Breathers from infinity in the anti-continuum limit

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The problem

The discrete Klein–Gordon (KG) equation in one dimension:

$$\ddot{u}_n + V'(u_n) = \gamma(u_{n+1} - 2u_n + u_{n-1}), \quad n \in \mathbb{Z},$$

where $\gamma > 0$ is the coupling constant and $V(u)$ is the nonlinear potential s.t.

P1 $V(x) \in C^4(\mathbb{R})$ and $V(-x) = V(x)$ for all $x \in \mathbb{R}$;

P2 $V(x) = \frac{1}{2}x^2 + \mathcal{O}(x^4)$ as $x \to 0$;

P3 $0 \leq V(x) \leq 1$ for all $x \in \mathbb{R}$;

$\gamma = 0$ is referred to as the *anti-continuum limit* of weakly coupled oscillators since the work of MacKay-Aubry (1994).

Discrete breathers

We would like to construct solutions in space

$$\mathbf{x}(t) \in H^2_{\rm per}((0,T); l^2(\mathbb{Z})),$$

so that

$$\mathbf{x}(t+T) = \mathbf{x}(t), \quad \lim_{|n|\to\infty} |x_n(t)| = 0, \quad t \in \mathbb{R}.$$

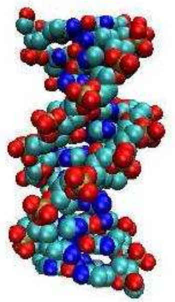
These solutions are referred to as the *discrete breathers*.

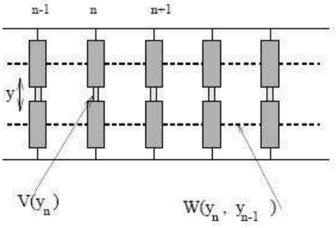
Additional simplifications thanks to reversibility in $t \in \mathbb{R}$ and $n \in \mathbb{Z}$:

$$x_n(-t) = x_n(t), \quad x_{-n}(t) = x_n(t), \quad n \in \mathbb{Z}, \;\; t \in \mathbb{R}.$$

Physical contexts

- Modeling of DNA (M. Peyrard, 2004)

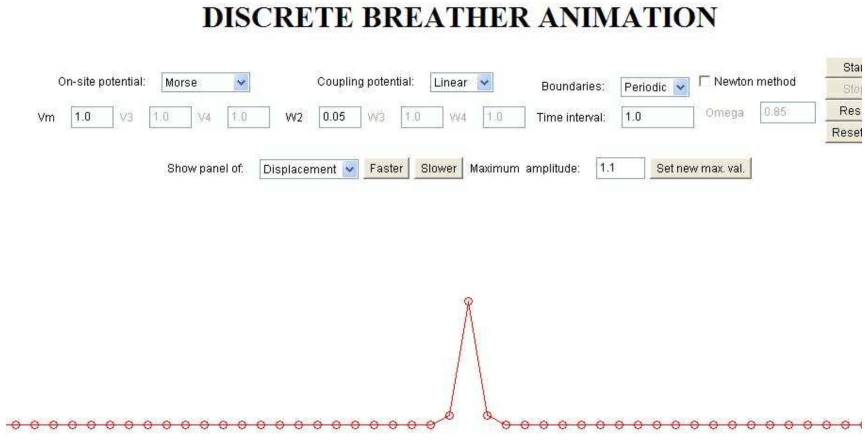




- Josephson junction arrays

- Solid state physics

http://www.mpipks-dresden.mpg.de/ andreym/dbanim/



Why anti-continuum limit?

The anti-continuum limit in KG and NLS lattices allows ...

- to continue uniquely solutions for small $\gamma > 0$ (MacKay-Aubry, 1994);
- to classify all solution branches for small $\gamma > 0$ from the limiting configuration for $\gamma = 0$ (Alfimov *et al.*, 2004)
- to count and approximate unstable eigenvalues in the spectral stability problem for small $\gamma > 0$ (Koukouloyannis, Kevrekidis, 2009)
- to study asymptotic stability and nonlinear dynamics analytically (P., Sakovich, in progress)

Oscillations at the central site

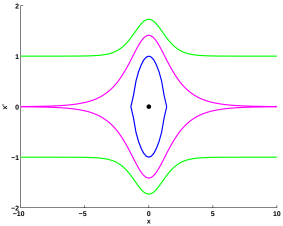
Let $\gamma = 0$ and consider the simplest discrete breather in the form

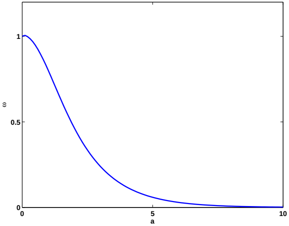
$$x_n(t) = 0, \quad n \in \mathbb{Z} \backslash \{0\}.$$

$x_0(t) \equiv x(t)$ is a T-periodic classical solution of

$$\ddot{x} + V'(x) = 0 \quad \Rightarrow \quad E = \frac{1}{2}\dot{x}^2 + V(x).$$

$V(x) = \tanh^2(x/\sqrt{2})$:





Small-amplitude and large-amplitude breathers

$E < 1$: There exist two T-periodic even solutions $x(t) \in H^2_{\rm per}(0,T)$ for $T > 2\pi$. The period $T = T(E)$ is at least C^1.

What if $E > 1$?

First answer: No T-periodic solutions exist at all.

Second answer:

$$\ddot{x}_0 + V'(x_0) = 2\gamma(x_1 - x_0) \quad \Rightarrow \quad \ddot{x}_0 + V'_\gamma(x_0) = 2\gamma x_1,$$

where $V_\gamma(x) = V(x) + \gamma x^2$, $\gamma > 0$.

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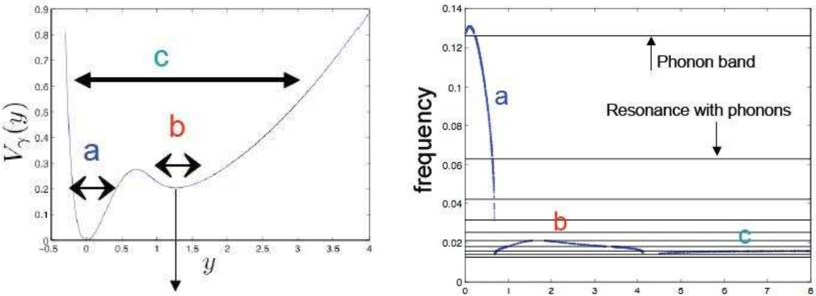
Large-amplitude breathers in $V_\gamma(x) = V(x) + \gamma x^2$

G. James, Levitt, Ferreira (Applicable Analysis, 2009) - large-amplitude breathers near large-amplitude stationary states



We would like to prove existence of large-amplitude breathers far from large-amplitude stationary states.

Review of MacKay-Aubry theory

Theorem: Fix $E < 1$ and assume that $T(E) \neq 2\pi\mathbb{N}$ and $T'(E) \neq 0$. There exists a small $\gamma_0(E) > 0$ such that for all $\gamma \in (0, \gamma_0)$ the dKG equation has a unique solution $\mathbf{x}(t) \in H^2_{\rm per}((0,T); l^2(\mathbb{Z}))$ such that $\gamma \mapsto \mathbf{x}(t)$ is C^1 and

$$\exists C > 0 : \quad \|\mathbf{x} - x\boldsymbol{\delta}_0\|_{H^2_{\rm per}} \leq C|\gamma|.$$

Here

$$(\boldsymbol{\delta}_0)_n = \begin{cases} 1, & n = 0, \\ 0, & n \neq 0 \end{cases}$$

and $x(t)$ is a solution of $\ddot{x} + V'(x) = 0$.

Two main steps in the proof:

- No resonances at other sites $n \neq 0$;
- No resonance at the central site $n = 0$.

No resonances at other sites $n \neq 0$

For $n \geq 1$, we have

$$\ddot{x}_n + x_n + N(x_n) = \gamma(x_{n+1} - 2x_n + x_{n-1}),$$

where $N(x) = V'(x) - x = \mathcal{O}(x^3)$ as $x \to 0$.

$H^2_{\rm per}(0,T)$ is a Banach algebra with respect to multiplication. For all $x \in B_\delta(H^2_{\rm per})$, there is $C(\delta) > 0$ such that

$$\|N(x)\|_{H^2_{\rm per}} \leq C(\delta)\|x\|^3_{H^2_{\rm per}}.$$

If linear operator L is invertible and there is $C > 0$ such that

$$\forall \mathbf{f} \in L^2_{\rm per}((0,T); l^2(\mathbb{N})) : \quad \|L^{-1}\mathbf{f}\|_{H^2_{\rm per}} \leq C\|\mathbf{f}\|_{L^2_{\rm per}},$$

the Implicit Function Theorem is applied. Therefore, there is a unique map $H^2_{\rm per}(0,T) \ni x_0 \mapsto \mathbf{x} \in H^2_{\rm per}((0,T); l^2(\mathbb{N}))$ for small $\gamma > 0$ so that for all $x_0 \in B_\delta(H^2_{\rm per})$

$$\exists C(\delta) > 0 : \quad \|\mathbf{x}\|_{H^2_{\rm per}} \leq C(\delta)\gamma.$$

Invertibility of the linear operator

We have

$$\ddot{x}_n + x_n - \gamma(x_{n+1} - 2x_n + x_{n-1}) = f_n, \quad n \geq 1$$

with $x_0 = 0$ and $\mathbf{f} \in L^2_{\rm per}((0,T); l^2(\mathbb{N}))$.

We can use the discrete sine-Fourier transform

$$x_n(t) = \int_{-\pi}^{\pi} \hat{x}(q,t)\sin(nq)dq, \quad n \in \mathbb{N}$$

and the Fourier series

$$\hat{x}(q,t) = \sum_{m\in\mathbb{Z}} \hat{x}_m(q)e^{im\omega t}, \quad \omega = \frac{2\pi}{T}.$$

Then, we have

$$\left(1 - m^2\omega^2 + 2\gamma - 2\gamma\cos(q)\right)\hat{x}_m(q) = \hat{f}_m(q), \quad q \in [-\pi,\pi], \;\; m \in \mathbb{Z}.$$

No resonances occur if $\omega^{-1} \notin \mathbb{N}$ and γ is small.

No resonances at the central site $n = 0$

For $n = 0$, we have

$$\ddot{x}_0 + V'(x_0) = 2\gamma(x_1 - x_0)$$

Let $x_0 = x + u$ and write

$$L_0 u + N_0(u) \equiv \ddot{u} + V''(x)u + \frac{1}{2}V'''(x)u^2 + ... = 2\gamma(x_1 - x - u)$$

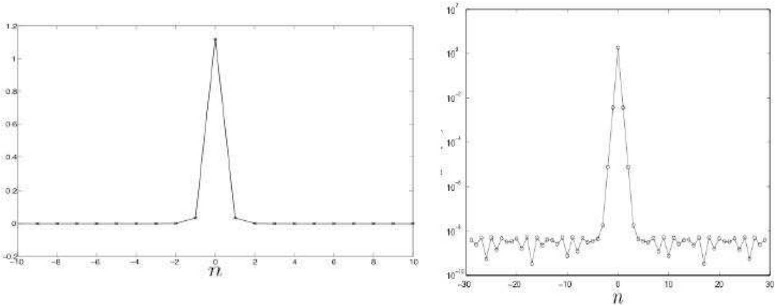
We have $L_0 \dot{x} = 0$ but $\dot{x}$ is odd. The second solution of $L_0 u = 0$ is even but not periodic if $T'(E) \neq 0$. Therefore, there is $C > 0$ such that

$$\forall f \in L^2_{\rm per}(0,T) : \quad \|L_0^{-1} f\|_{H^2_{\rm per}} \leq C \|f\|_{L^2_{\rm per}}.$$

By the Implicit Function Theorem, there is a unique map $\mathbb{R} \ni \gamma \mapsto u \in H^2_{\rm per}(0,T)$ such that

$$\exists C > 0 : \quad \|u\|_{H^2_{\rm per}} \leq C\gamma.$$

G. James, Levitt, Ferreira (Applicable Analysis, 2009) - large-amplitude breathers near large-amplitude stationary states



Left: the breather in the non-resonance domain;
Right: the breather in the resonance domain.

Suspense story for large-amplitude breathers

Let us add another assumption on $V(x)$:
(P4) $V'(x)$ is compactly supported on $[-a_0, a_0]$ and

(a) $\lim_{x\to\infty} V(x) = V_\infty \in (0,1)$
(b) $\int_0^{a_0} xV'(x)dx \neq 0$.

Theorem: Fix $E > 1$. Let $x(t)$ be a T-periodic solution of $\ddot{x} + V'_\gamma(x) = 0$ for small $\gamma > 0$. For sufficiently small γ, there exists a T-periodic solution $\mathbf{x}(t) \in H^1_{\rm per}((0,T); l^2(\mathbb{Z}))$ of the dKG equation such that

$$\exists C > 0 : \quad \sup_{t\in[0,T]} |x_0(t) - x(t)| \leq C\gamma^{-1/4}, \quad \sup_{n\geq 1} \sup_{t\in[0,T]} |x_n(t)| \leq C\gamma^{1/4}.$$

Remark: $\|x\|_{L^\infty_{\rm per}} = \mathcal{O}(\gamma^{-1/2})$.

Large-amplitude long-period breathers

Feature # 1: Large-amplitude oscillations in $-a \leq x(t) \leq a$, where

$$E = \gamma a^2 + V(a) \quad \Rightarrow \quad E - V_\infty \leq \gamma a^2 \leq E,$$

so that $a = \mathcal{O}(\gamma^{-1/2})$.

Feature # 2: Large period of oscillations

$$T = 2\sqrt{2} \int_0^a \frac{dx}{\sqrt{E - \gamma x^2 - V(x)}} = \frac{2\sqrt{2}}{\sqrt{\gamma}} \int_0^{\pi/2} \frac{d\theta}{\sqrt{1 + W(\theta)}},$$

where

$$\forall \theta \in (0, \pi/2] : \quad W(\theta) = \frac{V(a) - V(a \sin\theta)}{\gamma a^2 \cos^2\theta} \to 0 \quad \text{as} \quad \gamma \to 0.$$

Rescaling transformation

By the Dominant Convergence Theorem, $T = \mathcal{O}(\gamma^{-1/2})$.

Feature # 3: Scaling transformation brings about a linear oscillator with a singular nonlinear perturbation.

Let

$$x(t) = \frac{X(\tau)}{\gamma^{1/2}}, \quad \tau = \gamma^{1/2} t, \quad \Rightarrow \quad \|X\|_{L^\infty} = \mathcal{O}(1), \quad T_0 = \mathcal{O}(1).$$

New equations in rescaled variables

$$\ddot{X} + 2X + \gamma^{-1/2} V'(\gamma^{-1/2} X) = 0 \quad \Rightarrow \quad E = \frac{1}{2}\dot{X}^2 + X^2 + V(\gamma^{-1/2} X).$$

Therefore, $\|X\|_{H^1_{\rm per}} = \mathcal{O}(1)$ as $\gamma \to 0$, whereas $\|X\|_{H^2_{\rm per}} \to \infty$.

No resonance with other sites

Feature # 4: Proximity of resonances with other sites.

For $n \geq 1$, we have two systems

$$n \geq 2: \quad \gamma \ddot{X}_n + X_n + N(X_n) = \gamma (X_{n+1} - 2X_n + X_{n-1})$$

and

$$n = 1: \quad \gamma \ddot{X}_1 + X_1 + N(X_1) = \gamma (X_2 - 2X_1) + \gamma^{1/2} X_0,$$

where $N(X) = V'(X) - X = \mathcal{O}(X^3)$ as $X \to 0$.

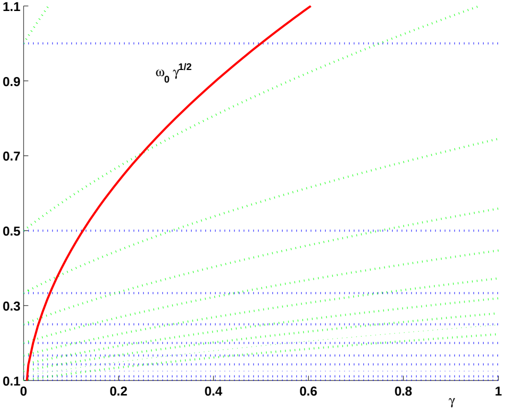
Using the same Fourier transforms for the linear part, we have

$$\left(1 - \gamma m^2 \omega_0^2 + 2\gamma - 2\gamma \cos(q)\right) \hat{X}_m(q) = \hat{F}_m(q), \quad q \in [-\pi, \pi], \;\; m \in \mathbb{Z},$$

where $\omega = \omega_0 \gamma^{1/2}$ is the breather frequency ($\omega_0 \sim \sqrt{2}$) and the phonon frequencies lie in the intervals

$$\frac{1}{m} \leq \omega \leq \frac{\sqrt{1 + 4\gamma}}{m}.$$

No resonance with other sites



No resonances occur in the disjoint set

$$C_{\omega_0} = \cup_{m \geq m_0} (\Gamma_m, \gamma_m), \quad \Gamma_m = \frac{\kappa^2}{\omega_0^2 (m+1)^2 - 4}, \quad \gamma_m = \frac{\kappa^2}{\omega_0^2 m^2}.$$

No resonance with other sites

Fix $\delta \in (0,1)$ and let $\tilde{C}_{\omega_0,\delta} = \cup_{m \geq m_0} (\tilde{\Gamma}_m, \tilde{\gamma}_m) \subset C_{\omega_0}$ with

$$\tilde{\Gamma}_m = \frac{\kappa^2}{\omega_0^2((m+1)^2 - \delta(m+1)) - 4}, \quad \tilde{\gamma}_m = \frac{\kappa^2}{\omega_0^2(m^2 + \delta m)}.$$

For any $\gamma \in \tilde{C}_{\omega_0,\delta}$, we have

$$\exists C > 0 : \quad \forall \mathbf{f} \in L^2_{\rm per}((0,T); l^2(\mathbb{N})) : \quad \|L^{-1}\mathbf{f}\|_{L^2_{\rm per}} \leq C\gamma^{-1/2}\|\mathbf{f}\|_{L^2_{\rm per}},$$

Back to equation

$$n = 1 : \quad \gamma\ddot{X}_1 + X_1 + N(X_1) = \gamma(X_2 - 2X_1) + \gamma^{1/2}X_0,$$

No fixed-point iterations are possible as $\|X_0\|_{H^1_{\rm per}} = \mathcal{O}(1)$!..

Normal form transformation

Feature # 5: Normal form transformation

$$X_1 = Y_1 + \gamma^{1/2} X_0, \quad X_n = Y_n, \;\; n \geq 2.$$

Then,

$$n = 1: \quad \gamma \ddot{Y}_1 + Y_1 + N(Y_1 + \gamma^{1/2} X_0) = \gamma (Y_2 - 2Y_1) - \gamma^{3/2} (\ddot{X}_0 + 2X_0).$$

Question: What do we know about $\|\ddot{X}_0 + 2X_0\|_{H^1_{\rm per}}$?

Bounds on $\ddot{X}_0 + 2X_0$

Let X_0 satisfy

$$\ddot{X}_0 + 2X_0 + \gamma^{-1/2} V'(\gamma^{-1/2} X_0) = 0.$$

Thanks to the compact support of $V'(x)$ on $[-a_0, a_0]$, we have $|X(\tau)| \leq a_0 \gamma^{1/2}$ for time interval $|\Delta T_0| = \mathcal{O}(\gamma^{1/2})$ as $\gamma \to 0$. As a result, we have

Feature # 6: growth of $\|\ddot{X}_0 + 2X_0\|_{H^1_{\rm per}}$:

$$\begin{aligned}
\int_0^{T_0} |\ddot{X}_0 + 2X_0|^2 d\tau &= \gamma^{-1} \int_0^{T_0} |V'(\gamma^{-1/2} X(\tau))|^2 d\tau \leq C_1 \gamma^{-1/2}, \\
\int_0^{T_0} |(\ddot{X}_0 + 2X_0)'|^2 d\tau &= \gamma^{-2} \int_0^{T_0} |\dot{X}(\tau)|^2 |V''(\gamma^{-1/2} X(\tau))|^2 d\tau \leq C_2 \gamma^{-3/2}.
\end{aligned}$$

Therefore,

$$\exists C > 0 : \quad \|\ddot{X}_0 + 2X_0\|_{H^1_{\rm per}} \leq C \gamma^{-3/4}.$$

No resonance at the central site $n = 0$

Back to equation

$$n = 1: \quad \gamma \ddot{Y}_1 + Y_1 + N(Y_1 + \gamma^{1/2} X_0) = \gamma(Y_2 - 2Y_1) - \gamma^{3/2}(\ddot{X}_0 + 2X_0).$$

Fixed-point arguments now give

$$\exists C > 0: \quad \forall X_0 \in H^1_{\rm per}(0, T_0): \quad \|Y_1\|_{H^1_{\rm per}} \leq C\gamma^{1/4} \|X_0\|_{H^1_{\rm per}}.$$

At the central site $n = 0$, we have

$$n = 0: \quad \ddot{X}_0 + 2X_0 + \gamma^{-1/2} V'(\gamma^{-1/2} X_0) = 2\gamma^{1/2} Y_1 + 2\gamma X_0.$$

Feature # 7: almost harmonic oscillations

$$T_0 = \sqrt{2}\pi \left(1 - \frac{\gamma^{1/2}}{\pi(E - V_\infty)^{3/2}} \int_0^{a_0} x V'(x) dx + o(\gamma^{1/2}) \right).$$

But

$$V'(\gamma^{-1/2} X_0) = V'(\gamma^{-1/2} X) + \gamma^{-1/2} V''(\gamma^{-1/2} X)(X_0 - X) + \ldots$$

and the nonlinear terms become too big for fixed-point arguments!..

No resonance at the central site $n = 0$

Let us use the Fourier cosine-series

$$\forall F \in L^2_{\rm per}(0,T_0): \quad F(\tau) = \sum_{m \in \mathbb{N}{\rm odd}} F_m \cos(m\omega_0 \tau), \quad \omega_0 = \frac{2\pi}{T_0}.$$

and consider the nonlinear equation

$$\ddot{Z}(\tau) + 2Z(\tau) + \gamma^{-1/2} V'(\gamma^{-1/2} Z(\tau)) = \gamma^{1/2} F(\tau),$$

Then, we have

$$(2 - m^2\omega_0^2) Z_m + W_m(\mathbf{Z}) = \gamma^{1/2} F_m, \quad m \in \mathbb{N},$$

where

$$W_m(\mathbf{Z}) = \frac{2}{T_0 \gamma^{1/2}} \int_0^{T_0} V'(\gamma^{-1/2} Z(\tau)) \cos(m\omega_0 \tau) d\tau.$$

No resonance at the central site $n = 0$

Thanks to the compact support of $V'(x)$ on $[-a_0, a_0]$, we have

$$\exists C > 0: \quad \forall Z \in H^1_{\rm per}(0, T_0): \quad |W_m(\mathbf{Z})| \leq C m \gamma^{1/2}, \quad m \in \mathbb{N} \text{ odd},$$

The vector $\mathbf{Z} = (Z_1, Z_3, Z_5, ...)$ is split into two parts Z_1 and $\tilde{\mathbf{Z}} = (Z_3, Z_5, ...)$. Then, we have a continuous map $\mathbb{R} \ni Z_1 \mapsto \tilde{\mathbf{Z}} \in l^2(\mathbb{N})$ such that

$$\exists C > 0: \quad \forall Z_1 \in \mathbb{R}: \quad \|\tilde{\mathbf{Z}}\|_{l^\infty_1} + \|\tilde{\mathbf{Z}}\|_{l^2} \leq C \gamma^{1/2} \left(1 + \|\mathbf{F}\|_{l^2}\right).$$

We need $\tilde{\mathbf{Z}} \in l^2_1(\mathbb{Z})$ to control

$$\tilde{Z}(\tau) = \sum_{m \geq 3} Z_m \cos(m \omega_0 \tau)!$$

Final step - projection to Z_1

Eliminating $\tilde{Z}$, we obtain

$$(2-\omega_0^2)Z_1 + \frac{\gamma^{1/2}}{\pi Z_1^2}\int_0^{a_0} \frac{xV'(x)}{(1-\frac{\gamma x^2}{Z_1^2})^{1/2}} dx = \gamma^{1/2} F_1.$$

By the Implicit Function Theorem, this gives

$$\exists C > 0 : \quad |Z_1 - (E - V_\infty)^{1/2}| \leq C \|F\|_{L^2} \text{ small.}$$

By fixed-point iterations, this construction finally gives

$$\|X_0 - X\|_{H^1_{\rm per}} \leq C\gamma^{1/4}.$$