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On the Bloch decomposition based spectral method for wave propagation in periodic media

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ABSTRACT

We extend the Bloch-decomposition based time-splitting spectral method introduced in an earlier paper [Z. Huang, S. Jin, P. Markowich, C. Sparber, A Bloch decomposition based split-step pseudo spectral method for quantum dynamics with periodic potentials, SIAM J. Sci. Comput. 29 (2007) 515–538] to the case of (non-)linear Klein–Gordon equations. This provides us with an unconditionally stable numerical method which achieves spectral convergence in space, even in the case where the periodic coefficients are highly oscillatory and/or discontinuous. A comparison to a traditional pseudo-spectral method and to a finite difference/volume scheme shows the superiority of our method. We further estimate the stability of our scheme in the presence of random perturbations and give numerical evidence for the well-known phenomenon of Anderson's localization.

1. Introduction

In this paper we consider the propagation of (nonlinear) *high frequency* waves in a one-dimensional medium with a *periodic microstructure*. Such problems arise, e.g., in the study of composite materials, photonic crystals, optic lattices [5]. For instance, the propagation of linearly polarized light in a fiber Bragg grating with intensity dependent refraction-index χ, i.e. a so-called Kerr medium, can be modelled by the nonlinear wave equation, cf. [6,26],

$$\frac{\partial^2 E}{\partial t^2} = \chi_{\text{lin}}(x)\frac{\partial^2 E}{\partial x^2} - \chi_{\text{lin}}(x)E - \chi_{\text{nl}}(x)E^3. \tag{1}$$

Here, E is the remaining (single) component of the electric field, χ_{lin} denotes the square of the linear index of refraction and χ_{nl} the corresponding nonlinear Kerr-susceptibility. Both coefficients are *spatially periodic* functions.

In the following we shall be interested in the case where the typical wavelength is comparable to the period of the medium, and both of which are assumed to be small on the length-scale of the considered physical domain, i.e. on the scale observation. This consequently leads us to a problem invoking *two-scales* where from now on we shall denote by $0 < \varepsilon \ll 1$ the small dimensionless parameter describing the microscopic/macroscopic scale ratio. In this paper we shall study of the following class of (one-dimensional) *Klein–Gordon type equations*

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$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} = \dfrac{\partial}{\partial x}\left(a_\Gamma\left(\dfrac{x}{\varepsilon}\right)\dfrac{\partial u}{\partial x}\right) - \dfrac{1}{\varepsilon^2}W_\Gamma\left(\dfrac{x}{\varepsilon}\right)u + f(x), \quad x \in \mathbb{R}, \ t > 0, \\ u|_{t=0} = u_0(x), \quad \dfrac{\partial u}{\partial t}|_{t=0} = v_0(x), \end{cases} \tag{2}$$

with given initial data $u_0(x),\ v_0(x) \in \mathbb{R}$ and $f(x) \in \mathbb{R}$ describing some slowly varying source term. A nonlinear version of this model, similar to Eq. (1), will also be considered later on (see Example 3.3). The highly oscillatory coefficients $a_\Gamma(y),\ W_\Gamma(y) \in \mathbb{R}$ are assumed to be *periodic* with respect to some *regular lattice* $\Gamma \simeq \mathbb{Z}$. Eq. (2) henceforth describes the propagation of waves on macroscopic length- and time-scales.

Concerning the numerical simulation of such problems, we note that in [8] Fogarty and LeVeque provided high-resolution finite-volume methods for acoustic waves propagation in periodic and random media. The reader can find more related works in [18,21]. Indeed, the main computational challenge in the simulations of equations like (2), stems from the fact that the computational grid size must be small enough to capture the microscopic details of the medium, or, equivalently, the shortest wavelength. Furthermore, having in mind the CFL conditions in traditional finite-difference or finite-volume schemes, also the time-steps have to be chosen small enough, i.e. $\mathcal{O}(\varepsilon)$. Therefore, the overall computational costs become prohibitively expensive.

One possibility to circumvent such problems is to entirely rely on *homogenized equations* which approximate (2) in the limit $\varepsilon \to 0$, cf. [1,5,10,11,25,26,28] for the derivation of such models. Numerical studies in this spirit can be found in [20,24] where the authors derive an effective dispersive model describing wave propagation in a periodic medium. Similarly, Kevorkian and Bosley [17] considered hyperbolic conservation laws with rapidly varying, spatially periodic fluctuations by multiple asymptotic analysis. Numerical approaches on the related problem of linear Schrödinger equation with a periodic potential were studied in [12,13]. However, by passing to an effective (homogenized) equation, one usually looses all details of the underlying microscopic dynamics. In particular this prohibits one to simulate and compare the behavior for different choices for $\varepsilon > 0$. It is therefore highly desirable to design a numerical method that, for any given wave-length, i.e. for any given choice of ε, allows for rather large mesh-size and/or time-steps. We have done so in our earlier works [14,15], where we considered (nonlinear) Schrödinger equations with periodic potentials. There, we developed a Bloch-decomposition based spectral method for which has been demonstrated to be superior to traditional Fourier spectral methods. The main advantages of our new method include: Spectral accuracy in space even in the case of discontinuous periodic coefficients and the possibility of choosing large time steps, i.e. of order $\mathcal{O}(1)$, even for small wave length. In the present work, we shall extend our Bloch-decomposition based time-splitting scheme to evolutionary problems of the above given Klein–Gordon type (including nonlinearities).

We outline the contents of the paper here. We first give a short review on the analytical background of the Bloch decomposition in Section 2 and we consequently show how to apply it numerically to equations of the form (2). Next, we compare our method with the more traditional pseudo-spectral method and with a finite-volume scheme in Section 3. In particular, we also include a (weakly) nonlinear case there. In Section 4 we shall also take into account *random coefficients* $a_\Gamma(\omega,y)$ to test the stability of our scheme with respect to random perturbations. Finally, we shall study the wave propagation in *random media* and give numerical evidence for the emergence of so-called *Anderson's localization*.

2. Description of the Bloch-decomposition based numerical method

In this section we will briefly recapitulate the numerical method developed in [14] and discuss its extension to the Klein–Gordon equation (2). For the convenience of the reader we shall first recall some basic definitions and important facts which are used when dealing with periodic operators.

2.1. Review of the Bloch decomposition

For definiteness, we shall assume from now on that

$$a_\Gamma(y + 2\pi) = a_\Gamma(y), \quad W_\Gamma(y + 2\pi) = W_\Gamma(y) \quad \forall y \in \mathbb{R}, \tag{3}$$

i.e. $\Gamma = 2\pi\mathbb{Z}$. Here, and in all what follows we shall always denote $y = x/\varepsilon$. Furthermore, we assume that

$$a_\Gamma(y) \geqslant a_0 > 0 \quad \forall y \in [0, 2\pi]. \tag{4}$$

In order to ensure ellipticity in the eigenvalue-problem (5). For $\Gamma = 2\pi\mathbb{Z}$, it holds [3]:

- The fundamental domain of our lattice is $\mathscr{C} = (0, 2\pi)$.
- The *dual lattice* Γ^* is simply given by $\Gamma^* = \mathbb{Z}$.
- The fundamental domain of the dual lattice $\mathscr{B} = \mathscr{C}^*$, i.e. the (first) *Brillouin zone*, is $\mathscr{B} = \left(-\frac{1}{2}, \frac{1}{2}\right)$.

Next, consider the eigenvalue problem,

$$\left(-\frac{\partial}{\partial_y}\left(a_\Gamma(y)\frac{\partial}{\partial_y}\right) + W_\Gamma(y)\right)\varphi_m(y,k) = \lambda_m(k)\varphi_m(y,k), \tag{5}$$