# Atomic-scale localization of high-energy solitary waves on lattices

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**Abstract**

One-dimensional monatomic lattices with Hamiltonian $H = \sum_{n\in \mathbb{Z}} (\frac{1}{2}p_n^2 + V(q_{n+1} - q_n))$ are known to carry localized travelling wave solutions, for generic nonlinear potentials $V$ [FW94]. In this paper we derive the asymptotic profile of these waves in the high-energy limit $H \to \infty$, for Lennard-Jones type interactions. The limit profile is proved to be a universal, highly discrete, piecewise linear wave concentrated on a single atomic spacing.

This shows that dispersionless energy transport in these systems is not confined to the long-wave regime on which the theoretical literature has hitherto focused, but also occurs at atomic-scale localization.

# 1 Introduction

One of the interesting properties of discrete nonlinear Hamiltonian chains is the possibility of dispersionless energy transport through localized solitary waves. For the model Hamiltonian

$$H = \sum_{n\in \mathbb{Z}} \Big(\frac{1}{2}p_n^2 + V(q_{n+1} - q_n)\Big) \tag{1.1}$$

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describing a one-dimensional monatomic chain (with $p_n$, $q_n$ denoting the momentum and displacement of the $n^{th}$ atom) such waves have been rigorously proven to exist for generic nonlinear potentials $V$ [FW94] (see also [FP99, Io00]).

In the low-energy regime $H \to 0$ these waves are by now well understood. In particular, the profile is known to be a small-amplitude long wave with sech$^2$ shape, amplitude $\sim H$ and wavelength $\sim H^{-1/2}$ (see [ZK65] for closely related formal asymptotic calculations valid for timescales $\sim H^{-3/2}$, [FP99] for a rigorous proof, [MM02] for higher order corrections, [FP01] for dynamic stability and [SW00] for collision behaviour). By contrast almost nothing is known in the high-energy regime.

The goal of this paper is to determine the limiting profile in the high-energy regime, for Lennard-Jones type interactions.

Since this regime is highly discrete and involves strong forces, neither classical continuum approximations (obtained by Taylor-expanding the difference terms in the governing profile equation) nor weak coupling approximations (as have allowed e.g. a rigorous understanding of highly-discrete breathers in certain discrete Hamiltonian systems [MA94]) are possible. Our approach is to derive the limit profile via a careful asymptotic analysis of an underlying minimum action principle.

To describe the result, we begin by recalling that Hamilton's equations give the dynamics as

$$\dot{q}_n = p_n, \quad \ddot{q}_n = \dot{p}_n = V'(q_{n+1} - q_n) - V'(q_n - q_{n-1}). \tag{1.2}$$

For travelling waves $q_n(t) = q(n - ct)$, the equations of motion reduce to the scalar second-order differential-difference equation

$$c^2 q''(x) = V'(q(x+1) - q(x)) - V'(q(x) - q(x-1)). \tag{1.3}$$

A key physical requirement of the interaction potential $V$ is that it is minimized when neighbouring particles are placed at some equilibrium distance $d > 0$, and that it tends to infinity as the neighbour distance tends to zero. Since the particle positions $x_n$ corresponding to displacements $q_n$ are $x_n = nd + q_n$ ($n \in \mathbb{Z}$), this means that $V(r)$ must have a minimum at $r = 0$ and that $V(r) \to \infty$ as $r \to -d$. More precisely we assume:

(H1) (Minimum at zero) $V \in C^3(-d, \infty)$, $V \geq 0$, $V(0) = 0$, $V''(0) > 0$
(H2) (Growth) $V(r) \geq c_0 (r + d)^{-1}$ for some $c_0 > 0$ and all $r$ close to $-d$
(H3) (Hardening) $V'''(r) < 0$ in $(-d, 0]$, $V(r) < V(-r)$ in $(0, d)$.

In particular, (H3) is satisfied if $V'''(r) < 0$ in $(-d, d)$. Prototypical are the standard Lennard-Jones potentials

$$V(r) = a\Big((r + d)^{-m} - d^{-m}\Big)^2, \quad a > 0, \ m \in \mathbb{N}.$$

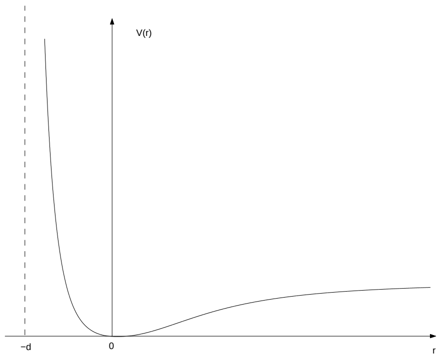



Figure 1: Typical interatomic potentials $V$ will satisfy the above hypotheses.

(In fact, the physically correct blow-up for small interatomic distances delivered by (Born-Oppenheimer-) quantum mechanics is $(r+d)^{-1}$, universally with respect to atomic number, as is equally covered by (H2).)

In our passage to the high energy limit, the property of the solitary waves of solving a naturally associated variational problem will play an important role:

$$\text{Minimize } T(q) := \frac{1}{2}\int_{\mathbb{R}} q'(x)^2 dx \text{ among } q \in W^{1,2}_{loc}(\mathbb{R}) \text{ satisfying}$$
$$q' \in L^2(\mathbb{R}),\ U(q) := \int_{\mathbb{R}} V(q(x+1)-q(x))dx = K. \tag{1.4}$$

This variational problem was introduced in [FW94] in order to establish existence and we briefly recall its derivation from Hamilton's principle: the action of a path of the form $q_n(t) = q(n-ct)$ taken over a time interval of length $1/c$ equals

$$\begin{aligned} S &= \int_{t_0}^{t_0+1/c} \sum_{n\in\mathbb{Z}} \Big(\frac{1}{2}\dot{q}_n^2(t) - V(q_{n+1}(t)-q_n(t))\Big)dt \\ &= \frac{1}{c}\int_{\mathbb{R}} \Big(\frac{c^2}{2}q'(x)^2 - V(q(x+1)-q(x))\Big)dx = c\,T(q) - \frac{1}{c}U(q). \end{aligned}$$

Hence (noting that any multiple of the constraint may be subtracted from the functional to be minimized) minimizing action among paths of the above form is equivalent to (1.4). Moreover the above calculation shows that for any travelling wave of speed $c$, $T(q) = c^{-2}\langle \textit{kinetic energy}\rangle$, $U(q) = \langle \textit{potential energy}\rangle$, where $\langle\cdot\rangle$ denotes the average over a time interval of length $1/c$.

The following existence result can be deduced from the existence theory in [FW94], by adapting their analysis to non-globally-defined potentials. The details are relegated to an appendix. We confine ourselves here to emphasizing that hardening assumptions such as (H3) are essential: for instance when $V$ is quadratic, solitary waves do not exist and the infimum of the variational problem (1.4) is not attained [FW94].

**Theorem 1** *(Existence, essentially [FW94]) Assume that the interaction potential satisfies (H1), (H2), (H3). For all* $K \in (0, \infty)$ *there exists a minimizer* $q_K$ *of (1.4). Moreover any minimizer has the following properties:*
*(i) (compression wave)* $q_K'(x) < 0$ *for all* $x$
*(ii) (collision avoidance)* $q_K(x+1) - q_K(x) > -d$ *for all* $x$
*(iii) (Euler-Lagrange equation)* $q_K$ *solves (1.3) for some* $c \neq 0$*;*
*in particular* $q_K \in C^4$ $(\in C^{k+1}$ *if* $V \in C^k)$
*(iv) (supersonicity)* $c^2 > V''(0)$.

We remark that property (ii) is not physically obvious. Intuitively one might have thought that the action could be lowered by formation of a singularity which would push $-U$ down without much expenditure of $T$. For an explanation why this does not happen see the Appendix.

The new result is

**Theorem 2** *(High-energy limit) Assume that the interaction potential satisfies (H1), (H2), (H3). For* $K \in (0, \infty)$*, let* $q_K$ *be any travelling wave (i.e. any solution to (1.3)) which is action-minimizing (i.e. solves (1.4)). Let* $q_\infty$ *denote the following ultra-short piecewise linear wave with width of a single atomic spacing (see Figure 2)*

$$q_\infty(x) := \begin{cases} 0, & x \leq 0 \\ -dx, & x \in [0,1] \\ -d, & x \geq 1. \end{cases}$$

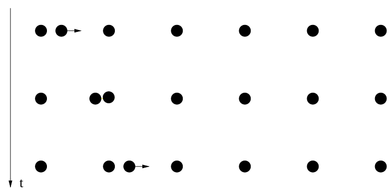
*There exist constants* $a_K$, $b_K \in \mathbb{R}$ *such that the translate* $\tilde{q}_K(x) := b_K + q_K(x - a_K)$ *satisfies the following convergences as* $K \to \infty$

$$\tilde{q}_K \to q_\infty \text{ uniformly on } \mathbb{R} \tag{1.5}$$

$$(\tilde{q}_K)' \to (q_\infty)' \text{ in } L^p(\mathbb{R}) \text{ for all } 1 \leq p < \infty. \tag{1.6}$$

**Remarks** 1) $L^p$ convergence in (1.6) cannot be improved to $L^\infty$ convergence, since the limit $(q_\infty)'$ is discontinuous but the $(\tilde{q}_K)'$ are smooth.

2) The limiting solitary wave corresponds to motion of the particle positions $x_n = nd + q_n(t) = nd + q_\infty(n - ct)$ via hard-sphere collision dynamics, with exactly one atom in motion at any time.



3) The above result makes explicit that solitary lattice waves are by no means confined to the long-wave regime on which the theoretical literature has hitherto focused (for an exception see [To78] but note the well known fact that at high energy the Toda soliton is unphysical as it does not respect the constraint that interpenetration of matter is forbidden). Instead we conclude that dispersionless energy transport is possible at atomic-scale localization. Such localized transport mechanisms are believed to play an important role in dislocation and domain wall motion in solids ([PK84] for a numerical studt of a relevant Frenkel-Kontorova model) and active biomolecules like DNA (see [Sa91]).

# 2 A-priori estimates

In this section we gather suitable a-priori estimates used in the passage to the high-energy limit.

**Proposition 2.1** *(A-priori estimates) Any minimizer $q_K$ of (1.4) with $U(q_K) = K$, $K \in (0,\infty)$, satisfies the following a-priori estimates:*
*i)* $||(q_K)'||_{L^2(\mathbb{R})} \le d_*(K)$ *for some* $d_*(K) < d$
*ii)* $\sup_{x\in\mathbb{R}} |q_K(x+1) - q_K(x)| \le d_*(K)$, $d_*(K)$ *as in i)*
*iii)* $||(q_K)'||_{L^1(\mathbb{R})} \le C_1(K)$, *for some* $C_1(K)$ *satisfying* $\limsup_{K\to\infty} C_1(K) \le d$
*iv)* $||(q_K)'||_{L^\infty(\mathbb{R})} \le C_\infty(K)$, *for some* $C_\infty$, *which is nonincreasing in* $K$

**Proof** Suppose $q_K$ is a solution to (1.4) with $U(q_K) = K$. Consider the trial function

$$\overline{q}_D := \begin{cases} 0, & x < 0 \\ -Dx, & x \in [0,1] \\ -D, & x > 1. \end{cases}$$

Consider its potential energy $U(\overline{q}_D) = 2\int_0^1 V(-D + Dx)dx$. It is zero when $D = 0$, and continuous and increasing for $D \in [0,d)$. We claim that $U(\overline{q}_D) \to \infty$ as $D \to d$. Indeed, by (H2) there exists $\delta > 0$ such that $V(r) \ge c_0/(r+d)$ for $r \in (-d, -d+\delta)$. Hence if $D > d - \delta/2$ and $x < \delta/2$, $V(-D+Dx) \ge c_0/(d-D+Dx)$, so

$$U(\overline{q}_D) \ge 2\int_0^{\delta/2} \frac{c_0}{d - D + Dx} dx \;\to\; \infty \;\text{ as } D \to d.$$

It follows from the intermediate value theorem that there exists $d_*(K) \in (0,d)$ such that $U(\overline{q}_{d_*(K)}) = K$. Using $\overline{q}_{d_*(K)}$ as a trial function in the variational principle gives $T(q_K) \le T(\overline{q}_{d_*(K)}) = \frac{1}{2}d_*(K)^2 < \frac{1}{2}d^2$, establishing i).

ii) is an immediate consequence of i) and the Cauchy-Schwarz inequality $|q_K(x+1) - q_K(x)| \le (\int_x^{x+1} q_K'(s)^2\, ds)^{1/2} \le ||q_K'||_{L^2(\mathbb{R})}$.

To show iii)-iv) we first estimate the wavespeed $c^2$ from below. To this end we use the Euler-Lagrange equation delivered by Theorem 1 iii) (which in turn follows from Proposition 2.1 ii) which implies that the relative displacement profile $r_K(x) := q_K(x+1) - q_K(x)$ stays away from the singular point $r = -d$ at which $V$ is not differentiable). Testing (1.3) with $q_K$ yields (see [FW94, eq. (24)])

$$c^2 = \frac{\int_{\mathbb{R}} V'(r_K(x)) r_K(x) dx}{2T(q_K)}. \tag{2.7}$$

Hence by i) and the fact that due to the hardening condition (H3) we have $V'(r)r \geq 2V(r)$ in $(-d, 0]$

$$c^2 \geq \frac{\int_{\mathbb{R}} V'(r_K) r_K}{d^2} \geq \frac{2K}{d^2}. \tag{2.8}$$

Next, we transform (1.3) into a first order equation for $q$, by using a nontrivial result of [FP99] that $r_K(x)$ tends to zero exponentially fast as $|x| \to \infty$. Hence so does $(q_K)''(x)$; in particular $\int_{\mathbb{R}} |(q_K)''| < \infty$. This allows to integrate (1.3) from $-\infty$ to $x$, yielding

$$(q_K)'(x) = \frac{1}{c^2} \int_{x-1}^{x} V'(r_K(s)) ds. \tag{2.9}$$

Hence using $(q_K)' \leq 0$, $r_K \leq 0$, $V'(r_K) \leq 0$, and (2.8), we have for any $\delta \in (0, d)$

$$\begin{aligned}
||(q_K)'||_{L^1(\mathbb{R})} &= \frac{1}{c^2} \int_{\mathbb{R}} \int_{[x-1,x]} |V'(r_K(s))| ds dx = \frac{1}{c^2} \int_{\mathbb{R}} |V'(r_K(x))| dx \\
&\leq \frac{d^2}{\int_{\mathbb{R}} V'(r_K) r_K} \Big[ \int_{\{x\,:\,|r_K(x)| > d-\delta\}} |V'(r_K(x))| dx + \int_{\{x\,:\,|r_K(x)| \leq d-\delta\}} |V'(r_K(x))| dx \Big] \\
&\leq \frac{d^2}{\int_{\mathbb{R}} V'(r_K) r_K} \Big[ \frac{1}{d-\delta} \int_{\{x\,:\,|r_K(x)| > d-\delta\}} V'(r_K(x)) r_K(x) dx + |V''(-d+\delta)| \, \|r_K\|_{L^1(\mathbb{R})} \Big] \\
&\leq \frac{d^2}{d-\delta} + \frac{d^2 |V''(-d+\delta)| \, ||r_K||_{L_1(\mathbb{R})}}{2K}.
\end{aligned} \tag{2.10}$$

Consequently, since $||r_K||_{L^1(\mathbb{R})} \leq ||(q_K)'||_{L^1(\mathbb{R})}$, we have

$$||r_K||_{L^1(\mathbb{R})} \Big( 1 - \frac{d^2 |V''(-d+\delta)|}{2K} \Big) \leq \frac{d^2}{d-\delta}$$

and hence $\limsup_{K\to\infty} ||r_K||_{L^1(\mathbb{R})} < \infty$. Back substitution into (2.10) yields $\limsup_{K\to\infty} ||(q_K)'||_{L^1(\mathbb{R})} \leq d^2/(d-\delta)$. Since $\delta$ was arbitrary, iii) follows.

Analogously to the above $L^1$ estimate we obtain an $L^\infty$ estimate:

$$|(q_K)'(x)|$$

$$= \frac{1}{c^2}\Big[\int_{[x-1,x]\cap\{s\,:\,|r_K(s)|>d-\delta\}} |V'(r_K(s))|ds + \int_{[x-1,x]\cap\{s\,:\,|r_K(s)|\le d-\delta\}} |V'(r_K(s))|ds\Big]$$
$$\le \frac{d^2}{\int_{\mathbb{R}} V'(r_K)r_K}\Big[\int_{[x-1,x]\cap\{s\,:\,|r_K(s)|>d-\delta\}} V'(r_K(s))r_K(s)ds + |V'(-d+\delta)|\Big]$$
$$\le \frac{d^2}{d-\delta} + \frac{d^2|V'(-d+\delta)|}{2K} =: C_\infty(K).$$

This is nonincreasing in $K$, proving iv) and completing the proof of Proposition 2.1.

# 3 High-energy limit

Here we prove Theorem 2 giving the asymptotic shape of the solitary wave profile. The proof combines the a-priori estimates of the previous section, standard weak convergence methods, and the following trivial lower bound on the kinetic energy which complements the upper bound of Proposition 2.1 i):

**Lemma 3.1** *Let $q \in W^{1,2}((0,1))$, $q(0) - q(1) = d$. Then $\int_0^1 (q')^2 dx \ge d^2$, with equality if and only if $q(x) = -dx + c$ for some constant $c \in \mathbb{R}$.*

**Proof of Lemma 3.1** By weak lower semicontinuity of the functional under investigation in $W^{1,2}((0,1))$, the infimum is attained. The assertion follows from the fact that the Euler-Lagrange equation is $q'' = 0$.

**Proof of Theorem 2** Choose the translates $\tilde{q}_K$ so that $\max_{x\in\mathbb{R}} |\tilde{r}_K(x)| = |\tilde{r}_K(0)|$, $\tilde{q}_K(0) = 0$. To simplify the notation we drop the tildes in the sequel. The first step is to show that $r_K := q_K(\cdot + 1) - q_K(\cdot)$ satisfies

$$r_K(0) \to -d \;\; (K \to \infty). \tag{3.11}$$

Suppose otherwise, i.e. $\limsup_{K\to\infty} r_K(0) > -d$ for a subsequence. Since on any compact subset of $(-d, \infty)$, $V(r) \le Cr^2$ for some constant $C$, it follows that

$$K = \int_{\mathbb{R}} V(r_K(x))dx \le C\int_{\mathbb{R}} r_K(x)^2 dx \le C\int_{\mathbb{R}}\int_x^{x+1} (q_K'(s))^2 ds\, dx = 2CT(q_K),$$

contradicting the fact that by Proposition 2.1, $T(q_K)$ remains bounded as $K \to \infty$. This establishes (3.11).

The a-priori bounds of Proposition 2.1 give the following subsequential convergences as $K \to \infty$:

$$q_K \to q \text{ weak* in } W^{1,\infty}(\mathbb{R}), \text{ weakly in } L^1(\mathbb{R}), \text{ and weakly in } L^2(\mathbb{R}) \tag{3.12}$$

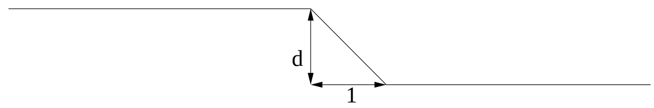



Figure 2: The limiting displacement profile $q_\infty$.

for some $q \in W^{1,\infty}(\mathbb{R})$ with $q' \in L^1(\mathbb{R})$, $q' \in L^2(\mathbb{R})$. In particular $q$ is continuous, hence so is $r := q(\cdot+1) - q(\cdot)$, and $q_K(x) \to q(x)$ for every (not just almost every) $x \in \mathbb{R}$.

We proceed to identify the limit $q$. By (3.11), $r(0) = -d$. Hence by Lemma 3.1 $\int_0^1 (q'(x))^2 dx \geq d^2$. On the other hand, by weak lower semicontinuity of the norm in $L^2(\mathbb{R})$ and Proposition 2.1 i), $\int_{\mathbb{R}} (q')^2 dx \leq \liminf_{K\to\infty} \int_{\mathbb{R}} (q_K')^2 dx \leq d^2$. Consequently $q' = 0$ in $\mathbb{R}\backslash(0,1)$ and (remembering the normalization $q(0) = 0$) $q(x) = -dx$ in $(0,1)$. Hence $q$ is equal to the function $q_\infty$ given in the statement of the Theorem. Moreover by uniqueness of the limit, the subsequential convergences (3.12) are valid for the whole sequence $q_K$. It remains to show that the convergences in fact occur in the strong norms asserted in the theorem. The preceding argument shows that $||q_K'||_{L^2(\mathbb{R})} \to ||q_\infty'||_{L^2(\mathbb{R})}$, which together with weak convergence of $q_K'$ to $q_\infty'$ in $L^2(\mathbb{R})$ implies strong convergence in $L^2(\mathbb{R})$. Next we show that

$$q_K' \to q_\infty' \text{ in } L^1(\mathbb{R}). \tag{3.13}$$

By the strong convergence of $q_K'$ in $L^2(\mathbb{R})$ and the fact that in bounded domains, $L^2$ convergence implies $L^1$ convergence, $q_K'|_{(0,1)} \to q_\infty'|_{(0,1)}$ strongly in $L^1((0,1))$, and so in particular $||q_K'||_{L^1((0,1))} \to ||q_\infty'||_{L^1((0,1))} = d$. On the other hand, by (3.12), weak lower semicontinuity of the norm in $L^1(\mathbb{R})$ and Proposition 2.1 iii),

$$d = ||q_\infty'||_{L^1(\mathbb{R})} \leq \liminf_{K\to\infty} ||q_K'||_{L^1(\mathbb{R})} \leq d.$$

Consequently all inequalities are equalities and $\lim_{K\to\infty} \int_{\mathbb{R}\backslash(0,1)} |q_K'| dx = 0$. This establishes (3.13). Finally, $L^p$ convergence of $q_K'$ follows from $L^1$ convergence and boundedness in $L^\infty$, and uniform convergence of $q_K$ follows from $L^1$ convergence of $q_K'$ and the fact that $q_K(0) = q_\infty(0) = 0$. The proof of Theorem 2 is complete.

# 4 Appendix

Here we prove the existence result of Theorem 1. This does not require to redo the concentration-compactness analysis of [FW94], but simply to make their result applicable to non-globally defined potentials with the help of a truncation argument.

**Proof of Theorem 1** We proceed in three steps. First, following [FW94] Section 6 we will introduce a globally defined potential $V^\epsilon$ which agrees with $V$ on $(-d+\epsilon, 0]$ for a suitably chosen $\epsilon > 0$, and appeal to [FW94, Theorem 1] to infer existence of a minimizer subject to the truncated and symmetrized constraint $U^\epsilon(q) := \int_{\mathbb{R}} V^\epsilon_{sym}(q(x+1)-q(x))dx = K$, where

$$V^\epsilon_{sym}(r) := V^\epsilon(-|r|).$$

Next we will show that this minimizer satisfies $|r(x)| \leq d-\epsilon$ for all $x \in \mathbb{R}$ and is hence a minimizer subject to the untruncated symmetrized constraint $U_{sym}(q) := \int_{\mathbb{R}} V_{sym}(q(x+1)-q(x))dx = K$, where

$$V_{sym}(r) := V(-|r|).$$

Finally, using (H3) we will show that $r(x) < 0$ and that it is a minimizer subject to the original constraint $U(q) = K$.

*Step 1.* For any $\epsilon \in (0, d)$, denote $m_\epsilon := \min_{[-d+\epsilon,0]} V'''$ and introduce the following function

$$M_\epsilon(u) := \begin{cases} m_\epsilon, & u \leq -d \\ \max\{m_\epsilon, V'''(u)\}, & u > -d \end{cases}$$

Then $M_\epsilon(u) \geq V'''(u)$ in $(-d, 0]$, $= V'''(u)$ in $[-d+\epsilon, \infty)$. Now define

$$V^\epsilon(r) := \int_0^r \int_0^s \Big[V''(0) + \int_0^t M_\epsilon(u)du\Big]dt\, ds.$$

Then $V^\epsilon(r) \leq V(r)$ in $(-d, \infty)$, $= V(r)$ in $[-d+\epsilon, \infty)$. Moreover, $V^\epsilon$ satisfies the requirements of [FW94] that $V^\epsilon \in C^2(\mathbb{R})$ and that $V^\epsilon(r)/r^2$ increases strictly with $|r|$ for $r < 0$. Hence for any given $K \in (0, \infty)$, [FW94] Theorem 1 yields existence of a minimizer $q = q^\epsilon$ (possibly depending on $\epsilon$) of $T$ subject to the constraint $U^\epsilon_{sym}(q) = K$, and gives the following properties for any minimizer: either $(q^\epsilon)' \leq 0$ or $(q^\epsilon)' \geq 0$; $q^\epsilon$ is a solution of (1.3) with $V$ replaced by $V^\epsilon_{sym}$, for some $c^\epsilon \neq 0$; $(c^\epsilon)^2 > V''(0)$.

*Step 2.* We now remove the truncation. Let $d_*(K) \in (0, d)$ be as defined in the proof of Proposition 2.1 and choose $\epsilon < d - d_*(K)$. Then the trial function $\overline{q}_{d_*(K)}$ from the proof of Proposition 2.1 satisfies $U^\epsilon_{sym}(\overline{q}_{d_*(K)}) = U_{sym}(\overline{q}_{d_*(K)}) = K$ and is hence admissible in both the truncated symmetrized variational problem and the untruncated symmetrized variational problem. Since $T(\overline{q}_{d_*(K)}) = \frac{d_*(K)^2}{2}$ but (see the Proof of Proposition 2.1 ii)) every function $q \in W^{1,2}_{loc}(\mathbb{R})$ satisfying $||q(\cdot+1)-q(\cdot)||_{L^\infty(\mathbb{R})} > d_*(K)$ has higher energy (i.e. $T(q) > \frac{d_*(K)^2}{2}$), it follows that the infimum of the untruncated symmetrized problem is attained, and that its set of minimizers equals the set of minimizers of the truncated symmetrized problem. Moreover we infer that every minimizer satisfies $||q(\cdot+1)-q(\cdot)||_{L^\infty(\mathbb{R})} < d$.

*Step 3.* It remains to undo the symmetrization. By the results of Step 1 and Step 2, there exists a minimizer $q_*$ to the symmetrized problem which satisfies $(q_*)' \leq 0$. Consequently this minimizer has unsymmetrized potential energy $U(q_*) = K$. We now claim the following:

$$\text{Whenever } q \text{ satisfies } U(q) = K \text{ and } T(q) \leq T(q_*) = \min_{U_{sym}(q)=K} T(q), \text{ then } r \leq 0. \tag{4.14}$$

Suppose not, i.e. suppose that for some such $q$, $r(x_0) > 0$ at some point $x_0 \in \mathbb{R}$. Since $q \in W^{1,2}_{loc}(\mathbb{R})$, $r$ is continuous and hence $r > 0$ on some interval. Moreover as in Step 2 we have $||r||_{L^\infty(\mathbb{R})} < d$. Since due to (H3) we have $V_{sym}(r) > V(r)$ for $r \in (0, d)$, it follows that $U_{sym}(q) > U(q)$. Hence there exists $\lambda < 1$ such that $U_{sym}(\lambda q) = K$. But now $T(\lambda q) = \lambda^2 T(q) < T(q) \leq \min_{U_{sym}(q)=K} T(q)$, a contradiction. This establishes (4.14). Consequently the infimum of the original problem is attained, and every minimizer of the original problem satisfies $r(x) \leq 0$ and is a minimizer of the symmetrized (and hence, by Step 2, also of the truncated symmetrized) problem. The results for solutions to these two problems derived Step 1 and Step 2 immediately imply Theorem 1 (ii), (iii) and (iv), and show that $(q_K)' \leq 0$. It remains to show that this latter inequality is sharp. This follows from the weak inequality, the fact that $r_K(x_0)$ must be strictly less than zero at some point $x_0$ (otherwise we would have $U(q_K) = 0$, contradicting the fact that $U(q_K) = K$), and iterative application of a simple lemma:

**Lemma 4.1** *Let $q \in W^{1,2}_{loc}(\mathbb{R})$ be any function with properties (ii), (iii) and (iv) of Theorem 1. If $r(x_0) < 0$ then $q'|_{(x_0,x_0+1)} < 0$ and $r|_{(x_0-1,x_0+1)} < 0$.*

**Proof of Lemma 4.1**. The first assertion follows from eq. (2.9) and the fact that for $x \in (x_0, x_0+1)$ the interval of integration $(x, x+1)$ intersects $\{x_0\}$. The second assertion follows from the definition of $r$ in terms of $q$, $r(x) = \int_x^{x+1} q'(s)ds$, and the fact that for $x \in (x_0-1, x_0+1)$ the interval of integration intersects the interval in which $q'$ has already been proven to be negative.

The proof of Lemma 4.1 and of Theorem 1 is complete.

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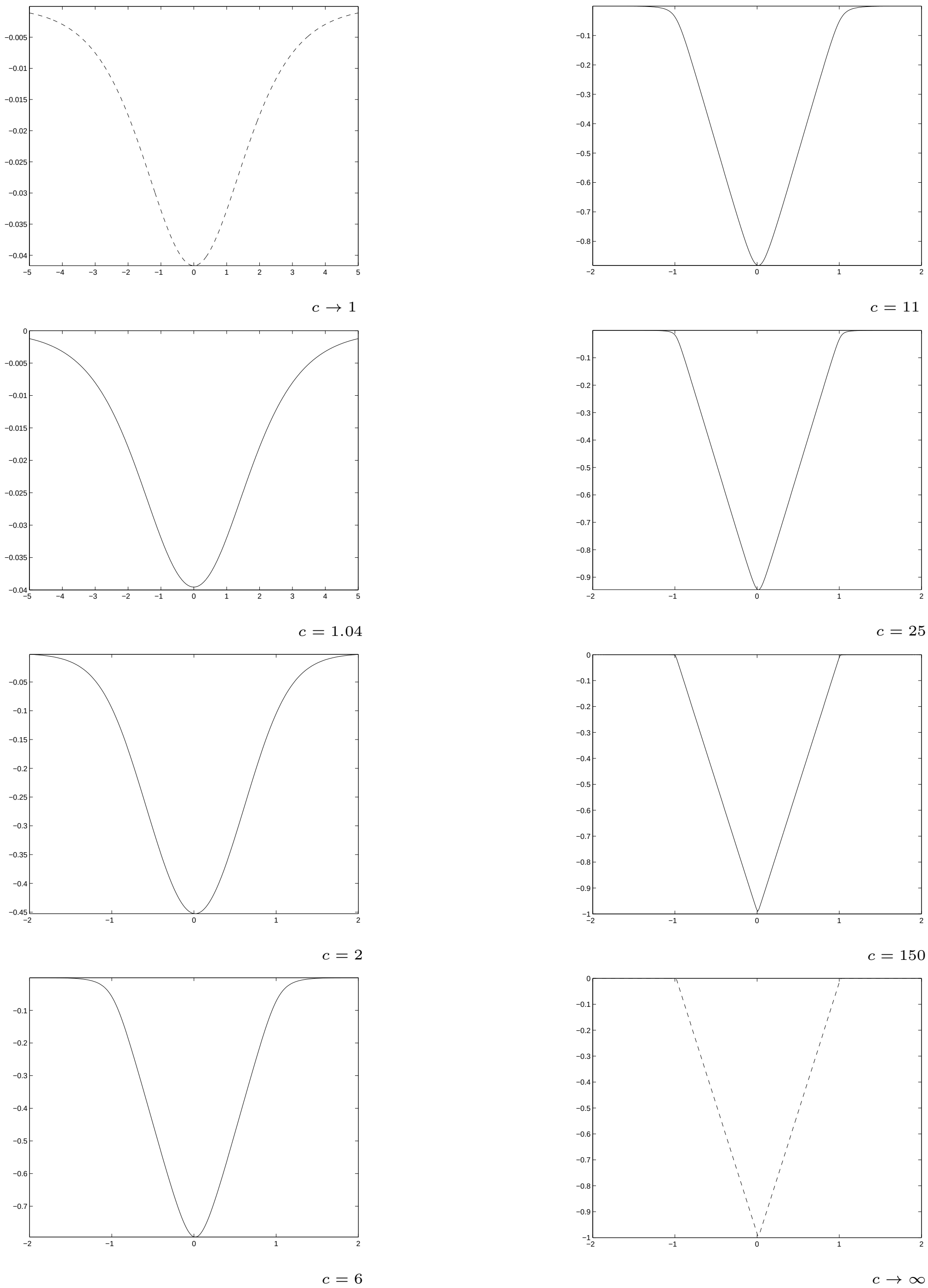


Figure 3: Theoretical and numerical profiles $r_c$ for $V(r) = \frac{1}{2}((r+1)^{-1} - 1)^2$ for several wave speeds $c$

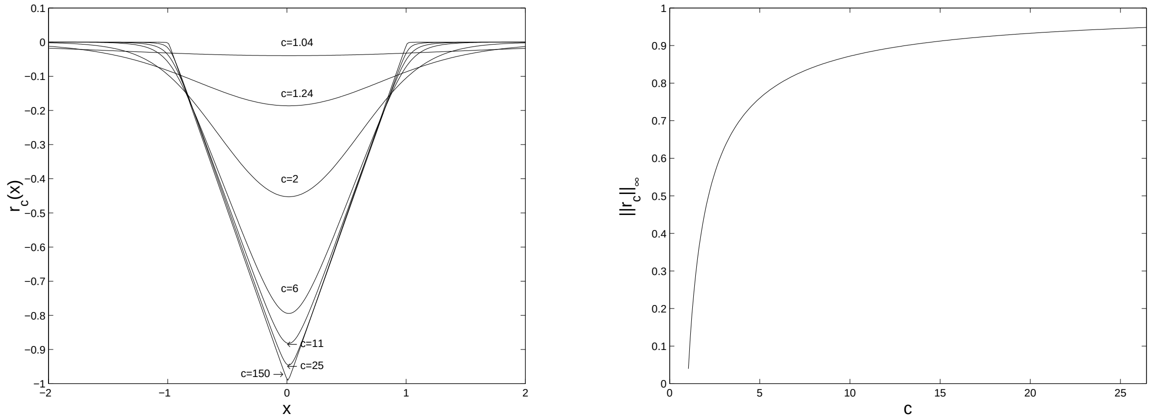


Figure 4: Comparison of different numerical profiles for $V(r) = \frac{1}{2}((r+1)^{-1} - 1)^2$ for changing speeds $c$ and their changing amplitude

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