MASS-IN-MASS LATTICES WITH SMALL INTERNAL RESONATORS

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Abstract. We consider the mass-in-mass (MiM) lattice when the internal resonators are very small. When there are no internal resonators the lattice reduces to a standard Fermi-Pasta-Ulam-Tsingou (FPUT) system. We show that the solution of the MiM system, with suitable initial data, shadows the FPUT system for long periods of time. Using some classical oscillatory integral estimates we can conclude that the error of the approximation is (in some settings) higher than one may expect.

Keywords: Fermi-Pasta-Ulam-Tsingou, mass-in-mass lattices, model equations justification, energy estimates.

1. The problem

We consider the mass-in-mass (MiM) variant of the Fermi-Pasta-Ulam-Tsingou (FPUT) lattice: infinitely many particles of unit mass (indexed by \( j \in \mathbb{Z} \)) are arranged on a line, each connected to its nearest neighbors by a “spring” with potential energy function \( V \) (which we assume is smooth\(^1\) and has \( V(0) = V'(0) = 0 \) \(< k := V''(0) \)). The displacement of the \( j \)th particle is \( U_j \). Additionally, each particle is connected by a linear spring (with spring constant \( \kappa \)) to an internal resonator (of mass \( \mu \)). The displacement of the \( j \)th resonator is \( u_j \). The equations of motion can be found using Newton’s second law:

\[
\ddot{U}_j = V'(U_{j+1} - U_j) - V'(U_j - U_{j-1}) + \kappa (u_j - U_j)
\]

\( \mu \ddot{u}_j = \kappa (U_j - u_j) \).

These sorts of lattices have been the subject of quite a bit of research of late, in large part because engineers have found a wide variety of applications for apparatus which are modeled by MiM systems. Applications range from shock absorption [4] to remote sensing [8] and in areas from medicine [9] to materials science [6].

Our interest is analytical and in this article we investigate the dynamics of (1) when \( 0 < \mu \ll 1 \), that is when the internal resonators have small mass. When \( \mu = 0 \) the second equation implies \( u_j = U_j \) and the first becomes

\[
\ddot{U}_j = V'(U_{j+1} - U_j) - V'(U_j - U_{j-1})
\]

These are the equations of motion for the standard FPUT. It takes little insight to conjecture that solutions of (1) shadow solutions of (2) when \( \mu \) is small. We prove a quantitative version of such a conjecture. However this is not a straightforward result: since \( \mu \) multiplies the highest order derivative in (1), the problem is one of singular perturbation. We also find something rather surprising: by slightly adjusting the potential in (2) and adding some

\(^1\)In this paper, when we say “smooth” we always mean \( C^\infty \).
restrictions to the initial conditions for the internal resonators, we can improve the accuracy of the approximation by more than an order of magnitude.

Before getting into the weeds, we make some remarks on a recent spate of articles on MiM and FPUT lattices and how they relate to our work. First we mention the article [5] by Kevrekidis, Stefanov & Xu. The authors use a variational argument to show that for the degenerate Hertzian potential \( V_H(h) := \frac{h^5}{2} \), there exists a countable number of choices for the internal mass \( \mu \), converging to zero, for which the MiM system admits spatially localized traveling wave solutions. This work was extended by Faver, Goodman & Wright in [3] to apply to more general, but non-degenerate, potentials. Again, for a sequence of choices of \( \mu \) converging to zero, there are spatially localized traveling waves. The argument in [3] is perturbative and in particular, uses the \( \mu = 0 \) FPUT traveling wave as the point of bifurcation. In [2], Faver proves that away from the countable collection of masses, the traveling waves are not spatially localized but instead converge at infinity to very small amplitude periodic waves, \( i.e. \) nanopterons [1]. The point here is that despite the relative simplicity of the system [1], from the standpoint of traveling wave solutions, the system depends subtly on the mass of the internal resonators. This paper is, in part, an attempt to address similar issues for the Cauchy problem. We also mention the article [7] by Pelinovsky & Schneider. In that paper the authors treat a diatomic FPUT lattice in the limit that the mass ratio tends to zero. They prove that the small mass ratio lattice is well-approximated by the limiting monatomic FPUT lattice. Their result directly inspired our work here. See Remark [1] for a more thorough comparison of their work and ours.

2. First order reformulation and existence of solutions

Let

\[
R_j := U_{j+1} - U_j, \quad P_j := \dot{U}_j, \quad r_j := u_j - U_j \quad \text{and} \quad p_j := \dot{u}_j.
\]

The variables are (in order): the relative displacement between adjacent external particles; the velocity of the external particles; the relative displacement between the internal resonators and their hosts; the velocity of the internal resonators. In these coordinates [1] reads:

\[
\begin{align*}
\dot{R} &= \delta^+ P \\
\dot{P} &= \delta^- [V'(R)] + \kappa r \\
\dot{r} &= p - P \\
\mu \dot{p} &= -\kappa r.
\end{align*}
\]

We suppress dependence on the lattice site \( j \) and use the notation \((\delta^\pm q)_j := \pm (q_{j+1} - q_j)\). In fact [3] is in classical hamiltonian form, though since we do not utilize this feature very strongly, we do not elaborate.

We view [3] as an ODE on the Hilbert space \((\ell^2)^4\). The right hand side can easily be shown to be a smooth map in that topology and thus the Cauchy problem is well-posed by Picard’s theorem and solutions exist for at least short periods of time. In fact solutions exist for all \( t \), at least if they are initially not too big. Before we state the result, we need to define
an appropriate norm for solutions. Let

$$(4) \| (R,P,r,p) \|_{\mu} := \sqrt{\frac{k}{2} \| R \|^2 + \frac{1}{2} \| P \|^2 + \frac{\kappa}{2} \| r \|^2 + \frac{\mu}{2} \| p \|^2}.$$ 

Here and throughout we use

$\| \cdot \| := \| \cdot \|_{\ell^2}.$

The norm $\| \cdot \|_{\mu}$ is just a scaling of the usual $(\ell^2)^4$ norm and is equal to the (square root of the) mechanical energy of the linearization of $(3)$; recall that $k := V''(0)$.

For a solution $(R,P,r,p)$ of (3), let

$$H(t) := \sum_{j \in \mathbb{Z}} \left( V(R_j) + \frac{1}{2} P_j^2 + \frac{1}{2} \kappa r_j^2 + \frac{1}{2} \mu p_j^2 \right).$$

If finite at $t = 0$, this quantity is constant for all $t$: it is just the mechanical energy of the lattice. Here is the calculation:

$$\dot{H}(t) = \sum_{j \in \mathbb{Z}} V'(R_j) \dot{R}_j + P_j \dot{P}_j + \kappa r_j \dot{r}_j + \mu p_j \dot{p}_j$$

$$= \sum_{j \in \mathbb{Z}} V'(R_j)(\delta^+ P)_j + P_j((\delta^- [V'(R)])_j + \kappa r_j) + \kappa r_j(p_j - P_j) - \kappa p_j r_j$$

$$= 0.$$

Since $\dot{H}(t) = 0$, $H(t)$ is constant. In the above we have made liberal use of the summation by parts identity, $\sum_{j \in \mathbb{Z}} (\delta^+ f)_j g_j = -\sum_{j \in \mathbb{Z}} f_j (\delta^- g)_j$.

The conservation of energy is crucial for proving:

**Theorem 1.** Fix $\kappa > 0$ and assume that $V : \mathbb{R} \to \mathbb{R}$ is smooth with $V(0) = V'(0) = 0$ and $V''(0) =: k > 0$. There exists $\rho_* = \rho_*(V) > 0$, such that, for any $\mu > 0$, if

$$\| (R_0, P_0, r_0, p_0) \|_{\mu} \leq \rho_*$$

then the unique solution of the MiM lattice (3) with initial data $(R_0, P_0, r_0, p_0)$ exists for all $t \in \mathbb{R}$ and

$$\| (R(t), P(t), r(t), p(t)) \|_{\mu} \leq 2 \| (R_0, P_0, r_0, p_0) \|_{\mu}.$$ 

**Proof.** The hypotheses on $V$ imply, by way of Taylor’s Theorem, the existence of $\sigma_* > 0$ for which $|h| \leq \sigma_*$ implies $\frac{k}{4} h^2 \leq V(h) \leq k h^2$. So if $\| R \|_{\ell^\infty} \leq \sigma_*$ we have $\sum_{j \in \mathbb{Z}} \frac{k}{4} R_j^2 \leq \sum_{j \in \mathbb{Z}} V(R_j) \leq \sum_{j \in \mathbb{Z}} \frac{k}{4} R_j^2$. This in turn implies

$$(5) \quad \frac{1}{2} \| (R, P, r, p) \|_{\mu}^2 \leq H \leq 2 \| (R, P, r, p) \|_{\mu}^2$$

when

$$(6) \quad \| R \|_{\ell^\infty} \leq \sigma_*.$$ 

That is to say when (6) holds, $\sqrt{H}$ and $\| (R, P, r, p) \|_{\mu}$ are equivalent.
Since $H$ is constant, (5) gives us:

$$\frac{1}{2} \| (R(t), P(t), r(t), p(t)) \|^2_\mu \leq H(t) = H(0) \leq 2 \| (R_0, P_0, r_0, p_0) \|^2_\mu.$$ 

If we cut out the middle terms and do some simple algebra we arrive at

(7) $$\| (R(t), P(t), r(t), p(t)) \|_\mu \leq 2 \| (R_0, P_0, r_0, p_0) \|_\mu.$$ 

This is the final estimate in the theorem but we are not yet done. The reason is that (7) only holds for those values of $t$ where (6) is true.

By restricting the initial data, we can ensure that (6) holds for all $t$ and thus so does (7). Here is the argument. We have the \"$\ell^2 \subset \ell^\infty$ embedding estimate\" $\| R \|_{\ell^\infty} \leq \| R \|$. Moreover, the definition of $\| (R, P, r, p) \|_\mu$ implies $\| R \| \leq \sqrt{2/k} \| (R, P, r, p) \|_\mu$. Putting these together with (6) we see that we have (7) for those $t$ when

(8) $$\| (R(t), P(t), r(t), p(t)) \|_\mu \leq \frac{1}{\sqrt{2}} \sigma_*.$$

Now assume

(9) $$\| (R_0, P_0, r_0, p_0) \|_\mu \leq \frac{1}{4} \sqrt{\frac{k}{2}} \sigma_* =: \rho_*.$$

Thus (8) holds initially and the inequality is strict. The solution of (3) with this initial data either satisfies (8) for all $t \in \mathbb{R}$ (in which case we have (7) for all $t \in \mathbb{R}$ and we are done) or it does not.

If it does not then, because the solution is continuous in $t$, there is a time $t_1$ for which

(10) $$\| (R(t_1), P(t_1), r(t_1), p(t_1)) \|_\mu = \sqrt{\frac{k}{2}} \sigma_*.$$

But note that at this time (8) is met and so we have (7). Putting (10), (7) and (9) together we obtain

$$\sqrt{\frac{k}{2}} \sigma_* = \| (R(t_1), P(t_1), r(t_1), p(t_1)) \|_\mu \leq 2 \| (R_0, P_0, r_0, p_0) \|_\mu \leq \frac{1}{2} \sqrt{\frac{k}{2}} \sigma_*.$$ 

This is an absurdity and thus (8) is met for all $t$ and we are done.

\[\square\]

3. The approximation theorem

In this section we prove a general approximation theorem for (3). Once this is done, we will turn our attention to the specific problem of approximating MiM by FPUT.

For any function

$$\tilde{\Phi}_j(t) = (\bar{R}_j(t), \bar{P}_j(t), \bar{r}_j(t), \bar{p}_j(t))$$
Definition 1. We say \( \tilde{\Phi} \) conditions on (12) \( \| \Phi \|_{\infty} \approximated by \) (D1) \( \sup_{O} \) of \( \Phi \) define the residuals. The residuals are identically zero if and only if \( \tilde{\Phi} \) holds when \( \mu \) for all (D3) \( \sup \). We additionally require that (D2) \( \sup \) \( \| \partial_t \tilde{R}^\mu \|_{\ell^\infty} \leq \beta_* \). Lastly, \( \tilde{R}^\mu \) and \( \partial_t \tilde{R}^\mu \) are not too big: there exist \( \alpha_*, \beta_*>0 \) so that \( \mu \in (0,\mu_0) \) implies (D2) \( \sup_{|t| \leq T_*} \| \tilde{R}^\mu \|_{\ell^\infty} \leq \alpha_* \) and \( \sup_{|t| \leq T_*} \| \partial_t \tilde{R}^\mu \|_{\ell^\infty} \leq \beta_* \). We additionally require that (D3) \( \alpha_* \leq \sup \{ \alpha : V''([-\alpha,\alpha]) \subset [k/2, 2k] \} \).

Here is our result:

Theorem 2. Fix \( \kappa > 0 \) and assume that \( V : \mathbb{R} \rightarrow \mathbb{R} \) is smooth with \( V(0) = V'(0) = 0 \) and \( V''(0) =: k > 0 \). Suppose that \( \{ \tilde{\Phi}^\mu = (\tilde{R}^\mu, \tilde{P}^\mu, \tilde{r}^\mu, \tilde{p}^\mu) \}_{\mu \in (0,\mu_0)} \) is a family of good approximators of \( \mathcal{O}(\mu^N) \) for (3) on the interval \([-T_*, T_*]\) where \( N > 0 \).

Then, for all \( K_* > 0 \), there exists positive constants \( \mu_* \) and \( C_* \) such that the following holds when \( \mu \in (0, \mu_*) \). If (12) \( \| \Phi^\mu_0 - \tilde{\Phi}^\mu(0) \|_{\mu} \leq K_* \mu^N \)

and \( \Phi^\mu \) is the solution of (3) with initial data \( \Phi^\mu_0 \) then (13) \( \| \Phi^\mu(t) - \tilde{\Phi}^\mu(t) \|_{\mu} \leq C_* \mu^N \)

for all \( t \in [-T_*, T_*] \).

That is to say, if \( \Phi^\mu \) and \( \tilde{\Phi}^\mu \) are initially \( \mathcal{O}(\mu^N) \) close then they are \( \mathcal{O}(\mu^N) \) close on all of \([-T_*, T_*]\).
Proof. Part 1—the Error Equations: Let

$$\Psi = (\psi_1, \psi_2, \psi_3, \psi_4) := \Phi^\mu - \tilde{\Phi}^\mu.$$  

This is the error between the true solution and the approximator. A direct calculation shows that $\Psi$ satisfies

$$
\begin{align*}
\dot{\psi}_1 &= \delta^+ \psi_2 + \text{Res}_1^\mu(\tilde{\Phi}^\mu) \\
\dot{\psi}_2 &= \delta^- [W'(\psi_1; t)] + \kappa \psi_3 + \text{Res}_2^\mu(\tilde{\Phi}^\mu) \\
\dot{\psi}_3 &= \psi_4 - \psi_2 + \text{Res}_3^\mu(\tilde{\Phi}^\mu) \\
\mu \dot{\psi}_4 &= -\kappa \psi_3 + \text{Res}_4^\mu(\tilde{\Phi}^\mu)
\end{align*}
\tag{14}
$$

where

$$W_j'(\zeta; t) := V'(\tilde{R}_j^\mu(t) + \zeta) - V'(\tilde{R}_j^\mu(t)).$$

Note that $W_j(\zeta; t) = \partial_t W_j(\zeta; t)$ with

$$W_j(\zeta; t) := V(\tilde{R}_j^\mu(t) + \zeta) - V(\tilde{R}_j^\mu(t)) - V'(\tilde{R}_j^\mu(t))\zeta.\tag{15}$$

We are done when we show that $\|\Psi(t)\|_\mu \leq C_s \mu^N$ for $t \in [-T_s, T_s]$.

Part 2—the Modified Energy: The heart of the proof is closely related to the conservation of the energy $H$. Let

$$E(t) := \sum_{j \in Z} \left( W(\psi_1; t) + \frac{1}{2} \psi_2^2 + \frac{1}{2} \kappa \psi_3^2 + \frac{1}{2} \mu \psi_4^2 \right).$$

This quantity is a modification of $H$ and, while it is not conserved, grows only slowly. Below, we will show that $\sqrt{E}$ is equivalent to $\|\Psi\|_\mu$, but first we compute its time derivative in order to develop the key energy estimate:

$$\dot{E}(t) = \sum_{j \in Z} \left( W'(\psi_1) \dot{\psi}_1 + \partial_t W(\psi_1; t) + \psi_2 \dot{\psi}_2 + \kappa \psi_3 \dot{\psi}_3 + \mu \psi_4 \dot{\psi}_4 \right).$$

Using (14)

$$\dot{E}(t) = \sum_{j \in Z} \left( W'(\psi_1; t) \left( \delta^+ \psi_2 + \text{Res}_1^\mu(\tilde{\Phi}^\mu) \right) + \psi_2 \left( \delta^- [W'(\psi_1; t)] + \kappa \psi_3 + \text{Res}_2^\mu(\tilde{\Phi}^\mu) \right) + \kappa \psi_3 \left( \psi_4 - \psi_2 + \text{Res}_3^\mu(\tilde{\Phi}^\mu) \right) + \psi_4 \left( -\kappa \psi_3 + \text{Res}_4^\mu(\tilde{\Phi}^\mu) \right) + \partial_t W(\psi_1; t) \right).$$

There are many cancelations:

$$\dot{E}(t) = \sum_{j \in Z} \left( W'(\psi_1; t) \text{Res}_1^\mu(\tilde{\Phi}^\mu) + \psi_2 \text{Res}_2^\mu(\tilde{\Phi}^\mu) + \kappa \psi_3 \text{Res}_3^\mu(\tilde{\Phi}^\mu) + \psi_4 \text{Res}_4^\mu(\tilde{\Phi}^\mu) + \partial_t W(\psi_1; t) \right).$$

Using the Cauchy-Schwarz inequality, Young’s inequality and (D1) we estimate the above:

$$\dot{E}(t) \leq \frac{1}{2} \|W'(\psi_1; t)\|^2 + \frac{1}{2} \|\psi_2\|^2 + \frac{\kappa^2}{2} \|\psi_3\|^2 + \frac{\mu}{2} \|\psi_4\|^2 + \|\partial_t W(\psi_1; t)\|_1 + \frac{1}{2} C_0^2 \mu^{2N}.\tag{16}$$

To go further than this, we need more information about $W$.  

Part 3—Estimates for $W$: Taylor’s theorem tells us that for $\zeta \in \mathbb{R}$ we have

$$W_j(\zeta; t) = \frac{1}{2} V''(z_j(t)) \zeta^2$$

where $z_j(t)$ lies between $\tilde{R}_j^\mu(t)$ and $\tilde{R}_j^\mu(t) + \zeta$. We have assumed (D2) and the condition (D3) on $\alpha_*$ tells us that $V''(\tilde{R}_j^\mu(t)) \in [k/2, 2k]$ for $j \in \mathbb{Z}$, $t \in [-T_*, T_*]$ and $\mu \in (0, \mu_0]$. Thus, since $V$ is smooth, there exists $\tau_* > 0$ so that $|\zeta| \leq \tau_*$ implies $V''(z_j(t)) \in [k/4, 4k]$ and as such

$$\frac{k}{8} \zeta^2 \leq W_j(\zeta; t) \leq 2k\zeta^2. \tag{17}$$

Now suppose that $\gamma \in \ell^2$ has $||\gamma|| \leq \tau_*$. Since $\ell^2 \subset \ell^\infty$ we have $||\gamma||_{\ell^\infty} \leq ||\gamma||$. Thus (17) gives us:

$$\frac{k}{8} \gamma_j^2 \leq W_j(\gamma_j; t) \leq 2k\gamma_j^2.$$ And so

$$||\gamma|| \leq \tau_* \implies \frac{k}{8} ||\gamma||^2 \leq \sum_{j \in \mathbb{Z}} W_j(\gamma_j; t) \leq 2k||\gamma||^2. \tag{18}$$

This estimate in turn implies that, for all $t \in [-T_*, T_*]$ and $\mu \in (0, \mu_0]$, $\mu$

$$||\psi_1|| \leq \tau_* \implies \frac{1}{4} ||\Psi||_\mu^2 \leq E(t) \leq 4||\Psi||_\mu^2. \tag{19}$$

This is the equivalence of $\sqrt{E}$ and $||\Psi||_\mu$ which was foretold. Completely analogous calculations can be used to show that

$$||\gamma|| \leq \tau_* \implies ||W'(\gamma; t)|| \leq 4k||\gamma||. \tag{20}$$

We also need an estimate on $\partial_t W$. Computing the derivative gets:

$$\partial_t W_j(\zeta; t) = \left[ V'(\tilde{R}_j^\mu(t) + \zeta) - V'(\tilde{R}_j^\mu(t)) - V''(\tilde{R}_j^\mu(t)) \zeta \right] \partial_t \tilde{R}_j^\mu.$$ Taylo-

r’s theorem tells us that

$$\partial_t W_j(\zeta; t) = \frac{1}{2} V'''(z_j(t)) \zeta^2 \partial_t \tilde{R}_j^\mu$$

with $z_j(t)$ in between $\tilde{R}_j^\mu$ and $\tilde{R}_j^\mu + \zeta$. Letting $\beta_0 := \max_{|\rho| \leq \tau_* + \alpha_*} |V'''(\rho)|$ and using the estimate for $\partial_t \tilde{R}_j^\mu$ in (D2) we now see that

$$|\partial_t W_j(\zeta; t)| \leq \frac{1}{2} \beta_0 \beta_\alpha \zeta^2$$

when $|\zeta| \leq \tau_*$. Thus we find that for all $t \in [-T_*, T_*]$ and $\mu \in (0, \mu_0]$

$$||\gamma|| \leq \tau_* \implies ||\partial_t W(\gamma; t)||_{\ell^2} \leq \beta_2 ||\gamma||^2 \tag{21}$$

where $\beta_2 := \beta_0 \beta_\alpha / 2$.

Part 4—Final Steps: Applying (19), (20) and (21) to (16) gets us

$$\dot{E} \leq \Gamma_* \left( E + \mu^2 \right)$$

so long as $||\psi_1|| \leq \tau_*$. The constant $\Gamma_* = \Gamma_* (V, \beta_*, \kappa, C_0) > 0$ is independent of $\mu$. 
We apply Grönwall’s inequality and get
\[ E(t) \leq e^{\Gamma_* t} \left( E(0) + \mu^2 N \right). \]

Then we use (19) again:
\[ \| \Psi(t) \|_\mu^2 \leq 16 e^{\Gamma_* t} \left( \| \Psi(0) \|_\mu^2 + \mu^2 N \right). \]

We have assumed that \( \| \Psi(0) \|_\mu \leq K_* \mu N \) and we know \( |t| \leq T_* \) so we have
\[ \| \Psi(t) \|_\mu \leq \frac{4e^{\Gamma_* T_*/2} \sqrt{K_*^2 + 1} \mu N}{C_*}. \]

The constant \( C_* \) does not depend on \( \mu \), but the above estimate holds only so long as \( \| \psi_1 \| \leq \tau_* \). But we can make the right hand side of this last displayed inequality (which controls \( \| \psi_1 \| \)) as small as we like, so this restriction is not a serious one. And so we find that there exists \( \mu_* > 0 \) so that \( \mu \in (0, \mu_*] \) implies \( \| \Psi(t) \| \leq C_* \mu^N \) for all \( |t| \leq T_* \) and we are done with the proof.

\[ \square \]

4. THE LEADING ORDER FPUT APPROXIMATION

In (3), if we put \( \mu = 0 \) we find that the last two equations become:
\begin{equation}
(22) \quad r = 0 \quad \text{and} \quad p = P.
\end{equation}

That is to say, as one may expect, the internal resonators are fixed at the center of their hosting particle and their velocity \( p \) is exactly equal to that of its host. Then we put (22) into the first two equations of (3):
\begin{equation}
(23) \quad \dot{R} = \delta^+ P \quad \text{and} \quad \dot{P} = \delta^- [V'(R)].
\end{equation}

Of course (23) is just a vanilla monatomic FPUT lattice, equivalent to (2). So our approximating system is
\begin{equation}
(24) \quad \tilde{\Phi}_{FPUT} := (\tilde{R}, \tilde{P}, 0, \tilde{P})
\end{equation}

where \( (\tilde{R}, \tilde{P}) \) solves (23).

Now we will show that \( \tilde{\Phi}_{FPUT} \) is a good approximator; note that it does not depend on \( \mu \), though the residuals will. An argument identical to that which led to Theorem 1 tells us that there is a positive constant \( \rho_1 \), such that \( \| \tilde{R}(0) \| + \| \tilde{P}(0) \| \leq \rho_1 \) implies
\begin{equation}
(25) \quad \| \tilde{R}(t) \| + \| \tilde{P}(t) \| \leq 2 \left( \| \tilde{R}(0) \| + \| \tilde{P}(0) \| \right)
\end{equation}

for all \( t \in \mathbb{R} \). Thus, so long as \( \| \tilde{R}(0) \| + \| \tilde{P}(0) \| \) is not too big, the conditions (D2) and (D3) are more or less automatically met and, moreover, they hold for all \( t \in \mathbb{R} \).

We compute directly that
\[ \text{Res}_1(\tilde{\Phi}_{FPUT}) = \text{Res}_2(\tilde{\Phi}_{FPUT}) = \text{Res}_3(\tilde{\Phi}_{FPUT}) = 0 \]

and
\[ \text{Res}_4(\tilde{\Phi}_{FPUT}) = -\mu \dot{\tilde{P}} = -\mu \delta^- [V'(\tilde{R})]. \]
Thus
\[
\sqrt{\| \text{Res}_1^\mu(\Phi_{FPUT}) \|^2 + \| \text{Res}_2^\mu(\Phi_{FPUT}) \|^2 + \| \text{Res}_3^\mu(\Phi_{FPUT}) \|^2 + \frac{1}{\mu} \| \text{Res}_4^\mu(\Phi_{FPUT}) \|^2}
\]
\[= \sqrt{\mu} \| \delta - [V'(\tilde{R})] \| .
\]

Standard estimates and (25) tell us that
\[
\sqrt{\mu} \| \delta - [V'(\tilde{R})] \| \leq C_0 \sqrt{\mu}
\]
for all \( t \in \mathbb{R} \). So we have (D1) with \( N = 1/2 \). We now call on Theorem 2 and get:

**Corollary 3.** Let \( \kappa > 0, K_* > 0, T_* > 0 \) and \( V : \mathbb{R} \to \mathbb{R} \) be smooth with \( V(0) = V'(0) = 0 \) and \( V''(0) =: k > 0 \). Then there exist \( \rho_* = \rho_*(V) > 0, \mu_* = \mu_*(K_*, T_*, \kappa, V) > 0 \) and \( C_* = C_*(K_*, T_*, \kappa, V) > 0 \) for which we have the following when \( \mu \in (0, \mu_*] \).

Suppose that \((\tilde{R}, \tilde{P})\) solves the FPUT system (23) with
\[
\| \tilde{R}(0) \| + \| \tilde{P}(0) \| \leq \rho_*
\]
and \((R, P, r, p)\) solves the MiM lattice (3) with
\[
\| (R(0), P(0), r(0), p(0)) - (\tilde{R}(0), \tilde{P}(0), 0, \tilde{P}(0)) \|_\mu \leq K_* \sqrt{\mu}.
\]

Then
\[
\| (R(t), P(t), r(t), p(t)) - (\tilde{R}(t), \tilde{P}(t), 0, \tilde{P}(t)) \|_\mu \leq C_* \sqrt{\mu}
\]
for all \( t \in [-T_*, T_*] \).

**Remark 1.** As we mentioned in the introduction, the article [7] treats the monatomic limit of a diatomic FPUT lattice in the case of small mass ratio. Their mass ratio is named \( \epsilon^2 \) and is most comparable to our internal mass \( \mu \). Their main result, Theorem 1, gives a rigorous error bound of \( O(\epsilon) \) on \( O(1) \) time scales. Given the comparison \( \epsilon^2 \sim \mu \), our result here is exactly the analogous one for MiM with small internal resonators.

## 5. Higher order expansions

The final two equations in (3) are solvable for \((r, p)\) in terms of \((R, P)\) with elementary ODE techniques. In this way we can eliminate \((r, p)\) from the system (almost) entirely and are left with what is a perturbation of FPUT with a continuous delay term. This delay term can then be approximated using classical oscillatory integral methods. Then we will use Theorem 2 to justify some of these approximations, which are of a higher order in \( \mu \) than what we saw in Corollary 3.

### 5.1. Delay equation reformulation

Take the time derivative of the equation for \( \dot{r} \) in (3) and get

\[
\dot{r} = -\omega_\mu^2 r - \dot{P}
\]
where
\[
\omega_\mu := \sqrt{\kappa/\mu}.
\]
We solve (26) using variation of parameters:

\[
\begin{aligned}
    r_j(t) &= r_j(0) \cos(\omega \mu t) + \frac{1}{\omega \mu} (p_j(0) - P_j(0)) \sin(\omega \mu t) - \frac{1}{\omega \mu} \int_0^t \sin(\omega \mu (t - t')) \dot{P}_j(t') dt'.
\end{aligned}
\]

\[\mu \Phi^\mu[r(0), p(0), P].\]

Though we do not use it, the equation for \( \dot{r} \) can be used to figure out \( p \):

\[
\begin{aligned}
    p_j(t) &= [P_j(t) - \omega \mu r_j(0) \sin(\omega \mu t) + (p_j(0) - P_j(0)) \cos(\omega \mu t)] - \int_0^t \cos(\omega \mu (t - t')) \dot{P}(t') dt'.
\end{aligned}
\]

Putting the solution for \( r \) back in the first two equations of (3) gets:

\[
\begin{aligned}
    \dot{R} &= \delta^+ P \\
    \dot{P} &= \delta^-[V'(R)] + \kappa \mu \Phi^\mu[r(0), p(0), P].
\end{aligned}
\]

This system is equivalent to (3); only the initial conditions of \( (r, p) \) still play a role. Because of the integral in \( \mu \Phi^\mu \), this is a continuous delay equation.

5.2. The general strategy. Suppose we have an approximation of \( \mu \Phi^\mu \):

\[
\mu \Phi^\mu[r(0), p(0), P] = \widetilde{\mu \Phi^\mu} + \mathcal{O}(\mu^N).
\]

Then we can make an approximating system easily:

\[
\begin{aligned}
    \dot{\tilde{R}} &= \delta^+ \tilde{P} \\
    \dot{\tilde{P}} &= \delta^- [V'(\tilde{R})] + \kappa \widetilde{\mu \Phi^\mu}
\end{aligned}
\]

(27)

(28)

For this approximating system we have

\[
\text{Res}_1^{\mu} (\tilde{\mu \Phi^\mu}) = \text{Res}_3^{\mu} (\tilde{\mu \Phi^\mu}) = \text{Res}_4^{\mu} (\tilde{\mu \Phi^\mu}) = 0
\]

and

\[
\text{Res}_2^{\mu} (\tilde{\mu \Phi^\mu}) = \kappa \mu \Phi^\mu[r(0), \tilde{p}(0), \tilde{P}] - \kappa \widetilde{\mu \Phi^\mu}.
\]

Thus, modulo some details, Theorem 2 tells us that the error made by this approximation is \( \mathcal{O}(\mu^N) \). The point here is that now all we have to do is find expansions of \( \mu \Phi^\mu \). Note that doing so does imply additional conditions on the initial data.

5.3. Oscillatory integral expansions. We put

\[
\begin{aligned}
    \mu \Phi^\mu[r(0), p(0), P] &= \left[ r(0) \cos(\omega \mu t) + \frac{1}{\omega \mu} (p(0) - P(0)) \sin(\omega \mu t) \right] + I^\mu[\dot{P}](t)
\end{aligned}
\]

where

\[
I^\mu[Q](t) := -\frac{1}{\omega \mu} \text{Im} \int_0^t e^{i\omega \mu (t-t')} Q(t') dt'.
\]

Since \( \omega \mu = \sqrt{\kappa/\mu} \), the frequency of the complex sinusoid is very high as \( \mu \to 0^+ \) and we can use classical oscillatory integral techniques to expand \( I^\mu \) in (negative) powers of
Specifically, we use the following lemma whose proof (which we omit) is obtained by integrating by parts many, many times:

**Lemma 4.** Suppose that \( f(t) \) is \( C^{n+1}(\mathbb{R}, \mathbb{C}) \) and \( \omega \neq 0 \). Then

\[
\int_0^t e^{i\omega(t-t')} f(t') dt' = i \sum_{j=0}^{n} \left( \frac{-i}{\omega} \right)^j f^{(j)}(t) - i e^{i\omega t} \sum_{j=0}^{n} \left( \frac{-i}{\omega} \right)^j f^{(j)}(0) \\
+ \left( \frac{-i}{\omega} \right)^{n+1} \int_0^t e^{i\omega(t-t')} f^{(n+1)}(t') dt'.
\]

In this lemma, the integral term and the \( j = n \) terms in the sums are \( O(1/\omega^{n+1}) \) and all other terms are lower order. Using this observation we get the expansion

\[
I_\mu[Q](t) = -\text{Im} \left( \frac{i}{\omega_\mu^2} \sum_{j=0}^{n-1} \left( \frac{-i}{\omega_\mu} \right)^j Q^{(j)}(t) - i e^{i\omega_\mu t} \sum_{j=0}^{n-1} \left( \frac{-i}{\omega_\mu} \right)^j Q^{(j)}(0) \right) + E_\mu^n[Q](t)
\]

where the estimate

\[
\|E_\mu^n[Q](t)\| \leq \frac{C}{\omega_\mu^{n+2}} \left( \|Q^{(n)}(t)\| + \|Q^{(n)}(0)\| + |t| \sup_{|t'| \leq |t|} \|Q^{(n+1)}(t')\| \right)
\]

is easily obtained. The above estimate tells us that we expect \( E_\mu^n = O(\mu^{n/2+1}) \).

If \( Q \) is purely real (as in our application), taking the imaginary part eliminates the odd values of \( j \) from the first sum in the expansion of \( I_\mu \). This, and the annoying but easily verified fact that

\[
\text{Im}(ie^{i\omega(-i)^j}) = \begin{cases} 
(-1)^{j/2} \cos(\omega t), & j \text{ is even} \\
(-1)^{(j-1)/2} \sin(\omega t), & j \text{ is odd}
\end{cases}
\]

lead us to:

\[
I_\mu[Q](t) = -\frac{1}{\omega_\mu^2} \sum_{j=0, \text{even}}^{n-1} \frac{(-1)^{j/2}}{\omega_\mu^2} Q^{(j)}(t) \\
+ \frac{1}{\omega_\mu^2} \left( \sum_{j=0, \text{even}}^{n-1} \frac{(-1)^{j/2}}{\omega_\mu^2} Q^{(j)}(0) \right) \cos(\omega_\mu t) \\
+ \frac{1}{\omega_\mu^2} \left( \sum_{j=1, \text{odd}}^{n-1} \frac{(-1)^{(j-1)/2}}{\omega_\mu^2} Q^{(j)}(0) \right) \sin(\omega_\mu t) \\
+ E_\mu^n[Q](t).
\]

The first sum is over evens and so only changes for every other \( n \). To squeeze the most out of the above expansion we therefore choose \( n = 2m \) for integers \( m \). A bit of reindexing
gives us:

\[
I_\mu[Q](t) = -\frac{1}{\omega_\mu^2} \sum_{k=0}^{m-1} \frac{(-1)^k}{\omega_\mu^{2k}} Q^{(2k)}(t) \\
+ \frac{1}{\omega_\mu^2} \left( \sum_{k=0}^{m-1} \frac{(-1)^k}{\omega_\mu^{2k}} Q^{(2k)}(0) \right) \cos(\omega_\mu t) \\
+ \frac{1}{\omega_\mu^2} \left( \sum_{k=0}^{m-1} \frac{(-1)^k}{\omega_\mu^{2k}} Q^{(2k+1)}(0) \right) \sin(\omega_\mu t) \\
+ \mathcal{E}_2^\mu[Q](t).
\] (32)

5.4. The FPUT approximation revisited. Now that we have our oscillatory integral expansions (32), we get back to approximating solutions of (3). Applying (32) with \(m = 0\) to \(F^\mu[r(0), p(0), P]\) yields

\[
F^\mu[r(0), p(0), P] = \left[ r(0) \cos(\omega_\mu t) + \frac{1}{\omega_\mu} (p(0) - P(0)) \sin(\omega_\mu t) \right] + \mathcal{E}_0^\mu[\tilde{P}](t).
\] (33)

Our computations above indicate that \(\mathcal{E}_0^\mu\) is \(O(\mu)\) and we can make the other terms above small by restrictions on the initial conditions. So we put

\[
\tilde{F}^\mu = 0.
\]

In which case the approximating system (28) consists of a standard FPUT

\[
\dot{\tilde{R}} = \delta^+ \tilde{P} \\
\dot{\tilde{P}} = \delta^- [V'(\tilde{R})]
\]

whose solution drives a simple harmonic oscillator

\[
\dot{\tilde{r}} = \tilde{p} - \tilde{P} \\
\mu \ddot{\tilde{r}} = -\kappa \tilde{r}.
\] (35)

This is very similar to the approximation from Section 4. The key difference is that instead of \(\tilde{r} = 0\) and \(\tilde{p} = \tilde{P}\) as in Corollary 3, the internal oscillators solve their equations of motion exactly with the caveat that they are driven by what is now an approximate version of \(P\).

As described in Section 5.2 all the residuals apart from the second are zero, which is \(\text{Res}_2^\mu(\tilde{\Phi}^\mu) = \kappa F^\mu[\tilde{r}(0), \tilde{p}(0), \tilde{P}]\). Using (31) and (33) we have:

\[
\| \text{Res}_2^\mu(\tilde{\Phi}^\mu(t)) \| \leq C \left( \| \tilde{r}(0) \| + \sqrt{\mu} \| \tilde{p}(0) - \tilde{P}(0) \| \right) \\
+ C \mu \left( \| \tilde{P}(t) \| + \| \dot{\tilde{P}}(0) \| + |t| \sup_{|t| \leq T_*} \| \tilde{P}(t) \| \right).
\]

Because it is part of the solution of FPUT, \(\tilde{P}\) satisfies a global in time estimate like (25). A routine bootstrap argument can be used to get global in time control of all higher order time derivatives of \(\tilde{P}\) as well. Therefore the final term above is genuinely \(O(\mu)\) for \(|t| \leq T_*\). If we
additionally demand that $\|\tilde{r}(0)\| + \sqrt{\mu}\|\tilde{p}(0) - \tilde{P}(0)\| \leq C\mu$ then we have $\|\text{Res}_2^\mu(\tilde{\Phi})\| \leq C\mu$ on $[-T_*, T_*]$. Theorem \[2\] tell us the error of the approximation \((34)-(35)\) is $O(\mu)$, a half power of $\mu$ better than in Corollary \[3\]. Here is the rigorous result:

**Corollary 5.** Let $\kappa > 0$, $K_* > 0$, $T_* > 0$ and $V : \mathbb{R} \to \mathbb{R}$ be smooth with $V(0) = V'(0) = 0$ and $V''(0) =: k > 0$. Then there exists $\rho_* = \rho_*(V) > 0$, $\mu_* = \mu_*(K_*, T_*, \kappa, V) > 0$ and $C_* = C_*(K_*, T_*, \kappa, V) > 0$ for which we have the following when $\mu \in (0, \mu_*]$. Suppose that $(\tilde{R}, \tilde{P})$ solves the FPUT system \((34)\) with $\|\tilde{R}(0)\| + \sqrt{\mu}\|\tilde{P}(0)\| \leq \rho_*$ and $(\tilde{r}, \tilde{p})$ solve the driven simple harmonic oscillator \((35)\) with $\|\tilde{r}(0)\| + \sqrt{\mu}\|\tilde{p}(0) - \tilde{P}(0)\| \leq K_*\mu$. Furthermore suppose that $(R, P, r, p)$ solves the MiM lattice \((3)\) with $\|(R(0), P(0), r(0), p(0)) - (\tilde{R}(0), \tilde{P}(0), \tilde{r}(0), \tilde{P}(0))\|_\mu \leq \mu$.

Then $\|(R(t), P(t), r(t), p(t)) - (\tilde{R}(t), \tilde{P}(t), \tilde{r}(t), \tilde{P}(t))\|_\mu \leq C_*\mu$ for all $t \in [-T_*, T_*]$.

5.5. **The higher order FPUT approximation.** Going to next order of the approximation has a surprising outcome: the approximation remains an FPUT approximation. Applying \((32)\) with $m = 1$ to $F_\mu[r(0), p(0), P]$ gets us, after some algebra,

$$F_\mu[r(0), p(0), P] = -\frac{1}{\omega_\mu^2} \dot{P}$$

$$+ \left(r(0) + \frac{1}{\omega_\mu^2} \dot{P}(0)\right) \cos(\omega_\mu t)$$

$$+ \frac{1}{\omega_\mu} \left(p(0) - P(0) + \frac{1}{\omega_\mu^2} \dot{P}(0)\right) \sin(\omega_\mu t)$$

$$+ \mathcal{E}_2^\mu[\dot{P}](t).$$

We can make the second two lines as small as we please by imposing restrictions on the initial data and the last line is expected to be $O(\mu^2)$. Thus we are lead to the choice of

$$\tilde{F}_\mu = -\frac{1}{\omega_\mu^2} \dot{P} = -\frac{\mu}{\kappa} \dot{P}.$$

With, this (and some really easy algebra) we form an approximating system from \((28)\). The variables $(\tilde{R}, \tilde{P})$ solve

$$\dot{\tilde{R}} = \delta^+ \tilde{P}$$

$$\dot{\tilde{P}} = \frac{1}{1 + \mu} \delta^- [V'(\tilde{R})].$$
and the variables \((\vec{r}, \vec{p})\) solve
\[
\begin{align*}
\dot{\vec{r}} &= \vec{p} - \vec{P} \\
\mu \dot{\vec{p}} &= -\kappa \vec{r}.
\end{align*}
\]
(38)
These are, again barely different that the FPUT approximations (28) or (31)-(35). The
\((\vec{R}, \vec{P})\) system (37) is once more FPUT, but the potential function is slightly modified by
the factor \(1/(1 + \mu)\), a roughly \(O(\mu)\) change.

To wit, we compute the residuals. As we saw above in Section 5.2 only \(\text{Res}_2(\vec{\Phi}^\mu)\) is
non-zero and in this setting is given by
\[
\begin{align*}
\text{Res}_2(\vec{\Phi}^\mu) &= \kappa \left( \vec{r}(0) + \frac{1}{\omega_\mu^2} \dot{\vec{P}}(0) \right) \cos(\omega_\mu t) \\
&\quad + \sqrt{\mu} \left( \vec{p}(0) - \vec{P}(0) + \frac{1}{\omega_\mu^2} \dot{\vec{P}}(0) \right) \sin(\omega_\mu t) \\
&\quad + \kappa \mathcal{E}_2^\mu[\vec{P}](t).
\end{align*}
\]
(39)
Since \((\vec{R}, \vec{P})\) satisfy an FPUT system, we get global in time estimates for them as in (25); that there is a mild \(\mu\) dependence in the equations for \((\vec{R}, \vec{P})\) does not effect this estimate in any way, so long as \(\mu\) is not too big. And, as in the previous section, it is elementary to
bootstrap and get \(\mu\)-uniform estimates on \(\vec{P}, \vec{P}\) and so on. Thus if we apply (31) we find
\[
\| \mathcal{E}_2^\mu[\vec{P}](t) \| \leq C \omega_\mu^{-n-2} \left( \| P^{(4)}(t) \| + \| P^{(4)}(0) \| + \| T_s \| \sup_{t' \leq |t|} \| P^{(5)}(t') \| \right) \leq C \mu^2.
\]
Then we demand
\[
\left\| \vec{r}(0) + \frac{1}{\omega_\mu^2} \dot{\vec{P}}(0) \right\| + \sqrt{\mu} \left\| \vec{p}(0) - \vec{P}(0) + \frac{1}{\omega_\mu^2} \dot{\vec{P}}(0) \right\| \leq C \mu^2.
\]
In which case we now have \(\| \text{Res}_2(\vec{\Phi}^\mu) \| \leq C \mu^2\). Since \(\dot{\vec{P}} = (1 + \mu)^{-1} \delta^{-}[V'(\vec{R})]\) we can rewrite
the above condition in a slightly more functional way as
\[
\left\| \vec{r}(0) + \frac{\mu}{\kappa (1 + \mu)} \delta^{-}[V'(\vec{R}(0))] \right\| + \sqrt{\mu} \left\| \vec{p}(0) - \vec{P}(0) + \frac{\mu}{\kappa (1 + \mu)} \delta^{-}[V''(\vec{R}(0))\delta^+ \vec{P}(0)] \right\| \leq C \mu^2.
\]
And the geometric series tells us that the above is implied by
\[
\left\| \vec{r}(0) + \frac{\mu}{\kappa} \delta^{-}[V'(\vec{R}(0))] \right\| + \sqrt{\mu} \left\| \vec{p}(0) - \vec{P}(0) + \frac{\mu}{\kappa} \delta^{-}[V''(\vec{R}(0))\delta^+ \vec{P}(0)] \right\| \leq K_s \mu^2.
\]
With all of the above considerations, we can invoke Theorem [2]

**Corollary 6.** Let \(\kappa > 0, K_s > 0, T_s > 0\) and \(V : \mathbb{R} \to \mathbb{R}\) be smooth with \(V(0) = V'(0) = 0\) and \(V''(0) =: k > 0\). Then there exists \(\rho_* = \rho_*(V) > 0, \mu_* = \mu_*(K_s, T_s, \kappa, V) > 0\) and \(C_*= C_*(K_s, T_s, \kappa, V) > 0\) for which we have the following when \(\mu \in (0, \mu_*]\).

Suppose that \((\vec{R}, \vec{P})\) solves the FPUT system (37) with
\[
\| \vec{R}(0) \| + \| \vec{P}(0) \| \leq \rho_*,
\]
and \((\tilde{r}, \tilde{p})\) solve the driven simple harmonic oscillator (35) subject to
\[
\left\| \tilde{r}(0) + \frac{\mu}{\kappa} \delta^{-}[V'(\tilde{R}(0))] \right\| + \sqrt{\mu} \left\| \tilde{p}(0) - \tilde{P}(0) + \frac{\mu}{\kappa} \delta^{-} [V''(\tilde{R}(0)) \delta^+ \tilde{P}(0)] \right\| \leq K_* \mu^2.
\]
Furthermore suppose that \((R, P, r, p)\) solves the MiM lattice (3) with
\[
\| (R(0), P(0), r(0), p(0)) - (\tilde{R}(0), \tilde{P}(0), \tilde{r}(0), \tilde{P}(0)) \|_\mu \leq K_* \mu^2.
\]
Then
\[
\| (R(t), P(t), r(t), p(t)) - (\tilde{R}(t), \tilde{P}(t), \tilde{r}(t), \tilde{P}(t)) \|_\mu \leq C_* \mu^2
\]
for all \(t \in [-T_*, T_*]\).

5.6. Challenges at the next order. Does this strategy always yield an FPUT system whose solutions drive the internal oscillators? Put \(m = 2\) into (32).

\[
F^\mu[r(0), p(0), P] = -\frac{1}{\omega_\mu^2} \dot{P} + \frac{1}{\omega_\mu^4} \partial^3_t P
\]
\[
+ \left( r(0) + \frac{1}{\omega_\mu^4} \dot{P}(0) - \frac{1}{\omega_\mu^4} \partial^3_t P(0) \right) \cos(\omega_\mu t)
\]
\[
+ \frac{1}{\omega_\mu} \left( p(0) - P(0) + \frac{1}{\omega_\mu^2} \dot{P}(0) - \frac{1}{\omega_\mu^4} \partial^3_t P(0) \right) \sin(\omega_\mu t)
\]
\[
+ \mathcal{E}_2^\mu(\dot{P})(t).
\]

(40)

If we followed the earlier strategy, we would truncate after the first line and use initial data restriction and (31) to control errors from the last two. Imagine that we do this now, then our approximating system reads:
\[
\dot{\tilde{R}} = \delta^+ \tilde{P}
\]
\[
-\frac{\mu^2}{\kappa} \partial^3_t \tilde{P} + (1 + \mu) \dot{\tilde{P}} = \delta^{-}[V'(\tilde{R})]
\]
\[
\dot{\tilde{r}} = \tilde{p} - \tilde{P}
\]
\[
\dot{\mu} \tilde{p} = -\kappa \tilde{r}.
\]

(41)

Again the first two lines are self-contained, but are not an FPUT system—they are a singularly perturbed FPUT equation. It is not at all obvious that such an approximation is useful, since the approximating system is now as complex as the original. We go no further.

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