)^k Y\right] = -(c_1 + 4c_2) N^2 A \left[(N^2A)^k Y\right] + \frac{c_2}{N^2} (N^2 A)^2 \left[(N^2A)^k Y\right]. \tag{79}$$

We next define the following norm for Y:

$$\forall Y \in \mathbb{R}^N, \quad \mathcal{N}_N(Y) = \left(\sum_{k\geq 0} \left(\frac{\delta}{N}\right)^{2k} \left\| \left(N^2 A\right)^{(k+1)/2} Y \right\|_{L^2}^2 \right)^{1/2}, \tag{80}$$

where $\delta > 0$ is some fixed constant which will be chosen later on (see (83) and (84) below). The scalar product of (79) with $\frac{dY}{d\tau}$ gives

$$\begin{aligned} \frac{1}{2}\frac{d}{d\tau} \left\| (N^2A)^{k/2} \frac{dY}{d\tau} \right\|^2 &= -(c_1 + 4c_2) \left((N^2A)^{k+1} Y, \frac{dY}{d\tau} \right) \\ &\quad + \frac{c_2}{N^2} \left((N^2A)^{k+2} Y, \frac{dY}{d\tau} \right) \\ &= -\frac{c_1 + 4c_2}{2} \frac{d}{d\tau} \left\| (N^2A)^{(k+1)/2} Y \right\|^2 \\ &\quad + \frac{c_2}{2N^2} \frac{d}{d\tau} \left\| (N^2A)^{(k+2)/2} Y \right\|^2. \end{aligned}$$

Hence, setting

$$\gamma_k = \left\| \left(N^2 A\right)^{k/2} Y \right\|_{L^2}^2,$$

we have

$$\left\|(N^2A)^{k/2}\frac{dY}{d\tau}\right\|^2+(c_1+4c_2)\gamma_{k+1}(t)-\frac{c_2}{N^2}\gamma_{k+2}(t)$$
$$=\left\|(N^2A)^{k/2}V^0\right\|^2+(c_1+4c_2)\gamma_{k+1}(0)-\frac{c_2}{N^2}\gamma_{k+2}(0). \quad (81)$$

Then, we use the definition (72) and (74) of X^0 and V^0, which allow to write

$$\gamma_k(0)\leq C\sum_{1\leq p\leq Na}|p|^{2k}\left|\widehat{\phi^0}(p)\right|^2,$$

and

$$\left\|(N^2A)^{k/2}V^0\right\|^2\leq C\sum_{1\leq p\leq Na}|p|^{2k}\left|\widehat{\phi^1}(p)\right|^2,$$

for some constant C independent of N. Summing this with respect to k, we thus have (recall that $\mathcal{N}_N$ is defined by (80))

$$\begin{aligned}\mathcal{N}_N(X^0)+\mathcal{N}_N(V^0) &\leq C\sum_{1\leq p\leq Na}\frac{1}{1-\frac{|p|^2\delta^2}{N^2}}\left(\left|\widehat{\phi^0}(p)\right|^2+\left|\widehat{\phi^1}(p)\right|^2\right)\\ &\leq \frac{C}{1-a^2\delta^2}\sum_{1\leq p\leq Na}\left|\widehat{\phi^0}(p)\right|^2+\left|\widehat{\phi^1}(p)\right|^2, \quad (82)\end{aligned}$$

if

$$a\delta<1. \quad (83)$$

We next sum (81) over k and insert (82) into the result:

$$\begin{aligned}\mathcal{N}_N(X)^2 &= \sum_{k\geq 0}\left(\frac{\delta}{N}\right)^{2k}\gamma_{k+1}\\ &\leq \frac{c_2}{c_1+4c_2}\sum_{k\geq 0}\frac{1}{N^2}\left(\frac{\delta}{N}\right)^{2k}\gamma_{k+2}+\mathcal{N}_N(X^0)^2+\frac{1}{(c_1+4c_2)N^2}\mathcal{N}_N(V^0)^2\\ &\leq \frac{1}{\delta^2}\frac{c_2}{c_1+4c_2}\sum_{k\geq 1}\left(\frac{\delta}{N}\right)^{2k}\gamma_{k+1}+\frac{C}{1-a^2\delta^2}\\ &\leq \frac{1}{\delta^2}\frac{c_2}{c_1+4c_2}\mathcal{N}_N(X)^2+\frac{C}{1-a^2\delta^2}.\end{aligned}$$

Hence, assuming that

$$\delta>\sqrt{\frac{c_2}{c_1+4c_2}}, \quad (84)$$

we find that

$$\mathcal{N}_N(X)\leq C,$$

for some constant C independent of N.

We then point out that $\mathcal{N}_N(X)\geq\left\|A^{1/2}Y\right\|_{L^2}=\|\nabla_N Y\|_{L^2}$. Using a discrete Poincaré inequality [3, 8], we also have

$$\frac{1}{N}\sum_{i=0}^{N}Y_i^2\leq\frac{C}{N}\sum_{i=0}^{N-1}N^2\left(Y_{i+1}-Y_i\right)^2\leq C\mathcal{N}_N(Y)^2,$$

where C does not depend on N. Applying Lemma B.1, we thus have strong convergence in L^2, up to extracting a subsequence:

$$Y \longrightarrow \eta \text{ in } L^2, \tag{85}$$

for some $\eta \in L^2(0,1)$, where the L^2 norm is defined by (64). Moreover, since $\nabla_N Y$ is also bounded in L^2, it converges weakly in L^2, up to extracting a subsequence:

$$\nabla_N Y \rightharpoonup \zeta \text{ in } L^2, \tag{86}$$

in the sense of (65). Finally, using (85) and (86), one easily proves that $\zeta = \partial_x \eta$. Using again these convergences, and the fact that X satisfies (40) a simple computation proves that $\eta = \phi$, the solution to (41). Hence:

$$Y \longrightarrow \phi \text{ in } L^2, \quad \text{and} \quad \nabla_N Y \rightharpoonup \partial_x \phi \text{ in } L^2. \tag{87}$$

The uniqueness of ϕ implies that this convergence holds for the whole sequence, and not only for a subsequence.
Third step: convergence of the energy.
We use the energy conservation for (40), namely, (81) with $k = 0$:

$$\left\| \frac{dY}{d\tau} \right\|^2 + (c_1 + 4c_2) \left\| N A^{1/2} Y \right\|^2 - \frac{c_2}{N^2} \left\| N^2 A Y \right\|^2 \\ = \left\| V^0 \right\|^2 + (c_1 + 4c_2) \left\| N A^{1/2} Y^0 \right\|^2 - \frac{c_2}{N^2} \left\| N^2 A Y^0 \right\|^2 \tag{88}$$

Similarly, the solution ϕ of (41) satisfies

$$\int_0^1 \left[\left(\frac{\partial \phi}{\partial \tau} \right)^2 + (c_1 + 4c_2) \left(\frac{\partial \phi}{\partial x} \right)^2 \right] dx = \int_0^1 \left[\left(\frac{\partial \phi^0}{\partial \tau} \right)^2 + (c_1 + 4c_2) \left(\frac{\partial \phi^0}{\partial x} \right)^2 \right] dx. \tag{89}$$

Since, according to (67) and (77), the right-hand side of (88) converges to the right-hand side of (89), we thus have

$$\forall \tau \geq 0, \quad \left\| \frac{dY}{d\tau} \right\|^2 + (c_1 + 4c_2) \left\| N A^{1/2} Y \right\|^2 - \frac{c_2}{N^2} \left\| N^2 A Y \right\|^2 \\ \underset{N \to \infty}{\longrightarrow} \int_0^1 \left[\left(\frac{\partial \phi}{\partial \tau} \right)^2 + (c_1 + 4c_2) \left(\frac{\partial \phi}{\partial x} \right)^2 \right] dx. \tag{90}$$

We need to prove that the last term of the left-hand side of (90) converges to zero. In order to do so, we return to (81), and sum over $k \geq 1$. Repeating the same argument as above, one easily proves that

$$\begin{aligned} \sum_{k \geq 1} \left(\frac{\delta}{N} \right)^{2k} \gamma_{k+1} &\leq \frac{1}{\delta^2} \frac{c_2}{c_1 + 4c_2} \sum_{k \geq 1} \left(\frac{\delta}{N} \right)^{2k} \gamma_{k+1} \\ &\quad + C \sum_{1 \leq p \leq Na} \sum_{k \geq 1} \left(\frac{|p|\delta}{N} \right)^{2k} \left(\left| \widehat{\phi^0}(p) \right|^2 + \left| \widehat{\phi^1}(p) \right|^2 \right) \\ &\leq \frac{1}{\delta^2} \frac{c_2}{c_1 + 4c_2} \sum_{k \geq 1} \left(\frac{\delta}{N} \right)^{2k} \gamma_{k+1} \\ &\quad + \frac{C}{1 - a^2 \delta^2} \frac{\delta^2}{N^2} \sum_{p \geq 1} |p|^2 \left(\left| \widehat{\phi^0}(p) \right|^2 + \left| \widehat{\phi^1}(p) \right|^2 \right), \end{aligned}$$

from which we deduce, with the same hypotheses as above, that

$$\frac{\delta^2}{N^2}\gamma_2 \leq \sum_{k\geq 1}\left(\frac{\delta}{N}\right)^{2k}\gamma_{k+1} \leq \frac{C}{N^2},$$

for some constant C depending only on a, δ, ϕ^0 and ϕ^1. Inserting this inequality into (90), we thus have, $\forall \tau \geq 0$

$$\left\|\frac{dY}{d\tau}\right\|^2 + (c_1+4c_2)\left\|NA^{1/2}Y\right\|^2 \underset{N\to\infty}{\longrightarrow} \int_0^1 \left[\left(\frac{\partial\phi}{\partial\tau}\right)^2 + (c_1+4c_2)\left(\frac{\partial\phi}{\partial x}\right)^2\right]dx. \quad (91)$$

Fourth step: strong convergence.
The weak convergences of $NA^{1/2}Y$ and $\frac{dY}{d\tau}$ imply that

$$\liminf_{N\to\infty}\left\|\frac{dY}{d\tau}\right\|^2 \geq \int_0^1\left(\frac{\partial\phi}{\partial\tau}\right)^2 dx,$$

and that

$$\liminf_{N\to\infty}\left\|NA^{1/2}Y\right\|^2 \geq \int_0^1\left(\frac{\partial\phi}{\partial x}\right)^2 dx.$$

This, together with (91), implies the convergences

$$\left\|\frac{dY}{d\tau}\right\|^2 \underset{N\to\infty}{\longrightarrow} \int_0^1\left(\frac{\partial\phi}{\partial\tau}\right)^2 dx, \quad \left\|NA^{1/2}Y\right\|^2 \underset{N\to\infty}{\longrightarrow} \int_0^1\left(\frac{\partial\phi}{\partial x}\right)^2 dx.$$

Since $\|NA^{1/2}Y\| = \|\nabla_N Y\|$, this in turn implies strong convergence of $\nabla_N Y$. In order to prove (68), we now write (recall $Y_0 = 0$):

$$\begin{aligned}
\left|Y_i - \phi\left(\frac{i}{N}\right)\right| &= \left|\frac{1}{N}\sum_{j=0}^{i-1} N\left(Y_{j+1}-Y_j\right) - \int_0^{i/N}\frac{\partial\phi}{\partial x}dx\right| \\
&\leq \sum_{j=0}^{i-1}\int_{j/N}^{(j+1)/N}\left|N\left(Y_{j+1}-Y_j\right) - \frac{\partial\phi}{\partial x}\right|dx \\
&\leq \left(\sum_{j=0}^{i-1}\frac{1}{N}\right)^{1/2}\left(\sum_{j=0}^{i-1}\int_{j/N}^{(j+1)/N}\left(N\left(Y_{j+1}-Y_j\right)-\frac{\partial\phi}{\partial x}\right)^2 dx\right)^{1/2} \\
&\leq \left\|\nabla_N Y - \frac{\partial\phi}{\partial x}\right\| \underset{N\to\infty}{\longrightarrow} 0.
\end{aligned}$$

Finally, it is easy to reproduce the above proof for $\frac{dY}{d\tau}$ instead of Y, thereby proving (69). □

Remark 8. The above proof readily applies to any finite range interaction. Indeed, if one allows for interaction to p neighbours, then the corresponding term in the equation may be rewritten as a polynomial of the discrete Laplacian, with the corresponding power of N in factor of each term. Hence, an adapted norm of the same type as $\mathcal{N}_N$ may be employed to obtain weak convergence, and next strong convergence using convergence of the energy.

Remark 9. In the proof of Proposition 5, we have applied a filter to the initial data (see equations (72) and (74)). As pointed out at the end of Section 3.2.1, without this filtering strategy, the result does not hold.

Remark 10. The proof of Proposition 5 is easily adapted to the case of coefficients c_1 and c_2 depending on i, as far as they are bounded and satisfy $c_1^i + 4c_2^i \geq \alpha$ for $\alpha > 0$ independent of i. In such a case, one needs to also use a filtering strategy for the coefficients c_p^i, as it was performed above for the initial data.

For the remainder of this article, we turn to nonlinear problems. As mentioned in the introduction, the only case where we are able to prove convergence without an additional linearization is the case when all potentials are convex. It is studied in our next subsection. In Subsection 3.4, we will have to consider a different regime.

3.3. **Nonlinear convex case.** Using the same strategy as in Section 2.2, we are able to prove the following result:

Proposition 6. *Assume that $V_1, V_2 \in C^4$ and that $V_1'', V_2'' \geq \alpha > 0$ for some constant α. Let $\phi \in C^0\left([0,T), C^4([0,1])\right)$ be a solution to (9). Let $N \in \mathbb{N}$, and define, for all $1 \leq i \leq N$,*

$$X_i^0 = N\phi^0\left(\frac{i}{N}\right), \quad V_i^0 = \phi^1\left(\frac{i}{N}\right).$$

Let $X_i(t)$ be the unique solution to (8), with the convention $X_0 = 0,\ X_{N+1} = 0$. Then, we have the convergences

$$\forall \tau \in (0,T), \qquad \sup_{1\leq i\leq N}\left|\frac{1}{N}X_i(N\tau) - \phi\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0,$$

and

$$\forall \tau \in (0,T), \qquad \sup_{1\leq i\leq N}\left|\frac{dX_i}{dt}(N\tau) - \frac{\partial\phi}{\partial\tau}\left(\frac{i}{N},\tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0.$$

Proof. This is an easy adaptation of the proof of Proposition 2.2. □

3.4. **Nonlinear non-convex case.** We consider throughout this section the Newton equations normalized in a a different regime, namely (10) and (12) with $\gamma \in (0,1)$. To begin with and for pedagogic purposes, we first return to the NN case, where we perform the detailed proof of convergence. The convergence of the NNN case is then proven by a simple adaptation, outlined in our final paragraph. For both cases, our proof follows the lines of the proof by weak convergence we employed above in the linear setting. The additional feature of a different normalization is useful for dealing with the nonlinearity. As above, let us briefly explain, using the discrete differentiation (19), our normalization procedure. Formally, we consider

$$\frac{\partial^2\Phi_\varepsilon}{\partial\tau^2} - \varepsilon^{-\gamma}D_\varepsilon\nabla V(\varepsilon^\gamma D_\varepsilon\Phi_\varepsilon) = 0, \tag{92}$$

When $\gamma \in (0,1)$, we observe that, still formally, Φ_ε converges to the solution Φ to

$$\frac{\partial^2\Phi}{\partial\tau^2} - \nabla V(0).D^2\Phi = 0.$$

This linearization procedure is formalized below in our proof. When $\gamma = 1$, (92) reads $\dfrac{\partial^2\Phi_\varepsilon}{\partial t^2} - D_\varepsilon\nabla V(D_\varepsilon\Phi_\varepsilon) = 0$. It is beyond our reach, without assuming convexity and thus simply using weak convergence arguments, to determine the limit of a term like $D_\varepsilon\nabla V(D_\varepsilon\Phi_\varepsilon)$ unless ∇V is linear, in which case the above equation in turn reduces to (20). This explains why, in the present state of our understanding, we need to resort to the specific normalization using $\gamma \in (0,1)$.

3.4.1. *Back to the nearest-neighbour case.* We first consider the NN case, and prove the following proposition, announced at the end of Subsection 2.2.

Proposition 7. *Assume that $\gamma \in (0,1)$, and that $V \in C^4$ is such that $V(1) = V'(1) = 0$, $V^{(3)}$ is bounded and*

$$\exists \alpha_1 > 0, \quad \exists \alpha_2 > 0, \quad \text{such that} \quad \forall x \in \mathbb{R}, \quad \alpha_1 (x-1)^2 \leq V(x) \leq \alpha_2 (x-1)^2. \tag{93}$$

Let $\phi \in C^0\left([0,T), H^1([0,1])\right)$ be a solution to (11), with $\phi^0 \in H^s(0,1), \phi^1 \in H^1(0,1)$, with $s > 7/6$. Consider the initial conditions $N\phi^0\left(\frac{i}{N}\right)$ and $\phi^1\left(\frac{i}{N}\right)$ for (10). Let

$$X_i^0 = N\phi^0\left(\frac{i}{N}\right) \quad V_i^0 = \phi^1\left(\frac{i}{N}\right), \tag{94}$$

and let $X_i(t)$ be the unique solution to (10), with the convention $X_0 = 0$, $X_{N+1} = 0$. Then, we have

$$\forall \tau \in (0,T), \quad \sup_{1\leq i\leq N} \left| \frac{1}{N} X_i(N\tau) - \phi\left(\frac{i}{N}, \tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0,$$

and

$$\forall \tau \in (0,T), \quad \sup_{1\leq i\leq N} \left| \frac{dX_i}{dt}(N\tau) - \frac{\partial \phi}{\partial \tau}\left(\frac{i}{N}, \tau\right)\right| \underset{N\to\infty}{\longrightarrow} 0.$$

Proof fo Proposition 7. First step: choice of the initial condition. Contrary to Proposition 5, the energy of the discrete system is convex, so no filtering is needed. Hence, the initial condition is simply given by (94).
Second step: weak convergence.
Here, the strategy is somewhat different: we write the conservation of the energy for the discrete system, that is, setting $Y_i(\tau) = \frac{1}{N} X_i(N\tau)$,

$$\frac{1}{2}\left\|\frac{dY}{d\tau}\right\|^2 + N^{2\gamma}\frac{1}{N}\sum_{i=1}^N V\left(1 + \frac{(\nabla_N Y)_i}{N^\gamma}\right) = \frac{1}{2}\left\|V^0\right\|^2 + N^{2\gamma}\frac{1}{N}\sum_{i=1}^N V\left(1 + \frac{(\nabla_N Y^0)_i}{N^\gamma}\right), \tag{95}$$

where we recall that the norm in (95) is defined by (64). Therefore, using the bounds (93) for V, we infer that

$$\left\|\frac{dY}{d\tau}\right\|_{L^2} \leq C, \quad \|\nabla_N Y\|_{L^2} \leq C, \tag{96}$$

for some constant $C > 0$ independent of N. Here again, we use a discrete Poincaré inequality [3, 8] to prove that Y is bounded in L^2, so that (87) holds, that is,

$$Y \longrightarrow \phi \text{ in } L^2, \quad \text{and} \quad \nabla_N Y \rightharpoonup \frac{\partial \phi}{\partial x} \text{ in } L^2, \tag{97}$$

where $\phi \in H^1((0,1)\times(0,T))$. We are now going to prove that ϕ is the solution to (11). For this purpose, we set $G(\tau) = \nabla_N Y(N\tau)$. Hence, we have, for any $\theta \in \mathcal{D}(0,1)$,

$$\left(\frac{d^2Y}{d\tau^2}, \theta\right) = NN^\gamma \sum_{i=0}^N \left[V'\left(1 + \frac{G_i}{N^\gamma}\right) - V'\left(1 + \frac{G_{i-1}}{N^\gamma}\right)\right] \int_{\frac{i-1/2}{N}}^{\frac{i+1/2}{N}} \theta(x)dx. \tag{98}$$

Using a Taylor expansion, we have

$$\left| V'\left(1+\frac{G_i}{N^\gamma}\right) - V''(1)\frac{G_i}{N^\gamma}\right| \leq \|V^{(3)}\|_{L^\infty}\frac{|G_i|^2}{N^{2\gamma}}.$$

Inserting this into (98), we thus have

$$\begin{aligned}\left|\left(\frac{d^2Y}{d\tau^2},\theta\right) - N\sum_{i=0}^N V''(1)\left(G_i-G_{i-1}\right)\int_{\frac{i-1/2}{N}}^{\frac{i+1/2}{N}}\theta(x)dx\right| &\leq N\|V^{(3)}\|_{L^\infty} \\ \times \sum_{i=0}^N \frac{G_i^2+G_{i-1}^2}{N^{2\gamma}}\int_{\frac{i-1/2}{N}}^{\frac{i+1/2}{N}}|\theta(x)|dx& \\ \leq 2\|V^{(3)}\|_{L^\infty}\|\theta\|_{L^\infty}\frac{\|G\|_{L^2}^2}{N^{2\gamma}} \underset{N\to\infty}{\longrightarrow} 0.& \quad (99)\end{aligned}$$

We compute the second term of the left-hand side:

$$\begin{aligned}&\sum_{i=0}^N V''(1)\left(G_i-G_{i-1}\right)\int_{\frac{i-1/2}{N}}^{\frac{i+1/2}{N}}\theta(x)dx \\ &\qquad = -\sum_{i=0}^N V''(1)G_i\underbrace{\left(\int_{\frac{i+1/2}{N}}^{\frac{i+3/2}{N}}\theta(x)dx - \int_{\frac{i-1/2}{N}}^{\frac{i+1/2}{N}}\theta(x)dx\right)}_{=\frac{\theta\left(\frac{i+1}{N}\right)-\theta\left(\frac{i}{N}\right)}{N}+O\left(\frac{1}{N^3}\right)},\end{aligned}$$

where $O(1/N^3)$ depends only on $\|\theta^{(3)}\|_{L^\infty}$. Thus,

$$\begin{aligned}&\sum_{i=0}^N V''(1)\left(G_i-G_{i-1}\right)\int_{\frac{i-1/2}{N}}^{\frac{i+1/2}{N}}\theta(x)dx \\ = \quad & -\sum_{i=0}^N V''(1)G_i\frac{\theta\left(\frac{i+1}{N}\right)-\theta\left(\frac{i}{N}\right)}{N} \\ & +O\left(\frac{\|G\|_{L^1}}{N^3}\right) \\ = \quad & -\sum_{i=0}^N V''(1)G_i\frac{\theta'\left(\frac{i}{N}\right)}{N^2} + O\left(\frac{1}{N^2}\right), \qquad (100)\end{aligned}$$

where we have used Cauchy-Schwarz inequality and the bound (96), together with a Taylor expansion of θ. Finally, the convergence (97) implies

$$\frac{1}{N}\sum_{i=0}^N V''(1)G_i\theta'\left(\frac{i}{N}\right) \underset{N\to\infty}{\longrightarrow} V''(1)\int_0^1\frac{\partial\phi}{\partial x}\theta'(x)dx. \qquad (101)$$

Collecting (99), (100), (101), we thus have

$$\left(\frac{d^2Y}{d\tau^2},\theta\right) + V''(1)\int_0^1\frac{\partial\phi}{\partial x}\theta'(x)dx \underset{N\to\infty}{\longrightarrow} 0.$$

This implies that ϕ defined by (97) is a solution to (11).

Third step: convergence of the energy. This step is actually simpler than the corresponding one in the proof of Proposition 5. Indeed, (95) and the following energy conservation:

$$\int_0^1 \left(\frac{\partial \phi}{\partial \tau}\right)^2 dx + V''(1)\int_0^1 \left(\frac{\partial \phi}{\partial x}\right)^2 dx = \int_0^1 \left(\phi^1\right)^2 dx + V''(1)\int_0^1 \left(\frac{\partial \phi^0}{\partial x}\right)^2 dx,$$

allow to prove convergence of the energy provided that it holds at $t=0$, that is,

$$\left\|V^0\right\|^2 + 2N^{2\gamma}\left(V\left(1+\frac{\nabla_N Y^0}{N^\gamma}\right),1\right) \underset{N\to\infty}{\longrightarrow} \int_0^1 \left(\phi^1\right)^2 dx + V''(1)\int_0^1 \left(\frac{\partial \phi^0}{\partial x}\right)^2 dx. \tag{102}$$

The convergence of the first term is clear, so we concentrate on the second one. We thus write, using here again a Taylor expansion of V around 1,

$$\begin{aligned} V\left(1+\frac{\left(\nabla_N Y^0\right)_i}{N^\gamma}\right) &= V(1) + V'(1)\frac{\left(\nabla_N Y^0\right)_i}{N^\gamma} + \frac{1}{2}V''(1)\frac{\left(\nabla_N Y^0\right)_i^2}{N^{2\gamma}} \\ &\quad + O\left(\left\|V^{(3)}\right\|_{L^\infty}\frac{\left|\left(\nabla_N Y^0\right)_i\right|^3}{N^{3\gamma}}\right) \\ &= \frac{1}{2}V''(1)\frac{\left(\nabla_N Y_i^0\right)^2}{N^{2\gamma}} + O\left(\left\|V^{(3)}\right\|_{L^\infty}\frac{\left|\left(\nabla_N Y^0\right)_i\right|^3}{N^{3\gamma}}\right), \end{aligned}$$

hence

$$\begin{aligned} N^{2\gamma}\frac{1}{N}\sum_{i=0}^N V\left(1+\frac{\left(\nabla_N Y^0\right)_i}{N^\gamma}\right) &= \frac{1}{2}V''(1)\frac{1}{N}\sum_{i=0}^N \left(\nabla_N Y^0\right)_i^2 \\ &\quad + O\left(\|V^{(3)}\|_{L^\infty}\frac{1}{N^{1+\gamma}}\sum_{i=0}^N \left|\left(\nabla_N Y^0\right)_i\right|^3\right) \end{aligned} \tag{103}$$

In addition, using the Hölder inequality, we have

$$\begin{aligned} \frac{1}{N}\sum_{i=0}^N \left|\left(\nabla_N Y^0\right)_i\right|^3 &= \frac{1}{N}\sum_{i=0}^N \left|N\left(\phi_N^0\left(\frac{i+1}{N}\right) - \phi_N^0\left(\frac{i}{N}\right)\right)\right|^3 \\ &= \frac{1}{N}\sum_{i=0}^N \left|N\int_{\frac{i}{N}}^{\frac{i+1}{N}} \frac{d\phi_N^0}{dx}(x)dx\right|^3 \\ &\le N^2\sum_{i=0}^N \frac{1}{N^2}\int_{\frac{i}{N}}^{\frac{i+1}{N}} \left|\frac{d\phi_N^0}{dx}\right|^3 = \int_0^1 \left|\frac{d\phi_N^0}{dx}\right|^3. \end{aligned}$$

Inserting this inequality into (103), we thus have

$$\begin{aligned} N^{2\gamma}\frac{1}{N}\sum_{i=0}^N V\left(1+\frac{\left(\nabla_N Y^0\right)_i}{N^\gamma}\right) &= \frac{1}{2}V''(1)\frac{1}{N}\sum_{i=0}^N \left(\nabla_N Y^0\right)_i^2 \\ &\quad + O\left(\|V^{(3)}\|_{L^\infty}\frac{\left\|\frac{d\phi_N^0}{dx}\right\|_{L^3}^3}{N^\gamma}\right). \end{aligned} \tag{104}$$

Standard Sobolev imbeddings (see for instance [1]) imply that, since $s > 7/6$,

$$\left\| \frac{d\phi_N^0}{dx} \right\|_{L^3} \leq \left\| \phi^0 \right\|_{H^s},$$

by definition of ϕ_N^0. Hence, the remainder of (104) vanishes as $N \to \infty$. The same argument as in the proof of Proposition 5 shows

$$\frac{1}{2} V''(1) \frac{1}{N} \sum_{i=0}^{N} \left(\nabla_N Y^0\right)_i^2 \underset{N\to\infty}{\longrightarrow} \frac{1}{2} V''(1) \int_0^1 \left(\frac{\partial \phi^0}{\partial x} \right)^2 dx.$$

This proves (102), hence the convergence of the energy, namely:

$$\frac{1}{2} \left\| \frac{dY}{dt}(N\tau) \right\|^2 + N^{2\gamma} \sum_{i=0}^{N} V\left(1 + \frac{(\nabla_N Y)_i}{N^\gamma}\right) \underset{N\to\infty}{\longrightarrow} \frac{1}{2} \int_0^1 \left(\frac{\partial \phi}{\partial \tau} \right)^2 dx + \frac{1}{2} V''(1) \int_0^1 \left(\frac{\partial \phi}{\partial x} \right)^2 dx, \quad (105)$$

for any $\tau \geq 0$.

Fourth step: strong convergence. In order to prove strong convergence, we need to prove convergence of each term of the energy. For this purpose, we cannot use the same argument as in the proof of Proposition 5, since V is not convex. Hence, we need to apply a special treatment to the term involving V. For this purpose, we split the indices into two sets, depending on the size of $(\nabla_N Y)_i$:

$$\mathcal{A}_N^+ = \left\{ 1 \leq i \leq N, \quad \left|(\nabla_N Y)_i\right| \geq N^{\gamma/2} \right\},$$

and

$$\mathcal{A}_N^- = \left\{ 1 \leq i \leq N, \quad \left|(\nabla_N Y)_i\right| < N^{\gamma/2} \right\}.$$

Note that, since $\nabla_N Y$ is bounded in L^2, we have

$$\# \mathcal{A}_N^+ \leq C N^{1-\gamma}. \quad (106)$$

We then write the potential energy as

$$\begin{aligned} 2N^{2\gamma} \sum_{i=0}^{N} V\left(1 + \frac{(\nabla_N Y)_i}{N^\gamma}\right) &= 2N^{2\gamma} \sum_{i \in \mathcal{A}_N^-} V\left(1 + \frac{(\nabla_N Y)_i}{N^\gamma}\right) \\ &\quad + 2N^{2\gamma} \sum_{i \in \mathcal{A}_N^+} V\left(1 + \frac{(\nabla_N Y)_i}{N^\gamma}\right) \\ &\geq 2N^{2\gamma} \sum_{i \in \mathcal{A}_N^-} V\left(1 + \frac{(\nabla_N Y)_i}{N^\gamma}\right). \end{aligned}$$

We then use a Taylor expansion of V around 0, writing

$$2N^{2\gamma} V\left(1 + \frac{(\nabla_N Y)_i}{N^\gamma}\right) = V''(1) \left(\nabla_N Y\right)_i^2 + O\left(\left\| V^{(3)} \right\|_{L^\infty} \frac{\left|(\nabla_N Y)_i\right|^3}{N^\gamma} \right).$$

Summing this equality with respect to i, and inserting it into the above inequality, gives

$$2N^{2\gamma}\sum_{i=0}^{N} V\left(1+\frac{(\nabla_N Y)_i}{N^\gamma}\right) \geq V''(1)\sum_{i\in\mathcal{A}_N^-}(\nabla_N Y)_i^2 \\ - C\left\|V^{(3)}\right\|_{L^\infty}\frac{1}{N^{\gamma/2}}\sum_{i\in\mathcal{A}_N^-}(\nabla_N Y)_i^2 .$$

Since $\|\nabla_N Y\|_{L^2}$ is bounded, the last term vanishes in the limit $N\to\infty$. Thus,

$$\liminf_{N\to\infty}\left[2N^{2\gamma}\frac{1}{N}\sum_{i=0}^{N} V\left(1+\frac{(\nabla_N Y)_i}{N^\gamma}\right)\right] \geq \liminf_{N\to\infty}\left[\frac{1}{N}V''(1)\sum_{i\in\mathcal{A}_N^-}(\nabla_N Y)_i^2\right] \tag{107}$$

In addition, defining

$$\tilde{G}_i = \begin{cases}(\nabla_N Y)_i & \text{if } i\in\mathcal{A}_N^-,\\ 0 & \text{if } i\in\mathcal{A}_N^+,\end{cases}$$

we have, for any $\theta\in\mathcal{D}(0,1)$, we have

$$\left(\tilde{G}-\nabla_N Y,\theta\right) = -\frac{1}{N}\sum_{i\in\mathcal{A}_N^+}(\nabla_N Y)_i\int_{\frac{i-1/2}{N}}^{\frac{i+1/2}{N}}\theta(x)dx,$$

whence

$$\left|\left(\tilde{G}-\nabla_N Y,\theta\right)\right| \leq \|\nabla_N Y\|_{L^2}\left(\int_{\mathcal{B}_N^+}\theta(x)^2dx\right)^{1/2}, \tag{108}$$

where $\mathcal{B}_N^+ = \bigcup_{i\in\mathcal{A}_N^+}\left[\frac{i-1/2}{N},\frac{i+1/2}{N}\right]$. Equation (106) implies that $\left|\mathcal{B}_N^+\right|\to 0$, hence the right-hand side of (108) vanishes as $N\to\infty$. Thus,

$$\tilde{G}\underset{N\to\infty}{\rightharpoonup}\frac{\partial\phi}{\partial x}.$$

Using this property and (107), we have

$$\liminf_{N\to\infty}\left[2N^{2\gamma}\frac{1}{N}\sum_{i=0}^{N} V\left(1+\frac{(\nabla_N Y)_i}{N^\gamma}\right)\right] \geq V''(1)\int_0^1\left(\frac{\partial\phi}{\partial x}\right)^2. \tag{109}$$

We note that, in view of the convergence of $dY/d\tau$, we also have

$$\liminf_{N\to\infty}\left\|\frac{dY}{d\tau}\right\|^2 \geq \int_0^1\left(\frac{\partial\phi}{\partial\tau}\right)^2dx.$$

These lower bounds and (105) imply that each term converges. Thus,

$$\frac{dY}{d\tau}(N\tau)\underset{N\to\infty}{\longrightarrow}\frac{\partial\phi}{\partial\tau}\quad\text{in}\quad L^2$$

In order to prove strong convergence of $\nabla_N Y$, we point out that the above argument implies that in (107) and (109), we can replace lim inf by lim and inequalities by equalities:

$$\lim_{N\to\infty}\left[2N^{2\gamma}\frac{1}{N}\sum_{i=0}^{N}V\left(1+\frac{(\nabla_N Y)_i}{N^\gamma}\right)\right]=\lim_{N\to\infty}\left[\frac{1}{N}V''(1)\sum_{i\in\mathcal{A}_N^-}(\nabla_N Y)_i^2\right],\quad(110)$$

$$\lim_{N\to\infty}\left[2N^{2\gamma}\frac{1}{N}\sum_{i=0}^{N}V\left(1+\frac{(\nabla_N Y)_i}{N^\gamma}\right)\right]=V''(1)\int_0^1\left(\frac{\partial\phi}{\partial x}\right)^2.\quad(111)$$

Thus,

$$\lim_{N\to\infty}\left(2N^{2\gamma}\frac{1}{N}\sum_{i\in\mathcal{A}_N^+}V\left(1+\frac{(\nabla_N Y)_i}{N^\gamma}\right)\right)=0.$$

Hence, the lower bound in (93) implies

$$\lim_{N\to\infty}\left(\frac{1}{N}\sum_{i\in\mathcal{A}_N^+}(\nabla_N Y)_i^2\right)=0.$$

Hence, still using (110) and (111), we infer

$$\|\nabla_N Y\|\underset{N\to\infty}{\longrightarrow}\left\|\frac{\partial\phi}{\partial x}\right\|,$$

so that we have strong convergence of $\nabla_N Y$. The end of the proof is similar to that of Proposition 5. □

3.4.2. *Next-to-nearest-neighbour nonlinear non-convex case.* The above proof can be adapted to prove convergence in the NNN nonlinear case.

Proposition 8. *Let $\gamma\in(0,1)$, and assume that $V_1,V_2\in C^4$ are such that $V_1(1)=V_2(2)=0$, $V_1^{(3)}$ and $V_2^{(3)}$ are bounded, that*

$$\exists\alpha_1>0,\quad\forall(x,y)\in\mathbb{R}^2,\quad V_1(1+x)+V_1(1+y)+2V_2(2+x+y)\geq\alpha_1\left(x^2+y^2\right),\quad(112)$$

and

$$\exists\alpha_2>0,\quad\exists\beta\geq0,\quad\text{such that}\quad\forall x\in\mathbb{R},\quad V_i(x)\leq\beta+\alpha_2(x-i)^2,\quad(113)$$

with $i=1,2$. Let $\phi\in C^0\left([0,T),H^1([0,1])\right)$ be a solution to (13), with $\phi^0\in H^s(0,1)$ and $\phi^1\in H^1(0,1)$, where $s>7/6$. Consider the initial conditions

$$X_i^0=N\phi^0\left(\frac{i}{N}\right),\quad V_i^0=\phi^1\left(\frac{i}{N}\right),\quad(114)$$

and let $X_i(t)$ be the unique solution to (12), with the convention $X_0=0$, $X_{N+1}=N+1$. Then,

$$\forall\tau\in(0,T),\quad\sup_{1\leq i\leq N}\left|\frac{1}{N}X_i(N\tau)-\phi\left(\frac{i}{N},\tau\right)\right|\underset{N\to\infty}{\longrightarrow}0,$$

and

$$\sup_{0<\tau<T}\left[\sup_{1\leq i\leq N}\left|\frac{dX_i}{dt}(N\tau)-\frac{\partial\phi}{\partial\tau}\left(\frac{i}{N},\tau\right)\right|\right]\underset{N\to\infty}{\longrightarrow}0.$$

Proof. The proof is adapted from that of Proposition 7. We follow the same steps, pointing out the necessary changes.

First step: choice of the initial condition. Here again, no filtering is needed. So we simply choose (114) as an initial condition. See Remark 11 below for a comment on this fact.

Second step: weak convergence. As in the proof of Proposition 7, we write the conservation of the energy, namely (here again, $Y(\tau) = (1/N)X(N\tau)$)

$$\begin{aligned}\frac{1}{2}\left\|\frac{dY}{d\tau}\right\|^2 + N^{2\gamma}\frac{1}{N}\sum_{i=0}^{N} V_1\left(1+\frac{N\left(Y_{i+1}-Y_i\right)}{N^\gamma}\right) \\ + N^{2\gamma}\frac{1}{N}\sum_{i=0}^{N+1} V_2\left(2+\frac{N\left(Y_{i+1}-Y_{i-1}\right)}{N^\gamma}\right) \\ = \frac{1}{2}\left\|V^0\right\|^2 + N^{2\gamma}\frac{1}{N}\sum_{i=0}^{N} V_1\left(1+\frac{N\left(Y^0_{i+1}-Y^0_i\right)}{N^\gamma}\right) \\ + N^{2\gamma}\frac{1}{N}\sum_{i=0}^{N+1} V_2\left(2+\frac{N\left(Y^0_{i+1}-Y^0_{i-1}\right)}{N^\gamma}\right)\end{aligned} \tag{115}$$

We use (112), and find (recall that $Y_i = 0$ if $i \le 0$ or $i \ge N+1$):

$$\begin{aligned}N^{2\gamma}\frac{1}{N}\sum_{i=0}^{N} V_1\left(1+\frac{N\left(Y_{i+1}-Y_i\right)}{N^\gamma}\right) + N^{2\gamma}\frac{1}{N}\sum_{i=0}^{N+1} V_2\left(2+\frac{N\left(Y_{i+1}-Y_{i-1}\right)}{N^\gamma}\right) \\ = N^{2\gamma-1}\sum_{i=0}^{N+1}\frac{1}{2}V_1\left(1+\frac{N\left(Y_{i+1}-Y_i\right)}{N^\gamma}\right) + \frac{1}{2}V_1\left(1+\frac{N\left(Y_i-Y_{i-1}\right)}{N^\gamma}\right) \\ + V_2\left(2+\frac{N\left(Y_{i+1}-Y_{i-1}\right)}{N^\gamma}\right) \\ \ge N\frac{\alpha_1}{2}\sum_{i=0}^{N+1}\left(Y_{i+1}-Y_i\right)^2 + \left(Y_i-Y_{i-1}\right)^2 = \alpha_1\frac{1}{N}\sum_{i=0}^{N} N^2\left(Y_{i+1}-Y_i\right)^2\end{aligned}$$

Inserting this inequality into (115), we prove that $\nabla_N Y$ is bounded in L^2, and we thus have weak convergence:

$$Y \longrightarrow \phi \text{ in } L^2, \quad \text{and} \quad \nabla_N Y \rightharpoonup \frac{\partial\phi}{\partial x} \text{ in } L^2,$$

where $\phi \in H^1((0,1)\times(0,T))$. The proof that ϕ is a solution to (13) is essentially similar to that for Proposition 7. The only difference is the presence of the term involving V_2. This term is dealt with exactly as that involving V_1, using (113).

Third step: convergence of the energy. Here again, we first write the energy conservation both for the discrete system and for the continuous one, reducing the problem to the convergence of the energy for the sequence of initial data. The strategy of the proof of Proposition 7 used to deal with the terms in V_1 is easily adapted to the terms involving V_2.

Fourth step: strong convergence. This last step is also a simple adaptation of the one in the proof of Proposition 7. □

Remark 11. It is interesting to make specific the condition (112) to the case of quadratic potentials $V_1(x) = \frac{c_1}{2}(x-1)^2$ and $V_2(x) = \frac{c_2}{2}(x-2)^2$. In that case, condition (112) reads

$$\forall (x,y) \in \mathbb{R}^2, \quad (c_1 + 2c_2)(x^2 + y^2) + 4c_2 xy \geq 0,$$

and this amounts to

$$c_1 + 2c_2 > 0, \quad c_1(c_1 + 4c_2) > 0.$$

It is easily seen that an equivalent condition is

$$c_1 > 0, \quad c_1 + 4c_2 > 0.$$

Evidently, this condition is more general than the "full convexity" ($c_1 > 0$, $c_2 > 0$). However, it rules out the case we considered as interesting in Section 3.2, that is, the case $c_1 < 0$ with $c_1 + 4c_2 > 0$, where negative eigenvalues exist for the underlying discrete differential operator. This observation formally explains why no dedicated filtering of the initial condition is necessary for Proposition 8. It remains that in the non-quadratic case, condition (112) is far more general than convexity and covers a large set of relevant cases.

Appendix A. **A few results on Fourier series.** We collect here the results on Fourier coefficients which we have used in the proof of Proposition 3. We recall that the definition of Fourier coefficients is given in Definition 3.1.

Lemma A.1. *Let $p \geq 1$, and let $\phi \in C^p(0,1)$ be such that $\phi(0) = \phi(1) = 0$. Assume that there exists $C > 0$ and $\theta > 0$ such that*

$$\forall k \in \mathbb{N}^*, \quad \left|\widehat{\phi}(k)\right| \leq Ce^{-\theta k}. \tag{116}$$

Then, defining, for all $N \in \mathbb{N}$ and all $k \leq N$,

$$u_j^k = \frac{1}{\sqrt{N}} \sin\left(\frac{jk\pi}{N}\right),$$

and, for $Q \in \mathbb{R}[X]$,

$$D_j = N \int_{j/N}^{(j+1)/N} Q(Nx - j)\phi^{(p)}(x)dx,$$

we have

$$|\left(u^k, D\right)| \leq C'\sqrt{N}k^p e^{-\theta k}, \tag{117}$$

for some constant C' independent of N and k.

Proof. We first define a function $\psi \in C^1(-1,1)$ by

$$\psi(x) = \begin{cases} \phi(x) & \text{if } x \in (0,1), \\ -\phi(-x) & \text{if } x \in (-1,0). \end{cases}$$

We next extend this function by periodicity, so as to obtain a function, still denoted by ψ, which is 2-periodic, and of class C^1. Hence, this function is equal to the sum of its Fourier series:

$$\psi(x) = \frac{1}{2}\sum_{m\in\mathbb{Z}} \left(e^{im\pi x}\int_{-1}^{1} \psi(y)e^{-im\pi y}dy\right) = 2\sum_{m\geq 1} \widehat{\phi}(m)\sin(m\pi x).$$

Since $\phi = \psi$ on $(0,1)$, we have

$$D_j = iN \sum_{m\geq 1} \int_{j/N}^{(j+1)/N} Q(Nx-j)\widehat{\phi}(m) \left[(-im\pi)^p \, e^{-im\pi x} - (im\pi)^p \, e^{im\pi x}\right] dx$$
$$= 2 \sum_{m\geq 1} \int_0^1 Q(y)\widehat{\phi}(m) \, \mathrm{Im}\left[(im\pi)^p e^{im\pi \frac{j+y}{N}}\right] dy,$$

where $\mathrm{Im}(z)$ denotes the imaginary part of z. Thus,

$$\begin{aligned}\left(u^k, D\right) &= \sum_{j=1}^N u_j^k D_j \\ &= \frac{2}{\sqrt{N}} \mathrm{Im}\left[\sum_{m\geq 1} \int_0^1 Q(y)(im\pi)^p \widehat{\phi}(m) e^{im\pi \frac{y}{N}} \sum_{j=1}^N e^{im\pi \frac{j}{N}} \sin\left(\frac{jk\pi}{N}\right) dy\right]\end{aligned}$$

We compute

$$\begin{aligned}\sum_{j=1}^N e^{im\pi \frac{j}{N}} \sin\left(\frac{jk\pi}{N}\right) &= \frac{1}{2i}\sum_{j=1}^N e^{i\pi\frac{(m+k)j}{N}} - \frac{1}{2i}\sum_{j=1}^N e^{i\pi\frac{(m-k)j}{N}} \\ &= \frac{N}{2i}(\delta_{m+k} - \delta_{m-k}),\end{aligned}$$

where δ is the Kronecker symbol ($\delta_n = 1$ if $n = 0$, $\delta_n = 0$ otherwise). Since both m and k are non-negative,

$$\begin{aligned}\left|\left(u^k, D\right)\right| &= \left|\sqrt{N}\int_0^1 Q(y)\,\mathrm{Im}\left[i\left((ik\pi)^p \widehat{\phi}(k) e^{ik\pi\frac{y}{N}}\right)\right] dy\right| \\ &\leq \sqrt{N}\int_0^1 |Q(y)| dy |k\pi|^p \left|\widehat{\phi}(k)\right|.\end{aligned}$$

Applying (116), we find (117). □

Lemma A.2. *Assume that ϕ^0 and ϕ^1 satisfy the hypotheses of Proposition 4, and assume that ϕ is the unique solution to (41) (with $c_1 + 4c_2 > 0$). Then, for any $\tau \geq 0$, $x \mapsto \phi(\tau, x)$ satisfies (116).*

Proof. Because of the boundary condition in (41), ϕ clearly satisfies $\phi(\tau, 0) = \phi(\tau, 1) = 0$. Computing the Fourier coefficient of order k of this equation, we find that

$$\frac{d^2}{d\tau^2}\widehat{\phi}(\tau, k) = -\pi^2 k^2 \widehat{\phi}(\tau, k),$$

hence

$$\widehat{\phi}(\tau, k) = \widehat{\phi^0}(k)\cos(\pi|k|\tau) + \widehat{\phi^1}(k)\sin(\pi|k|\tau).$$

Applying (46), we conclude the proof. □

Appendix B. Discrete convergence properties.

Lemma B.1. *Let $(Y_i)_{0\leq i\leq N}$ be a vector of $\mathbb{R}^{N+1}$, and assume that*

$$|Y_0| + N\sum_{i=0}^{N-1}(Y_{i+1} - Y_i)^2 \leq C,$$

where C does not depend on N. Then, there exists $g \in L^2(0,1)$ such that, up to the extraction of a subsequence,

$$Y \underset{N\to\infty}{\longrightarrow} g \text{ in } L^2,$$

in the sense

$$\int_0^{\frac{1}{2N}} (g(x)-Y_0)^2\,dx + \sum_{i=1}^{N-1} \int_{\frac{i-\frac12}{N}}^{\frac{i+\frac12}{N}} (g(x)-Y_i)^2\,dx + \int_{1-\frac{1}{2N}}^1 (g(x)-Y_N)^2\,dx \underset{N\to\infty}{\longrightarrow} 0.$$

Proof. Let h_N be a continuous, piecewise affine function such that h_N' is equal to $Y_{i+1}-Y_i$ on each interval $\left[\frac{i}{N},\frac{i+1}{N}\right]$, that is

$$\forall x \in \left[0,\frac{1}{N}\right], \qquad h_N(x) = Y_0 + (Y_1-Y_0)Nx, \tag{118}$$

$$\forall x \in \left[\frac{i}{N},\frac{i+1}{N}\right], \qquad h_N(x) = h_N\left(\frac{i}{N}\right) + (Y_{i+1}-Y_i)\,N\left(x-\frac{i}{N}\right), \tag{119}$$

where (119) is valid for any $1 \le i \le N-1$. Then, h_N is such that h_N' is bounded in L^2 and $h_N(0)$ is bounded. This implies that the sequence $(h_N)_{N\in\mathbb{N}}$ is compact in L^2. Hence it converges, up to the extraction of a subsequence, to some $g \in H^1$.

In order to complete the proof, we need to prove that $\|Y-h_N\|_{L^2} \underset{N\to\infty}{\longrightarrow} 0$, that is,

$$\int_0^{\frac{1}{2N}} (h_N(x)-Y_0)^2\,dx + \sum_{i=1}^{N-1} \int_{\frac{i-\frac12}{N}}^{\frac{i+\frac12}{N}} (h_N(x)-Y_i)^2\,dx + \int_{1-\frac{1}{2N}}^1 (h_N(x)-Y_N)^2\,dx \underset{N\to\infty}{\longrightarrow} 0. \tag{120}$$

For this purpose, we first point out that (118) and (119) imply that

$$\forall 0 \le i \le N, \quad h_N\left(\frac{i}{N}\right) = Y_i.$$

Next, we compute each term of (120) separately:

$$\int_0^{\frac{1}{2N}} (h_N(x)-Y_0)^2\,dx = N^2\int_0^{\frac{1}{2N}} (Y_1-Y_0)^2x^2dx = \frac{1}{24}\frac{(Y_1-Y_0)^2}{N},$$

and

$$\int_{1-\frac{1}{2N}}^1 (h_N(x)-Y_N)^2\,dx = N^2\int_0^{\frac{1}{2N}} (Y_N-Y_{N-1})^2x^2dx = \frac{1}{24}\frac{(Y_N-Y_{N-1})^2}{N}.$$

For $1 \le i \le N$,

$$\begin{aligned}
\int_{\frac{i-\frac12}{N}}^{\frac{i+\frac12}{N}} (h_N(x)-Y_i)^2\,dx &= \int_{\frac{i-\frac12}{N}}^{\frac{i}{N}} (Y_i-Y_{i-1})^2\,N^2\left(x-\frac{i}{N}\right)^2dx \\
&\quad + \int_{\frac{i}{N}}^{\frac{i+\frac12}{N}} (Y_{i+1}-Y_i)^2\,N^2\left(x-\frac{i}{N}\right)^2dx \\
&= \frac{1}{24}\frac{(Y_i-Y_{i-1})^2}{N} + \frac{1}{24}\frac{(Y_{i+1}-Y_i)^2}{N}.
\end{aligned}$$

Summing up all these equalities, we find (120), which concludes the proof. ∎

Appendix C. **Proof of Lemma 3.2.** We give here the proof of Lemma 3.2, which we recall here:

Lemma C.1. *Assume that $c_1 = -1$ and $c_2 = \frac{1}{2}$, so that $c_1 + 4c_2 = 1 > 0$. There exist $\phi^0 \in C^4(0,1)$ and $\phi^1 \in C^4(0,1)$ such that, if $(X_i)_{1\leq i\leq N}$ is the solution to (40), with $\left(X_i^0\right)_{1\leq i\leq N}$ and $\left(V_i^0\right)_{1\leq i\leq N}$ defined by (47), then the convergences (48) and (49) do not hold.*

Proof. Let us define

$$\phi^0(x) = \sum_{k\geq 1} \frac{1}{k^6}\sin(k\pi x), \quad \text{and} \quad \phi^1 = 0, \tag{121}$$

which are clearly of class C^4. Then, the solution ϕ to (41) is equal to

$$\phi(x,\tau) = \sum_{k\leq 1} \frac{1}{k^6}\sin(k\pi x)\cos(k\pi\tau)$$

Moreover, according to (47),

$$X_i^0 = \sum_{k\geq 1}\frac{1}{k^6}\sin\left(\frac{ik\pi}{N}\right),$$

and $V^0 = 0$. We thus have

$$\begin{aligned} X_{i+1}^0 - 2X_i^0 + X_{i-1}^0 &= \sum_{k\geq 1}\frac{1}{k^6}\left[\sin\left(\frac{ik\pi}{N}+\frac{k\pi}{N}\right) - 2\sin\left(\frac{ik\pi}{N}\right)\right. \\ &\qquad \left. + \sin\left(\frac{ik\pi}{N}-\frac{k\pi}{N}\right)\right] \\ &= -\sum_{k\geq 1}\frac{4}{k^6}\sin^2\left(\frac{k\pi}{2N}\right)\sin\left(\frac{ik\pi}{N}\right), \end{aligned}$$

and similarly

$$X_{i+2}^0 - 2X_i^0 + X_{i-2}^0 = -\sum_{k\geq 1}\frac{4}{k^6}\sin^2\left(\frac{k\pi}{N}\right)\sin\left(\frac{ik\pi}{N}\right).$$

Hence,

$$\begin{aligned} &c_1\left(X_{i+1}^0 - 2X_i^0 + X_{i-1}^0\right) + c_2\left(X_{i+2}^0 - 2X_i^0 + X_{i-2}^0\right) \\ &\quad = -X_{i+1}^0 + 2X_i^0 - X_{i-1}^0 + \frac{1}{2}\left(X_{i+2}^0 - 2X_i^0 + X_{i-2}^0\right) \\ &\quad = \sum_{k\geq 1}\frac{2}{k^6}\left[2\sin^2\left(\frac{k\pi}{2N}\right) - \sin^2\left(\frac{k\pi}{N}\right)\right]\sin\left(\frac{ik\pi}{N}\right) \\ &\quad = -\sum_{k\geq 1}\frac{4}{k^6}\cos\left(\frac{k\pi}{N}\right)\sin^2\left(\frac{k\pi}{2N}\right)\sin\left(\frac{ik\pi}{N}\right). \end{aligned}$$

As a consequence, the solution X_i to (40) is equal to

$$X_i(t) = \sum_{k\geq 1}\frac{1}{k^6}\cosh\left[2\sqrt{-\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}\right)t\right]\sin\left(\frac{ik\pi}{N}\right). \tag{122}$$

In (122), we use the convention that, if $-\cos\left(\frac{k\pi}{N}\right) < 0$, then $\sqrt{-\cos\left(\frac{k\pi}{N}\right)} = i\sqrt{\left|\cos\left(\frac{k\pi}{N}\right)\right|}$, and that $\cosh(i\alpha) = \cos(\alpha)$ for any $\alpha \in \mathbb{R}$. It should be noted that we have assumed that $\cos\left(\frac{k\pi}{N}\right)$ never vanishes, which is indeed that case if N is odd. We thus assume from now on that

$$N \notin 2\mathbb{Z}.$$

Next, we compute the L^2 norm of $X(t)$:

$$\begin{aligned}
\|X(t)\|_{L^2}^2 &= \frac{1}{N}\sum_{i=1}^{N} X_i(t)^2 \\
&= \frac{1}{N}\sum_{i=1}^{N}\sum_{k\geq 1}\sum_{k'\geq 1}\frac{1}{k^6}\frac{1}{k'^6}\sin\left(\frac{ik\pi}{N}\right)\sin\left(\frac{ik'\pi}{N}\right) \\
&\quad\times\cosh\left[2\sqrt{-\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}\right)t\right] \\
&\quad\times\cosh\left[2\sqrt{-\cos\left(\frac{k'\pi}{N}\right)}\sin\left(\frac{k'\pi}{2N}\right)t\right] \\
&= \frac{1}{N}\sum_{i=1}^{N}\sum_{k\geq 1}\frac{1}{k^{12}}\sin^2\left(\frac{ik\pi}{N}\right)\cosh^2\left[2\sqrt{-\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}\right)t\right] \\
&\quad+\frac{2}{N}\sum_{i=1}^{N}\sum_{k\geq 1}\sum_{k'\geq k+1}\frac{1}{k^6}\frac{1}{k'^6}\sin\left(\frac{ik\pi}{N}\right)\sin\left(\frac{ik'\pi}{N}\right) \\
&\quad\times\cosh\left[2\sqrt{-\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}\right)t\right] \\
&\quad\times\cosh\left[2\sqrt{-\cos\left(\frac{k'\pi}{N}\right)}\sin\left(\frac{k'\pi}{2N}\right)t\right].
\end{aligned} \tag{123}$$

We note that

$$\sum_{i=1}^{N}\sin\left(\frac{ik\pi}{N}\right)\sin\left(\frac{ik'\pi}{N}\right) = \begin{cases}\frac{N}{2}(-1)^p & \text{if } k' = k + Np,\ p\in\mathbb{Z},\\ 0 & \text{otherwise.}\end{cases}$$

Inserting this property into (123), we thus have

$$\begin{aligned}
\|X(t)\|_{L^2}^2 &= \frac{1}{2}\sum_{k\geq 1}\frac{1}{k^{12}}\cosh^2\left[2\sqrt{-\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}\right)t\right] \\
&\quad+\sum_{k\geq 1}\sum_{p\geq 1}\frac{(-1)^p}{k^6}\frac{1}{(k+Np)^6}\cosh\left[2\sqrt{-\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}\right)t\right] \\
&\quad\times\cosh\left[2\sqrt{-(-1)^p\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}+\frac{p\pi}{2}\right)t\right].
\end{aligned}$$

The above expression simplifies depending on p being odd or even: grouping the terms $p = 2q$ and $p = 2q+1$, we find

$$
\begin{aligned}
\|X(t)\|_{L^2}^2 &= \frac{1}{2}\sum_{k\geq 1}\frac{1}{k^{12}}\cosh^2\left[2\sqrt{-\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}\right)t\right] \\
&\quad -\sum_{k\geq 1}\frac{1}{k^6}\frac{1}{(k+N)^6}\cosh\left[2\sqrt{-\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}\right)t\right] \\
&\quad \times\cosh\left[2\sqrt{\cos\left(\frac{k\pi}{N}\right)}\cos\left(\frac{k\pi}{2N}\right)t\right] \\
&\quad +\sum_{k\geq 1}\sum_{q\geq 0}\alpha(k,q), \qquad (124)
\end{aligned}
$$

where

$$
\begin{aligned}
\alpha(k,q) &= \frac{1}{k^6}\frac{1}{(k+2Nq)^6}\cosh^2\left[2\sqrt{-\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}\right)t\right] \\
&\quad -\frac{1}{k^6}\frac{1}{(k+2Nq+N)^6}\cosh\left[2\sqrt{-\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}\right)t\right] \\
&\quad \times\cosh\left[2\sqrt{\cos\left(\frac{k\pi}{N}\right)}\cos\left(\frac{k\pi}{2N}\right)t\right] \\
&= \frac{1}{k^6}\cosh^2\left[2\sqrt{-\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}\right)t\right] \\
&\quad \times\left[\frac{1}{(k+2Nq)^6}-\frac{1}{(k+2Nq+N)^6}\frac{\cosh\left[2\sqrt{\cos\left(\frac{k\pi}{N}\right)}\cos\left(\frac{k\pi}{2N}\right)t\right]}{\cosh\left[2\sqrt{-\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}\right)t\right]}\right].
\end{aligned}
$$

Next, we study the sign of $\cos\left(\frac{k\pi}{N}\right)$ as a function of k:

$$
\cos\left(\frac{k\pi}{N}\right) \text{ is } \begin{cases}\text{positive} & \text{if } \left(2r-\frac{1}{2}\right)N < k < \left(2r+\frac{1}{2}\right)N,\ r\in\mathbb{Z}, \\ \text{negative} & \text{if } \left(2r+\frac{1}{2}\right)N < k < \left(2r+\frac{3}{2}\right)N,\ r\in\mathbb{Z}.\end{cases}
$$

Therefore, we have

$$\alpha(k,q) = \frac{1}{k^6}\cos^2\left[2\sqrt{\left|\cos\left(\frac{k\pi}{N}\right)\right|}\sin\left(\frac{k\pi}{2N}\right)t\right] \times \left[\frac{1}{(k+2Nq)^6} - \frac{1}{(k+2Nq+N)^6}\frac{\cosh\left[2\sqrt{\left|\cos\left(\frac{k\pi}{N}\right)\right|}\cos\left(\frac{k\pi}{2N}\right)t\right]}{\cos\left[2\sqrt{\left|\cos\left(\frac{k\pi}{N}\right)\right|}\sin\left(\frac{k\pi}{2N}\right)t\right]}\right]$$
$$\geq -\frac{1}{k^6}\frac{1}{(k+2Nq+N)^6}\left|\cos\left[2\sqrt{\left|\cos\left(\frac{k\pi}{N}\right)\right|}\sin\left(\frac{k\pi}{2N}\right)t\right]\right| \times \cosh\left[2\sqrt{\left|\cos\left(\frac{k\pi}{N}\right)\right|}\cos\left(\frac{k\pi}{2N}\right)t\right] \quad (125)$$

if $\left(2r-\frac{1}{2}\right)N < k < \left(2r+\frac{1}{2}\right)N,\ r\in\mathbb{Z}$, and

$$\alpha(k,q) = \frac{1}{k^6}\cosh^2\left[2\sqrt{\left|\cos\left(\frac{k\pi}{N}\right)\right|}\sin\left(\frac{k\pi}{2N}\right)t\right] \times \left[\frac{1}{(k+2Nq)^6} - \frac{1}{(k+2Nq+N)^6}\frac{\cos\left[2\sqrt{\left|\cos\left(\frac{k\pi}{N}\right)\right|}\cos\left(\frac{k\pi}{2N}\right)t\right]}{\cosh\left[2\sqrt{\left|\cos\left(\frac{k\pi}{N}\right)\right|}\sin\left(\frac{k\pi}{2N}\right)t\right]}\right]$$
$$\geq \frac{1}{k^6}\cosh^2\left[2\sqrt{\left|\cos\left(\frac{k\pi}{N}\right)\right|}\sin\left(\frac{k\pi}{2N}\right)t\right]\left[\frac{1}{(k+2Nq)^6} - \frac{1}{(k+2Nq+N)^6}\right] \quad (126)$$

if $\left(2r+\frac{1}{2}\right)N < k < \left(2r+\frac{3}{2}\right)N,\ r\in\mathbb{Z}$. We insert these estimates into (124), and, retaining only the terms $N/2 < k < 3N/2$ for (126) (recall that N is odd), we find

$$\begin{aligned}\|X(t)\|_{L^2}^2 \geq\ & \frac{1}{2}\sum_{k\geq 1}\frac{1}{k^{12}}\cosh^2\left[2\sqrt{-\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}\right)t\right] \\ & -\sum_{k\geq 1}\frac{1}{k^6}\frac{1}{(k+N)^6}\cosh\left[2\sqrt{-\cos\left(\frac{k\pi}{N}\right)}\sin\left(\frac{k\pi}{2N}\right)t\right] \\ & \times\cosh\left[2\sqrt{\cos\left(\frac{k\pi}{N}\right)}\cos\left(\frac{k\pi}{2N}\right)t\right] \\ & +\sum_{k=\frac{N+1}{2}}^{\frac{3N-1}{2}}\frac{1}{k^{12}}\cosh^2\left[2\sqrt{\left|\cos\left(\frac{k\pi}{N}\right)\right|}\sin\left(\frac{k\pi}{2N}\right)t\right] \\ & -\sum_{k\geq 1}\frac{1}{k^6}\left(\sum_{q\geq 0}\frac{1}{(k+2Nq+N)^6}\right)\cosh\left[2\sqrt{\left|\cos\left(\frac{k\pi}{N}\right)\right|}\cos\left(\frac{k\pi}{2N}\right)t\right]\end{aligned}$$

The first sum is non-negative, so we bound it by 0, and the second one is dealt with using estimate (125). Finally, we retain only the term $k = N$ in the third sum. We thus have:

$$\begin{aligned}\|X(t)\|_{L^2}^2 \quad &\geq \quad \left(\frac{1}{N}\right)^{12} \cosh^2\left[2\sqrt{|\cos(\pi)|}\sin\left(\frac{\pi}{2}\right)t\right] \\ &\quad -\sum_{k\geq 1}\frac{1}{k^6}\left[\frac{1}{(k+N)^6}+\sum_{q\geq 0}\frac{1}{(k+2Nq+N)^6}\right]\cosh(2t) \\ &\geq \quad \frac{C}{N^{12}}e^{2\sqrt{2}t} - Ce^{2t},\end{aligned}$$

where C does not depend on N. Hence, we have

$$\forall \tau > 0, \quad \|X(N\tau)\|_{L^2} \underset{N\to\infty}{\longrightarrow} +\infty,$$

which contradicts the convergence (48). A similar argument proves that (49) cannot hold either. □

Remark 12. The above proof gives only a particular example of an initial data for which converge does not hold. The power 6 in (121) may be replaced by any power ensuring convergence of the Fourier series. Moreover, it is also possible to adapt the proof, at the price of technical difficulties, to functions of the form

$$\phi^0(x) = \sum_{k\geq 1}\frac{\alpha_k}{k^p}\sin(k\pi x),$$

where $p > 2$ and α_k is a bounded sequence such that $\alpha_k \geq \alpha > 0$. Hence, non convergence occurs for a large set of initial data.

REFERENCES

[1] Robert A. Adams, "Sobolev Spaces," Pure and Applied Mathematics, **65**, Academic Press [A subsidiary of Harcourt Brace Jovanovich, Publishers], New York-London, 1975.

[2] M. Berezhnyy and L. Berlyand, *Continuum limit for three-dimensional mass-spring networks and discrete Korn's inequality*, J. Mech. Phys. Solids, **54** (2006), 635–669.

[3] Susanne C. Brenner, *Poincaré-Friedrichs inequalities for piecewise H^1 functions*, SIAM J. Numer. Anal., **41** (2003), 306–324 (electronic).

[4] Constantine M. Dafermos and William J. Hrusa, *Energy methods for quasilinear hyperbolic initial-boundary value problems. Applications to elastodynamics*, Arch. Ration. Mech. Anal., **87** (1985), 267–292.

[5] Wei-nan E and Ping-bing Ming, *Cauchy-Born rule and the stability of crystalline solids: Dynamic problems*, Acta Math. Appl. Sin. Engl. Ser., **23** (2007), 529–550.

[6] P. Joly, *Finite element methods with continuous displacement*, in "Effective Computational Methods for Wave Propagation," Numer. Insights, **5**, Chapman & Hall/CRC, Boca Raton, FL, (2008), 267–329.

[7] Tosio Kato, *The Cauchy problem for quasi-linear symmetric hyperbolic systems*, Archive for Rational Mechanics and Analysis, **58** (1975), 181–205.

[8] B. G. Pachpatte, *On discrete inequalities of the Poincaré type*, Period. Math. Hungar., **19** (1988), 227–233.

[9] Denis Serre, "Systems of Conservation Laws. 1. Hyperbolicity, Entropies, Shock Waves," Translated from the French by I. N. Sneddon, Cambridge University Press, Cambridge, 1999.

[10] Antoni Zygmund, "Trigonometrical Series," Dover Publications, New York, 1955.

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