Supplementary Material for
An energy-based stability criterion for solitary traveling waves in Hamiltonian lattices

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I. PROOFS OF SOME RESULTS IN THE MAIN TEXT

In this section, we prove Propositions 4.1 and 4.2 and Lemma 5.1 in the main text.

A. Proof of Proposition 4.1

Proof. Suppose $\tilde{S}_+\mathcal{E}_2(1,0)Y_0 = \mu Y_0$. Letting $Y(\tau) = \mathcal{E}_2(\tau,0)Y_0$, we have

$$\begin{aligned}Y(\tau+1) &= \mathcal{E}_2(\tau+1,1)\mathcal{E}_2(1,0)Y_0 = \mathcal{E}_2(\tau+1,1)\tilde{S}_-\mu Y_0 = \tilde{S}_-\mathcal{E}_2(\tau,0)\tilde{S}_+\tilde{S}_-\mu Y_0\\ &= \tilde{S}_-\mu\mathcal{E}_2(\tau,0)Y_0 = \tilde{S}_-\mu Y(\tau),\end{aligned}$$

where we used the fact that $X_{tw}(\tau+1) = \tilde{S}_- X_{tw}(\tau)$ and that the operator $D\mathcal{A}$ in

$$\begin{aligned}c\frac{d}{d\tau}Y(\tau) &= D\mathcal{A}(X_{tw}(\tau))Y(\tau), \quad \tau\in[\tau_0,\tau_1]\\ Y(\tau_0) &= Y_0.\end{aligned} \tag{1}$$

satisfies $D\mathcal{A}(\tilde{S}_\pm x) = \tilde{S}_\pm D\mathcal{A}(x)\tilde{S}_\mp$. Thus $Z_{tw}(\tau) = e^{-\log(\mu)\tau}Y(\tau)$ is a traveling wave solution of

$$\lambda Z_{tw} = \mathcal{L}Z_{tw}, \qquad \mathcal{L} = \frac{1}{c}D\mathcal{A}(X_{tw}) - \frac{d}{d\tau} = \frac{1}{c}J\frac{\partial^2\mathcal{H}}{\partial X^2}\bigg|_{X=X_{tw}} - \frac{d}{d\tau}, \tag{2}$$

with $\lambda = \log(\mu)$, satisfying $Z_{tw}(\tau+1) = \tilde{S}_- Z_{tw}(\tau)$.

Conversely, if $Y(\tau) = Z_{tw}(\tau)e^{\lambda\tau}$ solves

$$\frac{d}{d\tau}Y(\tau) = \frac{1}{c}D\mathcal{A}(X_{tw}(\tau))Y(\tau) = \frac{1}{c}J\frac{\partial^2\mathcal{H}}{\partial X^2}\bigg|_{X=X_{tw}}Y(\tau). \tag{3}$$

and $Z_{tw}(\tau)$ solves (2), we set $Y_0 = Y(0) = Z_{tw}(0)$, so that

$$\mathcal{E}_2(1,0)Y_0 = Y(1) = e^{\lambda}Z_{tw}(1) = e^{\lambda}\tilde{S}_- Z_{tw}(0) = \tilde{S}_-\mu Y_0,$$

so Y_0 is an eigenfunction of $\tilde{S}_+\mathcal{E}_2(\tau_1,\tau_0)$ associated with the eigenvalue $\mu = \mathrm{e}^{\lambda}$. $\square$

B. Proof of Proposition 4.2

Proof. Note that if $\lambda Z_0 = \mathcal{L}Z_0$ and $(\mathcal{L} - \lambda I)Z_1 = Z_0$, then $\tilde{Y}_1(\tau) = e^{\lambda\tau}(Z_1(\tau) + \tau Z_0(\tau))$ solves (3). Similarly, if

$$(\mathcal{L} - \lambda I)^k Z_{k-1} = (\mathcal{L} - \lambda I)^{k-1} Z_{k-1} = ... = (\mathcal{L} - \lambda I)Z_1 = Z_0, \tag{4}$$

then $\tilde{Y}_k(\tau) = e^{\lambda\tau}(\sum_{j=0}^{k} \frac{1}{j!}\tau^j Z_{k-j}(\tau))$ solves (3). Let $\tilde{Y}_1 = \tilde{Y}_1(0) = Z_1(0)$, then

$$\mathcal{E}_2(1, 0)\tilde{Y}_1 = \tilde{Y}_1(1) = e^{\lambda}(Z_0(1) + Z_1(1)) = \mu\tilde{S}_-(Z_0(0) + Z_1(0)),$$

where $\mu = e^{\lambda}$, and thus $(\tilde{S}_+\mathcal{E}_2(1, 0) - \mu I)\tilde{Y}_1 = \mu\tilde{Y}_0$. Using mathematical induction, we can show that if $\tilde{Y}_j = \tilde{Y}_j(0) = Z_j(0)$ for $1 \leq j \leq k$, then $(\tilde{S}_+\mathcal{E}_2(1, 0) - \mu I)\tilde{Y}_j = \mu(\sum_{i=0}^{j-1} \frac{1}{(j-i)!}\tilde{Y}_i)$. We claim that there exists a (non-unique) lower triangular matrix $\Omega = (\Omega_{ij})_{0\leq i,j\leq k}$ such that for $\tilde{Y}_0 = Z_0(0)$ and $Y_j = \sum_{i=0}^{j} \Omega_{ji}\tilde{Y}_i$ for $0 \leq j \leq k$ we have

$$(\tilde{S}_+\mathcal{E}_2(\tau_1, \tau_0) - \mu I)^k Y_k = (\tilde{S}_+\mathcal{E}_2(\tau_1, \tau_0) - \mu I)^{k-1} Y_{k-1} = ... = (\tilde{S}_+\mathcal{E}_2(\tau_1, \tau_0) - \mu I)Y_1 = Y_0. \tag{5}$$

To prove the existence of such Ω, let $R_1 = (R_{1,j,i})_{0\leq j,i\leq k}$ and $R_2 = (R_{2,j,i})_{0\leq j,i\leq k}$ be such that

$$R_{1,ji} = \begin{cases} 0, & i \geq j, \\ \frac{1}{(j-i)!}, & i < j \end{cases}, \qquad R_{2,ji} = \begin{cases} 1, & i = j-1, \\ 0, & i \neq j-1. \end{cases}$$

Then we have

$$(\tilde{S}_+\mathcal{E}_2(1, 0) - \mu I)\tilde{Y} = \mu R_1\tilde{Y}, \quad (\tilde{S}_+\mathcal{E}_2(1, 0) - \mu I)Y = R_2 Y,$$

where $Y = \Omega\tilde{Y}$, which implies

$$\mu\Omega R_1 = R_2\Omega.$$

By comparing the terms on both sides, one can verify that given Ω_{00}, one can compute the other diagonal terms $\Omega_{11}, \Omega_{22}, \ldots, \Omega_{kk}$. Once all diagonal terms are known, given Ω_{10}, one can solve for $\Omega_{21}, \Omega_{32}, ..., \Omega_{k(k-1)}$. Assuming Ω_{ji} are known for any $j - i < m$ and given Ω_{m0}, one can then obtain $\Omega_{(m+1)1}, \Omega_{(m+2)2}, \ldots, \Omega_{k(k-m)}$. Following this procedure, a matrix Ω can be found for given constants Ω_{j0}, $0 \leq j \leq k$. In particular, for $k = 3$ one choice of Ω is

$$\Omega = \begin{pmatrix} \mu^3 & 0 & 0 & 0 \\ 0 & \mu & 0 & 0 \\ 0 & \frac{1}{2}\mu & \mu & 0 \\ 0 & \frac{1}{3} & -1 & 1 \end{pmatrix}.$$

To prove the converse, we assume that (5) holds and let $\tilde{Y}_j = \sum_{i=0}^{k} \Omega^{-1}_{ji} Y_i$ for $0 \leq j \leq k$, with Ω defined above. Then for $1 \leq j \leq k$, $(\tilde{S}_+\mathcal{E}_2(1, 0) - \mu I)\tilde{Y}_j = \mu(\sum_{i=0}^{j-1} \frac{1}{(j-i)!}\tilde{Y}_i)$. Let $\tilde{Y}_0(\tau) = \mathcal{E}_2(\tau, 0)\tilde{Y}_0$ and $\tilde{Y}_j(\tau) = \mathcal{E}_2(\tau, 0)\tilde{Y}_j$ for $1 \leq j \leq k$, then $\tilde{Y}_j(\tau + 1) = \tilde{S}_-\mu(\sum_{i=0}^{j} \frac{1}{(j-i)!}\tilde{Y}_i(\tau))$. Using mathematical induction, one can show that $\tilde{Y}_j(\tau)$ has the form $\tilde{Y}_j(\tau) = e^{\lambda\tau}(\sum_{i=0}^{j} \frac{1}{i!}\tau^j Z_{j-i}(\tau))$, where $Z_j(\tau)$ are traveling waves, i.e., satisfy $Z_j(\tau+1) = \tilde{S}_- Z_j(\tau)$, for $0 \leq j \leq k$. Moreover, since $\tilde{Y}_j(\tau)$ solves (3), one can show $\lambda Z_0 = \mathcal{L}Z_0$ and (4) hold. □

C. Proof of Lemma 5.1.

Proof. Using the arguments similar to the ones leading to Propositions 5.1 and 5.2, one can show that $\lambda = \mathcal{O}(\epsilon^{1/(n-2)})$ in this case. To be more specific, using

$$\mathcal{L}(\partial_\tau X_{tw}(\tau; c)) = 0 \tag{6}$$

and

$$\mathcal{L}(c\partial_c X_{tw}(\tau; c)) = \partial_\tau X_{tw}(\tau; c), \tag{7}$$

we can similarly obtain the coefficients g_j and f_j (as well as the analogs of h_j defined in (23)). Moreover, from $0 = Q_0 g_1 + Q_1 g_0$ we can derive the n-dimensional version of $K_{00} = 0$, which eliminates the possibility of $\lambda \sim \mathcal{O}(\epsilon^{1/n})$. Using symmetries or $K_{10} = K_{01}$ we rule out the case $\lambda \sim \mathcal{O}(\epsilon^{1/(n-1)})$. Below we show that $2K_{20} \neq K_{11}$ is satisfied, so that $\lambda = \mathcal{O}(\epsilon^{1/(n-2)})$ can be achieved. Substituting $\lambda = \epsilon^{1/(n-2)}\lambda_1 + \epsilon^{2/(n-2)}\lambda_2 + \epsilon^{3/(n-2)}\lambda_3 + \ldots$ and $Z = Z_0 + \epsilon^{1/(n-2)} Z_1 + \epsilon^{2/(n-2)} Z_2 + \epsilon^{3/(n-2)} Z_3 + \ldots$ into $\lambda Z = \mathcal{L} Z$, we obtain

$$\begin{aligned}
\mathcal{L}_0 Z_j &= \sum_{k=1}^{j} \lambda_k Z_{j-k}, \quad j = 0,1,...,n-3 \\
\mathcal{L}_0 Z_{n-2} + \mathcal{L}_1 Z_0 &= \sum_{k=1}^{n-2} \lambda_k Z_{n-2-k} \\
\mathcal{L}_0 Z_{n-1} + \mathcal{L}_1 Z_1 &= \sum_{k=1}^{n-1} \lambda_k Z_{n-1-k} \\
\mathcal{L}_0 Z_n + \mathcal{L}_1 Z_2 &= \sum_{k=1}^{n} \lambda_k Z_{n-k}.
\end{aligned}$$

Let $Z_j = \sum_{k=0}^{n-1} (C_{jk} e_k) + (Z_j)^{\#}$, where $(Z_j)^{\#} \in G_n^{\perp}$. Then the above equations are equivalent to

$$\begin{aligned}
A_0 C_j &= \sum_{k=1}^{j} \lambda_k C_{j-k}, \quad j = 0,1,...,n-3 && (8) \\
A_0 C_{n-2} + M^{-1} Q_1 C_0 &= \sum_{k=1}^{n-2} \lambda_k C_{n-2-k} && (9) \\
A_0 C_{n-1} + M^{-1} Q_1 C_1 &= \sum_{k=1}^{n-1} \lambda_k C_{n-1-k} && (10) \\
A_0 C_n + M^{-1} Q_1 C_2 &= \sum_{k=1}^{n} \lambda_k C_{n-k}, && (11)
\end{aligned}$$

where C_j and n-dimensional vectors with components C_{jk} and $M = (\langle J^{-1} e_j, e_k \rangle)$, $Q_0 = (\langle J^{-1} e_j, \mathcal{L}_0 e_k \rangle)$ and $Q_1 = K = (\langle J^{-1} e_j, \mathcal{L}_1 e_k \rangle)$ are $n \times n$ matrices, with $j, k = 0, \ldots, n-1$. As before, we have $Q_0 = M A_0$, where A_0 is the $n \times n$ matrix whose only nonzero entries are ones along the superdiagonal (generalization of the previous 4-by-4 matrix A_0), Q_0 and Q_1 are symmetric, and M is a skew-symmetric invertible matrix (recall that n is even). Setting $g_0 = (1, 0, 0, ..., 0)^T$, we obtain

$$\begin{aligned}
C_j &= \sum_{k=1}^{j} \lambda_k A_0^T C_{j-k} + C_{j,0} g_0, \quad j = 0,1,...,n-3 && (12) \\
C_{n-2} &= \sum_{k=1}^{n-2} \lambda_k A_0^T C_{n-2-k} - A_0^T M^{-1} Q_1 C_0 + C_{n-2,0} g_0, && (13) \\
C_{n-1} &= \sum_{k=1}^{n-1} \lambda_k A_0^T C_{n-1-k} - A_0^T M^{-1} Q_1 C_1 + C_{n-1,0} g_0, && (14) \\
C_n &= \sum_{k=1}^{n} \lambda_k A_0^T C_{n-k} - A_0^T M^{-1} Q_1 C_2 + C_{n,0} g_0. && (15)
\end{aligned}$$

With $C_{00} = 1$, we get $C_{j,j} = \lambda_1^j$ and $C_{j,k} = 0$ for $0 \leq j \leq (n-3)$ and $j < k$. The last row of (13) is $K_{00} = 0$; the last row of (14) can be directly verified by using symmetries.

The last row of (11) is the same as the last row of $M^{-1} Q_1 C_2 = \lambda_1 C_{n-1}$, which yields

$$\alpha_1 \lambda_1^n + (2K_{20} - K_{11}) \lambda_1^2 = 0. \qquad (16)$$

Similar to (5.32) in the main text, we can show that the coefficient in front of λ_1^2 equals $-H''(c_0)$. Indeed, using $\nabla\mathcal{H}$ and $\nabla^2\mathcal{H}$ to simplify notation and recalling the symmetry of K, we have

$$\begin{aligned}
H''(c_0) &= 2\langle \nabla\mathcal{H}, U_2\rangle + \langle U_1, \nabla^2\mathcal{H} U_1\rangle \\
&= 2c_0\langle J^{-1}e_0, U_2\rangle + c_0\langle U_1, J^{-1}\mathcal{L}_0 U_1\rangle + c_0\langle U_1, J^{-1}\partial_\tau U_1\rangle \\
&= \langle e_1, J^{-1}(\partial_\tau U_1 - c_0\mathcal{L}_1 U_1)\rangle + \langle U_1, J^{-1}e_0\rangle + c_0\langle (f_{10}e_0 + \frac{1}{c_0}e_1), J^{-1}\partial_\tau U_1\rangle \\
&= \langle e_2, J^{-1}\mathcal{L}_1 e_0\rangle - \langle e_1, J^{-1}\mathcal{L}_1 e_1\rangle + 0 - c_0 f_{10}\langle e_1, J^{-1}\mathcal{L}_1 e_0\rangle + \langle (c_0 f_{10}e_1 + e_2), J^{-1}\mathcal{L}_1 e_0\rangle \\
&= -K_{20} + K_{11} + f_{10}c_0K_{10} - f_{10}c_0K_{10} - K_{20} \\
&= K_{11} - 2K_{20}.
\end{aligned} \tag{17}$$

Thus, nonzero roots of (16) satisfy

$$\lambda_1^{n-2} = \frac{K_{11} - 2K_{20}}{\alpha_1} = \frac{H''(c_0)}{\alpha_1}.$$

□

II. PROJECTION COEFFICIENTS

In this section, we provide some additional expressions for the projection coefficients arising in

$$\partial_\tau U_j = \sum_{k=0}^{3}(g_{jk}e_k) + (\partial_\tau U_j)^\#, \quad (\partial_\tau U_j)^\# \in G_4^\perp \tag{18}$$

and

$$U_j = \sum_{k=0}^{3}(f_{jk}e_k) + (U_j)^\#, \quad (U_j)^\# \in G_4^\perp. \tag{19}$$

We start with (18). Recall that $g_{0j} = \delta_{1,0}$ and that g_{1j} coefficients are given by (5.21). Using $0 = Q_0g_2 + Q_1g_1 + Q_2g_0$, we obtain $\sum_{j=1}^3 g_{1j}K_{0j} + L_{00} = 0$, and, recalling $g_1 = -A_0^TM^{-1}Q_1g_0 + g_{10}g_0$, we have

$$\begin{aligned}
g_2 &= -A_0^TM^{-1}Q_1g_1 - A_0^TM^{-1}Q_2g_0 + g_{20}g_0 \\
&= [(-A_0^TM^{-1}Q_1)^2 + (-A_0^TM^{-1}Q_2)]g_0 + (-A_0^TM^{-1}Q_1)g_{10}g_0 + g_{20}g_0.
\end{aligned} \tag{20}$$

This yields

$$\begin{aligned}
g_{21} &= \frac{\alpha_2^2K_{10}K_{11} - \alpha_1\alpha_2(-K_{12}K_{20} + K_{11}K_{30} + 2K_{10}K_{31})}{\alpha_1^4} \\
&\quad + \frac{K_{30}K_{31} - K_{20}K_{32} + K_{10}K_{33} + \alpha_2(g_{10}K_{10} + L_{00})}{\alpha_1^2} - \frac{g_{10}K_{30} + L_{30}}{\alpha_1} \\
g_{22} &= \frac{\alpha_1\alpha_2K_{10}K_{21} - \alpha_1^2(-K_{20}K_{22} + K_{10}K_{23} + K_{21}K_{30})}{\alpha_1^4} + \frac{g_{10}K_{20} + L_{20}}{\alpha_1} \\
g_{23} &= \frac{\alpha_2(-K_{10}K_{11}) + \alpha_1(K_{10}K_{13} - K_{12}K_{20} + K_{11}K_{30}) - \alpha_1^2(g_{10}K_{10} + L_{10})}{\alpha_1^3}.
\end{aligned} \tag{21}$$

Condition $\sum_{j=1}^3 g_{2j}K_{0j} + \sum_{j=0}^3 g_{1j}L_{0j} + B_{00} = 0$ follows from $0 = Q_0g_3 + Q_1g_2 + Q_2g_1 + Q_3g_0$, which together with g_1 and g_2 also yields

$$\begin{aligned}
g_3 &= -A_0^TM^{-1}Q_1g_2 - A_0^TM^{-1}Q_2g_1 - A_0^TM^{-1}Q_3g_0 + g_{30}g_0 \\
&= [(-A_0^TM^{-1}Q_1)^3 + (-A_0^TM^{-1}Q_1)(-A_0^TM^{-1}Q_2) \\
&\quad + (-A_0^TM^{-1}Q_2)(-A_0^TM^{-1}Q_1) + (-A_0^TM^{-1}Q_3)]g_0 \\
&\quad + [(-A_0^TM^{-1}Q_1)^2 + (-A_0^TM^{-1}Q_2)]g_{10}g_0 + (-A_0^TM^{-1}Q_1)g_{20}g_0 + g_{30}g_0,
\end{aligned}$$

resulting in

$$
\begin{aligned}
g_{31} &= -\frac{\sum_{j=0}^{3} g_{2j}K_{3j} + \sum_{j=0}^{3} g_{1j}L_{3j} + B_{30}}{\alpha_1} - \frac{\alpha_2}{\alpha_1} g_{33} \\
g_{32} &= \frac{\sum_{j=0}^{3} g_{2j}K_{2j} + \sum_{j=0}^{3} g_{1j}L_{2j} + B_{20}}{\alpha_1} \\
g_{33} &= -\frac{\sum_{j=0}^{3} g_{2j}K_{1j} + \sum_{j=0}^{3} g_{1j}L_{1j} + B_{10}}{\alpha_1}
\end{aligned}
\tag{22}
$$

To summarize, (5.21), (21) and (22) determine the projection coefficients g_{ij}, $i, j = 1, 2, 3$, in (18).

Considering now the coefficients in (19), (5.26)-(5.28) yield

$$
\begin{aligned}
f_1 &= \frac{1}{c_0} A_0^T g_0 + f_{10} g_0, \\
f_2 &= \frac{1}{2c_0}[A_0^T g_1 - A_0^T M^{-1}(Q_0 + c_0 Q_1) f_1] + f_{20} g_0 \\
&= \frac{1}{2c_0}[A_0^T g_1 - A_0^T M^{-1} Q_1 A_0^T g_0 - c_0 A_0^T M^{-1} Q_1 f_{10} g_0 - \frac{1}{c_0} A_0^T g_0] + f_{20} g_0, \\
f_3 &= \frac{1}{3c_0}[A_0^T g_2 - A_0^T M^{-1}(Q_1 + c_0 Q_2) f_1 - A_0^T M^{-1}(Q_0 + c_0 Q_1) 2 f_2] + f_{30} g_0 \\
&= \frac{1}{3c_0}[A_0^T g_2 - A_0^T M^{-1}(Q_1 + c_0 Q_2)(\frac{1}{c_0} A_0^T g_0 + f_{10} g_0) \\
&\quad -A_0^T M^{-1}(Q_0 + c_0 Q_1)(\frac{1}{c_0} A_0^T g_1 - \frac{1}{c_0} A_0^T M^{-1} Q_1 A_0^T g_0 - A_0^T M^{-1} Q_1 f_{10} g_0 \\
&\quad -\frac{1}{c_0^2} A_0^T g_0 + f_{20} g_0)] + f_{30} g_0.
\end{aligned}
$$

Using (5.26), we find that $f_1 = (f_{10}, \frac{1}{c_0}, 0, 0)^T$, which together with (5.27) yields

$$
\begin{aligned}
f_{21} &= \frac{\alpha_1^2(c_0 g_{10} - 1) + \alpha_2 c_0 (K_{11} + c_0 f_{10} K_{10}) - \alpha_1 c_0 (c_0 f_{10} K_{30} + K_{31})}{2\alpha_1^2 c_0^2} \\
f_{22} &= \frac{c_0 f_{10} K_{20} + K_{21} - K_{30}}{2\alpha_1 c_0}.
\end{aligned}
$$

and f_{23} in (5.30). Using (5.28) we obtain

$$
\begin{aligned}
f_{31} &= \frac{1}{3c_0}[g_{20} - \sum_{j=0}^{3} \frac{1}{\alpha_1}(K_{3j} + c_0 L_{3j}) f_{1j} - \sum_{j=0}^{3} c_0 \frac{1}{\alpha_1} K_{3j} 2 f_{2j} - 2 f_{21} - 2\frac{\alpha_2}{\alpha_1} f_{23}] - \frac{\alpha_2}{\alpha_1} f_{33} + \frac{g_{22}}{3c_0} + f_{30} \\
f_{32} &= \frac{1}{3c_0}[g_{21} - \sum_{j=0}^{3}(\frac{\alpha_2}{\alpha_1^2}(K_{0j} + c_0 L_{0j}) - \frac{1}{\alpha_1}(K_{2j} + c_0 L_{2j})) f_{1j} - \sum_{j=0}^{3} c_0 (\frac{\alpha_2}{\alpha_1^2} K_{0j} - \frac{1}{\alpha_1} K_{2j}) 2 f_{2j} - 2 f_{22}] \\
f_{33} &= \frac{1}{3c_0}[g_{22} - \frac{1}{\alpha_1}\sum_{j=0}^{3}(K_{1j} + c_0 L_{1j}) f_{1j} - \frac{1}{\alpha_1}\sum_{j=0}^{3} c_0 K_{1j} 2 f_{2j} - 2 f_{23}]
\end{aligned}
$$

To simplify some calculations, it is convenient to define $h_j = c_0 j f_j + (j-1) f_{j-1}$ for $j = 1, 2, 3$, so that

$$
\begin{aligned}
h_1 &= A_0^T g_0 + h_{10} g_0 \\
h_2 &= A_0^T g_1 - A_0^T M^{-1} Q_1 h_1 + h_{20} g_0 \\
h_3 &= A_0^T g_2 - A_0^T M^{-1} Q_2 h_1 - A_0^T M^{-1} Q_1 h_2 + h_{30} g_0
\end{aligned}
\tag{23}
$$

We note that the last rows of the equations (5.36)-(5.38) are closely connected to the constraints (6)–(7), one of the reasons for which is as follows:

Remark 1. *If the constant term in C_{2k} is given by g_k with $C_{2k,0} = g_{k,0}$, then the constant term in C_{2k+2} will be g_{k+1} with $C_{2k+2,0} = g_{k+1,0}$.*

Remark 2. *If the constant term in C_{2k-2} is given by g_{k-1} with $C_{2k-2,0} = g_{k-1,0}$ and the coefficient for λ_1 in C_{2k-1} is given by h_k with $h_{k,0} = 0$, then the coefficient for λ_1 in C_{2k+1} will be h_{k+1} with $h_{k+1,0} = 0$.*

By these two remarks, the constant terms in the last rows of (5.36)-(5.38) are always zero. A more involved calculation, omitted here, shows that the coefficients for λ_1 in the last rows of these equations also vanish. Similar techniques can be used in other cases, including the one considered in Sec. 5, to show the constant terms and λ_1 coefficients vanish in the last rows of the equations.

III. THE DEGENERATE CASE $H'(c_0) = H''(c_0) = 0$

In this section, we briefly discuss the degenerate case when $H'(c_0) = H''(c_0) = 0$ but $H'''(c_0) \neq 0$. For simplicity, we assume that $\dim(\mathrm{gker}(\mathcal{L}_0)) = 4$. Following the arguments in Proposition 5.1 and Proposition 5.2, one can show that the near-zero eigenvalues are at most $O(\epsilon)$. Proceeding as before, one obtains the following equation for λ_1:

$$\lambda_1^4 - b\lambda_1^2 = 0,$$

where

$$\begin{aligned} b = -\frac{1}{\alpha_1}\Bigg[&\frac{-2K_{01}K_{32} + 2K_{02}K_{22} - K_{03}^2 + K_{11}K_{31} - K_{12}^2}{\alpha_1} \\ &+ \frac{\alpha_2(2K_{21}K_{10} + K_{20}^2 - K_{11}^2)}{\alpha_1^2} + 2L_{02} - L_{11}\Bigg]. \end{aligned} \tag{24}$$

We omit the details. This yields

Lemma III.1. *Suppose all the assumptions in Theorem 5.1 hold except that $\partial_c^3(X_{tw,j}(\tau;c)) \in D^0([0,1])$ ($D_a^0([0,1])$ if weighted spaces are used), $H''(c_0) = 0$ and b defined in (24) is nonzero. Then there exist $c_1 < c_0$ and $c_2 > c_0$ such that for $c \in (c_1, c_2)$, the leading-order terms of nonzero eigenvalues of $\mathcal{L}$ will be*

$$\lambda = \pm\sqrt{b}(c - c_0) + o(|c - c_0|).$$

It is not clear whether the coefficient b is related to $H'''(c_0)$, which is given by

$$\begin{aligned} H'''(c_0) = 2\Bigg[&\frac{1}{\alpha_1}(-3K_{13}K_{20} + K_{12}^2 - 4K_{20}K_{22} + 4K_{10}K_{23} + 3K_{21}K_{30} \\ &+ 2c_0 f_{10}(K_{10}K_{13} - K_{12}K_{20} + K_{11}K_{30})) \\ &+ \frac{\alpha_2}{\alpha_1^2}(K_{11}^2 - 4K_{10}K_{21} - 4c_0 f_{10}K_{10}K_{11}) - 2g_{10}K_{20} - \frac{K_{20}}{c_0} + L_{11} - 4L_{20} \\ &+ c_0(2f_{20}K_{10} - 3f_{10}g_{10}K_{10} - 2f_{10}L_{10})\Bigg]. \end{aligned}$$

We note that it is possible to make $f_{10} = f_{20} = 0$ with a careful choice of $\{e_0, e_1, e_2, e_3\}$. While this case has an intrinsic theoretical value, we have not yet identified any Hamiltonian lattice models for which this degeneracy condition is satisfied.

IV. NUMERICAL PROCEDURES

In this section we describe the numerical procedures we used to obtain the solitary traveling waves and analyze their stability. More specifically, to identify the solitary wave structures, we use the procedure followed in [1]. To this end, we seek solutions of (6.3) in the co-traveling frame corresponding to velocity c:

$$r_n(t) = \Phi(\xi, t), \quad \xi = n - ct, \tag{25}$$

obtaining the advance-delay partial differential equation

$$\begin{aligned} &\Phi_{tt} + c^2\Phi_{\xi\xi} - 2c\Phi_{\xi t} + 2V'(\Phi(\xi,t)) - V'(\Phi(\xi+1,t)) - V'(\Phi(\xi-1,t)) \\ &+ \sum_{m=1}^{\infty} \Lambda(m)(2\Phi(\xi,t) - \Phi(\xi+m,t) - \Phi(\xi-m,t)) = 0. \end{aligned} \tag{26}$$

Solitary traveling waves $\phi(\xi)$ are stationary solutions of (26). They satisfy the advance-delay differential equation (6.4) and (6.5).

Following the approach in [2], we assume that $\phi(\xi) = o(1/\xi)$ and $\phi'(\xi) = o(1/\xi^2)$ as $|\xi| \to \infty$, multiply Eq. (6.4) by ξ^2 and integrate by parts to derive the identity

$$\left[c^2 - \sum_{m=1}^{\infty} m^2 \Lambda(m)\right] \int_{-\infty}^{\infty} \phi(\xi) \mathrm{d}\xi - \int_{-\infty}^{\infty} V'(\phi(\xi)) \mathrm{d}\xi = 0, \tag{27}$$

which imposes the constraint (6.5) on the traveling wave solutions. Here we assume that $\Lambda(m)$ decays faster than $1/m^3$ at infinity, so that the series on the left hand side converges.

To solve Eq. (6.4) numerically, we introduce a discrete mesh with step $\Delta\xi$, where $1/\Delta\xi$ is an integer, so that the advance and delay terms $\phi(\xi \pm m)$ are well defined on the mesh. We then use a Fourier spectral collocation method for the resulting system with periodic boundary conditions [3] with large period l. Implementation of this method requires an even number $\mathcal{N}$ of collocation points $\xi_j \equiv j\Delta\xi$, with $j = -\mathcal{N}/2 + 1, \ldots, \mathcal{N}/2$, yielding a system for ξ in the domain $(l/2, l/2]$, with $l = \mathcal{N}\Delta\xi$ being an even number, and the long-range interactions are appropriately truncated. To ensure that the solutions satisfy (6.5), we additionally impose a trapezoidal approximation of (27) on the truncated interval at the collocation points. This procedure is independent of the potential and the interaction range. However, the choices of $\Delta\xi$ and l depend on the nature of the problem.

To investigate spectral stability of a traveling wave $\phi(\xi)$, we substitute

$$\Phi(\xi, t) = \phi(\xi) + \epsilon a(\xi) \exp(\lambda c t), \tag{28}$$

into (26) and consider $O(\epsilon)$ terms resulting from this perturbation. This yields the following quadratic eigenvalue problem:

$$\begin{aligned} c^2\lambda^2 a(\xi) &= -c^2 a''(\xi) + 2\lambda c^2 a'(\xi) - 2V''(\phi(\xi))a(\xi) + V''(\phi(\xi+1))a(\xi+1) \\ &+ V''(\phi(\xi-1))a(\xi-1) - \sum_{m=1}^{\infty} \Lambda(m)(2a(\xi) - a(\xi+m) - a(\xi-m)). \end{aligned} \tag{29}$$

By defining $b(\xi) = c\lambda a(\xi)$, we transform this equation into the regular eigenvalue problem

$$c\lambda \begin{pmatrix} a(\xi) \\ b(\xi) \end{pmatrix} = \mathcal{M} \begin{pmatrix} a(\xi) \\ b(\xi) \end{pmatrix} \tag{30}$$

for the corresponding linear advance-delay differential operator $\mathcal{M}$. Note that this problem is equivalent to the eigenvalue problem (3.5) via the transformation $\xi = -\tau$ and $(a(\xi), b(\xi)) = (\Gamma_a(-\tau), \Gamma_b(-\tau) - c\Gamma_a'(-\tau))$. Spectral stability can be determined by analyzing the spectrum of the operator $\mathcal{M}$ after discretizing the eigenvalue problem the same way as the nonlinear Eq. (6.4) and again using periodic boundary conditions. A traveling wave solution is spectrally stable when the spectrum contains no real eigenvalues.

To analyze the dependence of the eigenvalues spectrum obtained using this procedure on the grid size $\Delta\xi$ and the size l of the lattice, we consider as an example an α-FPU lattice with $V(r) = r^2/2 - r^3/3$ and without long-range interaction ($\Lambda(m) \equiv 0$). In this case, $H'(c) > 0$ for every c, and one expects all waves to be stable (see, e.g., [4]). However, the numerically obtained spectra show mild oscillatory instabilities, which are associated with complex-valued eigenvalues with nonzero imaginary parts and small but nonzero real parts. As one can see in the example shown in Fig. 1, corresponding to $c = 1.3$, the real part of the eigenvalues does not change when $\Delta\xi$ is varied (only their imaginary parts are affected, given that smaller $\Delta\xi$ enables accessing higher wavenumbers); however, when the system's length l is increased, the real parts of the eigenvalues decrease. This suggests that the oscillatory instabilities are a numerical artifact due to the finite length of the lattice that can, in principle, be expected to disappear in the infinite lattice limit.

An alternative method for determining the spectral stability of the traveling waves is to use Floquet analysis. To this end, we cast traveling waves $\phi(\xi)$ as fixed points of the map

$$\begin{bmatrix} \{r_{n+1}(T)\} \\ \{\dot{r}_{n+1}(T)\} \end{bmatrix} \to \begin{bmatrix} \{r_n(0)\} \\ \{\dot{r}_n(0)\} \end{bmatrix}, \tag{31}$$

which is periodic modulo shift by one lattice point, with period $T = 1/c$. Indeed, one easily checks that $\hat{r}_n(t) = \phi(n - ct) = \phi(n - t/T)$ satisfies $\hat{r}_{n+1}(T) = \hat{y}_n(0) = \phi(n)$ and $\dot{\hat{r}}_{n+1}(T) = \dot{\hat{r}}_n(0) = -c\phi'(n)$. To apply the Floquet

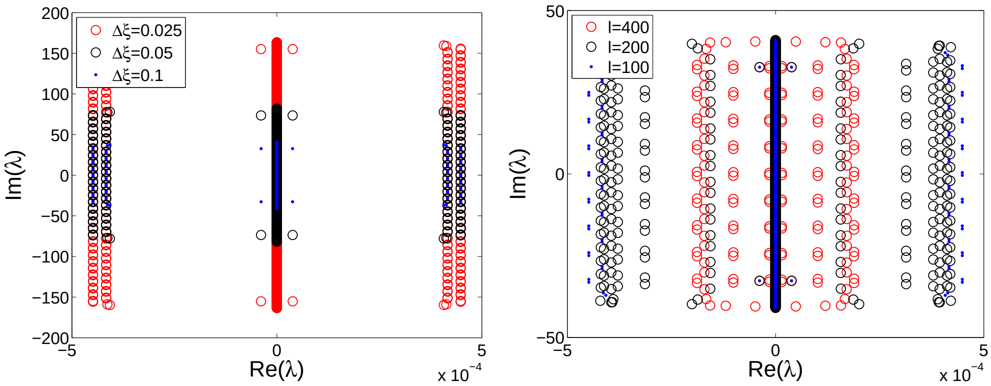

FIG. 1: Dependence of the linearization operator spectrum with the discretization parameter (left panel, with fixed $l = 100$) and the system length (right panel, with fixed $\Delta\xi = 0.1$) for a stable solitary traveling wave solution with $c = 1.3$ of the problem with the α-FPU potential governing nearest-neighbor interactions and no long-range interaction.

analysis, we trace time evolution of a small perturbation $\epsilon w_n(t)$ of the periodic-modulo-shift (traveling wave) solution $\hat{r}_n(t)$. This perturbation is introduced in (6.3) via $r_n(t) = \hat{r}_n(t) + \epsilon w_n(t)$. The resulting $O(\epsilon)$ equation reads

$$\begin{aligned} &\ddot{w}_n + 2V''(\hat{r}_n)w_n - V''(\hat{r}_{n+1})w_{n+1} - V''(\hat{r}_{n-1})w_{n-1} \\ &+ \sum_{m=1}^{\infty} \Lambda(m)(2w_n - w_{n+m} - w_{n-m}) = 0. \end{aligned} \tag{32}$$

Then, in the framework of Floquet analysis, the stability properties of periodic orbits are resolved by diagonalizing the monodromy matrix $\mathcal{F}$ (representation of the Floquet operator at finite systems), which is defined as:

$$\begin{bmatrix} \{w_{n+1}(T)\} \\ \{\dot{w}_{n+1}(T)\} \end{bmatrix} = \mathcal{F} \begin{bmatrix} \{w_n(0)\} \\ \{\dot{w}_n(0)\} \end{bmatrix}. \tag{33}$$

For the symplectic Hamiltonian systems we consider in this work, the linear stability of the solutions requires that the monodromy eigenvalues μ (also called Floquet multipliers) lie on the unit circle. The Floquet multipliers can thus written as $\mu = \exp(i\theta)$, with Floquet exponent θ (note that it coincides with $-i\lambda$).

The results were complemented by numerical simulations of the ODE system (6.3), performed using the fourth-order explicit and symplectic Runge-Kutta-Nyström method developed in [5], with time step equal to 10^{-3}. In particular, to explore the evolution of unstable waves, we used initial conditions with such waves perturbed along the direction of the Floquet mode causing the instability.

V. DISCUSSION: CONNECTION TO EXISTING ENERGY CRITERIA

In this section, we discuss connections between the energy-based stability criterion we derived and analyzed for solitary traveling waves in Hamiltonian lattices and related criteria for such waves in continuum systems and for discrete breathers.

A. Energy criteria for discrete breathers in Hamiltonian lattices

As we discuseed in Section 4, solitary traveling wave solutions in lattices can be viewed as time-periodic solutions (or discrete breathers, if they are exponentially localized) modulo an integer shift. In particular, suppose (2.1) has a family of time-periodic solutions $x_{per}(t;\omega)$ parametrized by the frequency ω and satisfying $x_{per}(t+\frac{1}{\omega};\omega) = x_{per}(t;\omega)$. Setting $\tau = \omega t$ and $X_{per}(\tau;\omega) = x_{per}(t;\omega)$, one can similarly define the linear operator

$$\mathcal{L} = \frac{1}{c} D\mathcal{A}(X_{per}) - \frac{d}{d\tau} = \frac{1}{c} J \frac{\partial^2 \mathcal{H}}{\partial X^2}|_{X=X_{per}} - \frac{d}{d\tau}.$$

With ω playing the role of c for traveling waves, almost all of the results in this work, including Theorem 5.1, Lemma 5.1 and Lemma III.1, can also be applied to discrete breathers; see [6] for details and a number of examples.

B. Energy criteria for solitary waves in continuum Hamiltonian systems

Stability of solitary waves in continuum Hamiltonian systems with symmetry (e.g $U(1)$-invariance) was analyzed in [7, 8]. Solitary traveling waves in such systems possess translational invariance in space, which breaks down in the case of lattice dynamical systems. However, in what follows, we rewrite the energy-based stability criteria obtained in [7, 8] to identify the similarities with our criterion for solitary traveling waves in lattices.

Following the formulation in [7], we consider a continuum Hamiltonian system

$$\frac{\partial u}{\partial t} = JE'(u), \quad u(x,t) = \begin{pmatrix} q(x,t) \\ p(x,t) \end{pmatrix}, \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \tag{34}$$

where E is the energy functional, while $q(x,t)$ and $p(x,t)$ are the displacement and momentum fields, respectively. Let $\mathcal{T}(s)$ be a one-parameter unitary operator group with the infinitesimal generator $\mathcal{T}'(0)$, i.e. $\mathcal{T}(s) = \exp(s\mathcal{T}'(0))$. We assume that E is invariant under $\mathcal{T}(s)$ for any s, i.e., $E(u) = E(T(s)u)$. This invariance corresponds to the symmetry of the system. In particular, $\mathcal{T}(s)u(x) = e^{s\partial_x}u(x) = u(x+s)$ corresponds to the translational symmetry.

Assuming that $\mathcal{T}(s)J\mathcal{T}^*(s) = J$ and differentiating it with respect to s at $s = 0$ gives $\mathcal{T}'(0)J = -J(\mathcal{T}'(0))^*$, so that $J^{-1}\mathcal{T}'(0)$ is self-adjoint. As a result, there exists a self-adjoint bounded linear operator $\mathcal{B}$ such that $J\mathcal{B}$ extends $\mathcal{T}'(0)$. This implies that $Q(u) = \frac{1}{2}\langle u, \mathcal{B}u\rangle$ is also invariant under $\mathcal{T}(s)$, i.e., $Q(u) = Q(\mathcal{T}(s)u)$.

Observe that if $\phi_\omega(x)$ satisfies $E'(\phi_\omega) = \omega Q'(\phi_\omega)$, then $u(x,t) = \mathcal{T}(\omega t)\phi_\omega(x)$ is a solitary solution of (34). In fact, the converse also holds. Indeed, if $u(x,t) = \mathcal{T}(\omega t)\phi_\omega(x)$ solves (34), then

$$\begin{aligned} JE'(\phi_\omega) &= J\mathcal{T}(\omega t)^* E'(\mathcal{T}(\omega t)\phi_\omega) = J\mathcal{T}(\omega t)^* J^{-1}\frac{\partial}{\partial t}(\mathcal{T}(\omega t)\phi_\omega) \\ &= J\mathcal{T}(\omega t)^* J^{-1}\frac{\partial}{\partial t}(\mathcal{T}(\omega t)\phi_\omega) = \mathcal{T}(-\omega t)\omega\mathcal{T}'(0)\mathcal{T}(\omega t)\phi_\omega \\ &= \omega\mathcal{T}'(0)\phi_\omega = J\omega Q'(\phi_\omega). \end{aligned} \tag{35}$$

Here we used the fact that $\mathcal{T}'(0)\mathcal{T}(\omega t) = \mathcal{T}(\omega t)\mathcal{T}'(0)$.

We now define the "free energy" $d(\omega) = E(\phi_\omega) - \omega Q(\phi_\omega)$ and the associated Hessian $H_\omega = E''(\phi_\omega) - \omega Q''(\phi_\omega)$. Observe that they satisfy

$$\begin{aligned} &H_\omega(\mathcal{T}'(0)\phi_\omega) = 0, \quad H_\omega(\partial_\omega\phi_\omega) = Q'(\phi_\omega) = J^{-1}\mathcal{T}'(0)\phi_\omega, \quad d'(\omega) = -Q(\phi_\omega), \\ &d''(\omega) = -\langle\partial_\omega\phi_\omega, Q'(\phi_\omega)\rangle = -\langle\partial_\omega\phi_\omega, H_\omega(\partial_\omega\phi_\omega)\rangle = -\frac{d}{d\omega}Q(\phi_\omega) = -\frac{1}{\omega}\frac{d}{d\omega}E(\phi_\omega). \end{aligned} \tag{36}$$

As stated in [7], if H_ω has at most one negative eigenvalue, $\ker(H_\omega)$ is spanned by $\mathcal{T}'(0)\phi_\omega$ and the rest of its spectrum is bounded below from zero, then $d''(\omega) > 0$ implies that ϕ_ω-orbit $\{\mathcal{T}(\omega t)\phi_\omega,\ t \in \mathbb{R}\}$ is stable. On the other hand, $d''(\omega) < 0$ implies instability. In other words,

$$d''(\omega) = 0 = -\frac{1}{\omega}\frac{d}{d\omega}E(\phi_\omega)$$

implies the change of stability, which is similar to our energy-based criterion $H'(c_0) = 0$ (and to the corresponding one for discrete breathers).

On the one hand, the solutions in our lattice problems are discrete in space and the translation operator $\mathcal{T}(s) = e^{s\partial_x}$ cannot be directly applied – except in the quasi-continuum, advance-delay variant of the problem. However, the nature of the traveling waves implies that the time dynamics on all sites is connected to a continuous profile function and one can easily replace the translation in space by translation in time by going to the co-moving frame. In fact, replacing $\mathcal{T}(s) = e^{s\partial_x}$ by $\mathcal{T}(s) = e^{\frac{1}{\omega}s\partial_t}$, we can similarly define

$$Q(u) = \frac{1}{2}\langle u, \mathcal{B}u\rangle = \frac{1}{2}\langle u, \frac{1}{\omega}J^{-1}\partial_t u\rangle, \quad H_\omega = E''(\phi_\omega) - \omega Q''(\phi_\omega) = E''(\phi_\omega) - J^{-1}\partial_t$$

and derive (36) where $u(t) = \mathcal{T}(\omega t)\phi_\omega$ is a solitary traveling wave solution of the lattice system with $E'(\phi_\omega) = \omega Q'(\phi_\omega)$. Note also the relation $\mathcal{L} = \omega J H_\omega$, with $\omega = c$ and $x_{tw}(c) = \phi_\omega$.

A more complete understanding of the relationship between the energy-based criteria in discrete and continuum systems remains a challenging problem to be considered in the future work.

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[1] Yasuda H, Chong C, Charalampidis EG, Kevrekidis PG, Yang J. 2016 Formation of rarefaction waves in origami-based metamaterials. *Phys. Rev. E* **93**, 043004.

[2] Eilbeck JC, Flesch R. 1990 Calculation of families of solitary waves on discrete lattices. *Phys. Lett. A* **149**, 200–202.

[3] Trefethen LN. 2000 *Spectral methods in MATLAB.* SIAM.

[4] Cuevas-Maraver J, Kevrekidis PG, Vainchtein A, Xu H. 2017 Unifying perspective: Solitary traveling waves as discrete breathers in Hamiltonian lattices and energy criteria for their stability. *Phys. Rev. E* **96**, 032214.

[5] Calvo MP, Sanz-Serna JM. 1993 The development of variable-step symplectic integrators, with application to the two-body problem. *SIAM J. Sci. Comp.* **14**, 936–952.

[6] Kevrekidis PG, Cuevas-Maraver J, Pelinovsky DE. 2016 Energy criterion for the spectral stability of discrete breathers. *Phys. Rev. Lett.* **117**, 094101.

[7] Grillakis M, Shatah J, Strauss W. 1987 Stability theory of solitary waves in the presence of symmetry, I. *J. Funct. Anal.* **74**, 160–197.

[8] Vakhitov NG, Kolokolov AA. 1973 Stationary solutions of the wave equation in a medium with nonlinearity saturation. *Radiophys. Quantum Electron.* **16**, 783–789.