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Two-scale modeling for Hamiltonian systems: formal and rigorous results

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We study how Hamiltonian structures reduce from a microscopic lattice model under the transition to a macroscopic continuum model. Thus, we provide tools for constructing effective macroscopic Hamiltonians. In particular, we are interested in the case of modulations of plane waves having a microscopic structure. Embedding the discrete system into a continuum one and using additional microscopic phase variables we are led to a completely equivalent continuous system that has additional first integrals associated with the translationally invariants in space and phase variables. The phase velocity of the microstructure and the group velocity of modulating pulse can then be factored out and suitable scalings lead to a singularly perturbed system. Arguing formally the Hamiltonian converges to a generalized Γ-limit that governs the macroscopic modulation equation. Only for a system without microstructure we are able to make the limit rigorous in showing weak convergence to a nonlinear Klein-Gordon equation.

The derivation of macroscopic equations for discrete models (or continuous models with microstructure) can be seen as a kind of reduction of the infinite dimensional system to a simpler subclass. If we choose well-prepared initial conditions, we hope that the solution will stay in this form and evolve according to a slow evolution with macroscopic effects only. We may interprete this as a kind of (approximate) invariant manifold, and the macroscopic equation describes the evolution on this manifold, the functions A defining kind of coordinates. We refer to [Mie91] for exact reductions of Hamiltonian systems and to [DHM06, GHM06a, Mie06b, GHM06b] for the full details.

1. Derivation of nlS via Hamiltonian two-scale reduction

As the easiest example we consider the one-dimensional Klein-Gordon chain

$$\ddot{x}_j = x_{j+1} - 2x_j + x_{j-1} - ax_j - bx_j^3, \quad j \in \mathbb{Z}.$$

The sum of the kinetic and potential energy gives the Hamiltonian

$$H(\mathbf{x}, \dot{\mathbf{x}}) = \textstyle\sum_{j\in\mathbb{Z}} \left(\frac{1}{2}\dot{x}_j^2 + \frac{1}{2}(x_{j+1}-x_j)^2 + \frac{a}{2}x_j^2 + \frac{b}{4}x_j^4\right).$$

We embed the discrete chain on $\mathbb{Z}$ into the cylinder $\Xi = \mathbb{R}\times\mathbb{S}^1$, where $\mathbb{S}^1$ contains the additional microscopic phase variable. The continuous Hamiltonian system is

$$\begin{aligned} &\partial_t^2 u = \Delta_{(1,0)}u - au + bu^3 \quad \text{with } a > 0, \quad u \in \mathrm{L}^2(\Xi), \\ &\text{and } \Delta_{(\varepsilon,\delta)}u(\eta,\phi) := u(\eta{+}\varepsilon, \phi{+}\delta) - 2u(\eta,\phi) + u(\eta{-}\varepsilon, \phi{-}\delta). \end{aligned} \tag{1}$$

Introducing $p = \partial_\tau u$ this is a canonical Hamiltonian system with

$$H^{\mathrm{cont}}(u,p) = \textstyle\int_\Xi \frac{1}{2}p^2 + \frac{1}{2}\big(\nabla_{(1,0)}u\big)^2 + \frac{a}{2}u^2 + \frac{b}{4}u^4 \,\mathrm{d}\eta\,\mathrm{d}\phi.$$

This system contains the KG chain exactly, because it decouples completely into an uncountable family of KG chains just displaced by $(\eta, \phi) \in [0,1) \times \mathbb{S}^1$. Moreover, (1) is invariant under translations in the spatial direction η as well as in the phase direction ϕ. This leads to the two first integrals $I^{\mathrm{sp}}(u,p) = \int_\Xi p\, \partial_\eta u \,\mathrm{d}\eta\, \mathrm{d}\phi$ and $I^{\mathrm{ph}}(u,p) = \int_\Xi p\, \partial_\phi u \,\mathrm{d}\eta \,\mathrm{d}\phi$. Using the symmetry transformation

$$(\widetilde{u}, \widetilde{p}) = T^{\mathrm{sp}}_{ct} T^{\mathrm{ph}}_{(\omega - c\theta)t}(u,p), \qquad \widetilde{\mathcal{H}} = \mathcal{H} - cI^{\mathrm{sp}} - (\omega - c\theta) I^{\mathrm{ph}}$$

the associated canonical Hamiltonian system $\mathbf{\Omega}^{\mathrm{can}}(\widetilde{u}_t, \widetilde{p}_t) = \mathrm{D}\widetilde{\mathcal{H}}(\widetilde{u}, \widetilde{p})$ on $\mathrm{L}(\Xi)^2$ is still fully equivalent to a family of uncoupled KG chains.

Introducing a suitable scaling, which anticipates the desired microscopic and macroscopic behavior, will exposes the desired limit. For this we let

$$(\widetilde{u}(\eta, \phi), \widetilde{p}(\eta, \phi)) = (\varepsilon U(\varepsilon \eta, \phi - \theta\eta), \varepsilon P(\varepsilon\eta, \phi - \theta\eta)),$$

which keeps the canonical structure (after moving a factor ε arising from $\mathrm{d}y = \varepsilon\, \mathrm{d}\eta$ into the time parametrization $\tau = \varepsilon^2 t$). We obtain the new Hamiltonian

$$\begin{aligned} \mathcal{H}_\varepsilon(U,P) = \int_\Xi \tfrac{1}{2\varepsilon^2} \Big(& \big[P - \omega U_\phi - \varepsilon c U_y\big]^2 + \big(\nabla_{(\varepsilon,\theta)} U\big)^2 \\ & + aU^2 - \big[\omega P U_\phi + \varepsilon c P U_y\big]^2 \Big) + \tfrac{b}{4} U^4 \,\mathrm{d}y\, \mathrm{d}\phi, \end{aligned}$$

where $\nabla_{(\varepsilon,\theta)} U(y,\phi) = U(y+\varepsilon, \phi+\theta) - U(y,\phi)$. The modulation ansatz now reads

$$(U(y,\phi), P(y,\phi)) = R_\varepsilon(A)(y,\phi) = (\mathrm{Re}\, A(y)\mathrm{e}^{\mathrm{i}\phi}, \omega\, \mathrm{Re}\, A(y) \mathrm{e}^{\mathrm{i}\phi}) + O(\varepsilon),$$

and leads to $\mathcal{H}_\varepsilon(R_\varepsilon(A)) = \mathbb{H}_{\mathrm{nlS}}(A) + O(\varepsilon)$ and $\mathrm{D}R_\varepsilon(A)^* \mathbf{\Omega}^{\mathrm{can}} \mathrm{D}R_\varepsilon(A) = \mathbf{\Omega}^{\mathrm{red}} + O(\varepsilon)$ with

$$\mathbb{H}_{\mathrm{nlS}}(A) = \int_{\mathbb{R}} \omega\omega'' |A_y|^2 + \tfrac{3b}{8} |A|^4 \,\mathrm{d}y \qquad \text{and} \qquad \mathbf{\Omega}^{\mathrm{red}} = 2\mathrm{i}\omega.$$

Thus, the macroscopic limit is the one-dimensional nonlinear Schrödinger equation

$$2\mathrm{i}\omega A_\tau = -2\omega\omega'' A_{yy} + \tfrac{3}{2} b |A|^2 A.$$

A rigorous justification of this micro-macro transition is given in [GM04, GM06].

2. A weak convergence result

For static problems there is a rich literature concerning the Γ-convergence of potential energy functionals of discrete models to continuum models (cf. [FJ00, FT02, BG02, BLM06]). Here we want to summarize some first results for dynamic problems that rely on weak convergence. In [Mie06a] it was shown that linear elastodynamics can be derived from a general linear lattice model. However, this result used exact periodicity and linearity in an essential way. The abstract approach presented in [Mie06b] has its main advantage in the flexibility, which allows for applications in nonlinear and macroscopically heterogeneous settings.

In particular, it can be applied to polyatomic Klein–Gordon chains, which we also allow to have large-scale variations in the stiffness and masses. The KG chains under consideration are assumed to have a periodicity of N on the microscopic level, may change also on the macroscopic scale $y = \varepsilon j$, and are all bounded from below by a positive constant. The KG chain is then given by the canonical Hamiltonian system on $\ell^2 \times \ell^2$ via

$$(2) \qquad \mathcal{H}_\varepsilon^{\rm discr}(\mathbf{x},\mathbf{p}) = \sum_{j\in\mathbb{Z}} \Big(\frac{p_j^2}{2m_{[j]}(\varepsilon j)} + \frac{a_{[j]}(\varepsilon j)}{2}(x_{j+1}-x_j)^2 + \frac{\varepsilon^2 b_{[j]}(\varepsilon j)}{2} x_j^2 + \frac{\varepsilon^2 c_{[j]}(\varepsilon j)}{4} x_j^4 \Big),$$

where $[j] = j \bmod N$. To derive a suitable continuum model we embed $\ell^2 \times \ell^2$ into $Z_\varepsilon \subset Z = Z_0 = \mathrm{H}^1(\mathbb{R}) \times \mathrm{L}^2(\mathbb{R})$ via

$$\begin{aligned} &(u,v) = E_\varepsilon(\mathbf{x},\mathbf{p}) \text{ with } (u(\varepsilon j), v(\varepsilon j)) = (x_j, p_j) \text{ for all } j \in \mathbb{Z} \\ &\text{with } Z_\varepsilon = \{\, (u,v) \in Z \mid u|_{[\varepsilon j, \varepsilon j+\varepsilon]} \text{ affine}, v|_{(\varepsilon j-\varepsilon/2,\ \varepsilon j+\varepsilon/2)} \text{ constant} \,\} \end{aligned}$$

Theorem [Mie06b] *Let $(x^\varepsilon, p^\varepsilon) : [0, T/\varepsilon] \to \ell^2 \times \ell^2$ be solutions of the canonical Hamiltonian system associated with $\mathcal{H}_\varepsilon^{\rm discr}$ in (2). If for $\tau = 0$ we have*

$$\begin{pmatrix} I & 0 \\ 0 & M(\cdot, \cdot/\varepsilon) \end{pmatrix} E_\varepsilon \begin{pmatrix} \mathbf{x}^\varepsilon(\tau/\varepsilon) \\ \varepsilon \mathbf{p}^\varepsilon(\tau/\varepsilon) \end{pmatrix} \rightharpoonup \begin{pmatrix} u(\tau) \\ M^*(\cdot) v(\tau) \end{pmatrix} \quad \text{in } Z,$$

then this convergence holds for all $\tau \in [0,T]$, where $(u,v) : [0,T] \to Z$ is a solution of the macroscopic wave equation arising from the canonical Hamiltonian system with $\mathcal{H}_0(u,v) = \int_\mathbb{R} \frac{1}{2M^*(y)} v^2 + \frac{A^*(y)}{2}(u')^2 + \frac{B^*(y)}{2} u^2 + \frac{C^*(y)}{4} u^4 \,\mathrm{d}y$, where $M^*(y) = \frac{1}{N}\sum_{k=1}^N m_k(y)$ and similarly for $B^*(y)$ and $C^*(y)$, whereas $A_*(y) = 1/\sum_{k=1}^N \frac{1}{a_k(y)}$ is the harmonic mean.

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