INSTITUTE OF PHYSICS PUBLISHING WAVES IN RANDOM MEDIA

Waves Random Media **11** (2001) R31–R102 www.iop.org/Journals/wr PII: S0959-7174(01)15886-6

TOPICAL REVIEW

Nonlinear photonic crystals: I. Quadratic nonlinearity

A Babin and A Figotin

University of California at Irvine, Irvine, CA 92697-3875, USA

Received 24 July 2000

Abstract

We develop a consistent mathematical theory of weakly nonlinear periodic dielectric media for the dimensions one, two and three. The theory is based on the Maxwell equations with classical quadratic and cubic constitutive relations. In particular, we give a complete classification of different nonlinear interactions between Floquet–Bloch modes based on indices which measure the strength of the interactions. The indices take on a small number of prescribed values which are collected in a table. The theory rests on the asymptotic analysis of oscillatory integrals describing the nonlinear interactions.

(Some figures in this article are in colour only in the electronic version; see www.iop.org)

Contents

0959-7174/01/020031+72$30.00

1. Introduction

We study here the effects of spatial periodic variation of the refractive index on nonlinear optical processes under the condition that the nonlinearity is small. One of the known ultimate results of the spatial periodicity is a substantial decrease in the nonlinear mode coupling, and weakening of the effect of the nonlinearity on the wave propagation. In particular, the spatial periodicity of the dielectric medium can significantly modify nonlinear processes such as second-mode generation, third-harmonic generation and four-wave mixing [1, 64, 69]. A simplified explanation of the effect is that the spatial periodicity causes Bragg scattering which, in turn, alters and destroys the phase matching needed for the nonlinear wave coupling to occur. The scattering selects a few strongly interacting modes, these modes are found from the equations (selection rules) we explicitly write. The effect of the spatial periodicity on nonlinear optical processes has been a subject of intensive studies in the physical literature [1, 7, 10, 14, 44, 58, 82]. In [82] one can also find recent experimental results on nonlinear phenomena in photonic crystals.

We make an effort here to develop a consistent mathematical theory of the electromagnetic wave propagation in weakly nonlinear periodic dielectric media based on Maxwell equations and classical nonlinear optics for one, two and three dimensions. In the case of a weak nonlinearity, the underlying linear periodic dielectric medium plays a key role in the analysis of the nonlinear response on the wave propagation. Periodic dielectric structures, often called *photonic crystals*, have attracted a great deal of attention because of their numerous potential applications in novel optical devices. Linear photonic crystals have been a subject of intensive studies for the last decade (see [36, 47, 65, 68, 77] and reference therein). The rigorous mathematical and computational studies in the theory of photonic crystals is a rather new area [8, 20, 25–32, 53, 54, 57]. The quoted papers consider the linear photonic crystals and their spectral properties. For a variety of phenomena in nonlinear photonic crystals see the following list and references therein [7, 9, 10, 17–19, 34, 40, 41, 43, 44, 55, 60, 62, 67, 73, 75, 79, 80, 82]. In this paper we show that basic components of classical nonlinear optics theory can be obtained via an asymptotic analysis of wavepacket solutions of the nonlinear Maxwell equations. We provide the framework for the rigorous treatment of basic nonlinear phenomena such as three-wave interactions and second-harmonic generation (SHG), in particular we show how few strongly interacting waves are selected from the ensemble of waves.

We thoroughly discuss the crucial elements of the theory and carry out calculations of the leading terms of asymptotics of oscillatory integrals describing the nonlinear interactions.

Recall that the main ingredients of the linear theory of electromagnetic waves in a homogeneous dispersive media are *dispersion relations, wavepackets* and *group velocities* of wavepackets. A standard way to build a relation between the linear and nonlinear wave theory is to study solutions to the relevant wave equations of the form $\boldsymbol{f}(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)$, where $\boldsymbol{k}$ is the wavevector and ω is the frequency. The dispersion relation $\omega=\omega(\boldsymbol{k})$ for the linear medium can be derived from the requirement that $\boldsymbol{f}(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)$ solves the corresponding linear equation, for instance, the Maxwell linear equations. When the wave equation becomes nonlinear and the space homogeneity is preserved one can still find exact solutions of the form $\boldsymbol{f}(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)$ and construct a nonlinear theory. Examples of such nonlinear theories can be found in [78], section 17.10. Unfortunately, for inhomogeneous media there are no simple forms for exact solutions analogous to $\boldsymbol{f}(\boldsymbol{k}\cdot\boldsymbol{r}-\omega t)$ that are preserved when we introduce a nonlinearity, and a way to study the nonlinear wave propagation is by applying asymptotic methods.

The nonlinear effects we intend to study, including second-mode generation, third-harmonic generation and four-wave mixing, can be explained in terms of the evolution properties of wavepackets which are slowly modulated time-harmonic waves and have frequencies in narrow bands. As to the spatial distribution, the wavepackets may have a spatial scale which is comparable with the spatial period of the medium. The nonlinear effects of the interest arise as the wavepacket passes through many period cells. Here we do not study wavepackets on length scales substantially smaller than the spatial period of the medium.

The standard description of waves in linear periodic media is based on the Floquet–Bloch spectral theory with *Bloch eigenmodes* replacing plane waves. In the periodic case, the role of the wavevector $\boldsymbol{k}$ (varying over the whole space for a homogeneous medium) is played by the quasimomentum $\boldsymbol{k}$ which lies in the *Brillouin zone* determined by the lattice period. The spectrum of the periodic medium consists of intervals (which may be overlapping), called bands, numbered by the index $n=1,2,\ldots$, and every band has its own *dispersion relation* $\omega=\omega_n(\boldsymbol{k})$ and corresponding Bloch eigenmode $\boldsymbol{G}_n(\boldsymbol{k})$. Similarly to the spatially homogeneous case, one can use the Floquet–Bloch representation in place of the Fourier representation, and introduce *wavepackets* and *group velocities* $\nabla\omega_n(\boldsymbol{k})$ of the wavepackets in the periodic medium. When defining the wavepackets we introduce an important parameter $\varrho\sim\frac{\Delta\omega}{\omega_0}$, where ω_0 is the carrier frequency and $\Delta\omega$ is the frequency bandwidth of the wavepacket (it can also be viewed as the typical frequency of the slowly varying envelope of the wavepacket). In other words, *one can think of the parameter ϱ as the relative frequency bandwidth of the wavepacket.*

One of the results of our theory is the classification of the nonlinear interactions based on their relative intensity. A simplified description of our approach to the classification in the case of a quadratic nonlinearity is as follows. Suppose that we have a wavepacket $V^{(0)}$ in the underlying linear medium. When a weak nonlinearity is introduced in the medium, the wavepacket becomes $V=V^{(0)}+V^{(1)}+\cdots$, where $V^{(1)}$ is the first nonlinear response. Then we introduce the modal expansions of all the waves based on the Bloch eigenmodes. In particular, we study the amplitudes $V_n^{(1)}(\boldsymbol{k})$ of the first nonlinear response. For the quadratic nonlinearity a triple of modes with the spectral indices $(n,\boldsymbol{k})$, $\left(n',\boldsymbol{k}'\right)$ and $\left(n'',\boldsymbol{k}''\right)$ can interact nonlinearly, and there are infinitely many possible interacting triples. One of implications of our theory is that for any fixed $(n,\boldsymbol{k})$ there will be only a few pairs of modes $\left(n_l',\boldsymbol{k}_l'\right)$ and $\left(n_l'',\boldsymbol{k}_l''\right)$ that can have a significant impact on $V_n^{(1)}(\boldsymbol{k})$. Those few modes can be found using the derived selection rules formulated in terms of dispersion relations $\omega_n(\boldsymbol{k})$. One of corollaries of our analysis shows that the nonlinear response $V_n^{(1)}(\boldsymbol{k}, t)$ for non-dimensional time $t \gg 1$ can be expressed by the formula

$$V_n^{(1)}(\boldsymbol{k}, t) = \sum_{l=1}^{N(\boldsymbol{k})} \beta_l t^{\xi_l} \qquad \xi_{l+1} \leqslant \xi_l \tag{1}$$

where the amplitudes β_l and indices ξ_l depend on interacting modes, i.e.

$$\beta_l = b_l(\vec{n}_l, \vec{\boldsymbol{k}}_l) V_{n'}^{(0)}(\boldsymbol{k}'_l, \cdot)\, V_{n''}^{(0)}(\boldsymbol{k}''_l, \cdot) \qquad \xi_l = \xi(\vec{n}_l, \vec{\boldsymbol{k}}_l) \tag{2}$$

and can be found explicitly for $l = 1, \ldots, N - 1$. The last term with the smallest power $\xi_N < \xi_{N-1}$ includes the approximation error. Formula (1) holds for appropriately chosen wavepackets, and the conditions of its applicability are discussed later. Evidently, the right-hand side of (1) has terms which are growing or decaying at different rates depending on the indices ξ_l. One can interpret this as the energy exchange between the modes of the wavepacket due to nonlinear interactions of different intensity. The indices ξ_l can be used for the classification of the nonlinear interactions. Clearly, larger indices ξ_l correspond to stronger and more significant nonlinear interactions, and the corresponding spectral indices $\vec{n} = (n, n', n'')$, $\vec{\boldsymbol{k}}_l = (\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{k}'')$ indicate the corresponding interacting modes.

The main features of the theory of weakly nonlinear media we construct are as follows. Let a parameter α characterize the relative magnitude of the nonlinearity. The field evolution equations become linear for $\alpha = 0$. Since there are no exact solutions to the Maxwell equations in general nonlinear periodic media in the form of wavepackets we proceed as follows. First, we introduce solutions to the nonlinear equations that turn into wavepackets for $\alpha = 0$, and then we study the solutions for small α. When doing that we would like to keep a certain regularity of solutions as a function of α. To construct the solutions with the described properties, we employ excitation currents $\boldsymbol{J}$ such that:

(a) they excite wavepackets in the linear case $\alpha = 0$; and
(b) they yield nonlinear solutions that are well approximated by wavepackets for small α.

We use the linear spectral theory as a reference frame and rewrite the Maxwell equations in the Floquet–Bloch eigenbasis. It is well known that there is no energy transfer between the Bloch eigenmodes in the linear case. However, when a weak nonlinearity is introduced, the nonlinear interactions may initiate a slow energy transfer between the normal modes, resulting over long times in noticeable changes. Hence, the most important nonlinear effects should be associated with a nonlinear interaction with the most intensive energy transfer. To single out those important interactions, we study the behaviour of wavepackets asymptotically as $\varrho \to 0$, $\alpha \to 0$. The asymptotic analysis yields, in particular, the well known nonlinear phenomena such as the frequency matching condition, second-harmonic generation, third-harmonic generation, three- and four-wave mixing. In addition to that, our asymptotic analysis shows new features of nonlinear mode coupling for periodic media which have no analogues in the case of homogeneously nonlinear media. For example, one of these features of coupling requires *the group velocities to match for interacting modes*. In essence, this is a new selection rule which determines the triples of modes (quadruples in the cubic case) of stronger nonlinear coupling. The matching condition selects the strongest nonlinearly coupled directions and velocities of wave propagation. A simple physical explanation of this '*group velocity matching*' selection rule is that, first, it takes time for modes to interact nonlinearly, and, second, the mode energy exchange is more efficient and constructive if the interacting waves move together as a group. Our analysis also shows that the strongest interaction in a generic quadratic media between all the matched wavepackets yields the phenomenon known as the second harmonic generation (third-harmonic generation in a cubic media), and, in addition to that, the most strongly involved modes in the interactions are a few of them that are selected by an additional degeneracy condition.

Carrying out the asymptotic analysis of the Maxwell equations with spatially periodic nonlinear constitutive relations we find that the main features of the wave propagation in the medium are determined by multidimensional *oscillatory integrals* that describe the nonlinear coupling between the Bloch modes of the underlying periodic linear medium. The asymptotic behaviour of the oscillatory integrals becomes central to the theory. The analysis of these integrals suggests, in particular, the use of *wavepackets, i.e. waves whose frequencies and wavevectors vary continuously in narrow bands* (see, for instance, [33], section 1.6, [64], section 2g), as an appropriate tool for the quantitative studies of the nonlinear wave coupling and interaction. The rise of these oscillatory integrals, of course, is not accidental. It reflects the fundamental role of fine constructive and destructive Bloch mode interference in a wavepacket as it propagates through the dispersive nonlinear medium. Mathematically our analysis has a lot in common with the well known geometrical (ray) optics approximation within wave theory ([33], section 1.6), and the long-time–distance evolution of wavepackets in a medium of weakly coupled oscillators ([64], section 6). The common ground with geometrical optics is provided, first, by the use of wavepackets and oscillatory integrals to account for wave interference, and, second, by the use of the stationary phase method to determine the modes giving the major contributions to the oscillatory integrals. The similarity of our theory with geometrical optics is limited though by the phenomena studied as well as the basic physical conditions needed for their occurrence. For example, geometrical optics is the approximation which arises when the wavelength of the carrier wave is significantly smaller than the characteristic scale of the medium spatial inhomogeneity. In that situation the medium can be treated as being homogeneous on the length scale corresponding to the carrier wave, and, hence, locally one can use wavepackets constructed from plane waves and study the propagation of spatially localized wavepackets. This approach leads to geometrical optics (see, for example, [33]). To some extent it can be generalized to nonlinear equations, yielding a nonlinear version of the geometrical optics [37–39, 45, 46].

In our theory the spatial scale of the medium inhomogeneity is the size of the periodic cell which can be of the same order as the wavelength of the carrier wave. Keeping this in mind, we construct wavepackets based on the relevant Bloch waves rather than plane waves. In addition to that, we study those phenomena related to a weak nonlinearity which develop during sufficiently long times. One of the important results of the study is the selection rules for nonlinearly interacting modes. The mathematical techniques used to obtain the selection rules are based on oscillatory integrals and are very similar to those in geometrical optics which produce eikonal equations.

In view of the above, the nonlinear interaction oscillatory integrals become the central objects of the quantitative studies of nonlinear effects in periodic media. We find asymptotics of the oscillatory integrals using the *stationary phase method* (see, for instance, [6], theorem 6.3, [21], section 4.5, [24], section 8, [71], section 5.5). According to the method the main contributions to the integral are given by small neighbourhoods of a few so-called *critical points* of the relevant phase function. Ultimately, the critical points, first, determine which the modes are involved in significant nonlinear interactions, and, second, classify the interactions according to the level of their intensity. We have also found that the strongest nonlinear coupling comes from *degenerate critical points*. In particular, the theory we develop singles out the phenomenon of *second-harmonic generation* (see [3], section 3.1, [16], section 1.2, [81], section 12.4) as the one associated with the most degenerate points. We would like to note that asymptotic approximations related to degenerate critical points are not covered by the standard classical theory of oscillatory integrals, but it is rather a subject of recent studies, see [5, 6].

Constructing the theory we consider a generic periodic dielectric medium assuming that the dispersion relations are generic functions. That is a pretty common assumption which means, in particular, that there are no hidden symmetries in the dispersion relations. Consequently, we consider only robust (generic) singularities of the phase functions, which cannot be removed by small perturbations. Our analysis of the degenerate and non-degenerate phase function critical points is carried out within the general framework of dispersion relations of the linear periodic media which imposes a substantial and crucial impact on the analysis. We have done this analysis for all the space dimensions one, two and three, and for both quadratic and cubic nonlinearities.

In this paper we give a general framework for the theory of weakly nonlinear photonic crystals, and apply it primarily to the case of the quadratic nonlinearity. To give a more complete account of the theory we also formulate some statements for the cubic nonlinearity, though, its detailed analysis as well as other issues related to weakly nonlinear photonic crystals are left for subsequent papers. We do not give detailed mathematical proofs here, since such proofs would significantly increase the length of the paper. Nevertheless, we have proved the main results we present here under appropriate assumptions. We have proved the existence of the exact solutions of the nonlinear Maxwell equations on time intervals t of order $1/\alpha$. The asymptotic expansions we obtained are also rigorously proven on time intervals t of order $1/\alpha$ when $\alpha \ll \varrho \ll 1$. Since $\alpha \to 0$ this allows us to compare terms of order t^q and ϱ^q with different q. We make the assumption that the linear Maxwell operator M is an operator in the Hilbert space H, which has generic dispersion relations $\omega_{\bar{n}}(\boldsymbol{k})$. One can get such an operator as a generic self-adjoint perturbation of the differential Maxwell operator with periodic coefficients. Such a perturbation may be not a differential operator, but for our analysis that is not important. The rigorous detailed proofs will be given in a subsequent paper. On longer intervals of order $1/\alpha^p$, $p > 0$, we give some arguments showing that the asymptotics still hold (see subsection 7.6), but we cannot prove it rigorously right now.

For the reader's convenience we provide the notation index at the end of the paper.

2. Basic concepts of weakly nonlinear periodic dielectrics

Let us list and discuss the basic ingredients of the theory of weakly nonlinear dielectric media. We develop and shape these ingredients based on:

(a) the well studied and understood properties of simpler systems such as weakly nonlinear oscillators or arrays of weakly nonlinear coupled oscillators [12, 51, 59, 63];
(b) basic properties of waves propagating in continuous dispersive inhomogeneous media [33, 78, 81];
(c) classical nonlinear optics [3, 15, 16, 69, 70].

The primary manifestation of a weak nonlinearity is a slow accumulation of small incremental changes over a long period of time ([51], sections 4.1, 4.2, [64], sections 1 and 6.g). To account for this accumulation it is necessary to set up the 'right' solution representation or, in other words, to choose suitable variables. If the choices are made correctly we get a satisfactory approximation for long times. The strategy for producing this representation is to find first for the unperturbed system the variables that are decoupled and, hence, do not exchange energy. This is a well known and popular method in physics of the decomposition of a dynamical system into a set of *decoupled oscillators*, or *normal modes*. The expectation then is that weak nonlinear interactions will initiate a slow energy exchange between the normal modes resulting over long times in noticeable changes. This factor is accounted for by allowing the amplitudes of the normal modes which are constant under unperturbed dynamics to vary slowly in time. There are two intimately related approaches which are often used to study the long-time effect of nonlinear oscillations mathematically:

(a) *the two-scale (multiscale) method* when we treat the regular time t as fast and the slow time $\tau = \varrho t$, where $\varrho \ll 1$;
(b) *the averaging method.*

The main idea of the two-scale (multiscale) method is, first, to appropriately introduce multiple scales in time by setting up 'new' time variables (the same can be done in the space), and, then, to treat the variables of different scales as independent up to a point after which to account for the relations between the scales (see [51], section 4, [61], section 6.1, [64], section 6.g and references therein). The averaging method focuses on another side of the phenomenon. It singles out the significant terms of the solution, neglecting the terms vanishing because of the destructive (incoherent) interference (see [12, 56], section 5, [61], section 5.2, [59], section 6 and references therein).

Accurate approximations for long times. The requirement for the approximations to be accurate for long times comes from the fact that a weak nonlinearity induces small and slow incremental changes, and, hence, rather long times are needed for the changes to accumulate to a significant level. The relative size of the nonlinearity is characterized by a scalar dimensionless parameter $\alpha \geqslant 0$ such that the weak nonlinearity corresponds to small values of α, and $\alpha = 0$ corresponds to the unperturbed linear case. The introduced coefficient ϱ determines the 'slow time' scale, and it is often set to satisfy $\varrho \sim \alpha$. We can set it that way too but it is not necessary.

The essence of the phenomenon of small nonlinearity is that even for small values α the nonlinearity can have a significant effect on the evolution process if it evolves for sufficiently long times, which are normally of the order of or substantially larger than α^{-1}. Hence, a satisfactory asymptotic theory is expected to accurately describe the evolution for the times at least of order α^{-1} and longer ([51], section 4, [64], section 6.g, [61], section 5.2). Our asymptotic approximation holds as long as, first, the electric field $\boldsymbol{E}^{(0)}(\boldsymbol{r}, t)$ of the linear medium stays bounded, and, second, the electric field $\boldsymbol{E}^{(1)}(\boldsymbol{r}, t)$ of the first nonlinear response stays small on time intervals $t = \mathrm{O}\left(\alpha^{-2}\right)$ in the case $d = 1$, $t = \mathrm{O}\left(\alpha^{-3}\right)$ in the case $d = 2$. For $d = 3$ there is no restriction in terms of α, the main condition is the boundedness of $\boldsymbol{E}^{(0)}(\boldsymbol{r}, t)$ and the smallness of $\boldsymbol{E}^{(1)}(\boldsymbol{r}, t)$ (see section 7.6 for details). Note that we consider generic periodic media, and one cannot, for example, consider two-dimensional (2D) periodic media as a generic subclass of three-dimensional (3D) periodic media. 2D periodic media form a very special, more symmetric subclass of 3D periodic media; in 2D media properties of the media and electromagnetic fields do not depend on the third variable.

Time shift invariance and the initial-value problem. We have found that it is very beneficial to deal with the wavepackets defined for all negative times $-\infty < t < T$, where $T \gg 1$ is not explicitly specified, and vanishing as $t \to -\infty$ rather then with a wave defined by the initial-value problem with the wave state given explicitly, say, at time $t = 0$. Such a setting is invariant with respect to time shifts. In the case of a linear medium the differences between solutions defined at all times and solutions of the initial-value problem are not that essential. However, in the presence of a nonlinearity the difference becomes quite significant. First of all, the classical optics expressions for the susceptibilities tensors χ (see [15], see also section 6 below) include time delays and are given in the time shift invariant form which also takes time dispersion into account. The time shift invariance, of course, is a very important principle that we want to preserve, especially when dealing with a nonlinear problem. Second of all, there are examples of additional complications in asymptotic analysis brought about by the initial-value problems [50]. One of reasons for complications is that initial conditions impose a strong influence on the short-time behaviour of solutions, whereas we are interested in a different kind of wave phenomena, namely wave interactions over large time intervals, and separating these different effects in a consistent way may be very technical.

We want all the fields to vanish as $t \to -\infty$ for the following reasons. It may be very difficult, if possible at all, to restrict ourselves to the analysis of small solutions to nonlinear equations for all times if they have a small, but non-zero magnitude at $-\infty$. Indeed, in the latter case it may be impossible to rule out a 'blow up' since even a small nonlinearity acting for a very long time can cause a significant impact on the wave. One possibility for a consistent analysis is to study solutions explicitly given for all times, similar, for example, to waves of the form $\boldsymbol{f}(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t)$ in spatially homogenous equations; unfortunately, such solutions are not available in periodic media. Alternatively, one may consider waves satisfying some general restrictions consistent with the equations and allowing a sufficiently detailed analysis. That can get very complicated, or even prohibitively complex, for spatially inhomogeneous equations with general classes of nonlinearities occurring in nonlinear optics. A physically sound way to avoid these difficulties is to deal with waves and excitation currents vanishing as $t \to -\infty$. An additional 'bonus' we get taking that approach is the natural way to single out the special class of waves, namely wavepackets, producing them by appropriately chosen current excitations. This approach is equally efficient in both linear and nonlinear media. It also allows one to control the regularity of the solutions to the nonlinear equations with respect to the parameter α, and, consequently, to study the properties of the exact solutions using perturbation methods over long time intervals. *Thus, we will work with the waves defined for all negative times*, and our natural substitute for the initial-value problem will be a wave in the underlying linear dielectric medium vanishing for $t \to -\infty$, and which is produced by currents vanishing for all negative times. Finally, we would like to note that the vanishing of wavepackets for all $t \leqslant 0$ is not imposed forcefully, but rather it follows automatically from the choice of the excitement currents which are zero for negative times.

Wave interference and oscillatory integrals. Oscillatory integrals that express the nonlinear interactions arise in the theory as the ultimate mathematical manifestations of constructive and destructive interference. One of the important results of the asymptotic analysis of the oscillatory integrals is the derivation of the selection rules allowing one to single out the modes of significant nonlinear interactions.

Dispersion relations of the linear periodic medium. The dispersion relations $\omega_n(\boldsymbol{k})$ relating quasimomenta $\boldsymbol{k}$ to the frequencies ω play the central role in the theory. In particular, the phases of the interaction oscillatory integrals and the selection rules are expressed explicitly in terms of $\omega_n(\boldsymbol{k})$. When constructing the theory we assume that we know the dispersion relations $\omega_n(\boldsymbol{k})$, and we use their basic properties which follow from Floquet–Bloch theory [2, 52, 66, 81]. This approach is common in both physical and mathematical studies.

2.1. Maxwell equations in periodic nonlinear media

We assume that the propagation of electromagnetic waves is described by the classical Maxwell equations (see, for instance, [35], section 6.12, and [42], sections I-4, I-12)

$$\nabla \times \boldsymbol{E}(\boldsymbol{r}, t) = -\frac{1}{c}\partial_t \boldsymbol{B}(\boldsymbol{r}, t) - \frac{4\pi}{c}\boldsymbol{J}_M(\boldsymbol{r}, t) \qquad \nabla \cdot \boldsymbol{B}(\boldsymbol{r}, t) = 0 \tag{3}$$

$$\nabla \times \boldsymbol{H}(\boldsymbol{r}, t) = \frac{1}{c}\partial_t \boldsymbol{D}(\boldsymbol{r}, t) + \frac{4\pi}{c}\boldsymbol{J}_E(\boldsymbol{r}, t) \qquad \nabla \cdot \boldsymbol{D}(\boldsymbol{r}, t) = 0 \tag{4}$$

where $\boldsymbol{H}$, $\boldsymbol{E}$, $\boldsymbol{B}$ and $\boldsymbol{D}$ are, respectively, the magnetic and electric fields, magnetic and electric inductions, and $\boldsymbol{J}_E$ and $\boldsymbol{J}_M$ are impressed electric and, so-called, impressed magnetic currents (current sources). We also assume that *there is no free electric and magnetic charges*, and, hence, the fields $\boldsymbol{B}$ and $\boldsymbol{D}$ are divergence-free as indicated in equations (3) and (4). Equations (3) and (4) imply that the impressed electric and magnetic currents are also divergence-free, i.e.

$$\nabla \cdot \boldsymbol{J}_E(\boldsymbol{r}, t) = 0 \qquad \nabla \cdot \boldsymbol{J}_M(\boldsymbol{r}, t) = 0. \tag{5}$$

We introduce the impressed currents primarily as a tool to generate wavepackets, the role of which is discussed in the following section.

To take into account the dielectric properties of the medium the Maxwell equations (3) and (4) are complemented with the constitutive relations between the fields $\boldsymbol{E}$ and $\boldsymbol{D}$, and $\boldsymbol{H}$ and $\boldsymbol{B}$. Depending on whether these relations are linear or nonlinear the medium is called linear or nonlinear ([35], section 1.4, [15], sections 1 and 2). As to the constitutive relations between $\boldsymbol{H}$ and $\boldsymbol{B}$, we consider for simplicity the case of non-magnetic media, i.e.

$$\boldsymbol{B}(\boldsymbol{r}, t) = \mu \boldsymbol{H}(\boldsymbol{r}, t) \qquad \mu = 1. \tag{6}$$

We assume the constitutive relations to be of the form standard in classical nonlinear optics, [15],

$$\boldsymbol{D} = \boldsymbol{E} + 4\pi \boldsymbol{P}(\boldsymbol{r}, t; \boldsymbol{E}) \tag{7}$$

and discuss them in more detail in section 6. The polarization $\boldsymbol{P}$ includes both the linear and the nonlinear parts

$$\boldsymbol{P}(\boldsymbol{r}, t; \boldsymbol{E}(\cdot)) = \boldsymbol{P}^{(1)}(\boldsymbol{r}, t; \boldsymbol{E}(\cdot)) + \boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{r}, t; \boldsymbol{E}(\cdot)) \tag{8}$$

and the nonlinear part $\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{r}, t; \boldsymbol{E}(\cdot))$ consists of the terms of homogeneity $h \geqslant 2$ and higher.

To quantify how weak the nonlinearity is, we recall that there exists the characteristic magnitude E_{ch} of $\boldsymbol{E}$ for which nonlinear part of the polarization $\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{r}, t; \boldsymbol{E})$ is comparable to its linear part. The value of E_{ch} depends on the physical mechanisms of nonlinear susceptibilities. It can be estimated theoretically [16], and a simple order-of-magnitude estimate yields $E_{\mathrm{ch}} = 2 \times 10^7$ esu ([16], section 1.1). Hence,

$$E_{\mathrm{ch}}^{-1} \boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{r}, t; \boldsymbol{E}) \simeq 1 \qquad \text{if} \quad \boldsymbol{E}/E_{\mathrm{ch}} \simeq 1.$$

For a weak nonlinearity the magnitude E_0 should be considerably smaller than E_{ch}, i.e.

$$E_0 = \alpha_0 E_{\mathrm{ch}} \qquad \alpha_0 \ll 1.$$

We introduce the rescaled dimensionless field $\tilde{\boldsymbol{E}}$ and $\tilde{\boldsymbol{B}}$ by the formulae

$$\boldsymbol{E} = \alpha_0 E_{\mathrm{ch}} \tilde{\boldsymbol{E}} \qquad \boldsymbol{B} = \alpha_0 B_{\mathrm{ch}} \tilde{\boldsymbol{B}}$$

where the magnitudes of $\tilde{\boldsymbol{E}}$ and $\tilde{\boldsymbol{B}}$ are of order 1. Then the magnitude of the nonlinearity $\tilde{\boldsymbol{P}}_{\mathrm{NL}}(\tilde{\boldsymbol{E}})$ (which is assumed to be homogeneous of order h, $h = 2$ for quadratic and $h = 3$ for cubic nonlinearity) is of order $\alpha = \alpha_0^{h-1}$, i.e.

$$\tilde{\boldsymbol{P}}_{\mathrm{NL}}(\tilde{\boldsymbol{E}}) = \alpha_0^{-1} E_{\mathrm{ch}}^{-1} \boldsymbol{P}_{\mathrm{NL}}\big(\alpha_0 E_{\mathrm{ch}} \tilde{\boldsymbol{E}}\big) \simeq \alpha_0^{h-1} = \alpha \qquad \text{if} \quad \tilde{\boldsymbol{E}} \simeq 1.$$

To simplify the notation we write below $\boldsymbol{E}$, $\boldsymbol{B}$ and $\boldsymbol{P}_{\mathrm{NL}}$ in place of $\tilde{\boldsymbol{E}}$, $\tilde{\boldsymbol{B}}$ and $\tilde{\boldsymbol{P}}_{\mathrm{NL}}$ remembering that from now on $\boldsymbol{E}$, $\boldsymbol{B}$ and $\boldsymbol{P}_{\mathrm{NL}}$ will stand for the dimensionless quantities. After the rescaling the constitutive relation becomes

$$\boldsymbol{D} = \boldsymbol{E} + 4\pi \left(\boldsymbol{P}^{(1)}(\boldsymbol{r}, t; \boldsymbol{E}(\cdot)) + \alpha \boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{r}, t; \boldsymbol{E})\right) \tag{9}$$

where $\alpha \ll 1$ measures the relative magnitude of the nonlinearity. We remind the reader that $\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{r}, t; \boldsymbol{E}(\cdot))$ is a nonlinear operator (in general, it is not just a function and may include integration) acting on the fields $\boldsymbol{E}(\cdot)$ of the form described in nonlinear optics, see [15] and section 6. The linear part $\boldsymbol{P}^{(1)}(\boldsymbol{r}, t; \boldsymbol{E}(\cdot))$ represents the linear term of the total polarization field and is given by

$$\boldsymbol{P}^{(1)}(\boldsymbol{r}, t; \boldsymbol{E}(\cdot)) = \boldsymbol{\chi}^{(1)}(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r}, t) \tag{10}$$

where $\boldsymbol{\chi}^{(1)}(\boldsymbol{r})$ is the tensor of linear susceptibility. We solve (9) in terms of $\boldsymbol{D}$ for small α and get $\boldsymbol{E} = \boldsymbol{E}(\boldsymbol{r}, t; \boldsymbol{D})$. Keeping only the leading terms we recast the constitutive relations in the following form:

$$\boldsymbol{E}(\boldsymbol{r}, t) = \boldsymbol{\eta}^{(1)}(\boldsymbol{r})\boldsymbol{D}(\boldsymbol{r}, t) - \alpha \boldsymbol{S}_D(\boldsymbol{r}, t; \boldsymbol{D}) \tag{11}$$

$$\boldsymbol{\eta}^{(1)}(\boldsymbol{r}) = \left[\varepsilon^{(1)}(\boldsymbol{r})\right]^{-1} \qquad \varepsilon^{(1)}(\boldsymbol{r}) = 1 + 4\pi \boldsymbol{\chi}^{(1)}(\boldsymbol{r}) \tag{12}$$

where $\varepsilon^{(1)}(\boldsymbol{r})$ is the tensor of the dielectric constant. We prefer to write the constitutive relations between $\boldsymbol{E}$ and $\boldsymbol{D}$ in somewhat unusual form (11) since the field $\boldsymbol{D}$, not $\boldsymbol{E}$, is divergence-free and we systematically use eigenfunction expansions with divergence-free eigenfunctions. The tensor $\boldsymbol{\eta}^{(1)}$, called *impermeability*, is commonly used in the studies of the electro-optical effects (Pockels and Kerr effects) ([81], section 7, [69], section 6.3, 18.1).

The dielectric properties of the periodic medium are assumed to vary periodically in the space. In other words, the constitutive relations and, hence, the fields $\boldsymbol{\chi}^{(1)}(\boldsymbol{r})$, $\boldsymbol{\eta}^{(1)}(\boldsymbol{r})$ and $\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{r}, t; \boldsymbol{E})$, $\boldsymbol{S}(\boldsymbol{r}, t; \boldsymbol{D})$ are periodic functions of the spatial variable $\boldsymbol{r}$. For simplicity, we consider the case when the lattice of periods is cubic with the lattice constant L_0 [2]. Hence, in particular,

$$\boldsymbol{\eta}^{(1)}(\boldsymbol{r} + L_0\boldsymbol{n}) = \boldsymbol{\eta}^{(1)}(\boldsymbol{r}) \qquad \text{for every integer-valued } \boldsymbol{n}. \tag{13}$$

The lattice constant gives the natural space scale and it is convenient now to pass to dimensionless quantities as follows:

$$\tilde{t} = \frac{tc}{L_0} \qquad \tilde{\omega} = \frac{\omega L_0}{c} \qquad \tilde{\boldsymbol{r}} = \frac{\boldsymbol{r}}{L_0} \qquad \nabla_{\tilde{\boldsymbol{r}}} = L_0 \nabla_{\boldsymbol{r}}. \tag{14}$$

To keep the notation short we will use the original symbols t, ω, $\boldsymbol{r}$ in place of $\tilde{t}$, $\tilde{\omega}$, $\tilde{\boldsymbol{r}}$, remembering that from now on these symbols stand for the dimensionless quantities. In particular, the speed of light c and the lattice constant L_0 are both unity, i.e. $c = 1$, $L_0 = 1$. We consider the situation when the wavelength c/ω of the carrier wave with the frequency ω is of the same order as L_0, therefore the frequencies $\tilde{\omega}$ we consider are of the order of one. (In the eigenfunction representation $\mathcal{M}\boldsymbol{U} \simeq \tilde{\omega}\boldsymbol{U} \simeq \boldsymbol{U}$, where $\mathcal{M}$ is the Maxwell operator described below.)

Periodicity of the media should not be confused with the properties of the *solutions to the Maxwell equations (3) and (4) which, in general, are not periodic functions of* $\boldsymbol{r}$. In some cases one can introduce and study periodic solutions to nonlinear Maxwell equations but that is not our intention. *On the contrary, we study the nonlinear effects by probing the medium with wavepackets* which in a homogeneous media are the waves with the frequencies and wavenumbers lying in narrow bands.

Substituting $\boldsymbol{E}$ from (11) into (3) we rewrite the nonlinear Maxwell equations in a concise form

$$\partial_t \boldsymbol{U} = -\,\mathrm{i}\mathcal{M}\boldsymbol{U} + \alpha \boldsymbol{F}_{\mathrm{NL}}(\boldsymbol{U}) - \boldsymbol{J};\, \boldsymbol{U}(t) = 0 \qquad \text{for} \quad t \leqslant 0 \tag{15}$$

where

$$\boldsymbol{U} = \begin{bmatrix} \boldsymbol{D} \\ \boldsymbol{B} \end{bmatrix} \qquad \mathcal{M}\boldsymbol{U} = \mathrm{i}\begin{bmatrix} \mu^{-1}\nabla \times \boldsymbol{B} \\ -\nabla \times \left(\eta^{(1)}(\boldsymbol{r})\boldsymbol{D}\right) \end{bmatrix} \tag{16}$$

$$\boldsymbol{J} = 4\pi \begin{bmatrix} \boldsymbol{J}_E \\ \boldsymbol{J}_M \end{bmatrix} \qquad \boldsymbol{F}_{\mathrm{NL}}(\boldsymbol{U}) = \begin{bmatrix} \boldsymbol{0} \\ \nabla \times \boldsymbol{S}_D(\boldsymbol{r}, t; \boldsymbol{D}) \end{bmatrix} \tag{17}$$

we assume everywhere that $\boldsymbol{D}$, $\boldsymbol{B}$ $\boldsymbol{J}_E$, $\boldsymbol{J}_M$ are divergence-free. The vector $\boldsymbol{J}$ of the impressed currents can be viewed as an external excitation which is switched off for negative t, $\boldsymbol{J}(t) = 0$ for $t \leqslant 0$. As has been indicated we are interested in such currents $\boldsymbol{J}$ that can produce wavepackets described in the following section. If $\alpha = 0$ equation (15) evidently becomes linear.

2.2. *Wavetrains and wavepackets in a linear periodic medium*

The simplest solutions to the spatially homogeneous linear Maxwell equations have the form of plane waves

$$\boldsymbol{U} = \boldsymbol{U}_0 \mathrm{e}^{\mathrm{i}(\boldsymbol{r}\cdot\boldsymbol{k} - \omega(\boldsymbol{k})t)} = \mathrm{e}^{-\mathrm{i}\omega(\boldsymbol{k})t}\boldsymbol{U}_0 \mathrm{e}^{\mathrm{i}\boldsymbol{r}\cdot\boldsymbol{k}} \tag{18}$$

where $\boldsymbol{k}$ is the wavevector and $\omega(\boldsymbol{k}) = \text{constant} \times |\boldsymbol{k}|$ is the dispersion relation. These time and space harmonic waves defined for all times and over all space are often called *wavetrains*. Though wavetrains are the most elementary waves, it is wavepackets rather than wavetrains that are more useful in the nonlinear phenomena we study. We remind the reader that wavepackets are waves of frequencies and/or wavevectors belonging to narrow bands (see, for instance, [33], section 1.6, [64], section 2g). The *wavepackets*, also known as envelope or slowly varying amplitude approximations, are often used in the studies of a number of dispersive and nonlinear phenomena ([16], section 2.2, [33], sections 1.6, 1.7, [64], sections 2g and 6g).

A general solution to the linear Maxwell equations in periodic media in the absence of external excitation has the following representation based on the eigenmodes of the underlying linear periodic medium:

$$\boldsymbol{U}(\boldsymbol{r}, t) = \sum_{\bar{n}} \frac{1}{(2\pi)^d} \int \mathrm{d}\boldsymbol{k}\, \tilde{U}_{\bar{n}}(\boldsymbol{k}) \tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k})\, \mathrm{e}^{-\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})t} \tag{19}$$

where $\omega_{\bar{n}}(\boldsymbol{k})$ are the eigenvalues of the linear periodic Maxwell operator $\mathcal{M}$, also known as the dispersion relations, $\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k})$ are the Bloch eigenmodes and $\tilde{U}_{\bar{n}}(\boldsymbol{k})$ are the corresponding amplitudes. This representation can also be viewed as a linear combination of wavepackets. We remind the reader that the Bloch eigenmodes have the following form:

$$\tilde{\boldsymbol{G}}_n(\boldsymbol{r}, \boldsymbol{k}) = \tilde{\boldsymbol{g}}_n(\boldsymbol{r}, \boldsymbol{k}) \exp{(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{r})} \qquad \text{where} \quad \tilde{\boldsymbol{g}}_n(\boldsymbol{r}, \boldsymbol{k}) \text{ is periodic in } \boldsymbol{r} \tag{20}$$

and the quasimomentum $\boldsymbol{k}$ runs the Brillouin zone (which is a cube for a cubic lattice, see [2] and section 5 below), and the zone number $n = 1, 2, \ldots$ labels different bands. The indices n and $\boldsymbol{k}$ describe symbolically the discrete and the continuous spectral parameters. Note that together with a frequency ω_n and an eigenfunction $\tilde{\boldsymbol{G}}_n(\boldsymbol{r}, \boldsymbol{k})$ the frequency $-\omega_n$ and the corresponding eigenfunction is always present, therefore we use the extended index $\bar{n} = (\pm 1, n)$ and denote $\omega_{\bar{n}} = \pm 1\omega_n$.

To generate time wavepackets for which the structure of the expansion (19) is preserved we allow the coefficients $\tilde{U}_{\bar{n}}(\boldsymbol{k})$ to vary slowly in time according to the following formula:

$$\boldsymbol{U}(\boldsymbol{r}, t) = \sum_{\bar{n}} \frac{1}{(2\pi)^d} \int \mathrm{d}\boldsymbol{k}\, \tilde{U}_{\bar{n}}(\boldsymbol{k}, \tau) \tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k})\, \mathrm{e}^{-\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})t} \qquad \tau = \varrho t \qquad \varrho \ll 1. \tag{21}$$

We do not introduce the spatial variation of coefficients $\tilde{U}_n(\boldsymbol{k}, \varrho t)$ for a number of reasons: first, we want to keep the form of solutions as simple as possible; second, the dependence of $\tilde{\boldsymbol{G}}_n(\boldsymbol{r}, \boldsymbol{k})$ on $\boldsymbol{r}$ may be very complicated and it would be difficult to separate the variability of coefficients from the variability of the eigenmodes $\tilde{\boldsymbol{G}}_n(\boldsymbol{r}, \boldsymbol{k})$; third, for the phenomena we study it is not needed. Denoting the nth component of the Floquet–Bloch expansion by

$$\tilde{U}_{\bar{n}}(\boldsymbol{k}) \tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}) = \tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k})$$

we rewrite (21) in a more concise form

$$\boldsymbol{U}(\boldsymbol{r}, t) = \sum_{\bar{n}} \frac{1}{(2\pi)^d} \int \mathrm{d}\boldsymbol{k}\, \tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \varrho t)\, \mathrm{e}^{-\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})t}. \tag{22}$$

This shorter form has an important advantage based on the fact that though $\tilde{\boldsymbol{G}}_n(\boldsymbol{r}, \boldsymbol{k})$ is defined non-uniquely for every $\boldsymbol{k}$ (since the eigenfunctions can be multiplied by an arbitrary complex number) the component $\tilde{\boldsymbol{U}}_n(\boldsymbol{r}, \boldsymbol{k})$ is defined uniquely. That becomes especially important in vicinities of singular (band-crossing points) of $\omega_n(\boldsymbol{k})$ where the $\tilde{\boldsymbol{G}}_n(\boldsymbol{r}, \boldsymbol{k})$ branch, whereas $\tilde{\boldsymbol{U}}_n(\boldsymbol{r}, \boldsymbol{k})$ do not (see section 5.4 for details). Note that (22) determines real solutions since together with $\tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \varrho t)\, \mathrm{e}^{-\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})t}$, $\bar{n} = (1, n)$ it contains its complex conjugate term $\tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \varrho t)\, \mathrm{e}^{-\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})t}$, $\bar{n} = (-1, n)$ with $\tilde{\boldsymbol{U}}_{(-1,n)}(\boldsymbol{r}, \boldsymbol{k}, \varrho t) = \tilde{\boldsymbol{U}}^*_{(1,n)}(\boldsymbol{r}, \boldsymbol{k}, \varrho t)$.

Note that to generate wavepackets of the form (21) one has to use an external excitation, and we use the impressed currents $\boldsymbol{J}(\boldsymbol{r}, t, \varrho t)$ for that purpose.

According to Maxwell equations (15) and (16) the electromagnetic fields $\boldsymbol{D}$, $\boldsymbol{B}$, which are components of $\boldsymbol{U}$ are excited by the currents $\boldsymbol{J}_E$, $\boldsymbol{J}_M$ which are components of $\boldsymbol{J}$. We assume that the currents have a carrier frequency (or several frequencies) ω which vary around a given frequency ω_0 (or several given frequencies). The carrier wave is slowly modulated, the characteristic frequency of the modulation is of the order of $\varrho\omega_0$ where $\varrho \ll 1$. The carrier frequencies may vary so that the ratio ω/ω_0 is O(1), i.e. it is uniformly bounded from above and below by ϱ-independent constants when we vary ϱ.

To use the impressed currents $\boldsymbol{J}$ as the wavepacket generation instrument we assume that both currents $\boldsymbol{J}_E$ and $\boldsymbol{J}_M$ have the form

$$\boldsymbol{J}(\boldsymbol{r}, t) = \sum_{\bar{n}} \frac{1}{(2\pi)^d} \int \varrho \tilde{\boldsymbol{j}}_n(\boldsymbol{r}, \boldsymbol{k}, \tau)\, \mathrm{e}^{-\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})t}\, \mathrm{d}\boldsymbol{k} \qquad \tau = \varrho t \tag{23}$$

where $\boldsymbol{j}(\boldsymbol{r}, \varrho t)$ is a slow modulation of the time harmonic carrier waves. We also assume that the currents vanish for negative times, i.e.

$$\boldsymbol{J}(\boldsymbol{r}, t) = 0 \qquad \tilde{\boldsymbol{j}}_n(\boldsymbol{k}, \boldsymbol{r}, \varrho t) = 0 \qquad \text{if} \quad t \leqslant 0. \tag{24}$$

Then, the currents are gradually 'turned on' and, possibly, 'turned off'. The currents have carriers with time harmonic amplitudes $\mathrm{e}^{\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})t}$.

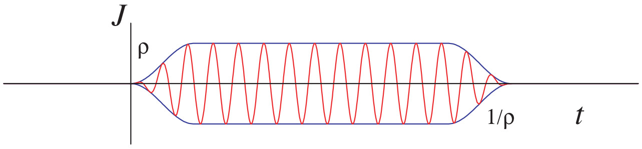

Figure 1. Impressed current J in the form of a time wavepacket of the amplitude of the order of ρ and of a time length of the order of $1/\rho$ generates the medium response which carries the information on the energy exchange between different modes.

The relation between slow amplitudes of currents which excite wavepackets and the linear wavepackets is very simple, one has just to integrate in time the slow amplitude $\boldsymbol{j}(\tau)$ of the current, see (28). Clearly, one can independently use modulation in different wavebands since solutions of linear equations are superposed.

Since the nonlinearity is small it may result in a considerable effect only after a long enough time. We consider interactions on the time interval of the order of $1/\varrho$ or much larger with a small ϱ. We consider solutions in the whole space, it is assumed that we have a solution of (15) which is smooth, decays fast enough as $\boldsymbol{r} \to \infty$ and is defined on a time interval $-\infty < t \leqslant T$. We do not study here the conditions under which such solutions exist. The existence theorems will be formulated and proven in a forthcoming paper.

2.3. *Asymptotics of solutions of nonlinear Maxwell equations*

In this section we give a simplified account of our approach to weakly nonlinear dielectric media. First of all, we recast the Maxwell equations in terms of the Bloch eigenmodes $\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k})$ representing the solution $\tilde{\boldsymbol{U}}$ to Maxwell equations in the form

$$\tilde{\boldsymbol{U}}(\boldsymbol{r}, \boldsymbol{k}, \tau) = \sum_{\bar{n}} \tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \tau) \tag{25}$$

$$\tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \tau) = \mathrm{e}^{-\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})\tau/\varrho} \tilde{V}_{\bar{n}}(\boldsymbol{k}, \tau) \tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}) = \mathrm{e}^{-\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})\tau/\varrho} \tilde{\boldsymbol{V}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \tau) \qquad \tau = \varrho t \tag{26}$$

where the extended index $\bar{n}$ is defined by

$$\bar{n} = (\zeta, n) \qquad n = 1, 2, \ldots \qquad \zeta = \pm 1 \qquad \omega_{\bar{n}} = \zeta \omega_n. \tag{27}$$

In the linear case, $\alpha = 0$, when $\boldsymbol{J}$ is given by (23), the solution $\boldsymbol{V}^{(0)}$ to the Maxwell equations (15) takes the form

$$\tilde{\boldsymbol{V}}_{\bar{n}}^{(0)}(\boldsymbol{r}, \boldsymbol{k}, \tau) = -\int_0^\tau \tilde{\boldsymbol{j}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \tau_1)\, \mathrm{d}\tau_1 \tag{28}$$

where the currents $\boldsymbol{j}_{\bar{n}}$ are defined in (23). If $\boldsymbol{V}$ is the corresponding solution to the nonlinear Maxwell equation for $\alpha > 0$ we introduce

$$\boldsymbol{W} = \boldsymbol{V} - \boldsymbol{V}^{(0)} \qquad \tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \tau) = \tilde{\boldsymbol{V}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \tau) - \tilde{\boldsymbol{V}}_{\bar{n}}^{(0)}(\boldsymbol{r}, \boldsymbol{k}, \tau). \tag{29}$$

In view of the condition (24) the waves $\boldsymbol{W}$, $\boldsymbol{V}$ and $\boldsymbol{V}^{(0)}$ vanish for negative times as well as their Floquet–Bloch components, i.e.

$$\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \tau) = \tilde{\boldsymbol{V}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \tau) = \tilde{\boldsymbol{V}}_{\bar{n}}^{(0)}(\boldsymbol{r}, \boldsymbol{k}, \tau) = 0 \qquad \tau \leqslant 0. \tag{30}$$

As follows from the definition (29), the wave $\boldsymbol{W}$ is a part of the wave related to the nonlinearity of the medium. The evolution equation for $\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \tau)$ is equivalent to the original Maxwell equations and by (22) it takes the form

$$\partial_t \tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \tau) = \frac{\alpha}{\varrho} \sum_{\bar{n}', \bar{n}''} \int_{[-\pi,\pi]^d} \mathrm{e}^{\mathrm{i}\phi_{\bar{n}}(\boldsymbol{k}, \boldsymbol{k}')\tau/\varrho} \tilde{Q}_{\bar{n}}\big[\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)} | \boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}', \tau\big]\, \mathrm{d}\boldsymbol{k}' \tag{31}$$

with the phase $\phi_{\vec{n}}$ and quadratic tensor $\tilde{Q}_{\vec{n}}$ defined for every $\vec{n} = (\bar{n}, \bar{n}', \bar{n}'')$, respectively, by

$$\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}') = \omega_{\bar{n}}(\boldsymbol{k}) - \omega_{\bar{n}'}(\boldsymbol{k}') - \omega_{\bar{n}''}(\boldsymbol{k} - \boldsymbol{k}') \tag{32}$$

$$\tilde{Q}_{\vec{n}}\big[\tilde{\boldsymbol{v}}|\,\boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}', \tau\big] = \tilde{Q}_{\vec{n}}\big[\tilde{\boldsymbol{v}}, \tilde{\boldsymbol{v}}\big] = \frac{1}{(2\pi)^d}\tilde{\Pi}_{\bar{n}} \times \begin{bmatrix} 0 \\ \nabla_{\boldsymbol{r}} \times \left(\chi_D^{(2)}\left(\boldsymbol{r}, \omega_{\bar{n}'}(\boldsymbol{k}'), \omega_{\bar{n}''}(\boldsymbol{k} - \boldsymbol{k}')\right) \vdots\, \tilde{\boldsymbol{v}}_{\bar{n}'}\left(\boldsymbol{r}, \boldsymbol{k}', \tau\right) \tilde{\boldsymbol{v}}_{\bar{n}''}(\boldsymbol{r}, \boldsymbol{k} - \boldsymbol{k}', \tau)\right) \end{bmatrix} \tag{33}$$

where $\tilde{\Pi}_{\bar{n}}$ is a projector on the corresponding Bloch eigenmode, and $\chi_D^{(2)}$ is the quadratic susceptibility described in section 6.1, (260). Equation (31) can be rewritten in the integral form

$$\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \tau) = \frac{\alpha}{\varrho}\sum_{\bar{n}', \bar{n}''}\int_0^\tau \int_{[-\pi,\pi]^d} \mathrm{e}^{\mathrm{i}\phi_{\vec{n}}(\boldsymbol{k},\boldsymbol{k}')\tau_1/\varrho}\, \tilde{Q}_{\vec{n}}\big[\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)}|\,\boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}', \tau_1\big]\, \mathrm{d}\boldsymbol{k}'\, \mathrm{d}\tau_1. \tag{34}$$

Our goal now is to single out the triples $\vec{n} = (\overline{n}, \overline{n}', \overline{n}'')$ and $(\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{k}'')$ yielding dominant contributions to the oscillatory integrals in (34). In turns out that those significant triples must satisfy the *frequency matching condition*

$$\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}') = \omega_{\bar{n}}(\boldsymbol{k}) - \omega_{\bar{n}'}(\boldsymbol{k}') - \omega_{\bar{n}''}(\boldsymbol{k} - \boldsymbol{k}') = 0 \tag{35}$$

and the *group velocity matching condition*

$$\nabla\omega_{\bar{n}'}(\boldsymbol{k}') = \nabla\omega_{\bar{n}''}(\boldsymbol{k} - \boldsymbol{k}'). \tag{36}$$

If we denote the points $\boldsymbol{k}'$ that satisfy (35) and (36) by $\boldsymbol{k}'_{*l}$ and the corresponding indices by $\vec{n}_l$ then the evolution equation (34) can be rewritten as

$$\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \tau) = \frac{\alpha}{\varrho}\varrho^{q_0(\boldsymbol{k})}\sum_l \int_0^\tau \bar{Q}_{\vec{n}_l}\big[\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)}|\,\boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}'_{*l}, \tau_1\big]\,\mathrm{d}\tau_1 + \frac{\alpha}{\varrho}\mathrm{O}\left(\varrho^{q_1(\boldsymbol{k})}\right) \tag{37}$$

where $q_1(\boldsymbol{k}) > q_0(\boldsymbol{k})$, the tensor $\bar{Q}_{\vec{n}_l}$ is determined by $\tilde{Q}_{\vec{n}}$ and by the type of the point $\boldsymbol{k}'_{*l}$. This equation indicates that there are only a few modes that can have significant nonlinear interaction. Those modes are related to the points $\boldsymbol{k}'_{*l}$ yielding the corresponding zones $\overline{n}'_l, \overline{n}''_l$ and quasimomenta $\boldsymbol{k}'_{*l}, \boldsymbol{k} - \boldsymbol{k}'_{*l}$. An additional important simplification in equation (37) comes from the observation that $|\tilde{\boldsymbol{W}}| \ll |\tilde{\boldsymbol{V}}^{(0)}|$. This allows one to omit $\tilde{\boldsymbol{W}}$ in the right-hand side of (37), yielding

$$\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, \tau) = \frac{\alpha}{\varrho}\varrho^{q_0(\boldsymbol{k})}\sum_l \int_0^\tau \bar{Q}_{\vec{n}_l}\big[\tilde{\boldsymbol{V}}^{(0)}|\,\boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}'_{*l}, \tau_1\big]\,\mathrm{d}\tau_1 + \frac{\alpha}{\varrho}\left[\mathrm{O}\left(\varrho^{q_1(\boldsymbol{k})}\right) + \sum \mathrm{O}\left(\varrho^{q_0(\boldsymbol{k}'_{*l}) + q_0(\boldsymbol{k})}\right)\right]. \tag{38}$$

The first sum in (38) which we denote $\tilde{\boldsymbol{V}}^{(1)}$,

$$\tilde{\boldsymbol{V}}^{(1)} = \frac{\alpha}{\varrho}\varrho^{q_0(\boldsymbol{k})}\sum_l \int_0^\tau \bar{Q}_{\vec{n}_l}\big[\tilde{\boldsymbol{V}}^{(0)}|\,\boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}'_{*l}, \tau_1\big]\,\mathrm{d}\tau_1 \tag{39}$$

gives the main contribution and is called the first nonlinear response. The sum $\tilde{\boldsymbol{V}}^{(0)} + \tilde{\boldsymbol{V}}^{(1)}$, often called the *first Born approximation*, turns out to be sufficient in capturing such important phenomena as the second- and the third-harmonic generations, three-wave mixing, frequency conversion, self-phase modulation and more [69, sections 19.1–19.3]. Keeping this in mind, we now define *the nonlinearity as weak if the first Born approximation* $\tilde{\boldsymbol{V}}^{(0)} + \tilde{\boldsymbol{V}}^{(1)}$ *represents well the exact solution* $\tilde{\boldsymbol{U}}(\boldsymbol{r}, \boldsymbol{k}, \tau)$; see section 7.4 for details. A more detailed discussion of the above formulae is given in section 4.

3. Simpler models

As was discussed at the beginning of section 2, the nonlinear phenomena we study manifest themselves on relatively large time intervals, and, hence, 'straightforward' perturbation methods are not adequate. The adequate perturbation theory we develop is based on the following:

(a) Floquet–Bloch spectral theory for linear periodic media;
(b) the stationary phase method for the oscillatory integrals related to nonlinear interactions.

In the models below we explore and expose the main ingredients of the theory based on examples which are simpler than our main problem of the nonlinear Maxwell equations. We also use these examples to explain our notation in simple situations.

3.1. Field evolution equation

The nonlinear Maxwell equations and simpler models we consider are covered by the following general field evolution equation:

$$\frac{\mathrm{d}U}{\mathrm{d}t} = -\mathrm{i}MU + \alpha F[U] - J(t) \tag{40}$$

where $U = U(\mathbf{r}, t)$ is a field (for instance, the position and time-dependent electromagnetic field), M is a self-adjoint operator associated with the underlying linear medium (for instance, the linear Maxwell operator), J corresponds to sources (currents), $F(U)$ is a nonlinear term and α describes its relative magnitude. *We assume that the nonlinearity is weak, and that it is interpreted as the dominance of the linear term over the nonlinear one for sufficiently small fields U.* In other words, we assume that

$$\alpha \ll 1 \qquad F[U] = \mathrm{O}(1) \qquad \text{when} \quad U = \mathrm{O}(1). \tag{41}$$

For $\alpha = 0$ we obtain the linear medium with the evolution equation

$$\frac{\mathrm{d}U^{(0)}}{\mathrm{d}t} = -\mathrm{i}MU^{(0)} - J(t). \tag{42}$$

To single out unique solutions for both (40) and (42) we consider only the waves that vanish for all large negative times, i.e.

$$U(t) = 0 \qquad t \ll -1. \tag{43}$$

For the phenomena that we study the source (current) $J(t)$ is used to produce an appropriate wavepacket which then evolves in the nonlinear medium according to the evolution equation (40). By appropriate wavepackets we mean those that elucidate the nonlinear phenomena of interest. It is convenient to take wavepackets formed by harmonic oscillations with a slowly varying amplitude. It turns out that the proper wavepackets can be produced by the currents $J(t)$ of the form

$$J(t) = \varrho \mathrm{e}^{-\mathrm{i}Mt} j(\tau) = \varrho \exp\left[-\mathrm{i}\frac{M}{\varrho}\tau\right] j(\tau) \qquad \tau = \varrho t \tag{44}$$

$$\text{where } j(\tau) = 0 \qquad \text{for} \quad \tau \leqslant 0. \tag{45}$$

Note that the condition (45) implies

$$U(t) = 0 \qquad t \leqslant 0. \tag{46}$$

In other words for negative times everything is at rest. If a current of the form (44) and (45) is introduced in the linear medium it produces a wavepacket $U^{(0)}$ that satisfies the linear evolution equation (42) with the condition (46). Taking into account (44)–(46) we obtain the following representation:

$$U^{(0)} = \mathrm{e}^{-\mathrm{i}Mt} V^{(0)}(\tau) \qquad V^{(0)}(\tau) = -\int_0^\tau j(\tau_1)\,\mathrm{d}\tau_1 \tag{47}$$

and, evidently, $V^{(0)}(\tau) = 0$ if $\tau \leqslant 0$. Let us now introduce the following important representation for the field U satisfying the nonlinear equations (40) and (46):

$$U = \mathrm{e}^{-\mathrm{i}Mt} V(\tau) \qquad V(\tau) = W(\tau) + V^{(0)}(\tau) \tag{48}$$

where $V^{(0)}$ is defined by (47), clearly $U(\tau)$ and $W(\tau)$ vanish for negative times. It is evident from (48) that to find $U(\tau)$ it suffices to find $W(\tau)$. To obtain the evolution equation for $W(\tau)$ we substitute U in the form (48) into the original equation (40) which yields the following nonlinear equation which is equivalent to (40):

$$\begin{aligned} &\frac{\mathrm{d}W(\tau)}{\mathrm{d}\tau} = \frac{\alpha}{\varrho}\exp\left[\mathrm{i}\frac{M}{\varrho}\tau\right] F\left[\exp\left[-\mathrm{i}\frac{M}{\varrho}\tau\right]\left(W(\tau) + V^{(0)}(\tau)\right)\right] \\ &W(\tau) = 0 \qquad \text{for} \quad \tau \leqslant 0 \end{aligned} \tag{49}$$

where $V^{(0)}$ is defined by (47). The first nonlinear response $V^{(01)}(\tau)$ is obtained if, under the assumption $W \ll V^{(0)}$, we neglect $W(\tau)$ on the right-hand side of (49), obtaining

$$\begin{aligned} &\frac{\mathrm{d}V^{(01)}(\tau)}{\mathrm{d}t} = \frac{\alpha}{\varrho}\exp\left[\mathrm{i}\frac{M}{\varrho}\tau\right] F\left[\exp\left[-\mathrm{i}\frac{M}{\varrho}\tau V^{(0)}\right](\tau)\right] \\ &V^{(01)}(\tau) = 0 \qquad \text{for} \quad \tau \leqslant 0. \end{aligned} \tag{50}$$

In the general case $V^{(01)}(\tau)$ gives a good approximation on an interval $\tau = \mathrm{O}(1)$ as long as α/ϱ is small, that is for $t = \mathrm{O}\left(\alpha^{-1}\right)$. When we consider the Maxwell equations and several model equations in the following section we derive a reduced equation

$$\frac{\mathrm{d}V^{(1)}(\tau)}{\mathrm{d}t} = \frac{\alpha}{\varrho}\bar{F}\left[V^{(0)}(\tau)\right] \qquad V^{(1)}(\tau) = 0 \qquad \text{for} \quad \tau \leqslant 0 \tag{51}$$

where $\bar{F}$ is a simplified, reduced nonlinearity. In the general case $V^{(1)}(\tau) - V^{(01)}(\tau)$ is small when ϱ is small and $\tau = \mathrm{O}(1)$, $\alpha/\varrho = \mathrm{O}(1)$, so $V^{(1)}(\tau)$ gives a good approximation of $W(\tau)$ for $t = \mathrm{O}\left(\alpha^{-1}\right)$. We show in section 7.6 that thanks to the properties of the Maxwell equations in periodic media, the first nonlinear response $V^{(1)}(\tau)$ is a good approximation for exact wavepacket solutions $W(\tau)$ on much longer intervals $t = \mathrm{O}\left(\alpha^{-p}\right)$, where $p > 1$ depends on the spatial dimension d.

All the equations we consider, including the nonlinear Maxwell equations, will be reduced to equations of the form (49) and then analysed. To study the dependence of equation (49) on ϱ we will diagonalize the operator M in an appropriate eigenbasis.

3.2. Model 1. Van der Pol equation

An important condition which arises in the study of the nonlinear effects of wavepacket propagation in the underlying periodic dielectric linear medium is the *frequency matching condition*. In its simpler form imposition of this condition is equivalent to application of the *averaging method* known as the *Van der Pol technique and Krylov–Bogolubov technique* ([61], section 5.2). We discuss it for a weakly nonlinear second-order ordinary differential equation of the form

$$\frac{\mathrm{d}^2 Y}{\mathrm{d}t^2} + \omega_0^2 Y = \beta f\left(Y, \frac{\mathrm{d}Y}{\mathrm{d}t}\right) - J. \tag{52}$$

We assume for simplicity that the function f is h-homogeneous and take $h = 2$, which corresponds to the quadratic nonlinearity. Equation (52) can be reduced to a first-order system with the standard change of variables

$$\boldsymbol{U} = \begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix} = \begin{bmatrix} Y \\ \frac{1}{\omega_0}\frac{\mathrm{d}Y}{\mathrm{d}t} \end{bmatrix} \qquad \boldsymbol{f} = \begin{bmatrix} 0 \\ f \end{bmatrix} \tag{53}$$

$$\boldsymbol{J} = \begin{bmatrix} 0 \\ \frac{1}{\omega_0} J \end{bmatrix} \qquad \boldsymbol{M} = \begin{bmatrix} 0 & \mathrm{i}\omega_0 \\ -\mathrm{i}\omega_0 & 0 \end{bmatrix}. \tag{54}$$

Using the notation

$$Y_1 = [\boldsymbol{U}]_{(1)} \qquad Y_2 = [\boldsymbol{U}]_{(2)} \qquad \text{for} \quad \boldsymbol{U} = \begin{bmatrix} Y_1 \\ Y_2 \end{bmatrix} \tag{55}$$

we rewrite (52) in the form of a first-order system

$$\frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}t} = -\mathrm{i}\boldsymbol{M}\boldsymbol{U} + \alpha \boldsymbol{f}(\boldsymbol{U}) - \boldsymbol{J} \qquad \boldsymbol{f}(\boldsymbol{U}) = \begin{bmatrix} 0 \\ f\left([\boldsymbol{U}]_{(1)}, \omega_0\, [\boldsymbol{U}]_{(2)}\right) \end{bmatrix} \qquad \alpha = \frac{\beta}{\omega_0}. \tag{56}$$

Applying the general approach discussed in the previous subsection we take $\boldsymbol{J}$ in the form of slowly modulated free oscillations:

$$\boldsymbol{J} = \varrho \mathrm{e}^{-\mathrm{i}\boldsymbol{M}t} \boldsymbol{j}(\varrho t) \qquad \boldsymbol{j}(t) = \boldsymbol{0} \quad \text{when } t \leqslant 0 \tag{57}$$

where $0 < \varrho \ll 1$, $\alpha = \beta/\omega_0$ is a small parameter and α/ϱ is bounded. To proceed further we need the eigenmodes $\boldsymbol{G}_{\pm 1}$ of the 2×2 matrix $\boldsymbol{M}$:

$$\boldsymbol{M}\boldsymbol{G}_{+1} = \omega_0 \boldsymbol{G}_{+1} \qquad \boldsymbol{M}\boldsymbol{G}_{-1} = -\omega_0 \boldsymbol{G}_{-1}. \tag{58}$$

Using the explicit form (54) of $\boldsymbol{M}$ we readily find

$$\boldsymbol{G}_{\pm 1} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \pm\mathrm{i} \end{bmatrix}. \tag{59}$$

Let us introduce an index $\zeta = \pm 1$ and set

$$\omega_{\zeta,0} = \zeta \omega_0. \tag{60}$$

Then (58) takes the form

$$\boldsymbol{M}\boldsymbol{G}_\zeta = \omega_{\zeta,0} \boldsymbol{G}_\zeta \qquad \zeta = \pm 1. \tag{61}$$

In addition to that, using $\boldsymbol{G}_{\pm 1}$ as a basis we represent every vector $\boldsymbol{U}$ as follows:

$$\boldsymbol{U} = \sum_{\zeta=\pm 1} U_\zeta \boldsymbol{G}_\zeta = \sum_{\zeta=\pm 1} \boldsymbol{U}_\zeta. \tag{62}$$

Note that in our notation $U_1 \neq [\boldsymbol{U}]_{(1)} = Y_1 \neq \boldsymbol{U}_1 = U_1\boldsymbol{G}_1$. It is convenient to introduce a so-called *slow time* $\tau = \varrho t$ where ϱ is a small parameter relating the slow time τ to the time t ([61], section 5.2). The solution to the linear equation when $\alpha = 0$ is given by

$$\boldsymbol{U}^{(0)} = \mathrm{e}^{-\mathrm{i}Mt}\boldsymbol{V}^{(0)}(\tau) \qquad \boldsymbol{V}^{(0)}(\tau) = -\int_0^\tau \boldsymbol{j}(s)\,\mathrm{d}s \qquad \tau = \varrho t. \tag{63}$$

Following the general settings of section 3.1, we seek the solution to the nonlinear equation (56) in the form

$$\boldsymbol{U} = \mathrm{e}^{-\mathrm{i}Mt}\boldsymbol{V}(\tau) \qquad \boldsymbol{V}(\tau) = \boldsymbol{W}(\tau) + \boldsymbol{V}^{(0)}(\tau). \tag{64}$$

Then an equivalent form of the original equation (56) is

$$\frac{\mathrm{d}\boldsymbol{W}}{\mathrm{d}\tau} = \frac{\alpha}{\varrho}\mathrm{e}^{\mathrm{i}M\tau/\varrho}\boldsymbol{f}\left\{\mathrm{e}^{-\mathrm{i}M\tau/\varrho}\left[\boldsymbol{W}(\tau) + \boldsymbol{V}^{(0)}(\tau)\right]\right\}. \tag{65}$$

This equation involves explicitly the rapidly oscillating term $\mathrm{e}^{\pm\mathrm{i}\omega_0\tau/\varrho}$. Finding the solution $\boldsymbol{W}$ to equation (65) by integrating its right-hand side with respect to τ, we observe that the time integrals of rapidly oscillating terms are insignificant compare to the non-oscillating terms. This simple observation is a basis of the classical averaging method. The method is also called the Van der Pol and Krylov–Bogolubov–Mitropolski method (see [12, 59, 61, 63]).

Note that on time intervals of the length $t = \mathrm{O}(1)$ one may use the straightforward power expansions in α in the original equation. It is well known though, beginning from classical results in celestial mechanics, that because of the so-called *secular terms* these elementary expansions become inadequate on the time intervals of the order of $1/\alpha$ for $\alpha \ll 1$. To obtain an adequate approximation over large time intervals of the order of $1/\alpha$ or higher one has to use the averaging method or the closely related two-scale method ([51], section 4, [64], section 6.g, [61], section 5.2).

We will now discuss the main ingredients of the averaging method for this model which will also be useful for more complicated infinite-dimensional systems. Separating resonant terms we form the *averaged nonlinearity* $\overline{\boldsymbol{f}}$ and rewrite the equation in the integral form

$$\boldsymbol{W}(\tau) = \boldsymbol{W}(0) + \frac{\alpha}{\varrho}\int_0^\tau \overline{\boldsymbol{f}}\left[\boldsymbol{W}(\tau_1) + \boldsymbol{V}^{(0)}(\tau_1)\right]\mathrm{d}\tau_1 + \mathrm{O}(\alpha) \tag{66}$$

where the averaged nonlinearity $\overline{\boldsymbol{f}}(\boldsymbol{W})$ is defined as the time average

$$\overline{\boldsymbol{f}}(\boldsymbol{W}) = \lim_{T\to\infty}\frac{1}{T}\int_0^T \mathrm{e}^{\mathrm{i}M\tau}\boldsymbol{f}\left[\mathrm{e}^{-\mathrm{i}M\tau}\boldsymbol{W}\right]\mathrm{d}\tau. \tag{67}$$

In formula (67) $\boldsymbol{W}$ is treated as a fixed parameter. In (66) $\mathrm{O}(\alpha)$ includes terms obtained by integration of rapidly oscillating terms $\frac{\alpha}{\varrho}\mathrm{e}^{\pm\mathrm{i}\varkappa\omega_0\tau/\varrho}$, $\varkappa = 1, 2, 3$. Formula (66) singles out the most important interactions in terms of the averaged nonlinearity $\overline{\boldsymbol{f}}$ which does not include fast oscillations. Later we obtain generalization of the (66) to the Maxwell equations.

Computation of $\overline{\boldsymbol{f}}\,(\boldsymbol{W})$ becomes especially simple when the nonlinearity $\boldsymbol{f}(\boldsymbol{W})$ is a tensor which is a homogeneous polynomial of degree h of the components of $\boldsymbol{W}$, such as, for instance, in the important cases of the quadratic, $h = 2$, and the cubic, $h = 3$, nonlinearities. To find $\overline{\boldsymbol{f}}(\boldsymbol{W})$ from (67) we expand the integrand into the sum of terms with time harmonic factors of the form

$$\exp\left\{\frac{\mathrm{i}\tau}{\varrho}\left(\mp_0\omega_0 \pm_1 \omega_0 \pm \cdots \pm_h \omega_0\right)\right\} \tag{68}$$

where $\pm_j$ denotes '+' or '−'. Evidently, these factors can be recast as

$$\exp\left\{\frac{\mathrm{i}\tau}{\varrho}\,(\mp_0\omega_0 \pm_1 \omega_0 \pm \cdots \pm_h \omega_0)\right\} = \exp\left\{\frac{\mathrm{i}\tau}{\varrho}\phi_{\vec{\zeta}}\right\} \qquad \phi_{\vec{\zeta}} = \omega_\zeta - \sum_{j=1}^{h}\omega_{\zeta^{(j)}} \tag{69}$$

where

$$\vec{\zeta} = (\zeta, \zeta^{(1)}, \ldots, \zeta^{(h)}) \qquad \zeta^{(j)} = \pm 1 \qquad \omega_{\zeta^{(j)}} = \zeta^{(j)}\omega_0. \tag{70}$$

The non-oscillating (resonance) factors are those with $\phi_{\vec{\zeta}} = 0$, and the oscillating (non-resonance) factors are those for which $\phi_{\vec{\zeta}} \neq 0$. Finally, summing up the terms associated with the resonance factors we obtain $\overline{\boldsymbol{f}}(\boldsymbol{W})$. Based on this and using (62) and (335) we obtain for the homogeneous $\boldsymbol{f}$

$$\overline{\boldsymbol{f}}(\boldsymbol{U})_\varsigma = \sum_{\omega_\zeta - \sum_{j=1}^{h}\omega_{\zeta^{(j)}} = 0} \left[\boldsymbol{f} \,\vdots\, \prod_{j=1}^{h} \boldsymbol{U}_{\zeta^{(j)}}\right]_\varsigma . \tag{71}$$

The selection rule

$$\omega_\zeta - \sum_{j=1}^{h}\omega_{\zeta^{(j)}} = 0 \tag{72}$$

for strongly interacting modes is called a *frequency matching condition*.

Now we continue the discussion of the averaging method. Let us introduce the first term in the asymptotic approximation of $\boldsymbol{W}$ by

$$\boldsymbol{W}(\tau) = \overline{\boldsymbol{W}}(\tau) + \mathrm{O}(\alpha). \tag{73}$$

The dominant term $\overline{\boldsymbol{W}}(\tau)$ has the property $\overline{\boldsymbol{W}}(\tau) = \mathrm{O}(1)$ for $\tau \geqslant \tau_0 > 0$ and is the solution of the following evolution equation for the averaged quantity $\overline{\boldsymbol{W}}$:

$$\frac{\mathrm{d}\overline{\boldsymbol{W}}(\tau)}{\mathrm{d}\tau} = \alpha_1 \overline{\boldsymbol{f}}\left[\overline{\boldsymbol{W}}(\tau) + \boldsymbol{V}^{(0)}(\tau)\right] \qquad \overline{\boldsymbol{W}}(0) = \boldsymbol{0} \qquad \alpha_1 = \frac{\alpha}{\varrho}. \tag{74}$$

Equation (74) can be recast as an integral equation

$$\overline{\boldsymbol{W}}(\tau) = \alpha_1 \int_0^\tau \overline{\boldsymbol{f}}\left[\overline{\boldsymbol{W}}(\tau_1) + \boldsymbol{V}^{(0)}(\tau_1)\right] \mathrm{d}\tau. \tag{75}$$

Expanding $\overline{\boldsymbol{W}}(\tau)$ in powers of α_1 we obtain

$$\overline{\boldsymbol{W}}(\tau) = \alpha_1 \overline{\boldsymbol{V}}^{(1)}(\tau) + \alpha_1^2 \overline{\boldsymbol{V}}^{(2)}(\tau) + \cdots \tag{76}$$

and we obtain

$$\overline{\boldsymbol{V}}^{(1)}(\tau) = \int_0^\tau \overline{\boldsymbol{f}} \,\vdots\, \boldsymbol{V}^{(0)}\left(\tau'\right)^h \,\mathrm{d}\tau'. \tag{77}$$

Therefore,

$$\overline{\boldsymbol{W}}(\tau) = \alpha_1 \overline{\boldsymbol{V}}^{(1)}(\tau) + \mathrm{O}(\alpha_1^2) \tag{78}$$

where $\overline{\boldsymbol{V}}^{(1)}(\tau)$ is given by (77). It is important to note that one obtains the same equation for $\overline{\boldsymbol{V}}^{(1)}$ expanding (66) with $\alpha = \varrho$ in powers of α and taking the first-order term. One more way to obtain (77) is by first expanding the solution of (65) in powers of α and obtaining a linear equation for $\boldsymbol{V}^{(1)}(\tau)$,

$$\frac{\mathrm{d}\boldsymbol{V}^{(01)}}{\mathrm{d}\tau} = \frac{\alpha}{\varrho}\mathrm{e}^{\mathrm{i}M\tau/\varrho} f\left\{\mathrm{e}^{-\mathrm{i}M\tau/\varrho}\left[\boldsymbol{V}^{(0)}(\tau)\right]\right\}, \boldsymbol{V}^{(01)}(0) = \mathbf{0} \tag{79}$$

and averaging the right-hand side of the linear equation after that. The simplicity of the representation (77) is partially due to the fact that the initial solution $\boldsymbol{V}^{(0)}(\tau)$ is defined for all times and vanishes for negative times, so we consider the averaging around a zero solution. We obtain analogues of the formulae (66) and (77) for nonlinear Maxwell equations. In this paper we do not consider a generalization of (74) to nonlinear Maxwell equations, it will be given in a separate paper.

3.3. Model 2. Nonlinear wave equation with discrete spectrum

The next model in terms of complexity to consider is one with infinitely many oscillatory modes. An example of such a multimode model is a wave equation similar to the nonlinear Klein–Gordon equation:

$$\partial_t^2 Y - \partial_x^2 Y = -\alpha\partial_x Y^2 - J \qquad J = J(x,t). \tag{80}$$

In this example we deal with a one-dimensional medium, $d = 1$, a solution Y and forcing J are assumed to be 2π-periodic in x with zero average. Here we take the quadratic nonlinearity $\partial_x Y^h = hY^{h-1}\partial_x Y$ with $h = 2$ as a prototype of the quadratic nonlinearity for the Maxwell equations. The cubic nonlinearity $h = 3$ can be approached in a similar fashion. For this model the eigenmodes of the linear part are plane waves, and, hence, we use the Fourier series expansion

$$Y(t,x) = \sum_n Y_n(t)\,\mathrm{e}^{\mathrm{i}k_n x} \qquad k_n = n \qquad n = \pm 1, \ldots \tag{81}$$

to rewrite the wave equation (80) as an infinite ordinary differential equation (ODE) system:

$$\frac{\mathrm{d}^2 Y_n}{\mathrm{d}t^2} + \omega_n^2 Y_n = -\mathrm{i}\alpha \sum_{k_{n'}+k_{n''}=k_n} k_n Y_{n'} Y_{n''} - J_n(t) \qquad \omega_n = |n|. \tag{82}$$

The analysis of equation (82) with $J_n = 0$ based on *Benjamin's approach* is carried out in [78], section 15.6.

As in the case of the Van der Pol equation (56) we recast (82) as the first-order ODE system

$$\frac{\mathrm{d}\boldsymbol{U}_n}{\mathrm{d}t} = -\mathrm{i}M_n\boldsymbol{U}_n - \alpha \sum_{k_{n'}+k_{n''}=k_n} Q_n\left[\boldsymbol{U}_{n'}, \boldsymbol{U}_{n''}\right] - \boldsymbol{J}_n(t) \tag{83}$$

$$M_n = \begin{bmatrix} 0 & \mathrm{i}\omega_n \\ -\mathrm{i}\omega_n & 0 \end{bmatrix} \qquad \boldsymbol{U}_n = \begin{bmatrix} Y_n \\ \dfrac{1}{\omega_n}\dfrac{\mathrm{d}Y_n}{\mathrm{d}t} \end{bmatrix} \qquad \boldsymbol{J}_n(t) = \begin{bmatrix} 0 \\ \dfrac{1}{\omega_n} J_n(t) \end{bmatrix} \tag{84}$$

where using the notation (55) like in (56) we define the bilinear tensor Q_n on Fourier coefficients by

$$Q_n\left[\boldsymbol{U}', \boldsymbol{U}''\right] = \frac{\mathrm{i}k_n}{\omega_n}\begin{bmatrix} 0 \\ \left[\boldsymbol{U}'\right]_{(1)}\left[\boldsymbol{U}''\right]_{(1)} \end{bmatrix}. \tag{85}$$

As in the previous model we take the current of the form (44) and (45),

$$\boldsymbol{J}_n(t) = \varrho \mathrm{e}^{-\mathrm{i}M_n t} \boldsymbol{j}_n(\tau) \qquad \tau = \varrho t \qquad \boldsymbol{j}_n(\tau) = 0 \quad \text{as } \tau \leqslant 0. \tag{86}$$

Using now (59) for every n we obtain

$$\boldsymbol{U}_n = \boldsymbol{U}_{1,n} + \boldsymbol{U}_{-1,n} = (\boldsymbol{G}_1 \cdot \boldsymbol{U}_n)\, \boldsymbol{G}_1 + (\boldsymbol{G}_{-1} \cdot \boldsymbol{U}_n)\, \boldsymbol{G}_{-1}. \tag{87}$$

It is convenient to introduce the following quantities:

$$\omega_{\bar{n}} = \zeta \omega_n \qquad \bar{n} = (\zeta, n) \qquad \bar{n} = (\zeta, n) \qquad \zeta = \pm 1 \qquad n = 0, \pm 1, \ldots \tag{88}$$

and, using (87),

$$\boldsymbol{U}_n(t) = \mathrm{e}^{-\mathrm{i}M_n \tau/\varrho} \left[\boldsymbol{W}_n(\tau) + \boldsymbol{V}_n^{(0)}(\tau)\right] \tag{89}$$

$$\boldsymbol{W}_n = \boldsymbol{W}_{1,n} + \boldsymbol{W}_{-1,n} \qquad \boldsymbol{V}_n^{(0)} = \boldsymbol{V}_{1,n}^{(0)} + \boldsymbol{V}_{-1,n}^{(0)}$$

$$\boldsymbol{U}_{\bar{n}}(t) = \mathrm{e}^{-\mathrm{i}\omega_{\bar{n}} \tau/\varrho} \left[\boldsymbol{W}_{\bar{n}}(\tau) + \boldsymbol{V}_{\bar{n}}^{(0)}(\tau)\right] \tag{90}$$

where according to (47)

$$\boldsymbol{V}_{\bar{n}}^{(0)}(\tau) = -\int_0^\tau \boldsymbol{j}_{\bar{n}}(\tau_1)\, \mathrm{d}\tau_1.$$

We rewrite $Q_n\left[\boldsymbol{U}', \boldsymbol{U}''\right]$ defined by (85) using the eigenbasis $\boldsymbol{G}_\varsigma$ for the expansion

$$\left[Q_n \vdots \left(\sum_{\zeta'} \boldsymbol{U}'_{\zeta'}\right)\left(\sum_{\zeta''} \boldsymbol{U}''_{\zeta''}\right)\right]_\varsigma = \sum_{\zeta', \zeta''} \left[Q_n\left[\boldsymbol{U}'_{\zeta'}, \boldsymbol{U}''_{\zeta''}\right]\right]_\varsigma = \sum_{\zeta', \zeta''} \tilde{Q}_{n\vec{\zeta}}\left[\boldsymbol{U}', \boldsymbol{U}''\right] \tag{91}$$

which determines tensors $\tilde{Q}_{n\vec{\zeta}}$, $\vec{\zeta} = (\zeta, \zeta', \zeta'')$. Then we denote

$$\tilde{Q}_{\vec{n}}\left[\boldsymbol{U}\right] = Q_n\left[\boldsymbol{U}_{(\zeta',n')}, \boldsymbol{U}_{(\zeta'',n'')}\right]_\varsigma = \tilde{Q}_{n\vec{\zeta}}\left[\boldsymbol{U}_{\bar{n}'}, \boldsymbol{U}_{\bar{n}''}\right] \qquad \vec{n} = (\bar{n}, \bar{n}', \bar{n}''). \tag{92}$$

Now let us introduce

$$\boldsymbol{W}(\tau) = \sum_{\bar{n}} \boldsymbol{W}_{\bar{n}}(\tau) \qquad \boldsymbol{V}^{(0)}(\tau) = \sum_{\bar{n}} \boldsymbol{V}_{\bar{n}}^{(0)}(\tau) \tag{93}$$

where $\bar{n} = (\zeta, n)$, $\zeta = \pm 1$, $n = \pm 1, \ldots$. Using (90) and (92) we recast the evolution equation (83) as follows:

$$\frac{\mathrm{d}\boldsymbol{W}_{\bar{n}}}{\mathrm{d}\tau} = \frac{\alpha}{\varrho} \sum_{\substack{\bar{n}', \bar{n}'': \\ k_{n'} + k_{n''} = k_n}} \exp\left\{\mathrm{i}\frac{\tau\left(\omega_{\bar{n}} - \omega_{\bar{n}'} - \omega_{\bar{n}''}\right)}{\varrho}\right\} \tilde{Q}_{\vec{n}}\left[\boldsymbol{W}(\tau) + \boldsymbol{V}^{(0)}(\tau)\right] \tag{94}$$

where the sum includes the summation over indices ζ' and ζ'' contained in $\bar{n}'$ and $\bar{n}''$. The evident difference from the Van der Pol equation is that here we have many frequencies $\omega_{\bar{n}}$, and that the equations for $\boldsymbol{W}_{\bar{n}}$ are coupled for different $\bar{n}$. Still we can use the averaging method here too, and obtain

$$\boldsymbol{W}_{\bar{n}}(\tau) = \frac{\alpha}{\varrho} \int_0^\tau \sum_{\substack{\bar{n}', \bar{n}'':\ k_{n'} + k_{n''} = k_n \\ \omega_{\bar{n}} - \omega_{\bar{n}'} - \omega_{\bar{n}''} = 0}} \tilde{Q}_{\vec{n}}\left[\boldsymbol{W}(\tau_1) + \boldsymbol{V}^{(0)}(\tau_1)\right] \mathrm{d}\tau_1 + \mathrm{O}(\alpha). \tag{95}$$

Comparing (94) with (95) we see that the summation in (95) is over a smaller set of indices because of the extra restriction (frequency matching condition) $\omega_{\bar{n}} - \omega_{\bar{n}'} - \omega_{\bar{n}''} = 0$, and the coefficients do not contain oscillating factors. The summation over the smaller set of indices is a consequence of the removal of oscillating terms, as in (71), in full compliance with the averaging method. The equality (73) holds here if $\overline{\boldsymbol{W}}(\tau)$ is a solution to the averaged evolution equation obtained by neglecting $\mathrm{O}(\alpha)$.

In summary, we observe that the averaging method selects the most significant terms in the sum in (94), resulting in a simpler equation (95). In addition to that, we learned that the waves of stronger nonlinear interaction can be attributed to the lesser oscillating factors in (94). The most significant terms and the related waves in (94) are selected by the following relations, called *selection rules*, for the modes labelled by the indices $\vec{n} = (\bar{n}, \bar{n}', \bar{n}'')$:

$$k_n = k_{n'} + k_{n''} \tag{96}$$

$$\omega_{\bar{n}} = \omega_{\bar{n}'} + \omega_{\bar{n}''} \tag{97}$$

where the former is often referred to as the *phase matching condition* (PhMC) (see [16], section 2.2, 2.7, [15], sections 7.2.1 and 7.2.2), and the latter is often called the *frequency matching condition* (FMC). Note that condition (96) stems directly from the space homogeneity which results in the convolution formula, whereas condition (97) requires a lack of oscillation of the exponential factors in (94).

As to the complete mathematical analysis to all the phenomena, we would like to note that though the treatment of the model (80) on the technical level is much more laborious than of the Van der Pol model, the difficulties are not 'fatal' and can be overcome (see [13] for a very detailed, mathematically rigorous treatment of a similar approach to the Euler equations for rotating fluids).

3.4. Model 3. Nonlinear wave equation with a continuous spectrum

In this model we want to incorporate the crucial factor of the spectral continuity presented in the Maxwell equations. To do that we use a wave equation over the entire space $\mathbb{R}^d$, $d = 2, 3$. As a simplified model for the Maxwell equations in homogeneous media we introduce the following scalar wave equation similar to the Klein–Gordon equation (80):

$$\frac{\partial^2 Y}{\partial t^2} - \Delta Y = -\alpha \partial_{x_1} Y^2 - J \qquad J = J(x,t) \qquad \Delta = \sum_{j=1}^{d} \frac{\partial^2}{\partial x_j^2} \qquad d = 2, 3. \tag{98}$$

In this case the linear part of equation (98) is spatially homogeneous, the corresponding dispersion relation is

$$\omega(\boldsymbol{k}) = |\boldsymbol{k}|. \tag{99}$$

It has the same form as for the Maxwell equations and the eigenmodes are plane waves. As for the preceding models using these waves as a basis we come up with the Fourier integral

$$Y(\boldsymbol{r}) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \tilde{Y}(\boldsymbol{k})\, \mathrm{e}^{\mathrm{i}\boldsymbol{r}\cdot\boldsymbol{k}}\, \mathrm{d}\boldsymbol{k} \qquad \boldsymbol{k} = (k_1, \ldots, k_d) \qquad \mathbf{d}\boldsymbol{k} = \mathrm{d}k_1 \ldots \mathrm{d}k_d \tag{100}$$

as the appropriate decomposition. Using (100) we now rewrite equation (98) as follows (compare with (83)):

$$\frac{\mathrm{d}\tilde{\boldsymbol{U}}(\boldsymbol{k})}{\mathrm{d}t} = -\mathrm{i}\boldsymbol{M}(\boldsymbol{k})\tilde{\boldsymbol{U}}(\boldsymbol{k}) - \alpha \int_{\mathbb{R}^d} Q\left[\tilde{\boldsymbol{U}}(\boldsymbol{k}'), \tilde{\boldsymbol{U}}\left(\boldsymbol{k}-\boldsymbol{k}'\right)\right] \mathrm{d}\boldsymbol{k}' - \boldsymbol{J}(\boldsymbol{k}, t) \tag{101}$$

$$\tilde{M}(\boldsymbol{k}) = \begin{bmatrix} 0 & \mathrm{i}\omega(\boldsymbol{k}) \\ -\mathrm{i}\omega(\boldsymbol{k}) & 0 \end{bmatrix} \qquad \tilde{\boldsymbol{U}}(\boldsymbol{k}) = \begin{bmatrix} \tilde{Y}(\boldsymbol{k}) \\ \dfrac{1}{\omega(\boldsymbol{k})}\dfrac{\mathrm{d}\tilde{Y}(\boldsymbol{k})}{\mathrm{d}t} \end{bmatrix} \tag{102}$$

$$\tilde{\boldsymbol{J}}(\boldsymbol{k}, t) = \begin{bmatrix} 0 \\ \dfrac{1}{\omega(\boldsymbol{k})}\tilde{J}(\boldsymbol{k}, t) \end{bmatrix} \qquad Q\left[\boldsymbol{U}', \boldsymbol{U}''\right] = \frac{\mathrm{i}k_1}{|\boldsymbol{k}|}\begin{bmatrix} 0 \\ \left[\boldsymbol{U}'\right]_{(1)}\left[\boldsymbol{U}''\right]_{(1)} \end{bmatrix}. \tag{103}$$

Now as in the preceding model we introduce

$$\omega_\zeta(\boldsymbol{k}) = \zeta|\boldsymbol{k}| \qquad \zeta = \pm 1 \tag{104}$$

and, using (59) and (87), the decomposition

$$\tilde{\boldsymbol{U}}(\boldsymbol{k}) = \tilde{\boldsymbol{U}}_1(\boldsymbol{k}) + \tilde{\boldsymbol{U}}_{-1}(\boldsymbol{k}) = \sum_{\zeta=\pm 1}\left(\boldsymbol{G}_\zeta, \tilde{\boldsymbol{U}}(\boldsymbol{k})\right)\boldsymbol{G}_\zeta = \sum_\zeta \tilde{\boldsymbol{U}}_\zeta(\boldsymbol{k}). \tag{105}$$

Following the guidelines of section 3.1 we set

$$\tilde{\boldsymbol{U}}_\zeta(\boldsymbol{k}) = \mathrm{e}^{-\mathrm{i}\omega_\zeta(\boldsymbol{k})t}\left[\tilde{\boldsymbol{W}}_\zeta(\boldsymbol{k}, \tau) + \tilde{\boldsymbol{V}}_\zeta^{(0)}(\boldsymbol{k}, \tau)\right] \qquad \tau = \varrho t \tag{106}$$

where $\tilde{\boldsymbol{V}}_\zeta^{(0)}(\boldsymbol{k}, \tau)$ is the solution to the linear equation (101) for $\alpha = 0$. Following again the guidelines of section 3.1 we take the current $\tilde{\boldsymbol{J}}_\zeta$ of the form

$$\tilde{\boldsymbol{J}}_\zeta(\boldsymbol{k}, t) = \varrho\mathrm{e}^{-\mathrm{i}\omega_\zeta(\boldsymbol{k})t}\tilde{\boldsymbol{j}}_\zeta(\boldsymbol{k}, \tau) \qquad \tau = \varrho t \tag{107}$$

then (47) yields

$$\tilde{\boldsymbol{V}}_\zeta^{(0)}(\boldsymbol{k}, \tau) = -\int_0^\tau \tilde{\boldsymbol{j}}_\zeta(\boldsymbol{k}, s)\,\mathrm{d}s. \tag{108}$$

Obviously, in the model (98) the continuous $\boldsymbol{k}$ plays the role of $k_n = n$ introduced in model 2. To obtain the evolution equation similar to (94) we introduce the notation

$$\vec{\zeta} = \left(\zeta, \zeta', \zeta''\right) \qquad \zeta, \zeta', \zeta'' = \pm 1. \tag{109}$$

Using (105) as in (91) and (92) we define

$$\tilde{Q}_{\vec{\zeta}}\left[\tilde{\boldsymbol{U}}|\,\boldsymbol{k}, \boldsymbol{k}', \tau\right] = Q\left[\tilde{\boldsymbol{U}}\left(\boldsymbol{k}', \tau\right)_{\zeta'}, \tilde{\boldsymbol{U}}\left(\boldsymbol{k}-\boldsymbol{k}', \tau\right)_{\zeta''}\right]_\zeta. \tag{110}$$

Then from (101) using (105) we obtain an evolution equation similar to (94):

$$\frac{\mathrm{d}\tilde{\boldsymbol{W}}_\zeta(\boldsymbol{k})}{\mathrm{d}\tau} = \frac{\alpha}{\varrho}\sum_{\zeta',\zeta''}\int_{\mathbb{R}^d} \exp\left[\mathrm{i}\frac{\tau}{\varrho}\phi_{\vec{\zeta}}(\boldsymbol{k}, \boldsymbol{k}')\right]\tilde{Q}_{\vec{\zeta}}\left[\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)}|\,\boldsymbol{k}, \boldsymbol{k}', \tau\right]\mathrm{d}\boldsymbol{k}' \tag{111}$$

where $\tau = \varrho t$, the phase $\phi_{\vec{\zeta}}(\boldsymbol{k}, \boldsymbol{k}')$ is defined by

$$\phi_{\vec{\zeta}}(\boldsymbol{k}, \boldsymbol{k}') = \omega_\zeta(\boldsymbol{k}) - \omega_{\zeta'}(\boldsymbol{k}') - \omega_{\zeta''}(\boldsymbol{k}-\boldsymbol{k}'). \tag{112}$$

Note that (111) is *equivalent* to (98) and is obtained by a change of variables.

Now $\boldsymbol{k}$ is a continuous variable in $\mathbb{R}^d$ and ζ is a discrete index. This equation describes the coupling between $\tilde{\boldsymbol{W}}_{\zeta'}(\boldsymbol{k}')$, $\tilde{\boldsymbol{W}}_{\zeta''}(\boldsymbol{k}'')$. Observe that the integral in (111) is an oscillatory integral of the form

$$I_{\bar{\zeta}}(\boldsymbol{k}, \tau, \varrho) = \int_{\mathbb{R}^d} \exp\left[\mathrm{i}\frac{\tau}{\varrho}\phi_{\bar{\zeta}}(\boldsymbol{k}, \boldsymbol{k}')\right] A_{\bar{\zeta}}(\boldsymbol{k}, \boldsymbol{k}', \tau)\, \mathrm{d}\boldsymbol{k}' \tag{113}$$

where $\phi_{\bar{\zeta}}$ is the *phase* defined by (141) and $A_{\bar{\zeta}}$ is called the *amplitude function*. The amplitude $A_{\bar{\zeta}}(\boldsymbol{k}, \boldsymbol{k}', \tau)$ is smooth in $\boldsymbol{k}'$ for well behaved wavepackets. The asymptotics of $I_{\bar{\zeta}}(\boldsymbol{k}, \tau, \varrho)$ for $\varrho \to 0$ can be found by the *stationary phase method* [6, 21, 23, 24, 71]. A detailed and insightful analysis of asymptotic approximations to oscillatory integrals in electrodynamics is given in [33].

According to the stationary phase method, the most significant contributions to the oscillatory integral $I_{\bar{\zeta}}(\boldsymbol{k}, \tau, \varrho)$ come from vicinities of so-called *critical points* where the phase is stationary, that is the following *stationary phase condition* is satisfied:

$$\nabla_{\boldsymbol{k}'}\phi_{\bar{\zeta}}(\boldsymbol{k}, \boldsymbol{k}') = 0. \tag{114}$$

For $\phi_{\bar{\zeta}}$ defined by (112) the stationary phase condition (114) yields

$$\nabla_{\boldsymbol{k}'}\omega_{\zeta'}(\boldsymbol{k}'_*) - \nabla_{\boldsymbol{k}''}\omega_{\zeta''}(\boldsymbol{k} - \boldsymbol{k}'_*) = 0. \tag{115}$$

The classical case for a critical point $\boldsymbol{k}'_*$ is when the Hessian of the phase function is not degenerate at it, i.e.

$$\det \nabla^2_{\boldsymbol{k}'}\phi_{\bar{\zeta}}(\boldsymbol{k}, \boldsymbol{k}'_*) \neq 0. \tag{116}$$

Critical points satisfying (116) are called critical points of the type A_1 [6]. *If $\phi_{\bar{\zeta}}(\boldsymbol{k}, \boldsymbol{k}'_*)$ is smooth at $\boldsymbol{k}'_*$ and the condition (116) is satisfied* then the critical $\boldsymbol{k}'_*$ is called a *simple non-degenerate critical point.* If all critical points were simple non-degenerate the following classical explicit formula would hold (see section 7 and references therein):

$$I_{\bar{\zeta}}(\boldsymbol{k}, \varrho) = \varrho^{d/2} \sum_l \bar{b}_{A_1}\left(\phi_{\bar{\zeta}}(\boldsymbol{k}, \boldsymbol{k}'_{*l}), \tau\right)\left[\exp\left[-\mathrm{i}\frac{\tau}{\varrho}\phi_{\bar{\zeta}}\right](\boldsymbol{k}, \boldsymbol{k}'_{*l}) A_{\bar{\zeta}}\left(\boldsymbol{k}, \boldsymbol{k}'_{*l}, \tau\right) + \mathrm{O}(\varrho)\right] \tag{117}$$

where

$$\bar{b}_{A_1}\left(\phi_{\bar{\zeta}}(\boldsymbol{k}, \boldsymbol{k}'_{*l}), \tau\right) = \left(\frac{2\pi}{\tau}\right)^{d/2} \left|\det \nabla^2_{\boldsymbol{k}'}\phi_{\bar{\zeta}}(\boldsymbol{k}, \boldsymbol{k}'_{*l})\right|^{-1/2} \exp\left\{\frac{\mathrm{i}\pi}{4}\,\mathrm{sign}\left[\nabla^2_{\boldsymbol{k}'}\phi_{\bar{\zeta}}(\boldsymbol{k}, \boldsymbol{k}'_{*l})\right]\right\}. \tag{118}$$

The summation in (117) is carried out over all critical points l, and $\mathrm{sign}[M]$ in (118) is the signature of the non-degenerate matrix M, i.e. the algebraic sum of the signs of the matrix eigenvalues. Note that passing to the limit $\tau \to 0$ does not create a difficulty since the condition $\boldsymbol{U}(\tau) = 0$ for $\tau \leqslant 0$ implies that as $\tau \to 0$ the amplitude $A_{\bar{\zeta}}\left(\boldsymbol{k}, \boldsymbol{k}'_{*l}, \tau\right)$ vanishes at a sufficiently high rate.

If the condition (116) held, then for $\tau > 0$ the asymptotic formula (117) would yield $I_{\bar{\zeta}}(\boldsymbol{k}, \varrho) \backsim$ constant $\varrho^{d/2}$ as $\varrho \to 0$. However, an analysis below shows that for this model the *determinant in (116) is zero and, hence, the integral $I_{\bar{\zeta}}(\boldsymbol{k}, \varrho)$ has an asymptotic approximation which is different from (117).* We also have for this model the relations analogous to the phase and frequency matching conditions (96) and (97). The phase matching condition here is

$$\boldsymbol{k}' + \boldsymbol{k}'' = \boldsymbol{k}. \tag{119}$$

Note that the phase matching condition (119) is just a fundamental consequence of the homogeneity of the linear and nonlinear medium. It arises because the pointwise multiplication *of functions commutes with translations and is expressed in terms of the convolution integral.* The frequency matching condition takes the form

$$\omega_{\zeta}(\boldsymbol{k}) - \omega_{\zeta'}(\boldsymbol{k}') - \omega_{\zeta''}(\boldsymbol{k}'') = 0 \tag{120}$$

with $\boldsymbol{k}'' = \boldsymbol{k} - \boldsymbol{k}'$. For the dispersion relation $\omega(\boldsymbol{k}) = |\boldsymbol{k}|$ the matching conditions (119) and (120) become the following:

$$\pm|\boldsymbol{k}| \pm |\boldsymbol{k}'| \pm |\boldsymbol{k}''| = 0 \qquad \boldsymbol{k}'' = \boldsymbol{k} - \boldsymbol{k}'. \tag{121}$$

If the vectors $\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{k}''$ satisfy (121) they are collinear,

$$\boldsymbol{k}' = s\boldsymbol{k} \qquad \boldsymbol{k}'' = \boldsymbol{k} - \boldsymbol{k}' = (1 - s)\boldsymbol{k} \tag{122}$$

and hence (122) is equivalent to (121). Note now that the stationary phase condition (115), stemming from (114), for $\omega(\boldsymbol{k}) = |\boldsymbol{k}|$ takes the form

$$\pm\frac{\boldsymbol{k}'}{|\boldsymbol{k}'|} \mp \frac{\boldsymbol{k} - \boldsymbol{k}'}{|\boldsymbol{k} - \boldsymbol{k}'|} = 0 \tag{123}$$

which is equivalent to (122). So the only triples $(\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{k}'')$ of the plane waves that are strongly coupled by the nonlinear interaction (or, we say, the only strongly interacting waves) are those for which the wavevectors $\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{k}''$ are parallel. Therefore, *for the dispersion relation $\omega(\boldsymbol{k}) = |\boldsymbol{k}|$ the stationary phase condition does not impose a new constraint in addition to the phase and frequency matching conditions (119) and (120).* This property, of course, is not just a coincidence, and can be ascribed to the rotational and dilational symmetry of the dispersion relation $\omega(\boldsymbol{k}) = |\boldsymbol{k}|$.

Now we consider the Hessian form $\nabla^2_{\boldsymbol{k}'}\phi_{\vec{\zeta}}$, we restrict ourselves to the case when $\zeta = \zeta' = \zeta'' = 1$, other cases are similar. We have

$$\phi_{\vec{\zeta}}(\boldsymbol{k}, \boldsymbol{k}') = |\boldsymbol{k}| - |\boldsymbol{k}'| - |\boldsymbol{k} - \boldsymbol{k}'| \equiv 0 \qquad \text{when} \quad \boldsymbol{k}' = s\boldsymbol{k} \quad 0 < s < 1. \tag{124}$$

Therefore, the Hessian quadratic form $\nabla^2_{\boldsymbol{k}'}\phi_{\vec{\zeta}}(\boldsymbol{k}, \boldsymbol{k}')$ vanishes in the direction $\boldsymbol{k}$ at every point of this segment. *This degeneration of the Hessian $\nabla^2_{\boldsymbol{k}'}\phi_{\vec{\zeta}}(\boldsymbol{k}, \boldsymbol{k}')$ on entire segments rather than in a few points can be ascribed to the rotational and dilational symmetry of the homogeneous media which is reflected in the homogeneous and rotation invariant dispersion relation $\omega(\boldsymbol{k}) = |\boldsymbol{k}|$.*

Carrying out elementary but tedious computations we find that the oscillatory integral $I_{\vec{\zeta}}(\boldsymbol{k}, \varrho)$ is of the order of $\varrho^{(d-1)/2}$. The resulting expression obtained by integration of (111) is of the form

$$\tilde{\boldsymbol{W}}_{\zeta}(\boldsymbol{k}, \tau) = \frac{\alpha}{\varrho}\varrho^{(d-1)/2} \sum_{\zeta',\zeta''} \int_0^{\tau} \int_{-\infty}^{\infty} \bar{b}^{(0)}\,(r, |\boldsymbol{k}|)\, \bar{Q}_{\vec{\zeta}} \left[\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)} | \, \boldsymbol{k}, r\frac{\boldsymbol{k}}{|\boldsymbol{k}|}, \tau_1\right] \mathrm{d}r\,\mathrm{d}\tau_1$$
$$+\mathrm{O}\left(\alpha\varrho^{(d-1)/2}\right) \tag{125}$$

where the function $\bar{b}^{(0)}\,(r, |\boldsymbol{k}|)$ is the factor determined by the phase function only. Clearly, the leading interactions in (125) are much more restricted than in (111), only $\boldsymbol{k}'$ collinear to $\boldsymbol{k}$ are included.

The first nonlinear response is again given by (77) which now takes the form

$$\tilde{\boldsymbol{V}}_{\zeta}^{(1)}(\boldsymbol{k}, \tau) = \frac{\alpha}{\varrho}\varrho^{(d-1)/2} \int_0^{\tau} \int_{-\infty}^{\infty} \overline{b}^{(0)}(r) \bar{Q}_{\vec{\zeta}} \left[\tilde{\boldsymbol{V}}^{(0)} | \, \boldsymbol{k}, \boldsymbol{k}', r\frac{\boldsymbol{k}}{|\boldsymbol{k}|}, \tau_1\right] \mathrm{d}r\,\mathrm{d}\tau_1 \tag{126}$$

with

$$\tilde{\boldsymbol{V}}_{\zeta}^{(0)}(\boldsymbol{k}, \tau) = -\int_0^{\tau} \tilde{\boldsymbol{j}}_{\zeta}\,(\boldsymbol{k}, \tau_1)\,\mathrm{d}\tau_1. \tag{127}$$

Formula (126) describes the three-wave mixing between two input waves with amplitudes $\tilde{\boldsymbol{V}}_{\zeta'}^{(0)}(\boldsymbol{k}')$, $\tilde{\boldsymbol{V}}_{\zeta''}^{(0)}(\boldsymbol{k}'')$ and one nonlinear response wave $\tilde{\boldsymbol{V}}_{\zeta}^{(1)}(\boldsymbol{k})$.

Spectral continuity factor. The main effect of the spectral continuity is a weakening of the nonlinear interactions. Indeed, the typical dominant nonlinear interactions for the discrete spectrum are of the order of O(1), whereas for a continuous spectrum in this example it is of order $O(\varrho^{(d-1)/2})$. A simplified explanation of the weakening is that in the continuous case the dominant modes are just a few of the continuum of modes, and the energy is distributed over this continuum. The quantified justification of this statement requires an analysis of the oscillatory integral in (111). This analysis based on the stationary phase method shows that the modes of significant nonlinear interaction lie in small vicinities of the wavenumbers $\boldsymbol{k}'$ solving the equation (selection rule) $\nabla_{\boldsymbol{k}'}\phi_{\bar{\zeta}}(\boldsymbol{k}, \boldsymbol{k}') = 0$. It is important to note that even in this simple example one cannot restrict the use of the stationary phase method just to the classical formula (117) which would yield $O(\varrho^{d/2})$, but rather one has to consider degenerate cases yielding $O(\varrho^{(d-1)/2})$ as an estimate of the strength of the nonlinear coupling.

4. Sketch of the theory for Maxwell equations

In the preliminary discussion in section 2.1 we recast the Maxwell equation into the operator form (15) and (16). The requirement for the field $\boldsymbol{U}(t)$ and the currents $\boldsymbol{J}(t)$ to vanish for negative times is part of the approach (see section 3.1 and the introductory part of section 2).

As we learned from simpler models in section 3 the spectral analysis of the linear Maxwell operator $\mathcal{M}$ defined by (16) is an important step in the analysis. Fourier analysis, appropriate for homogeneous media, ought to be replaced with the *Floquet–Bloch* analysis, since the *Bloch waves*, not the *plane waves*, are the eigenmodes of the underlying linear periodic medium. As we briefly discussed in the introductory part to section 2 (for more details see section 5) the spectrum of the operator $\mathcal{M}$ (also called the spectrum of the periodic medium) can be described in terms of the dispersion relations $\omega_n(\boldsymbol{k})$ where the discrete parameter $n = 1, 2, \ldots$ labels so-called spectral bands and $\boldsymbol{k}$ is the continuous quasimomentum which runs the *Brillouin zone* [2]. The Brillouin zone in our case is simply the cube $[-\pi, \pi]^d$. The numeration of the bands is chosen to satisfy $\omega_{n+1}(\boldsymbol{k}) \geqslant \omega_n(\boldsymbol{k})$. Then as in model 2 (see (88)) we introduce the dispersion relation with the extended index $\bar{n}$,

$$\omega_{\bar{n}}(\boldsymbol{k}) = \zeta\omega_n(\boldsymbol{k}) \qquad \bar{n} = (\zeta, n) \qquad \bar{n} = (\zeta, n) \qquad \zeta = \pm 1 \qquad n = 1, 2, \ldots \tag{128}$$

where $\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{k}, \boldsymbol{r})$ is the corresponding *Bloch eigenmode*:

$$\mathcal{M}\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{k}, \boldsymbol{r}) = \omega_{\bar{n}}(\boldsymbol{k})\,\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{k}, \boldsymbol{r}). \tag{129}$$

For every fixed $\boldsymbol{k}$ the set of all Bloch eigenmodes $\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{k}, \boldsymbol{r})$ as functions of $\boldsymbol{r}$ form an orthonormal basis in a Hilbert space $\mathcal{H}$ of square-integrable functions on $[0, 1]^d$ with an appropriate scalar product (see (174), (191) and section 5.2 for details). The orthogonal projection on $\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{k}, \boldsymbol{r})$ in $\mathcal{H}$ is denoted by $\tilde{\Pi}_{\bar{n}}(\boldsymbol{k})$. Now we have the following band decomposition:

$$\boldsymbol{U}(\boldsymbol{r}, t) = \sum_{\bar{n}} \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, t)\,\mathrm{d}\boldsymbol{k} \qquad \tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}, t) = \tilde{U}_{\bar{n}}(\boldsymbol{k}, t)\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}). \tag{130}$$

This representation combines the features of the Fourier series and the Fourier integral since we have both a discrete index $\bar{n}$, as in (81), and a continuous parameter $\boldsymbol{k}$ as in (100). The components $\tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{k}, \tau)$ of a solution are smooth for all $\boldsymbol{k}$ except for band-crossing points which are the points $\boldsymbol{k}_\otimes$ corresponding to multiple frequencies, when for some n $\omega_{n+1}(\boldsymbol{k}_\otimes) = \omega_n(\boldsymbol{k}_\otimes)$. We assume that singularities at the band-crossing points have a generic structure which is described in section 5.4. Note that the smoothness of $\tilde{\boldsymbol{U}}(\boldsymbol{k})$ in $\boldsymbol{k}$ is related to spatial localization of $\boldsymbol{U}(\boldsymbol{r})$ via the Paley–Wiener theorem.

Following now to the general set-up of section 3.1, in particular (48), we introduce first the currents of the form

$$\boldsymbol{J}(\boldsymbol{r},t)=\frac{1}{(2\pi)^d}\sum_{\bar{n}}\int_{[-\pi,\pi]^3}\tilde{\boldsymbol{J}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k},t)\,\mathrm{d}\boldsymbol{k} \tag{131}$$

$$\tilde{\boldsymbol{J}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k},t)=\varrho e_{\bar{n}}^{-\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})t}j(\boldsymbol{k},\tau)\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k}) \qquad j_{\bar{n}}(\boldsymbol{k},\tau)=0 \qquad \text{for} \quad \tau=\varrho t\leqslant 0. \tag{132}$$

We arrive at the following representation of the Floquet–Bloch components to the solution:

$$\tilde{\boldsymbol{U}}(\boldsymbol{r},\boldsymbol{k},\tau)=\sum_{\bar{n}}\tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k},\tau) \qquad \tau=\varrho t \tag{133}$$

$$\tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k},\tau)=\mathrm{e}^{-\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})\tau/\varrho}V_{\bar{n}}(\boldsymbol{k},\tau)\,\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k})=\mathrm{e}^{-\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})\tau/\varrho}\tilde{\boldsymbol{V}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k},\tau) \tag{134}$$

$$\tilde{\boldsymbol{V}}(\boldsymbol{r},\boldsymbol{k},\tau)=\sum_{\bar{n}}\tilde{\boldsymbol{V}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k},\tau). \tag{135}$$

Let us introduce

$$\tilde{\boldsymbol{V}}_{\bar{n}}^{(0)}(\boldsymbol{r},\boldsymbol{k},\tau)=-\int_0^\tau\tilde{\boldsymbol{j}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k},\tau_1)\,\mathrm{d}\tau_1 \qquad \tilde{\boldsymbol{j}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k},\tau_1)=j_{\bar{n}}(\boldsymbol{k},\tau)\,\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k}) \tag{136}$$

and

$$\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k},\tau)=\tilde{\boldsymbol{V}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k},\tau)-\tilde{\boldsymbol{V}}_{\bar{n}}^{(0)}(\boldsymbol{r},\boldsymbol{k},\tau). \tag{137}$$

Obviously, equation (132) implies that $\tilde{\boldsymbol{V}}_{\bar{n}}^{(0)}(\boldsymbol{r},\boldsymbol{k},\tau)=\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k},\tau)=0$ for $\tau\leqslant 0$. As in section 3.1, the problem of solving the nonlinear Maxwell equations is equivalent to the problem of finding $\boldsymbol{W}(\tau)$ or, equivalently, all of its components $\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{k},\tau)$. In the case of the Maxwell equations (15) the evolution equation (49) is written in the Floquet–Bloch form as follows:

$$\partial_\tau\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k},\tau)=\frac{\alpha}{\varrho}\sum_{\bar{n}',\bar{n}''}\int_{[-\pi,\pi]^d}\mathrm{e}^{\mathrm{i}\phi_{\vec{n}}(\boldsymbol{k},\boldsymbol{k}')\tau/\varrho}\tilde{Q}_{\vec{n}}\big[\tilde{\boldsymbol{W}}+\tilde{\boldsymbol{V}}^{(0)}|\,\boldsymbol{r},\boldsymbol{k},\boldsymbol{k}',\tau\big]\,\mathrm{d}\boldsymbol{k}' \tag{138}$$

with the functions ϕ and $\bar{Q}$ defined by the formulae

$$\phi_{\vec{n}}(\boldsymbol{k},\boldsymbol{k}')=\omega_{\bar{n}}(\boldsymbol{k})-\omega_{\bar{n}'}(\boldsymbol{k}')-\omega_{\bar{n}''}\big(\boldsymbol{k}-\boldsymbol{k}'\big) \qquad \vec{n}=\big(\bar{n},\bar{n}',\bar{n}''\big) \tag{139}$$

$$\tilde{Q}_{\vec{n}}\big[\tilde{\boldsymbol{V}}\,|\boldsymbol{r},\boldsymbol{k},\boldsymbol{k}',\tau\big] \\ =\frac{1}{(2\pi)^d}\begin{bmatrix}0\\ \tilde{\Pi}_{\bar{n}}(\boldsymbol{k})\boldsymbol{\chi}_D^{(2)}\big(\omega_{\bar{n}'}(\boldsymbol{k}'),\omega_{\bar{n}''}\big(\boldsymbol{k}-\boldsymbol{k}'\big)\big)\,\vdots\,\tilde{\boldsymbol{V}}_{\bar{n}'}\big(\boldsymbol{r},\boldsymbol{k}',\tau\big)\,\tilde{\boldsymbol{V}}_{\bar{n}''}(\boldsymbol{r},\boldsymbol{k}-\boldsymbol{k}',\tau)\end{bmatrix} \tag{140}$$

where $\tilde{\Pi}_{\bar{n}}(\boldsymbol{k})$ is the projection operator on the corresponding Bloch eigenmode and $\boldsymbol{\chi}_D^{(2)}$ is the quadratic susceptibility described below in section 6.1, (260). When writing the formulae (138)–(140) we have taken into account the phase matching condition

$$\boldsymbol{k}'+\boldsymbol{k}''=\boldsymbol{k}\mod(2\pi) \tag{141}$$

which stems from the periodicity of the medium and appears in the formulae in the form of the convolution operation.

Equation (138) can now be rewritten in the integral form

$$\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k},\tau)=\frac{\alpha}{\varrho}\sum_{\bar{n}',\bar{n}''}\int_0^\tau\int_{[-\pi,\pi]^d}\mathrm{e}^{\mathrm{i}\phi_{\vec{n}}(\boldsymbol{k},\boldsymbol{k}')\tau_1/\varrho}\tilde{Q}_{\vec{n}}\big[\tilde{\boldsymbol{W}}+\tilde{\boldsymbol{V}}^{(0)}|\,\boldsymbol{r},\boldsymbol{k},\boldsymbol{k}',\tau_1\big]\,\mathrm{d}\boldsymbol{k}'\,\mathrm{d}\tau_1. \tag{142}$$

Assuming that in the formula (142) $\tilde{\boldsymbol{W}} \ll \tilde{\boldsymbol{V}}^{(0)}$ we obtain the following expression for the first (non-reduced) nonlinear response:

$$\tilde{\boldsymbol{V}}_{\vec{n}}^{(01)}(\boldsymbol{r}, \boldsymbol{k}, \tau) = \frac{\alpha}{\varrho} \sum_{\vec{n}', \vec{n}''} \int_0^{\tau} \int_{[-\pi,\pi]^3} \exp\left\{ \mathrm{i}\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}') \frac{\tau_1}{\varrho} \right\} \tilde{Q}_{\vec{n}}\left[\tilde{\boldsymbol{V}}^{(0)} | \, \boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}', \tau_1\right] \mathrm{d}\boldsymbol{k}' \, \mathrm{d}\tau_1. \tag{143}$$

As in previous models we want to single out combined triples $\vec{n}$ and $(\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{k}'')$ that yield the dominant contributions to the oscillatory integrals in (142) and (143). The right-hand side of (142) is a sum of oscillatory integrals with given phase functions and amplitudes. Our analysis shows that

$$\tilde{\boldsymbol{W}}_{\vec{n}}(\boldsymbol{r}, \boldsymbol{k}, \tau) = \tilde{\boldsymbol{V}}_{\vec{n}}^{(1)}(\boldsymbol{r}, \boldsymbol{k}, \tau) + \mathrm{O}\left(\alpha \varrho^{q_1 - 1}\right) \tag{144}$$

where $\tilde{\boldsymbol{V}}_{\vec{n}}^{(1)}$ is the first nonlinear response which is obtained from (143) by application of selection rules. Expressions for $\tilde{\boldsymbol{V}}_{\vec{n}}^{(1)}$ are given in section 4.3, they are obtained by methods which we describe below; we only note here that $\tilde{\boldsymbol{V}}_{\vec{n}}^{(1)} = \mathrm{O}\left(\alpha \varrho^{q_0 - 1}\right)$ with $q_0 < q_1$.

Now we discuss the selection rules. Since faster oscillating terms on the right-hand side of (142) produce a smaller contribution to $\tilde{\boldsymbol{W}}_{\vec{n}}$, the leading terms correspond to those triples $\vec{n}$ and $(\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{k}'')$ for which the phases $\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{k}'')$ vanish. This yields the following *frequency matching condition*:

$$\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}') = \omega_{\bar{n}}(\boldsymbol{k}) - \omega_{\bar{n}'}(\boldsymbol{k}') - \omega_{\bar{n}''}\left(\boldsymbol{k} - \boldsymbol{k}'\right) = 0 \qquad \vec{n} = \left(\overline{n}, \overline{n}', \overline{n}''\right) \tag{145}$$

which is well known in nonlinear optics [69, section 19.4]. The condition is also called the *sum-frequency mixing condition* ([15], sections 2.3.3, 7.2.2, [16], section 1.3). The reason for the rise of this condition is discussed in section 3.2, and its more detailed analysis is given in section 7.2.

We can further narrow down the set of nonlinearly coupled modes labelled by the combined triples $\vec{n}$ and $(\boldsymbol{k}, \boldsymbol{k}', \boldsymbol{k}'')$ by applying the stationary phase method to the integral (142), see section 7. According to the method the asymptotics of the oscillatory integral (142) as $\varrho \to 0$ are determined by infinitesimally small vicinities of the critical points $\boldsymbol{k}'_*$ defined as solutions to the equation

$$\nabla_{\boldsymbol{k}'} \phi_{\vec{n}}\left(\boldsymbol{k}, \boldsymbol{k}'_*\right) = 0. \tag{146}$$

For ϕ defined by (140) equation (146) reduces to

$$\nabla \omega_{\bar{n}'}(\boldsymbol{k}'_*) = \nabla \omega_{\bar{n}''}(\boldsymbol{k} - \boldsymbol{k}'_*). \tag{147}$$

For the reasons explained below, we call (147) the *group velocity matching condition (GV). The GV condition (147) can be viewed as a selection rule for the modes yielding dominant contributions to the oscillatory integrals in (138).* Evidently, equations (146) and (147) are analogous to equations (114) and (115) which arise in the homogeneous case. *However, an important difference is that for the periodic dielectric medium the dispersion relations* $\omega_{\bar{n}}(\boldsymbol{k})$ *have no continuous groups of rotational or dilation symmetries, and equation (147) is an additional selection rule which is not reducible to (145) as happens for* $\omega_{\bar{n}}(\boldsymbol{k}) = \mathrm{constant} \times |\boldsymbol{k}|$ *(see (123) and (124)).*

Now observe that the selection rule (147) has a simple physical interpretation. Indeed, the oscillatory integrals in the evolution equation (138) describe the contributions of two (because the nonlinearity here is quadratic) nonlinearly interacting Bloch waves of the indices $(\bar{n}', \boldsymbol{k}')$ and $(\bar{n}'', \boldsymbol{k}'')$ to the amplitude growth of the Bloch wave with the index $(\bar{n}, \boldsymbol{k})$. In a medium with the dispersion relation $\omega = \omega(\boldsymbol{k})$ the group velocity is defined as $\nabla_{\boldsymbol{k}} \omega(\boldsymbol{k})$. Therefore, we may conclude that the selection rule (147) indicates that the dominant contributions and, hence, *the strongest nonlinear coupling occur when the group velocities of interacting modes are equal. In view of this interpretation we will refer to the selection rule (147) as a group velocity matching condition.*

An elementary calculation made in section 5.3 based on (142), (147), and the inverse Floquet–Bloch transform shows that the group velocity of the wavepacket $\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{k},\tau)\exp\left\{\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})\frac{\tau}{\varrho}\right\}$ corresponding to the nonlinear response $\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{k},\tau)$ is $\nabla\omega_{\bar{n}''}(\boldsymbol{k}-\boldsymbol{k}'_*)$. In other words, if the group velocities of two interacting modes $\left(\bar{n}',\boldsymbol{k}'_*\right)$ and $\left(\bar{n}'',\boldsymbol{k}-\boldsymbol{k}'_*\right)$ match according to (147), then

$$\nabla\omega_{\bar{n}'}(\boldsymbol{k}'_*)=\nabla\omega_{\bar{n}''}(\boldsymbol{k}-\boldsymbol{k}'_*)=\boldsymbol{v} \tag{148}$$

and the nonlinear response wave $\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{k},\tau)\exp\left\{\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})\frac{\tau}{\varrho}\right\}$ propagates with *the same* group velocity $\boldsymbol{v}$. *Note that the group velocity $\boldsymbol{v}=\nabla\omega_{\bar{n}''}(\boldsymbol{k}-\boldsymbol{k}'_*)$ of the nonlinear response $\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{k},\tau)$ of the $(\bar{n},\boldsymbol{k})$-mode differs from the group velocity $\nabla\omega_{\bar{n}}(\boldsymbol{k})$ of the $(\bar{n},\boldsymbol{k})$-mode as a linear wave.*

In summary, we conclude that two nonlinearly interacting waves significantly affect the third only if their group velocities match. Note that for a generic dispersion relation, for a given triplet $\vec{n}=\left(\bar{n},\bar{n}',\bar{n}''\right)$ of interacting bands, and for a given $\boldsymbol{k}$ there will be only a finite number of $\boldsymbol{k}'_*$ and the corresponding $\boldsymbol{k}''=\boldsymbol{k}-\boldsymbol{k}'_*$ that satisfy the group velocity matching condition (147). The importance of group velocity matching is known in the physical literature (see [73]).

As a result, applying the selection rules we obtain (37) in which the leading part of the nonlinear response $\boldsymbol{W}$ is singled out and also (38) and (39) in which the leading part of the first nonlinear response $\boldsymbol{V}^{(1)}$ is singled out.

Applicability of the first nonlinear response over long time intervals. Our analysis also shows that two types of condition have to hold on the time interval where the first nonlinear response gives a good approximation. The first condition is the boundedness of the linear and first nonlinear response over the whole interval. The second condition is a restriction on the length of the interval which arises from our analysis and takes the form

$$t\ll\alpha^{-2}\qquad\text{for}\quad d=1 \tag{149}$$

$$t\ll\alpha^{-3}\qquad\text{for}\quad d=2. \tag{150}$$

For $d=3$ there is no additional restriction on t. Recall that we always assume $\varrho\ll 1,\alpha\ll 1$. We always assume boundedness of the linear response $\boldsymbol{V}^{(0)}(t)$ and the first nonlinear response $\boldsymbol{V}^{(1)}(t)$ by a constant of order 1, and it is the only restriction for the case $d=3$. Note that to prove the results absolutely rigorously in addition to the above restrictions one has to impose technical conditions which imply restrictions $t\ll\alpha^{-1}\ln(1/\alpha)$.

We point out again that the linear dispersion theory and, in particular, the dispersion relations $\omega_n(\boldsymbol{k})$ play a key role in our analysis of the nonlinear wavepacket propagation as they do in the general theory of nonlinear optical phenomena [16, section 3.5]. For instance, evidently both the phase matching condition (141) and the frequency matching condition (145) are formulated entirely and explicitly in terms of the dispersion relations $\omega_n(\boldsymbol{k})$ and quasimomenta $\boldsymbol{k}$.

4.1. Classification of nonlinear interactions

As follows from the previous discussions, the nonlinear response is expressed by oscillatory integrals which describe nonlinear interactions between different modes. The asymptotic

Table 1. Abbreviations for the classes of nonlinear interactions. Every table entry indicates that the conditions in the corresponding row and the column are satisfied. The entry itself is an abbreviation used to refer to the related properties.

	Simple GV condition holds	BC condition holds
FMC holds: cumulative response	CGV	CBC
FMC does not hold: instantaneous response	IGV	IBC

behaviour of the interaction oscillatory integrals such as in (142) and (143) gives a base for the classification of the nonlinear interactions. We use the relative bandwidth $\varrho \sim \Delta\omega/\omega_0$ of the wavepacket as the small parameter, which is customary in the slow envelope approach. We have found that for well behaved wavepackets the nonlinear interaction oscillatory integrals decay according to the power law ϱ^q with positive indices q as $\varrho \to 0$. It is quite remarkable that nonlinear interactions become small even for fixed magnitude α of the nonlinearity provided that the relative bandwidth of wavepackets is small even if the excitation produces a linear response $\boldsymbol{V}^{(0)}$ of order one. This phenomenon is due to the destructive wave interference. Thus, we set the *asymptotic behaviour of the interaction oscillatory integrals as* $\varrho \to 0$ *to be the base of our classification of nonlinear interactions*, this choice singles out the class of wave phenomena we study here. One has to keep in mind, though, that there can be other approaches for the classification for other classes of phenomena.

The asymptotic analysis of the oscillatory interaction integrals in equation (142) or (143) as $\varrho \to 0$ with the phase function $\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}')$ defined by (139) is based on the stationary phase method. Ultimately, it is reduced to the study of two types of the phase critical points: simple and band-crossing ones. We define *simple critical points* or the points where a simple group velocity matching condition holds as points $\boldsymbol{k}'_*$ such that:

(a) both eigenfrequencies $\omega_{\zeta'}(\boldsymbol{k}'_*)$ and $\omega_{\zeta''}(\boldsymbol{k} - \boldsymbol{k}'_*)$ are simple, i.e. of multiplicity one, and, consequently, the phase $\phi_{\vec{\zeta}}(\boldsymbol{k}, \boldsymbol{k}')$ and the amplitude are smooth in $\boldsymbol{k}'$ at $\boldsymbol{k}' = \boldsymbol{k}'_*$;
(b) the *stationary phase condition* (146) is satisfied.

The second type of critical points are *band-crossing points* (BC points) where either $\omega_{\bar{n}'}(\boldsymbol{k}')$ or $\omega_{\bar{n}''}(\boldsymbol{k} - \boldsymbol{k}')$ is not differentiable. Such points $\boldsymbol{k}'_\otimes$ arise when $\omega_{\bar{n}'}\big(\boldsymbol{k}'_\otimes\big)$ is the eigenfrequency of multiplicity two or higher that is two or more bands meet; generic BC points have multiplicity two.

The first and the simplest classification of nonlinear interactions is based on the fulfilment of the frequency matching condition, group velocity matching condition (GVC) and band-crossing condition (BCC). There are three classes of interactions which may account for leading contributions; the fourth class (IBC) is always subordinate. Note that when the BC condition holds, a specific form of GV condition may hold too, but we do not single out this case in the table.

4.2. Asymptotic approximations of interaction integrals

The interaction integrals are represented by summands on the right-hand side of (142) or (143). Each summand shows the impact of the related modes from bands n', n'' and quasimomenta $\boldsymbol{k}'$, $\boldsymbol{k}'' = \boldsymbol{k} - \boldsymbol{k}'$ onto the mode from band n with quasimomentum $\boldsymbol{k}$. Our analysis singles out the leading terms (asymptotic approximations) for these integrals, they may have a different structure depending on the fulfilment of different conditions at corresponding critical points $\boldsymbol{k}'$.

Let us give a look at different types of asymptotic approximations for the nonlinear interactions. Note that considering the asymptotics in ϱ we assume everywhere that $\tau \geqslant \tau_0 > 0$ with an arbitrary small but fixed τ_0, this corresponds to $t \geqslant \tau_0/\varrho$.

Frequency and group velocity matching conditions hold (CGV). This class of interactions is the strongest. The asymptotic approximation to the corresponding integral is given by

$$I_{\mathrm{CGV}}\big(\vec{n}, \boldsymbol{k}, \boldsymbol{k}'_*, \tau, \tilde{\boldsymbol{V}}^{(0)}\big) = \frac{\alpha}{\varrho} B \varrho^{q_{\mathcal{T}}} \tag{151}$$

where

$$B = \bar{b}_{\mathcal{T}}\big[\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}'_*)\big] \int_0^\tau \tilde{Q}_{\vec{n}}\big[\tilde{\boldsymbol{V}}^{(0)} | \, \boldsymbol{k}, \boldsymbol{k}'_*, \tau_1\big] \tau_1^{-q_{\mathcal{T}}} \, \mathrm{d}\tau_1 \tag{152}$$

where $\tilde{Q}_{\vec{n}}$ is defined by (140), $\mathcal{T} = \mathcal{T}(\boldsymbol{k}'_*)$ is the type of critical point $\boldsymbol{k}'_*$. Since this expression for the value of the nonlinear response at time τ includes integration in $\tau_1 \leqslant \tau$ we call it *cumulative*. The scalar coefficient $\bar{b}_{\mathcal{T}}\left[\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}'_*)\right]$ is determined:

(a) by the phase $\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}')$;
(b) by its Hessian;
(c) for degenerate types of critical points by higher-order derivatives at the point $\boldsymbol{k}'_*$, and by the *type* $\mathcal{T}$ of the simple critical point $\boldsymbol{k}'_*$ of the phase function $\phi_{\vec{n}}$.

All the types of critical points which can occur for generic dispersion relations, namely the types $\mathcal{T} = A_p$ with $p = 1, 2, 3, 4$, are described in section 7 (see (287) and [5, 6] for more general types). The factor $\bar{b}_{\mathcal{T}}$ does not depend on $\tilde{\boldsymbol{W}}, \tilde{\boldsymbol{V}}^{(0)}$ and on the tensor $\tilde{Q}$. The coefficient $\bar{b}_{\mathcal{T}}\left[\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}'_*)\right]$ is given explicitly in (289) (in the case of a non-degenerate point it is given by (118)).

The exponent $q_{\mathcal{T}}$ depends only on the space dimension d and on the type $\mathcal{T}$ of the related point $\boldsymbol{k}'_*$. The possible values of $q_{\mathcal{T}}$ are equal to the leading index q_0 for cumulative terms. Their values are collected in table 2. The contribution due to cumulative terms is non-zero if $\vec{n}, \boldsymbol{k}, \boldsymbol{k}', \boldsymbol{k} - \boldsymbol{k}'$ satisfy both the frequency matching condition (145) and the group velocity matching condition (147). *If the cumulative contribution I_{CGV} is present, it is always dominant* and is of the order of ϱ^{q_0} with the smallest available q_0, whereas other types of contributions (I_{IGV} and I_{CBC}, see below) are of higher degrees in ϱ and, hence, are weaker for small ϱ.

The group velocity matching condition holds, whereas the frequency matching condition does not (IGV). In this case the leading term of the corresponding integral at a critical point $\boldsymbol{k}'_*$ is given by an instantaneous contribution

$$I_{\mathrm{IGV}}\big(\vec{n}, \boldsymbol{k}, \boldsymbol{k}'_*, \tau, \tilde{\boldsymbol{V}}^{(0)}\big) = \frac{\alpha}{\varrho} B \varrho^{1+q_{\mathcal{T}}} \tag{153}$$

where

$$B = \bar{b}_{\mathcal{T}}\left[\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}'_*)\right] \tilde{Q}^{\mathrm{in}}_{\vec{n}}\big[\tilde{\boldsymbol{V}}^{(0)} | \, \boldsymbol{k}, \boldsymbol{k}'_*, \tau\big] \, \mathrm{e}^{\mathrm{i}\phi_{\vec{n}}(\boldsymbol{k},\boldsymbol{k}'_*)\tau/\varrho} \tau^{-q_{\mathcal{T}}} \qquad \mathcal{T} = \mathcal{T}(\boldsymbol{k}'_*). \tag{154}$$

The coefficient $\bar{b}_{\mathcal{T}}\left[\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}'_*)\right]$ is the same as in the cumulative term. The instantaneous interaction couples $\tilde{W}_{\vec{n}}(\boldsymbol{k}, \tau)$ with $\tilde{\boldsymbol{V}}^{(0)}_{\vec{n}'}(\boldsymbol{k}'_*, \tau)$ and $\tilde{\boldsymbol{V}}^{(0)}_{\vec{n}''}(\boldsymbol{k} - \boldsymbol{k}'_*, \tau)$ at the same instant τ, and it does not involve the integration over time. The definition of $\tilde{Q}^{\mathrm{in}}_{\vec{n}}$ is given in (296).

Critical points $\boldsymbol{k}'_*$ producing instantaneous contributions can be more degenerate than cumulative. Therefore, the indices $q_{\mathcal{T}}$ may be smaller for the instantaneous terms, though the resulting exponent $1 + q_{\mathcal{T}}$ is always greater than the corresponding indices for the cumulative contribution (see table 2). Therefore, the instantaneous contributions can be of any significance only if the cumulative contribution for the same $\bar{n}, \boldsymbol{k}$ are not presented for all $\bar{n}', \bar{n}''$.

Band-crossing condition holds (CBC, IBC). We call points $\boldsymbol{k}' = \boldsymbol{k}'_\otimes$ *band-crossing points* (BC points) if eigenfrequencies $\omega_{\vec{n}'}(\boldsymbol{k}')$ or $\omega_{\vec{n}''}(\boldsymbol{k}-\boldsymbol{k}')$ are of multiplicity two or higher; generic BC points are of multiplicity two. For a band-crossing point $\boldsymbol{k}'_\otimes$ either $\omega_{\vec{n}'}(\boldsymbol{k}')$ or $\omega_{\vec{n}''}(\boldsymbol{k}-\boldsymbol{k}')$ is not differentiable. The condition of multiplicity, or the *band-crossing condition*, has the form

$$\omega_{(\zeta',n')}\big(\boldsymbol{k}'_\otimes\big) = \omega_{(\zeta',n'\pm1)}\big(\boldsymbol{k}'_\otimes\big) \qquad \text{or} \qquad \omega_{(\zeta'',n'')}\left(\boldsymbol{k}-\boldsymbol{k}'_\otimes\right) = \omega_{(\zeta'',n''\pm1)}\left(\boldsymbol{k}-\boldsymbol{k}'_\otimes\right). \tag{155}$$

For a more detailed discussion on band-crossing points see section 5.4. Now we only note that in our generic problems such points do not exist in the one-dimensional case $d = 1$, are isolated in the case $d = 2$, and form curves in the case $d = 3$. The interaction integral has to be treated separately. Near a generic BC point one can introduce polar (or cylindric in the 3D case) coordinates in which the dispersion relation becomes smooth; this allows analysis of the oscillating integrals. Band-crossing points can yield cumulative (CBC) or instantaneous (IBC) contributions depending on the fulfilment of the frequency matching condition at $\boldsymbol{k}'_\otimes$.

The instantaneous contribution from band-crossing points is always subordinate to the instantaneous contribution due to simple critical points, and, hence, it is never dominant. For that reason, we normally neglect them.

The cumulative contribution has the form

$$I_{\mathrm{CBC}}\big(\vec{n}_\otimes, \boldsymbol{k}, \boldsymbol{k}'_\otimes, \tau, \tilde{\boldsymbol{V}}^{(0)}\big) = \frac{\alpha}{\varrho} B \varrho^{q_{\mathcal{T}_\otimes}} \tag{156}$$

where

$$B = \int_0^\tau \bar{Q}^{\otimes}_{\vec{n}_\otimes}\big[\tilde{\boldsymbol{V}}^{(0)}|\, \boldsymbol{k}, \boldsymbol{k}'_\otimes, \tau_1\big]\tau_1^{-q_{\mathcal{T}_\otimes}}\,\mathrm{d}\tau_1 \qquad \mathcal{T}_\otimes = \mathcal{T}_\otimes\big(\boldsymbol{k}'_\otimes\big).$$

All possible values of $q_{\mathcal{T}_\otimes} = q_0$ are given in table 2. As in the case of simple critical points, BC points give the largest contribution when the group velocity matching condition (147) is fulfilled; but the computation of the gradients in (147) is more complicated. Now to find the gradient $\nabla\omega_{(\zeta',n')}\big(\boldsymbol{k}'_\otimes\big)$ at a BC point one has to use corresponding polar (or cylindric) coordinates (see section 5.3 and, in particular, formula (224)). The order of GVM contribution is $q_{\mathcal{T}_\otimes} = \frac{5}{4}$ when $d = 2$ and $q_{\mathcal{T}_\otimes} = \frac{3}{2}$ or $q_{\mathcal{T}_\otimes} = \frac{7}{4}$ when $d = 3$. Unlike in the case of simple critical points the BC points give a contribution of finite order even if the group velocity matching condition is not fulfilled. For instance, when the GVM condition does not hold, $q_{\mathcal{T}_\otimes} = 2$ when $d = 2$ and three values $q_{\mathcal{T}_\otimes} = \frac{9}{4}, \frac{7}{3}, \frac{5}{2}$ are possible for $d = 3$. Here the tensor $\bar{Q}^{\otimes}_{\vec{n}_\otimes}$ differs from $\tilde{Q}_{\vec{n}}$. For example, when $\omega_{(\zeta',n')}\big(\boldsymbol{k}'_\otimes\big) = \omega_{(\zeta',n'+1)}\big(\boldsymbol{k}'_\otimes\big)$ the second argument of the bilinear tensor $\bar{Q}^{\otimes}_{\vec{n}_\otimes}\big[\tilde{\boldsymbol{V}}^{(0)}|\, \boldsymbol{k}, \boldsymbol{k}'_\otimes, \tau_1\big]$ is $\tilde{\boldsymbol{V}}^{(0)}_{(\zeta'',n'')}\left(\boldsymbol{k}-\boldsymbol{k}'_\otimes\right)$ and the first one is not $\tilde{\boldsymbol{V}}^{(0)}_{(\zeta',n')}\big(\boldsymbol{k}'_\otimes\big)$, but rather a linear combination of $\tilde{\boldsymbol{V}}^{(0)}_{(\zeta',n')}\big(\boldsymbol{k}'_\otimes\big)$ and $\tilde{\boldsymbol{V}}^{(0)}_{(\zeta',n'+1)}\big(\boldsymbol{k}'_\otimes\big)$ of the amplitudes from two meeting bands. The coefficients of the linear combination are determined by values of the functions $\omega_{(\zeta',n')}(\boldsymbol{k}')$ and $\omega_{(\zeta'',n'')}(\boldsymbol{k}-\boldsymbol{k}')$ and their derivatives at $\boldsymbol{k}' = \boldsymbol{k}'_\otimes$. The computation and resulting expressions for the coefficients are rather technical, and we skip the detailed description which will be offered in a forthcoming paper.

One can ask a question: what causes the properties of band-crossing points to be different from the properties of simple points? A simplified answer is that there exist many (a continuum of) group velocities at any band-crossing point $\boldsymbol{k}'_\otimes$ which has a singularity for the dispersion relation (see section 5.3).

4.3. Asymptotic approximation of the first nonlinear response

For parameters $\bar{n}, \boldsymbol{k}$ which satisfy CGV (that is FMC and GVC both hold for some $\boldsymbol{k}'_{*l}$) the first nonlinear response (39) is a combination of I_{CGV} and takes the cumulative form

$$\tilde{\boldsymbol{V}}_{\bar{n}}^{(1)}(\boldsymbol{k},\tau)=\frac{\alpha}{\varrho}\varrho^{q_0(\bar{n},\boldsymbol{k})}\sum_l \bar{b}_{\mathcal{T}}\big[\phi_{\vec{n}(l)}\left(\boldsymbol{k},\boldsymbol{k}'_{*l}\right)\big]\int_0^\tau \bar{Q}_{\vec{n}(l)}\big[\tilde{\boldsymbol{V}}^{(0)}|\,\boldsymbol{k},\boldsymbol{k}'_{*l},\tau_1\big]\tau_1^{-q_{\mathcal{T}}}\,\mathrm{d}\tau_1 \tag{157}$$

where $\vec{n}=\vec{n}(l)$, $\boldsymbol{k}'_*=\boldsymbol{k}'_{*l}$ are solutions of the system of equations (145) and (147). The index $q_0(\bar{n},\boldsymbol{k})$ is the minimum of $q_{\mathcal{T}}=q_{\mathcal{T}}\left(\vec{n},\boldsymbol{k}'_*,\boldsymbol{k}\right)$ over all the solutions with fixed $\bar{n},\boldsymbol{k}$ and different $\boldsymbol{k}'_*$, $\bar{n}'$, $\bar{n}''$ for which the tensor $\bar{Q}_{\vec{n}}\big[\tilde{\boldsymbol{V}}^{(0)}|\,\boldsymbol{k},\boldsymbol{k}'_{*l},\tau_1\big]$ is not zero. All possible values of $q_{\mathcal{T}}$ are listed in table 2. Only points $\boldsymbol{k}'_*=\boldsymbol{k}'_{*l}$ having the minimal value of $q_{\mathcal{T}}\left(\vec{n},\boldsymbol{k}'_*,\boldsymbol{k}\right)=q_0(\bar{n},\boldsymbol{k})$ are included in the summation. The remaining contributions are collected in the smaller remainder $\frac{\alpha}{\varrho}\mathrm{O}\left(\varrho^{q_1(\bar{n},\boldsymbol{k})}\right)$ in (144). Note that smaller values of $q_{\mathcal{T}}\left(\vec{n},\boldsymbol{k}'_*,\boldsymbol{k}\right)$ corresponding to stronger nonlinear interactions are produced by critical points of higher degeneracy.

If the current $\boldsymbol{j}$ in (132) is chosen in a special way then (157) simplifies. Namely, if in (132) and (136) we set $\boldsymbol{j}_{\bar{n}}(\tau)=\boldsymbol{j}_{\bar{n}}^0/\varrho$, where $\boldsymbol{j}_{\bar{n}}^0$ is a constant for $\tau\geqslant 0$, then we obtain

$$\tilde{\boldsymbol{V}}^{(0)}(\tau)=a_0\boldsymbol{j}_{\bar{n}}^0\frac{\tau}{\varrho}\qquad\text{for}\quad\tau\geqslant 0 \tag{158}$$

and formula (151) takes the form

$$I_{\mathrm{CGV}}\big(\vec{n},\boldsymbol{k},\boldsymbol{k}'_*,\tau,\tilde{\boldsymbol{V}}^{(0)}\big)=\alpha p\varrho^{q_{\mathcal{T}(\boldsymbol{k}'_*)}-3}\tau^{3-q_{\mathcal{T}}(\boldsymbol{k}'_*)}=\alpha p t^{\xi}\qquad \xi=3-q_{\mathcal{T}}(\boldsymbol{k}'_*) \tag{159}$$

where p is a constant. The expressions (159) and (157) yield the time power asymptotic formula (1). If $\boldsymbol{j}_{\bar{n}}(\tau)=\boldsymbol{j}_{\bar{n}}^0$ for $\tau_2\geqslant\tau\geqslant\tau_1>0$, and $\boldsymbol{j}_{\bar{n}}(\tau)$ vanishes for $\tau\geqslant\tau_3>\tau_2$ then, again, we obtain (1) with $\xi=1-q_{\mathcal{T}}(\boldsymbol{k}'_*)$ for $t\gg\tau_3/\varrho$.

For the remaining $\bar{n},\boldsymbol{k}$ the first nonlinear response includes I_{IGV} and I_{CBC} and takes the form

$$\begin{aligned}\tilde{\boldsymbol{V}}_{\bar{n}}^{(1)}(\boldsymbol{k},\tau)&=\frac{\alpha}{\varrho}\varrho^{q_0(\bar{n},\boldsymbol{k})}\sum_l \bar{b}_{\mathcal{T}}\big[\phi_{\vec{n}(l)}(\boldsymbol{k},\boldsymbol{k}'_*)\big]\bar{Q}_{\vec{n}}\big[\tilde{\boldsymbol{V}}^{(0)}|\,\boldsymbol{k},\boldsymbol{k}'_*,\tau\big]\,\mathrm{e}^{\mathrm{i}\phi_{\vec{n}(l)}(\boldsymbol{k},\boldsymbol{k}'_*)\tau/\varrho}\tau^{-q_0(\bar{n},\boldsymbol{k})+1}\\&\quad+\frac{\alpha}{\varrho}\varrho^{q_{0\otimes}(\bar{n},\boldsymbol{k})}\sum_{l'}\int_0^\tau \bar{Q}^{\otimes}_{\vec{n}^{\otimes}(l')}\big[\tilde{\boldsymbol{V}}^{(0)}|\,\boldsymbol{k},\boldsymbol{k}'_{\otimes l'},\tau_1\big]\tau_1^{-q_{0\otimes}(\bar{n},\boldsymbol{k})}\,\mathrm{d}\tau_1\end{aligned} \tag{160}$$

where (a) $q_{0\otimes}(\bar{n},\boldsymbol{k})=q_0(\bar{n},\boldsymbol{k})$ if both sums are present; (b) $\boldsymbol{k}'_*=\boldsymbol{k}'_{*l}$ are solutions of (147), and $\boldsymbol{k}'_{\otimes l'},\vec{n}^{\otimes}(l')$ are solutions of (155) and (145); (c) $q_0(\bar{n},\boldsymbol{k})$ is the minimum of $q_{\mathcal{T}}=q_{\mathcal{T}}\left(\vec{n},\boldsymbol{k}'_*,\boldsymbol{k}\right)$ over all the solutions of (147) with fixed $\bar{n},\boldsymbol{k}$ for which the tensor $\bar{Q}_{\vec{n}}\big[\tilde{\boldsymbol{V}}^{(0)}|\,\boldsymbol{k},\boldsymbol{k}'_{*l},\tau_1\big]$ is not zero. Only points $\boldsymbol{k}'_*=\boldsymbol{k}'_{*l}$ having the minimal value of $1+q_{\mathcal{T}}\big(\vec{n},\boldsymbol{k}'_*,\boldsymbol{k}\big)=q_0(\bar{n},\boldsymbol{k})$ are included in the summation in l. Similarly, in the second sum counting the contributions of the band-crossing points, the index $q_{0\otimes}(\bar{n},\boldsymbol{k})$ is the minimum of $q_{\otimes}\left(\vec{n},\boldsymbol{k}'_{\otimes},\boldsymbol{k}\right)$. In the one-dimensional case, $d=1$, there is no sum over l'. In the two-dimensional case, $d=2$, if GVC does not always hold $q_{\otimes}^{(0)}=q_{\mathcal{T}\otimes}\left(\vec{n},\boldsymbol{k}'_{\otimes},\boldsymbol{k}\right)=2$. If GVC holds then one has to use (224) to evaluate GVC at a BC point that yields $q_{\otimes}^{(0)}=\frac{5}{4}$. Note that for most values of $\boldsymbol{k}$ the sum in l' is absent since the system of equations (145) and (155) has no solutions, whereas equation (147) always has solutions.

Let us analyse the terms in the asymptotic approximation in (160) and (157). Note that in (157) and (160) there are terms involving the integration with respect to the slow time τ_1. We call those terms *cumulative*. The remaining terms in (160) we refer to as *instantaneous* terms. Note also that the factor $\tau_1^{-q_0(\boldsymbol{k})}$ in the cumulative term in (160) does not create a

Table 2. Oscillatory indices of the critical points for the quadratic nonlinearity. The fractions in the entries indicate the permitted values of the index q_0. Since the interaction integral is of the order of ρ^{q_0} as $\rho \to 0$ the smaller values of q_0 correspond to stronger nonlinear interactions. The largest values of q_0 correspond to non-degenerate simple critical points with $q_{\mathcal{T}} = d/2$. Higher degeneracy yields smaller q_0 and, hence, stronger nonlinear interactions.

q_0	Cumulative CGV $q_0 = q_{\mathcal{T}}$	Instantaneous IGV $q_0 = q_{\mathcal{T}} + 1$	Cumulative CBC $q_0 = q_{\mathcal{T}\otimes}$
$d = 1$	$\frac{1}{2}$	$\frac{5}{4}; \frac{4}{3}; \frac{3}{2}$	None
$d = 2$	$\frac{3}{4}; \frac{5}{6}; 1$	$\frac{5}{3}; \frac{7}{4}; \frac{11}{6}; 2$	$\frac{5}{4}; 2$
$d = 3$	$\frac{7}{6}; \frac{5}{4}; \frac{4}{3}; \frac{3}{2}$	$2; \frac{17}{8}; \frac{13}{6}; \frac{11}{5}; \frac{9}{4}; \frac{7}{3}; \frac{5}{2}$	$\frac{3}{2}; \frac{7}{4}; \frac{9}{4}; \frac{7}{3}; \frac{5}{2}$

singularity at $\tau_1 = 0$ thanks to presence of another factor $\bar{Q}_{\vec{n}(l)}\big(\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)}, \boldsymbol{k}_l', \tau_1\big)$ and the equality $\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)} = 0$ at $\tau_1 = 0$. For the cumulative case the difference $q_1(\boldsymbol{k}) - q_0(\boldsymbol{k})$ in (144) is not less than $\frac{1}{4}$ for $d = 2$ and $\frac{1}{6}$ for $d = 3$. The oscillatory index $q_0(\boldsymbol{k}) > 0$ takes several fixed values (see the table 2) determined by the types $\mathcal{T}$ of the critical points $\boldsymbol{k}_l'$.

4.4. Summary of the classification of nonlinear interactions

The representations (157) and (160) for the nonlinear wave interactions together with the selection rules (145), (147) and (155) show, first of all, which components of the wavepacket play significant roles in the nonlinear medium response, and, second of all, that the contributions of these components are characterized by the oscillatory indices $q_0(\boldsymbol{k})$. We also would like to point out that the indices $q_0(\boldsymbol{k})$ depend on, first, the space dimension, which can be one, two or three, and, second, on the type of nonlinearity which can be quadratic or cubic.

We conclude that the *analysis of the phase critical points, especially degenerate ones, and the study of the asymptotic approximation (157) become the central problem of the quantitative analysis of the wavepacket propagation in weakly nonlinear media.* The contribution of non-degenerate critical points is evaluated with the aid of the *Morse lemma* leading to formula (117) (see [71], section 8, section 2.3.2). This case is part of the classical theory of oscillatory integrals, and we discuss it in section 7. The case of degenerate critical points is more complicated, and, to the best of our knowledge, a consistent theory for it has begun to be developed rather recently (see [5, 6] and references therein). As to the types of critical points, it turns out that for the cases of interest there are just a few different robust (generic) types of critical points, and we analysed all of them. *Since degenerate points yield larger contributions to the interaction integral than the non-degenerate ones, we carry out an exhaustive study of all possible generic cases of the degeneracy related to our problems covering the space dimensions one, two and three.*

In table 2 we list all possible values of the oscillatory index $q_0(\boldsymbol{k})$ for the quadratic nonlinearity.

Every entry in table 2 contains several values of q_0. Since the interaction integral is of the order of ϱ^{q_0} as $\varrho \to 0$, the smaller values of q_0 correspond to stronger nonlinear interactions. The largest values of q_0 for simple points correspond to non-degenerate simple critical points with $q_{\mathcal{T}} = d/2$. Higher degeneracy yields smaller q_0 and, hence, stronger nonlinear interactions. Note that the value $q_0 = \frac{1}{2}(d - 1)$ for the homogeneous medium considered in section 3.4 is smaller than all the values in table 2. This can be explained by the higher symmetry of a homogeneous medium and consequently the higher degeneracy of critical points compared with a periodic medium. One can see from the table that instantaneous interactions for which the FM condition (145) does not hold, are weaker than the simple cumulative interactions (CGV).

Observe that the dependence $\omega_{\bar{n}'}(\boldsymbol{k}')$ on $\boldsymbol{k}'$ from the Brillouin zone is periodic, and, hence, *there is no convexity restrictions on the dispersion relation as in the homogeneous case, which is a known obstacle to satisfying FMC*. It is well known that in homogeneous anisotropic media FMC can be satisfied because of the *birefringence* (the dependence of the refractive index on the direction of polarization of optical radiation) ([16], section 2.7, [3], section 3.1).

4.5. Degenerate critical points

Table 2 shows that the contribution of degenerate critical points to the relevant oscillatory integral is more significant than the contribution from non-degenerate critical points. This implies that *the degenerate critical points correspond to the stronger nonlinear interactions than non-degenerate ones*. Therefore, to study the most significant nonlinear interactions *we must study the degenerate critical points.*

Let us look in more detail at possible degeneracies. The necessary condition for a degeneracy is the vanishing of the determinant of the Hessian

$$\det \nabla^2_{\boldsymbol{k}'} \phi_{\bar{n}}(\boldsymbol{k}, \boldsymbol{k}') = 0. \tag{161}$$

For every fixed $\boldsymbol{k}$ this equation has a simple geometrical meaning: it determines points on the graph of $\phi_{\bar{n}}$ considered as a function of $\boldsymbol{k}'$ at which one of the principal curvatures of the graph vanishes; such points are called parabolic in differential geometry. The detail of the analysis of degenerate critical points depend on the space dimension d. Let us consider the dimensions one, two and three and discuss simple critical points. We do not discuss BC points here since their analysis is more technical and the contribution from BC points is not leading for most values of $\boldsymbol{k}$.

One-dimensional case $d = 1$. In this case we have two parameters $\boldsymbol{k}, \boldsymbol{k}'$ and two equations: the GV condition and the FMC hold generically together at a discrete set of points $\boldsymbol{k}, \boldsymbol{k}'$; the cumulative critical points are non-degenerate (type $\mathcal{T} = A_1$) which gives $q_0(\boldsymbol{k}) = \frac{1}{2}$. Generic instantaneous critical points can be degenerate of class $\mathcal{T} = A_2$ which gives $q_0(\boldsymbol{k}) = \frac{4}{3}$. Instantaneous degenerate SHG points are of class $\mathcal{T} = A_3$ which gives $q_0(\boldsymbol{k}) = \frac{5}{4}$.

Two-dimensional case $d = 2$. For any given $\boldsymbol{k}$ (147) has several solutions (maximum, minimum and saddle points of the periodic function $\omega_{\bar{n}'}(\boldsymbol{k}') + \omega_{\bar{n}''}(\boldsymbol{k} - \boldsymbol{k}')$ considered as a function of $\boldsymbol{k}'$ when it is smooth); but if these solutions do not satisfy the FMC they contribute to the instantaneous response only. In the last case $q_0(\boldsymbol{k}) = 2$, giving the order $\frac{\alpha}{\varrho}\varrho^2$. Nevertheless, we have a continuous parameter $\boldsymbol{k}$, and for some values of $\boldsymbol{k}$ we may have FMC and GVC satisfied simultaneously which results in the cumulative response. The GVC and the FMC impose three equations on four variables $\boldsymbol{k}, \boldsymbol{k}'$, which determine a curve in the four-dimensional $\boldsymbol{k}, \boldsymbol{k}'$ space. On the curve $q_0(\boldsymbol{k}) = 1$. The Hessian may change the sign along this curve. In such a case equation (161) must have a solution; generically (161) is satisfied for several values $\boldsymbol{k} = \boldsymbol{k}_*$. At such points the phase is degenerate, the degenerate point is generically of type $\mathcal{T} = A_2$ which gives $q_0(\boldsymbol{k}) = \frac{5}{6}$ when $n'' \neq n'$ or $\boldsymbol{k} - \boldsymbol{k}' \neq \boldsymbol{k}'$.

There are special cases, namely when $\bar{n}'' = \bar{n}'$, $\boldsymbol{k}' = \boldsymbol{k}/2 \pmod{2\pi}$, for which (147) obviously holds. In those cases the FMC then implies

$$\omega_{\bar{n}}(\boldsymbol{k}) = 2\omega_{\bar{n}'}(\boldsymbol{k}/2). \tag{162}$$

The equality (162) is the well known second-harmonic generation case. The FMC determines a curve in the $\boldsymbol{k}$-plane. It can happen that det $\nabla^2_{\boldsymbol{k}'}\phi_{\vec{n}}\,(\boldsymbol{k}, \boldsymbol{k}/2)$ changes sign on this curve. In this case we have a degeneracy at the point where the determinant vanishes. At a degenerate SHG point, which is generically of type $\mathcal{T} = A_3$, the index of the most significant nonlinear interaction is $q_0(\boldsymbol{k}) = \frac{3}{4}$.

Three-dimensional case $d = 3$. When the FM condition does not hold, we have the instantaneous response at the points which satisfy the GV condition (147) which produces $q_0(\boldsymbol{k}) = \frac{5}{2}$ for non-degenerate points, though more degenerate cases can occur. The cumulative response for $d = 3$ occurs when both the GV condition and the FM condition hold together imposing four equations on six variables, and, hence, we may have a two-dimensional surface of solutions in the six-dimensional $\boldsymbol{k}$, $\boldsymbol{k}'$-space. It is clear that for most of the triples n', n'', n there is no solution at all. Note that on the mentioned surface $q_0(\boldsymbol{k}) = \frac{3}{2}$ at almost all points. If the Hessian changes the sign on this surface its zero-level curve determines a curve of degenerate points of type $\mathcal{T} = A_2$ where (161) holds. For the points $\boldsymbol{k}$ on the curve we have $q_0(\boldsymbol{k}) = \frac{7}{3}$. Note also, that the zero eigenvector of the Hessian determines the null-direction at every point of this curve, and that generically the phase function is cubic in this direction. However, it is possible that the phase function degenerates to be of fourth order at several points. Then at the related points of class $\mathcal{T} = A_3$ we would have $q_0(\boldsymbol{k}) = \frac{5}{4}$.

Critical points associated with SHG are determined by the special SHG-FMC condition (162). This condition determines a two-dimensional surface in the three-dimensional $\boldsymbol{k}$-space. The Hessian degeneration condition (161) may give a curve on this surface, and on such a curve we would have points of the type $\mathcal{T} = A_3$ with $q_0(\boldsymbol{k}) = \frac{5}{4}$. For special points on this curve there may be a higher degeneration in the null-direction of the Hessian which will produce points of the type $\mathcal{T} = A_5$, yielding $q_0(\boldsymbol{k}) = \frac{7}{6}$. The value $q_0(\boldsymbol{k}) = \frac{7}{6}$ is the smallest possible in the generic case value for the index $q_0(\boldsymbol{k})$, and, consequently, it is associated with the strongest nonlinear interaction. Therefore, one can conclude that the second-harmonic generation appears as the strongest mechanism in nonlinear interactions.

We would like to point out that if one of the mentioned scenarios holds for a triple of generic dispersion relations $\omega_{\vec{n}}(\boldsymbol{k})$, $\omega_{\vec{n}'}(\boldsymbol{k}')$, $\omega_{\vec{n}''}(\boldsymbol{k}'')$ then it persists under a small smooth perturbation of the relations, indicating the *robustness* of all the scenarios.

We also add that since all generic points in cumulative integrals are of class $\mathcal{T} = A_p$, the corresponding integrals are given explicitly by formula (288) similar to (117) (for details see section 7).

4.6. Comparison of periodic and homogeneous media

The analysis of waves in spatially homogeneous linear media is based on Fourier analysis. For general periodic media it is appropriate to use the Bloch eigenmodes in the place of the plane waves and Fourier analysis. Interestingly enough, though the Bloch waves are more complex functions than trigonometric polynomials, it is possible to carry out a rather complete analysis of the phenomena under consideration. In addition to that, we have found that studies of periodic media can help to better understand the properties of homogeneous media.

The nonlinear phenomena in periodic and homogeneous media have many common properties, though, there are quite significant differences. In our studies homogeneous media can be viewed as an extremely symmetric case of periodic media. Since more symmetric situations produce higher degeneracies one can expect quite significant differences in the nonlinear phenomena for homogeneous and periodic media. Since a periodic medium has fewer symmetries than a homogeneous one, weaker interactions can be expected and this conclusion is supported by our analysis. Evidently, in homogeneous, isotropic media there are no selected directions of the wave propagation, whereas for a general periodic medium this degeneracy is removed, resulting in substantial modifications in the phenomena we study. In particular, we show that there is a discrete set of special directions related to the principal part of the nonlinear response. These directions (group velocities) are solutions to certain equations (called selection rules) based on which one also finds the corresponding frequencies.

The remarkable fact that the selection rules produce just a few special directions can be explained as follows. In a periodic medium there is much more scattering than in a homogeneous medium, and, hence, for a generic direction the waves interact destructively producing no significant results. However, for a few special directions that satisfy the selection rules the waves are 'in phase' and interact coherently, producing a noticeable nonlinear response. The reason why certain directions are selected in the periodic media can be explained as follows. *In the case of a generic periodic medium for an arbitrary* $\boldsymbol{k}$ *the group and frequency matching conditions (147) and (145) cannot be satisfied simultaneously.* Assuming that $\boldsymbol{k}$ and $\boldsymbol{k}'_*$ satisfy the group velocity matching condition (147) we may then view the frequency matching condition (145) as an additional equation on $\boldsymbol{k}$. In general, there will be no solutions $\boldsymbol{k}$ to this equation for most of the triples $\vec{n}$, but for some special triples $\vec{n}$ there may be solutions forming a $(d-1)$-dimensional surfaces in the d-dimensional Brillouin zone. These solutions correspond to modes which exhibit the most significant nonlinear interactions. The magnitude ϱ^{q_0} of nonlinear response with $q_0 > \frac{1}{2}(d-1)$ for periodic media is smaller than the corresponding factor $\varrho^{(d-1)/2}$ for homogeneous media. This fact shows that the introduction of periodic variations in the medium weakens most nonlinear interactions to some degree, but most important is that this weakening is different for different interactions and some selected interactions are much stronger then all the others.

We would also like to point out that the weakening of the nonlinear interactions is more significant for higher dimensions since there is more possibility for a wave to disperse. As to the constructive and destructive wave interference it is worth noting that:

(a) in homogeneous media the eigenmodes are plane waves and, hence, their wavefronts are planes; consequently, if the related phases are matched locally, they automatically match globally in the whole space;

(b) fine evaluations of the wave interference is carried out with the help of oscillatory integrals;

(c) in the evaluation of the oscillatory integrals corresponding to a general periodic media we systematically apply methods of singularity theory (see [6]).

As we have already pointed out, the symmetries of the medium have a strong impact on the level of nonlinear interactions. Every symmetry of the media has to be taken into account. To simplify the theory we make a pretty common assumption that there are no symmetries we 'do not know about', or, in other words, we assume that the dispersion relations are *generic*. However, we would like to point out that *there are symmetries that are naturally present in the phase function even for generic dispersion relations*. For instance, the phase

$$\omega_n(\boldsymbol{k}) + \omega_{n'}(\boldsymbol{k}') + \omega_{n'}(\boldsymbol{k} - \boldsymbol{k}')$$

is symmetric with respect to the change of variables $\boldsymbol{k}' \leftrightarrow \boldsymbol{k} - \boldsymbol{k}'$ for an arbitrary function $\omega_{n'}$. The fixed point of this symmetry is given by $\boldsymbol{k} - \boldsymbol{k}' = \boldsymbol{k}'$. This fact after some analysis implies that the second-harmonic generation is the strongest mechanism of generic nonlinear quadratic interaction with the smallest index q_0.

5. Linear dielectric periodic medium

The methods we develop are equally applicable to all the space dimensions $d = 1, 2, 3$. We often carry out the computations for the case $d = 3$. The cases of $d = 1, 2$ deal with three-component vector fields which do not depend, respectively, on x_2, x_3 and on x_3. These cases differ from $d = 3$ only in the concrete expressions for the Maxwell operator and the eigenmodes which can be obtained by a reduction; the general framework is the same.

5.1. Floquet–Bloch transformation

Suppose that we have a lattice in the space $\mathbb{R}^d$ and assume that the lattice is just the set $\mathbb{Z}^d$ of integer-valued vectors $\boldsymbol{m}$ in $\mathbb{R}^d$. Then for any square-integrable complex-valued function $v(\boldsymbol{r})$ from $L_2\left(\mathbb{R}^d\right)$ we introduce two types of Floquet–Bloch transformations [2, 52, 66, 81]:

$$\tilde{v}(\boldsymbol{r}, \boldsymbol{k}) = \sum_{\boldsymbol{m}\in\mathbb{Z}^d} v(\boldsymbol{r}+\boldsymbol{m}) \exp(-\mathrm{i}\boldsymbol{m}\cdot\boldsymbol{k}) \qquad \hat{v}(\boldsymbol{r}, \boldsymbol{k}) = \exp(-\mathrm{i}\boldsymbol{r}\cdot\boldsymbol{k})\, \tilde{v}(\boldsymbol{r}, \boldsymbol{k}). \tag{163}$$

Note that if $v(\boldsymbol{r})$ decays sufficiently fast at infinity then $\tilde{v}(\boldsymbol{r}, \boldsymbol{k})$ is a smooth function of $\boldsymbol{k}$. The equalities (163) readily imply the following identities which hold for any $\boldsymbol{m}$ in $\mathbb{Z}^d$ and $\boldsymbol{r}$ in $\mathbb{R}^d$:

$$\tilde{v}(\boldsymbol{r}, \boldsymbol{k}+2\pi\boldsymbol{m}) = \tilde{v}(\boldsymbol{r}; \boldsymbol{k}) \qquad \tilde{v}(\boldsymbol{r}+\boldsymbol{m}; \boldsymbol{k}) = \exp(\mathrm{i}\boldsymbol{m}\cdot\boldsymbol{k})\, \tilde{v}(\boldsymbol{r}; \boldsymbol{k}) \tag{164}$$

$$\hat{v}(\boldsymbol{r}, \boldsymbol{k}+2\pi\boldsymbol{m}) = \exp(-\mathrm{i}\boldsymbol{r}\cdot 2\pi\boldsymbol{m})\, \hat{v}(\boldsymbol{r}, \boldsymbol{k}) \qquad \hat{v}(\boldsymbol{r}+\boldsymbol{m}, \boldsymbol{k}) = \hat{v}(\boldsymbol{r}, \boldsymbol{k}). \tag{165}$$

The function $\tilde{v}(\boldsymbol{y}, \boldsymbol{k})$ is $2\pi\mathbb{Z}^d$-periodic in $\boldsymbol{k} = (k_1, \ldots, k_d)$ and the function $\hat{v}(\boldsymbol{r}, \boldsymbol{k})$ is $\mathbb{Z}^d$-periodic in $\boldsymbol{r} = (x_1, \ldots, x_d)$. Evidently, if a function in $\boldsymbol{r}$ is $\mathbb{Z}^d$-periodic it is uniquely defined by its values in the cube

$$Q = [0, 1]^d \tag{166}$$

called the primitive cell. The parameter $\boldsymbol{k}$, often called the *quasimomentum* or the *wavevector*, varies in d-dimensional reciprocal space $\mathbb{R}^d$. For functions which are $2\pi\mathbb{Z}^d$-periodic in $\boldsymbol{k}$ it is convenient to take the primitive cell, called the *Brillouin* zone [2, 52, 66, 81], to be

$$Q' = [-\pi, \pi]^d. \tag{167}$$

It is often appropriate to identify the opposite faces of the cube Q' and treat it as a torus. We will do it without introducing new notation.

The *inverse formula* is

$$v(\boldsymbol{r}+\boldsymbol{m}) = \frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d} \tilde{v}(\boldsymbol{r}, \boldsymbol{k}) \exp(\mathrm{i}\boldsymbol{m}\cdot\boldsymbol{k})\, \mathrm{d}\boldsymbol{k} \tag{168}$$

for every $\boldsymbol{m}$ in $\mathbb{Z}^d$. In particular,

$$v(\boldsymbol{r}) = \frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d} \tilde{v}(\boldsymbol{r}, \boldsymbol{k})\, \mathrm{d}\boldsymbol{k}. \tag{169}$$

The equalities (163) imply that if $a(\boldsymbol{r})$ is a bounded $\mathbb{Z}^3$-periodic function then

$$\widetilde{av}(\boldsymbol{r}, \boldsymbol{k}) = a(\boldsymbol{r})\tilde{v}(\boldsymbol{r}, \boldsymbol{k}) \qquad \widehat{av}(\boldsymbol{r}, \boldsymbol{k}) = a(\boldsymbol{r})\hat{v}(\boldsymbol{r}, \boldsymbol{k}). \tag{170}$$

We also have the following identity:

$$\widehat{\partial_{x_j} v}(\boldsymbol{r}, \boldsymbol{k}) = (\partial_{x_j} + \mathrm{i}k_j)\hat{v}(\boldsymbol{r}, \boldsymbol{k}). \tag{171}$$

The next *convolution formula* describes the pointwise multiplication of functions in the Bloch representation:

$$\tilde{vw}(\boldsymbol{r},\boldsymbol{k}) = \sum_{\boldsymbol{m}} vw(\boldsymbol{m}+\boldsymbol{r})\,\mathrm{e}^{-\mathrm{i}\boldsymbol{m}\boldsymbol{k}}$$
$$= (2\pi)^{-d}\int_{[-\pi,\pi]^d}\tilde{w}(\boldsymbol{r},\boldsymbol{k}')\tilde{v}(\boldsymbol{r},\boldsymbol{k}-\boldsymbol{k}')\,\mathrm{d}\boldsymbol{k}'. \tag{172}$$

This implies

$$\hat{vw}(\boldsymbol{y},\boldsymbol{k}) = \sum_{\boldsymbol{m}} vw(\boldsymbol{m}+\boldsymbol{y})\,\mathrm{e}^{-\mathrm{i}\boldsymbol{m}\boldsymbol{k}}\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\boldsymbol{y}}$$
$$= \frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d}\hat{w}(\boldsymbol{y},\boldsymbol{k}')\hat{v}(\boldsymbol{y},\boldsymbol{k}-\boldsymbol{k}')\,\mathrm{d}\boldsymbol{k}'. \tag{173}$$

Now we consider a situation which arises in applications to Maxwell equations. We consider for square-integrable vector-functions from $\left(L_2([0,1]^d)\right)^6$ a scalar product

$$(\boldsymbol{u},\boldsymbol{v})_{\mathcal{H}} = \int_{[0,1]^d}\boldsymbol{u}(\boldsymbol{r})\cdot\sigma(\boldsymbol{r})\boldsymbol{v}^*(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} \tag{174}$$

where $\boldsymbol{v}^*$ is a vector complex conjugate to $\boldsymbol{v}$ and $\sigma(\boldsymbol{r}) > 0$ is a positive symmetric matrix which is 1-periodic in $\boldsymbol{r}$. Suppose now that for every $\boldsymbol{k}$ we have a sequence of vectors $\tilde{\boldsymbol{g}}_n(\boldsymbol{r};\boldsymbol{k})$, $n = 1, 2, \ldots$ considered as functions of $\boldsymbol{r}$ that forms an orthogonal basis the Hilbert space $\mathcal{H}$ with respect to this scalar product. We also assume that the functions $\tilde{\boldsymbol{g}}_n(\boldsymbol{r};\boldsymbol{k})$ are defined for all $\boldsymbol{r}$ in $\mathbb{R}^d$ and satisfy the *Bloch cyclic condition*

$$\tilde{\boldsymbol{g}}_n(\boldsymbol{r}+\boldsymbol{m},\boldsymbol{k}) = \exp\{\mathrm{i}\boldsymbol{m}\cdot\boldsymbol{k}\}\tilde{\boldsymbol{g}}_n(\boldsymbol{r};\boldsymbol{k}) \qquad \boldsymbol{m} \text{ in } \mathbb{Z}^d \quad \boldsymbol{r} \text{ in } \mathbb{R}^d. \tag{175}$$

The basis satisfying the Bloch cyclic condition (175) naturally arises as an eigenbasis of a differential operator with periodic coefficients. Since $\{\tilde{\boldsymbol{g}}_n\}$ is the basis then for any square-integrable function $\boldsymbol{v}(\boldsymbol{r})$ with $\boldsymbol{r}$ in $\mathbb{R}^d$ we obtain for every $\boldsymbol{k}$ an expansion of its Bloch transform $\tilde{\boldsymbol{v}}(\boldsymbol{r},\boldsymbol{k})$:

$$\tilde{\boldsymbol{v}}(\boldsymbol{r},\boldsymbol{k}) = \sum_{n\geqslant 1}\tilde{v}_n(\boldsymbol{k})\tilde{\boldsymbol{g}}_n(\boldsymbol{r},\boldsymbol{k}) = \sum_{n\geqslant 1}\tilde{\boldsymbol{v}}_n(\boldsymbol{r},\boldsymbol{k}) \tag{176}$$

where

$$\tilde{v}_n(\boldsymbol{k}) = \frac{(\tilde{\boldsymbol{v}}(\cdot,\boldsymbol{k}),\tilde{\boldsymbol{g}}_n(\cdot,\boldsymbol{k}))_{\mathcal{H}}}{((\tilde{\boldsymbol{g}}_n(\cdot,\boldsymbol{k}),\tilde{\boldsymbol{g}}_n(\cdot,\boldsymbol{k}))_{\mathcal{H}})^{1/2}} \qquad \tilde{\boldsymbol{v}}_n(\boldsymbol{r},\boldsymbol{k}) = \tilde{v}_n(\boldsymbol{k})\tilde{\boldsymbol{g}}_n(\boldsymbol{r},\boldsymbol{k})$$
$$\tilde{\boldsymbol{v}}_n(\boldsymbol{r},\boldsymbol{k}) = \tilde{\Pi}_{g_n}(\boldsymbol{k})\hat{\boldsymbol{v}}(\boldsymbol{r},\boldsymbol{k}) \tag{177}$$

and $\tilde{\Pi}_{g_n}(\boldsymbol{k})$ is the orthogonal projection operator onto the function $\tilde{\boldsymbol{g}}_n(\boldsymbol{y},\boldsymbol{k})$. Using (169) we readily obtain the following relations (see also [66], theorem XIII.98):

$$\int_{\mathbb{R}^d}|\boldsymbol{v}(\boldsymbol{r})|^2\,\mathrm{d}\boldsymbol{r} = \frac{1}{(2\pi)^d}\sum_{n=1}^{\infty}\int_{[-\pi,\pi]^d}|\tilde{v}_n(\boldsymbol{k})|^2\,\mathrm{d}\boldsymbol{k} \tag{178}$$

$$\boldsymbol{v}(\boldsymbol{r}) = \frac{1}{(2\pi)^d}\sum_{n=1}^{\infty}\int_{[-\pi,\pi]^d}\tilde{v}_n(\boldsymbol{k})\tilde{\boldsymbol{g}}_n(\boldsymbol{r},\boldsymbol{k})\,\mathrm{d}\boldsymbol{k} \qquad \boldsymbol{r} \text{ in } \mathbb{R}^d. \tag{179}$$

Note that in formula (179) $\tilde{\boldsymbol{g}}_n(\boldsymbol{r},\boldsymbol{k})$ is considered as a function defined for all $\boldsymbol{r}$ in $\mathbb{R}^d$ and satisfying the cyclic (Bloch) conditions (175). One can readily verify that the projection $\tilde{\Pi}_g$

is $2\pi\mathbb{Z}^d$-periodic in $\boldsymbol{k}$. The relation between the projection $\tilde{\Pi}_g(\boldsymbol{k})$ and its other representation $\hat{\Pi}_g(\boldsymbol{k})$ is as follows:

$$\tilde{\Pi}_g(\boldsymbol{k})\tilde{\boldsymbol{v}}(\boldsymbol{r},\boldsymbol{k}) = \exp\{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}\}\,\hat{\Pi}_g(\boldsymbol{k})\exp\{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}\}\,\tilde{\boldsymbol{v}}(\boldsymbol{r},\boldsymbol{k}) = \exp\{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}\}\,\hat{\Pi}_g(\boldsymbol{k})\hat{\boldsymbol{v}}(\boldsymbol{r},\boldsymbol{k}). \tag{180}$$

Keeping in mind that nonlinear interactions are defined through products of field components we need to derive a formula for the Floquet–Bloch transforms of a product of two scalar functions. We denote the ith component of a vector $\boldsymbol{v}$ by $v_{(i)}$. The vector-valued quadratic nonlinearities we deal with are described by bilinear tensors $Q\,\vdots\,\boldsymbol{v}\boldsymbol{w}$ which can be written in coordinates as

$$\left(Q\,\vdots\,\boldsymbol{v}\boldsymbol{w}\right)_{(l)} = \sum_{i,j} Q_{ijl}v_{(i)}w_{(j)}. \tag{181}$$

Multilinear tensors are written in a similar way. Using the convolution formula (172) and assuming that the coefficients $\tilde{v}_n(\boldsymbol{k})$, $\tilde{w}_n(\boldsymbol{k})$ decay sufficiently fast as $n \to \infty$ we obtain the following formula for the pointwise product:

$$\widetilde{v_{(i)}w_{(j)}}(\boldsymbol{r},\boldsymbol{k}) = \sum_{n',n''\geqslant 1}\frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d}\tilde{v}_{n'(i)}(\boldsymbol{r},\boldsymbol{k}')\tilde{w}_{n''(j)}(\boldsymbol{r},\boldsymbol{k}-\boldsymbol{k}')\,\mathrm{d}\boldsymbol{k}'. \tag{182}$$

For a quadratic nonlinearity $\boldsymbol{Q}$ depending on the field components at the same point $\boldsymbol{r}$ the $(\boldsymbol{r},\boldsymbol{k})$-components of its Floquet–Bloch transform can be found from the expression

$$\left[\tilde{\boldsymbol{Q}}(\tilde{v},\tilde{w})\right]_n(\boldsymbol{r},\boldsymbol{k}) = \frac{1}{(2\pi)^d}\Pi_n(\boldsymbol{k})\sum_{n',n''}\int Q\,\vdots\,\tilde{\boldsymbol{v}}_{n'}(\boldsymbol{r},\boldsymbol{k}')\tilde{\boldsymbol{w}}_{n''}(\boldsymbol{r},\boldsymbol{k}-\boldsymbol{k}')\,\mathrm{d}\boldsymbol{k}' \tag{183}$$

where the tensor Q may depend 1-periodically on $\boldsymbol{r}$; we use the notation (181) and (170). The cubic case is similar and the related representation involves the double-convolution operation.

5.2. *Linear Maxwell operator*

Let us look closely at the linear version of the Maxwell equations introduced in section 2.1. Recall that the electric permittivity (dielectric constant) ε is a periodic tensor in the space, i.e.

$$\varepsilon^{(1)}(\boldsymbol{r}+\boldsymbol{m}) = \varepsilon^{(1)}(\boldsymbol{r}) \qquad \boldsymbol{m} \text{ in } \mathbb{Z}^3. \tag{184}$$

In the spatially inhomogeneous case, in particular for the periodic media, when ε depends on $\boldsymbol{r}$, there is an advantage in selecting the electric inductance $\boldsymbol{D}$ rather than the electric field $\boldsymbol{E}$ as the main field variable, because of the simplicity of the condition $\nabla\cdot\boldsymbol{D} = 0$ compared with $\nabla\cdot\left(\varepsilon^{(1)}(\boldsymbol{r})\boldsymbol{E}\right) = 0$. This advantage is even greater in the case of a nonlinear dielectric constant $\varepsilon = \varepsilon(\boldsymbol{r};\boldsymbol{E}(\cdot))$. Keeping that in mind we take $\boldsymbol{D}$ as the main field variable and write the linear constitutive relation in the form (compare with (11) and (12))

$$\boldsymbol{E}(\boldsymbol{r},t) = \boldsymbol{\eta}^{(1)}(\boldsymbol{r})\boldsymbol{D}(\boldsymbol{r},t) \qquad \boldsymbol{\eta}^{(1)}(\boldsymbol{r}) = \left[\varepsilon^{(1)}(\boldsymbol{r})\right]^{-1}. \tag{185}$$

The tensor $\boldsymbol{\eta}^{(1)}$ is called impermeability. Note also that (246) implies that $\varepsilon^{(1)}(\boldsymbol{r})$ and, hence, $\boldsymbol{\eta}^{(1)}(\boldsymbol{r})$ are symmetric tensors with real-valued entries, i.e.

$$\varepsilon^{(1)*}(\boldsymbol{r}) = \varepsilon^{(1)}(\boldsymbol{r}) \geqslant \mathbf{1} \qquad 0 < \boldsymbol{\eta}^{(1)}(\boldsymbol{r}) = \boldsymbol{\eta}^{(1)*}(\boldsymbol{r}) \leqslant \mathbf{1}. \tag{186}$$

In addition to that, in view of (184) $\boldsymbol{\eta}^{(1)}(\boldsymbol{r})$ is periodic, i.e.

$$\boldsymbol{\eta}^{(1)}(\boldsymbol{r}+\boldsymbol{m}) = \boldsymbol{\eta}^{(1)}(\boldsymbol{r}) \qquad \boldsymbol{m} \text{ in } \mathbb{Z}^3. \tag{187}$$

We also assume that $\boldsymbol{\eta}^{(1)}(\boldsymbol{r})$ is positive and bounded:

$$C_{-}\mathbf{1} \leqslant \boldsymbol{\eta}^{(1)}(\boldsymbol{r}) \leqslant C_{+}\mathbf{1} \qquad \text{where} \quad 0 < C_{-} \leqslant C_{+}. \tag{188}$$

According to (16) for the dimension $d = 3$ the linear Maxwell operator $\mathcal{M}$ and the field variable $\boldsymbol{U}$ are

$$\mathcal{M} = \mathrm{i}\begin{bmatrix} \mathbf{0} & \mu^{-1}\nabla\times \\ -\nabla\times\eta^{(1)}(\boldsymbol{r}) & \mathbf{0} \end{bmatrix} \qquad \boldsymbol{U} = \begin{bmatrix} \boldsymbol{D} \\ \boldsymbol{B} \end{bmatrix}. \tag{189}$$

We assume everywhere that $\nabla\cdot\boldsymbol{D} = 0$, $\nabla\cdot\boldsymbol{B} = 0$. Note that the electromagnetic energy is the following quadratic form of $\boldsymbol{U}(\boldsymbol{r}, t)$:

$$\mathcal{E}(\boldsymbol{U}, \boldsymbol{U}) = \tfrac{1}{2}\int \left[\boldsymbol{D}(\boldsymbol{r})\cdot\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\boldsymbol{D}(\boldsymbol{r}) + \mu^{-1}\boldsymbol{B}(\boldsymbol{r})\cdot\boldsymbol{B}(\boldsymbol{r})\right]\mathrm{d}\boldsymbol{r} \tag{190}$$

$$= \tfrac{1}{2}\int \boldsymbol{U}(\boldsymbol{r})\sigma(\boldsymbol{r})\boldsymbol{U}(\boldsymbol{r})\,\mathrm{d}\boldsymbol{r} \qquad \sigma(\boldsymbol{r}) = \begin{bmatrix} \boldsymbol{\eta}^{(1)}(\boldsymbol{r}) & \mathbf{0} \\ \mathbf{0} & \mu^{-1}\boldsymbol{I} \end{bmatrix} \tag{191}$$

where integration is over the whole space. One can easily verify that the Maxwell operator $\mathcal{M}$ satisfies the identity

$$\mathcal{E}\left(\boldsymbol{U}, \mathcal{M}\boldsymbol{W}\right) = \mathcal{E}\left(\mathcal{M}\boldsymbol{U}, \boldsymbol{W}\right) \tag{192}$$

and, hence, it is a self-adjoint (Hermitian) operator with respect to the bilinear energy form $\mathcal{E}(\boldsymbol{U}, \boldsymbol{V})$. This implies that $\mathrm{e}^{-\mathrm{i}\mathcal{M}t}$ is a unitary operator preserving $\mathcal{E}$.

It was discussed in section 2 that the analysis of the weakly nonlinear dielectric medium requires rather detailed information on the eigenvalues and eigenmodes of the linear medium described by the self-adjoint operator $\mathcal{M}$. Since the impermeability $\boldsymbol{\eta}(\boldsymbol{r})$ is a periodic function the spectral analysis of the first-order differential operator $\mathcal{M}$ can be carried our with the aid of the Floquet–Bloch theory (see [2, 52, 66, 81]).

Let us describe the basic spectral properties of the operator $\mathcal{M}$ for the dimension $d = 3$. First of all, the spectral analysis of the operator $\mathcal{M}$ acting on six-dimensional fields $\boldsymbol{U}$ can be reduced in a canonical fashion to a simpler operator $\mathfrak{m}$ acting on three-dimensional fields $\boldsymbol{B}$ by the formula

$$\mathfrak{m}\boldsymbol{B}(\boldsymbol{r}) = \nabla\times\mu^{-1}\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\nabla\times\boldsymbol{B}(\boldsymbol{r}). \tag{193}$$

The exact relation between the spectral data of operators $\mathcal{M}$ and $\mathfrak{m}$ is as follows [28]. Suppose that ω^2 and $\boldsymbol{g}_{\omega^2}(\boldsymbol{r})$ are, respectively, a positive eigenvalue and an eigenmode of $\mathfrak{m}$, i.e.

$$\mathfrak{m}\boldsymbol{g}_{\omega^2}(\boldsymbol{r}) = \omega^2\boldsymbol{g}_{\omega^2}(\boldsymbol{r}) \qquad \nabla\cdot\boldsymbol{g}_{\omega^2}(\boldsymbol{r}) = 0 \qquad \omega \geqslant 0. \tag{194}$$

Then the vector fields

$$\boldsymbol{G}_{\pm\omega}(\boldsymbol{r}) = \begin{bmatrix} \pm\mathrm{i}\,[\omega\mu]^{-1}\,\nabla\times\boldsymbol{g}_{\omega^2}(\boldsymbol{r}) \\ \boldsymbol{g}_{\omega^2}(\boldsymbol{r}) \end{bmatrix} \tag{195}$$

are the eigenmodes of the operator $\mathcal{M}$, namely

$$\mathcal{M}\boldsymbol{G}_{\pm\omega}(\boldsymbol{r}) = \pm\omega\boldsymbol{G}_{\pm\omega}(\boldsymbol{r}). \tag{196}$$

We recall that $\mu = \text{constant}$ and that both three-dimensional components of $\boldsymbol{G}_{\pm\omega}$ are divergence-free. In fact, all the eigenmodes of the operator $\mathcal{M}$ are represented by the formula (195) with the aid of an appropriate eigenmode of the operator $\mathfrak{m}$ [28].

Now we describe the spectral theory in more detail. In the case of a $\mathbb{Z}^3$-periodic $\boldsymbol{\eta}^{(1)}(\boldsymbol{r})$ the Floquet–Bloch theory [2, 52, 66, 81]), describes the spectrum and the eigenmodes of the operator $\mathfrak{m}$ as follows. Under the conditions (187) and (188) $\mathfrak{m}$ is a well defined self-adjoint operator. To find the Floquet–Bloch transformation of this operator we introduce the following operator:

$$\widetilde{\mathfrak{m}}(\boldsymbol{k})\tilde{\boldsymbol{\Psi}}(\boldsymbol{r}) = \nabla \times \mu^{-1}\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\nabla \times \tilde{\boldsymbol{\Psi}}(\boldsymbol{r}) \qquad \nabla \cdot \tilde{\boldsymbol{\Psi}}(\boldsymbol{r}) = 0 \qquad \boldsymbol{r} \text{ in } [0, 1]^3 \tag{197}$$

where $\tilde{\boldsymbol{\Psi}}(\boldsymbol{r})$ satisfies the following cyclic Bloch boundary conditions:

$$\begin{aligned} &\tilde{\boldsymbol{\Psi}}\,(\boldsymbol{r}+\boldsymbol{m}) = \exp\,(\mathrm{i}\boldsymbol{m}\cdot\boldsymbol{k})\,\tilde{\boldsymbol{\Psi}}(\boldsymbol{r}) \\ &\nabla\tilde{\boldsymbol{\Psi}}\,(\boldsymbol{r}+\boldsymbol{m}) = \exp\,(\mathrm{i}\boldsymbol{m}\cdot\boldsymbol{k})\,\nabla\tilde{\boldsymbol{\Psi}}(\boldsymbol{r}) \qquad \boldsymbol{m} \text{ in } \mathbb{Z}^3. \end{aligned} \tag{198}$$

Hence, the dependence of the operator $\mathfrak{m}(\boldsymbol{k})$ on $\boldsymbol{k}$ comes through the cyclic boundary condition (198). This definition is consistent with the Floquet–Bloch transformation $\boldsymbol{v} \to \tilde{\boldsymbol{v}}$, which transforms square-integrable functions $\boldsymbol{\Psi}(\boldsymbol{r})$ into functions $\tilde{\boldsymbol{\Psi}}(\boldsymbol{r}, \boldsymbol{k})$ satisfying the Bloch boundary conditions and depending on the parameter $\boldsymbol{k}$ in the Brillouin zone:

$$\widetilde{[\mathfrak{m}\boldsymbol{\Psi}]}(\boldsymbol{r}, \boldsymbol{k}) = \widetilde{\mathfrak{m}}(\boldsymbol{k})\tilde{\boldsymbol{\Psi}}(\boldsymbol{r}, \boldsymbol{k}) \qquad \boldsymbol{r} \text{ in } [0, 1]^3 \qquad \boldsymbol{k} \text{ in } [-\pi, \pi]^3\,. \tag{199}$$

Another unitary equivalent representation of the Maxwell operator is based on the second Floquet–Bloch transform $\boldsymbol{v} \to \hat{\boldsymbol{v}}$:

$$\begin{aligned} &\widehat{\mathfrak{m}}(\boldsymbol{k})\hat{\boldsymbol{\Psi}}(\boldsymbol{r}) = \hat{\nabla}_{\boldsymbol{k}} \times \boldsymbol{\eta}^{(1)}(\boldsymbol{r})\hat{\nabla}_{\boldsymbol{k}} \times \hat{\boldsymbol{\Psi}}(\boldsymbol{r}) \qquad \hat{\nabla}_{\boldsymbol{k}} = \nabla_{\boldsymbol{r}} - \mathrm{i}\boldsymbol{k} \\ &\hat{\nabla}_{\boldsymbol{k}} \cdot \hat{\boldsymbol{\Psi}}(\boldsymbol{r}) = 0 \qquad \boldsymbol{r} \text{ in } [0, 1]^3 \end{aligned} \tag{200}$$

where $\hat{\nabla}_{\boldsymbol{k}}$ is defined by (171) and $\hat{\boldsymbol{\Psi}}(\boldsymbol{r})$ satisfy the $\mathbb{Z}^3$-periodic boundary conditions

$$\hat{\boldsymbol{\Psi}}\,(\boldsymbol{r}+\boldsymbol{m}) = \hat{\boldsymbol{\Psi}}(\boldsymbol{r}) \qquad \nabla\hat{\boldsymbol{\Psi}}\,(\boldsymbol{r}+\boldsymbol{m}) = \nabla\hat{\boldsymbol{\Psi}}(\boldsymbol{r}) \qquad \boldsymbol{m} \text{ in } \mathbb{Z}^3. \tag{201}$$

This representation is consistent with the transformation $\boldsymbol{v} \to \hat{\boldsymbol{v}}$:

$$\widehat{[\mathfrak{m}\boldsymbol{\Psi}]}(\boldsymbol{r}, \boldsymbol{k}) = \hat{\mathfrak{m}}(\boldsymbol{k})\hat{\boldsymbol{\Psi}}(\boldsymbol{r}, \boldsymbol{k}) \qquad \boldsymbol{r} \text{ in } [0, 1]^3 \quad \boldsymbol{k} \text{ in } [-\pi, \pi]^3\,. \tag{202}$$

Remark. The rigorous proof of the representation (199) is the same as the proof of the similar representation for the periodic Schrödinger operator in [66] (theorem XIII.98) provided that the resolvent $[\widehat{\mathfrak{m}}(\boldsymbol{k}) + I]^{-1}$ is compact for every $\boldsymbol{k}$. The compactness of the resolvent follows from the inequalities

$$\mu^{-1}C_{+}^{-1}\big(\hat{\nabla}_{\boldsymbol{k}} \times \hat{\boldsymbol{\Psi}}, \hat{\nabla}_{\boldsymbol{k}} \times \hat{\boldsymbol{\Psi}}\big) \leqslant \big(\hat{\boldsymbol{\Psi}}, \widehat{\mathfrak{m}}(\boldsymbol{k})\hat{\boldsymbol{\Psi}}\big) \leqslant \mu^{-1}C_{-}^{-1}\big(\hat{\nabla}_{\boldsymbol{k}} \times \hat{\boldsymbol{\Psi}}, \hat{\nabla}_{\boldsymbol{k}} \times \hat{\boldsymbol{\Psi}}\big) \tag{203}$$

and the compactness of the resolvent of the operator $\hat{\nabla}_{\boldsymbol{k}} \times \hat{\nabla}_{\boldsymbol{k}} \times (\cdot)$ which, in turn, is a consequence of the compactness of the resolvent $[-\Delta + I]^{-1}$ of the Laplace operator on the torus $[0, 1]^3$ (see [28, 29]).

The compactness of the resolvent $[\widehat{\mathfrak{m}}(\boldsymbol{k}) + I]^{-1}$ for every $\boldsymbol{k}$ implies the existence of a complete set of $\mathbb{Z}^3$-periodic eigenmodes $\hat{g}_n(\boldsymbol{r}, \boldsymbol{k})$ with the corresponding eigenvalues $\omega_n^2(\boldsymbol{k})$ for the operator $\widehat{\mathfrak{m}}(\boldsymbol{k})$, i.e.

$$\widehat{\mathfrak{m}}(\boldsymbol{k})\hat{g}_n(\boldsymbol{r}, \boldsymbol{k}) = \omega_n^2(\boldsymbol{k})\hat{g}_n(\boldsymbol{r}, \boldsymbol{k}) \qquad \nabla \cdot \hat{g}_n(\boldsymbol{r}, \boldsymbol{k}) = 0 \quad \boldsymbol{r} \text{ in } [0, 1]^3. \tag{204}$$

The eigenmodes $\tilde{g}_n(\boldsymbol{r}, \boldsymbol{k})$ of the periodic operator $\widetilde{\mathfrak{m}}(\boldsymbol{k})$ have the Bloch form

$$\tilde{g}_n(\boldsymbol{r}, \boldsymbol{k}) = \exp\{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}\}\,\hat{g}_n(\boldsymbol{r}, \boldsymbol{k}) \qquad \text{where} \quad \hat{g} \text{ is a } \mathbb{Z}^3\text{-periodic function in } \boldsymbol{r}. \tag{205}$$

The eigenvalues for $\widetilde{\mathfrak{m}}(\boldsymbol{k})$ are the same as for $\hat{\mathfrak{m}}(\boldsymbol{k})$. Clearly, we obtain by complex conjugation

$$\tilde{g}_n(\boldsymbol{r}, \boldsymbol{k}) = \tilde{g}_n^*(\boldsymbol{r}, -\boldsymbol{k}) \qquad \hat{g}_n(\boldsymbol{r}, \boldsymbol{k}) = \hat{g}_n^*(\boldsymbol{r}, -\boldsymbol{k}) \tag{206}$$

$$\omega_n^2(\boldsymbol{k}) = \omega_n^2(-\boldsymbol{k}). \tag{207}$$

Summarizing, the set of all the eigenvalues and eigenmodes of the operator $\widetilde{\mathfrak{m}}$ can be parametrized by two indices $n = 1, 2, \ldots$, called the *zone number*, and the continuous $\boldsymbol{k}$, called the *quasimomentum*, from the *Brillouin zone* $[-\pi, \pi]^3$. The eigenvalue and the eigenmode of $\mathfrak{m}$ associated with a given n and $\boldsymbol{k}$ are, respectively, denoted by $\omega_n^2(\boldsymbol{k})$ (it is the square of the angular frequency) and $\tilde{g}_n(\boldsymbol{r}, \boldsymbol{k})$ of the Bloch form (205). They satisfy the equation

$$\widetilde{\mathfrak{m}}(\boldsymbol{k})\tilde{g}_n(\boldsymbol{r}, \boldsymbol{k}) = \omega_n^2(\boldsymbol{k})\tilde{g}_n(\boldsymbol{r}, \boldsymbol{k}) \qquad \nabla \cdot \tilde{g}_n(\boldsymbol{r}, \boldsymbol{k}) = 0 \quad \boldsymbol{r} \text{ in } [0, 1]^3 \tag{208}$$

where

$$\begin{aligned} &0 \leqslant \omega_1^2(\boldsymbol{k}) \leqslant \omega_2^2(\boldsymbol{k}) \leqslant \cdots \\ &\tilde{g}_n(\boldsymbol{r} + \boldsymbol{m}, \boldsymbol{k}) = \exp\{\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{m}\}\, \tilde{g}_n(\boldsymbol{r}, \boldsymbol{k}) \\ &\nabla\tilde{g}_n(\boldsymbol{r} + \boldsymbol{m}, \boldsymbol{k}) = \exp\{\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{m}\}\, \nabla\tilde{g}_n(\boldsymbol{r}, \boldsymbol{k}) \qquad \boldsymbol{m} \text{ in } \mathbb{Z}^3. \end{aligned} \tag{209}$$

Remark. As follows from the inequalities (203) $\omega_n(\boldsymbol{k}) = 0$ if the corresponding eigenmodes are zeros of the operator $\hat{\nabla}_{\boldsymbol{k}} \times \hat{\nabla}_{\boldsymbol{k}} \times (\cdot)$. Hence, $\omega_n(\boldsymbol{k}) = 0$ only when $\boldsymbol{k} = \boldsymbol{0}$ and the corresponding eigenmodes are constant fields.

Note that the parametrization by $\boldsymbol{k}$, which is possible due to the periodicity of the operator, reduces the original eigenvalue problem in the space $\mathbb{R}^3$ to the problem in the primitive cell $[0, 1]^3$. Note also that the representations $\widetilde{\mathfrak{m}}$ and $\widehat{\mathfrak{m}}$ related to the two Floquet–Bloch transforms (163) are unitarily equivalent and choosing one or other is a matter of convenience. Evidently, in the case of the operator $\widetilde{\mathfrak{m}}(\boldsymbol{k})$ its differential expression does not depend on $\boldsymbol{k}$ and the dependence on $\boldsymbol{k}$ comes through the cyclic boundary conditions (198). In the case of the operator $\widehat{\mathfrak{m}}(\boldsymbol{k})$, in contrast, the differential expression for it depends explicitly on $\boldsymbol{k}$ whereas the domain of $\widehat{\mathfrak{m}}(\boldsymbol{k})$ is fixed: it is the set of periodic functions (see the periodic boundary conditions (201)).

Using the decomposition (176) where $\tilde{g}_n$ are the described eigenmodes we obtain for an arbitrary square-integrable divergence-free function $\boldsymbol{\Psi}(\boldsymbol{r})$ the following *Floquet–Bloch expansions*:

$$\begin{aligned} \hat{\boldsymbol{\Psi}}(\boldsymbol{r}, \boldsymbol{k}) &= \sum_{n\geqslant 1} \hat{\Psi}_n(\boldsymbol{k})\hat{g}_n(\boldsymbol{r}, \boldsymbol{k}) = \sum_{n\geqslant 1} \hat{\boldsymbol{\Psi}}_n(\boldsymbol{k}, \boldsymbol{r}) \\ \tilde{\boldsymbol{\Psi}}(\boldsymbol{r}, \boldsymbol{k}) &= \sum_{n\geqslant 1} \tilde{\Psi}_n(\boldsymbol{k})\tilde{g}_n(\boldsymbol{r}, \boldsymbol{k}) = \sum_{n\geqslant 1} \tilde{\boldsymbol{\Psi}}_n(\boldsymbol{k}, \boldsymbol{r}). \end{aligned} \tag{210}$$

The relation between the eigendata (208) and (209) for the operator $\mathfrak{m}$ together with the general identities (194)–(196) readily yield

$$\mathcal{M}\tilde{\boldsymbol{G}}_{\pm 1,n}(\boldsymbol{r}, \boldsymbol{k}) = \pm\omega_n(\boldsymbol{k})\tilde{\boldsymbol{G}}_{\pm 1,n}(\boldsymbol{r}, \boldsymbol{k}) \qquad \nabla \cdot \tilde{\boldsymbol{G}}_{\pm 1,n}(\boldsymbol{r}, \boldsymbol{k}) = 0 \qquad \boldsymbol{r} \text{ in } [0, 1]^3 \tag{211}$$

$$\begin{aligned} &\tilde{\boldsymbol{G}}_{\pm 1,n}(\boldsymbol{r} + \boldsymbol{m}, \boldsymbol{k}) = \exp\{\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{m}\}\tilde{\boldsymbol{G}}_{\pm 1,n}(\boldsymbol{r}, \boldsymbol{k}) \\ &\nabla\tilde{\boldsymbol{G}}_{\pm 1,n}(\boldsymbol{r} + \boldsymbol{m}, \boldsymbol{k}) = \exp\{\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{m}\}\nabla\tilde{\boldsymbol{G}}_{\pm 1,n}(\boldsymbol{r}, \boldsymbol{k}) \qquad \boldsymbol{m} \text{ in } \mathbb{Z}^3. \end{aligned} \tag{212}$$

Note that $\omega_n(\boldsymbol{k})$ and $\tilde{g}_n(\boldsymbol{r}, \boldsymbol{k})$ are globally Lipschitz and, in addition to that, analytic in $\boldsymbol{k}$ almost everywhere except for band-crossing points at which the multiplicity of the related eigenfrequencies is two or more. At the band-crossing points all the functions of interest become analytic in appropriate polar coordinates (see section 5.4). Since the index of the eigenmodes $\tilde{\boldsymbol{G}}_{\pm 1,n}(\boldsymbol{r},\boldsymbol{k})$ is always a pair $\bar{n}=(\zeta,n)$ with $\zeta=\pm 1$, we abbreviate the notation by introducing

$$\bar{n}=(\zeta,n) \qquad \text{where} \quad \zeta=\pm 1 \quad n=1,2,\ldots \tag{213}$$

and setting

$$\omega_{\bar{n}}(\boldsymbol{k})=\zeta\omega_n(\boldsymbol{k}) \qquad \text{for} \quad \bar{n}=(\zeta,n). \tag{214}$$

Hence,

$$\mathcal{M}\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k})=\omega_{\bar{n}}(\boldsymbol{k})\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k}) \qquad \nabla\cdot\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k})=0 \qquad \boldsymbol{r}\text{ in }[0,1]^3 \tag{215}$$

$$\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r}+\boldsymbol{m},\boldsymbol{k})=\exp\{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{m}\}\,\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k}) \qquad \boldsymbol{m}\text{ in }\mathbb{Z}^3. \tag{216}$$

In view of (195) the vector fields $\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k})$ have the following $\boldsymbol{D}$ and $\boldsymbol{B}$ components:

$$\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k})=\begin{bmatrix}\tilde{\boldsymbol{D}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k})\\ \tilde{\boldsymbol{B}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k})\end{bmatrix}=\begin{bmatrix}\mathrm{i}\zeta\,[\omega_{\bar{n}}(\boldsymbol{k})\mu]^{-1}\,\nabla\times\tilde{\boldsymbol{g}}_n(\boldsymbol{r},\boldsymbol{k})\\ \tilde{\boldsymbol{g}}_n(\boldsymbol{r},\boldsymbol{k})\end{bmatrix}. \tag{217}$$

The eigenfunctions $\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k})$ with different $\bar{n}$ are orthogonal in the Hilbert space $\mathcal{H}$ of divergence-free vector fields with the scalar product defined by (174) where $\sigma(\boldsymbol{r})$ is defined in (191) and they form an orthogonal basis in this space for every $\boldsymbol{k}$. Using (210) and (177) we obtain the following representation for an arbitrary vector field $\boldsymbol{U}=\left[\begin{smallmatrix}\boldsymbol{D}\\ \boldsymbol{B}\end{smallmatrix}\right]$ with $\nabla\cdot\boldsymbol{D}=\boldsymbol{0}$, $\nabla\cdot\boldsymbol{B}=\boldsymbol{0}$ and finite energy:

$$\boldsymbol{U}(\boldsymbol{r})=\frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^3}\tilde{\boldsymbol{U}}(\boldsymbol{r},\boldsymbol{k})\,\mathrm{d}\boldsymbol{k}=\frac{1}{(2\pi)^d}\sum_{\bar{n}}\int_{[-\pi,\pi]^d}\tilde{U}_{\bar{n}}(\boldsymbol{k})\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k})\,\mathrm{d}\boldsymbol{k} \tag{218}$$

where

$$\begin{aligned}&\tilde{\boldsymbol{U}}(\boldsymbol{r},\boldsymbol{k})=\sum_{\bar{n}}\tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k}) \qquad \tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k})=\tilde{\Pi}_{\bar{n}}(\boldsymbol{k})\tilde{\boldsymbol{U}}(\boldsymbol{r},\boldsymbol{k})=\tilde{U}_{\bar{n}}(\boldsymbol{k})\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k})\\ &\tilde{U}_{\bar{n}}(\boldsymbol{k})=\left(\tilde{\boldsymbol{U}}(\cdot,\boldsymbol{k}),\tilde{\boldsymbol{G}}_{\bar{n}}(\cdot,\boldsymbol{k})\right)_{\mathcal{H}}\left(\left(\tilde{\boldsymbol{G}}_{\bar{n}}(\cdot,\boldsymbol{k}),\tilde{\boldsymbol{G}}_{\bar{n}}(\cdot,\boldsymbol{k})\right)_{\mathcal{H}}\right)^{-1/2}\end{aligned} \tag{219}$$

and $(\,,\,)_{\mathcal{H}}$ is defined by (174); when $d=3$ $\tilde{\boldsymbol{G}}_{\bar{n}}$ are defined by (217).

Remark. The boundary condition (212) still holds after adding 2π to k_j. This implies that $\tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k})$ are $2\pi\mathbb{Z}^3$-periodic functions of $\boldsymbol{k}$. They are uniformly Lipschitz continuous and they are analytic in $\boldsymbol{k}$ on a dense connected set. The singular points if any for a generic operator are conical points which can be regularized in polar coordinates (see section 5.4).

Remark. The components $\tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k})$ form the Floquet–Bloch transform of the field $\tilde{\boldsymbol{U}}(\boldsymbol{r})$. Evidently, the Floquet–Bloch transform for a periodic medium plays the role which the Fourier transform plays in the case of a homogeneous medium. We assume that the components $\boldsymbol{U}_n(\boldsymbol{k})$ are sufficiently smooth in $\boldsymbol{k}$ on the torus $[-\pi,\pi]^3$ (have only admissible singularities at band-crossing points) and that they decay sufficiently fast as $n\to\infty$. These conditions are analogous to the conditions of smoothness and decay of the Fourier transform of a wavepacket which are normally imposed to provide the basic properties of the wavepacket.

5.3. *Group velocity of wavepackets in periodic media*

Recall that the group velocity $\boldsymbol{v}_{\mathrm{g}}(\boldsymbol{k}^*)$ of a wavepacket localized about a point $\boldsymbol{k}^*$ is defined qualitatively as the velocity at which the wavepacket moves as a whole. In homogeneous media with the dispersion relation $\omega(\boldsymbol{k})$ it is given by $\boldsymbol{v}_{\mathrm{g}} = \nabla\omega(\boldsymbol{k}^*)$ [78], section 11.4. In particular, the group velocity of the $(\bar{n}', \boldsymbol{k}')$-mode of the linear wave

$$\tilde{\boldsymbol{V}}^{(0)}_{\bar{n}'}(\boldsymbol{k}')\exp\left\{\mathrm{i}\omega_{\bar{n}'}(\boldsymbol{k}')\frac{\tau}{\varrho}\right\}$$

is $\nabla\omega_{\bar{n}'}(\boldsymbol{k}')$. The group velocity can be alternatively defined as the amplitude, energy or wavenumber propagation velocity, and can be found in the case of homogeneous media by the stationary phase method ([78], section 11.4, [33], section 1.6a). The same definition is used in the case of periodic media as well (see [2, 81], section 6.7)

$$\boldsymbol{v}_{\mathrm{g}} = \nabla\omega_n(\boldsymbol{k}^*) \tag{220}$$

where $\boldsymbol{k}$ is the quasimomentum, and $\omega_n(\boldsymbol{k})$ is the dispersion relation for the nth band. The justification of the definition is similar to the case of homogeneous media. It is based on the inverse Floquet–Bloch transform in place of the inverse Fourier transform. Let us discuss it for completeness. Consider a wavepacket

$$\boldsymbol{U}_n(\boldsymbol{r}, t) = \frac{1}{(2\pi)^d}\int \tilde{\boldsymbol{U}}_n(\boldsymbol{r}, \boldsymbol{k}, \varrho t)\exp[-\mathrm{i}\omega_n(\boldsymbol{k})t]\,\mathrm{d}\boldsymbol{k}$$

where $\tilde{\boldsymbol{U}}_n(\boldsymbol{r}, \boldsymbol{k}, \varrho t)$ is non-zero only near a point $\boldsymbol{k}_*$. According to the formula for the inverse Floquet–Bloch transformation we obtain

$$\boldsymbol{U}_n(\boldsymbol{r}+\boldsymbol{m}, t) = \frac{1}{(2\pi)^d}\int \tilde{\boldsymbol{U}}_n(\boldsymbol{r}, \boldsymbol{k}, \varrho t)\exp[-\mathrm{i}\omega_n(\boldsymbol{k})t + (\mathrm{i}\boldsymbol{m}\cdot\boldsymbol{k})]\,\mathrm{d}\boldsymbol{k}. \tag{221}$$

For $\boldsymbol{m} = t\nabla\omega_n\,(\boldsymbol{k}_*)$ the phase $[-\mathrm{i}\omega_n(\boldsymbol{k})t + (\mathrm{i}\boldsymbol{m}\cdot\boldsymbol{k})]$ has a critical point at $\boldsymbol{k} = \boldsymbol{k}_*$, which determines the leading term of the asymptotics of the integral as $t = \tau/\varrho \to \infty$ as $\varrho \to 0$. This term is of the order of $\varrho^{d/2}$ in the non-degenerate case. Hence, the wavepacket is spatially localized near a point $t\nabla\omega_n\,(\boldsymbol{k}_*)$ where $\boldsymbol{r}+\boldsymbol{m} \sim \boldsymbol{m}$ since $\boldsymbol{r}$ is fixed. This justifies the expression $\nabla\omega_n\,(\boldsymbol{k}_*)$ as a group velocity $\boldsymbol{v}$ of the wavepacket at $\boldsymbol{k}_*$.

Note that this justification makes sense if ϱ is small and, hence, for large t, and as the wavepacket passes many period cells. One can see here that the discreteness of $\boldsymbol{m}$ is not essential.

A similar analysis of the wavepacket

$$\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{k}, \tau)\exp\left\{-\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})\frac{\tau}{\varrho}\right\}$$

where $\tilde{\boldsymbol{W}}_{\bar{n}}(\boldsymbol{k}, \tau)$ is the nonlinear response given by (34), produces the following representation for its group velocity:

$$\boldsymbol{v}_{\mathrm{gr}} = \nabla_{\boldsymbol{k}}\left(\omega_{\bar{n}}(\boldsymbol{k}) - \phi_{\bar{n}}(\boldsymbol{k}, \boldsymbol{k}')\right) = \nabla\omega_{\bar{n}''}(\boldsymbol{k} - \boldsymbol{k}'_*). \tag{222}$$

Evidently, the group velocity $\boldsymbol{v}_{\mathrm{gr}} = \nabla\omega_{\bar{n}''}(\boldsymbol{k} - \boldsymbol{k}'_*)$ *of the nonlinear response* $\tilde{W}_{\bar{n}}(\boldsymbol{k}, \tau)$ *of the* $(\bar{n}, \boldsymbol{k})$*-mode differs from the group velocity* $\nabla\omega_{\bar{n}}(\boldsymbol{k})$ *of the* $(\bar{n}, \boldsymbol{k})$*-mode as a linear wave.*

The dispersion relation $\omega(\boldsymbol{k})$ has singularities at band-crossing points $\boldsymbol{k}_\otimes$ for which $\omega_n(\boldsymbol{k}_\otimes) = \omega_{n-1}(\boldsymbol{k}_\otimes)$. It is shown in section 5.4 that in the two-dimensional case, $d = 2$, a generic dispersion relation $\omega(\boldsymbol{k})$, if rewritten in the polar coordinates

$$k_1 = k_{\otimes 1} + \eta\cos\theta \qquad k_2 = k_{\otimes 2} + \eta\sin\theta \tag{223}$$

becomes a smooth function of η, θ. If a function $f(\boldsymbol{k})$ is smooth at $\boldsymbol{k}_\otimes$ its gradient $\nabla f(\boldsymbol{k}_\otimes)$ in polar coordinates is

$$\nabla f(\boldsymbol{k}_\otimes) = \left(\cos\theta\,\partial_\eta f - \sin\theta\,\partial_\theta\partial_\eta f, \sin\theta\,\partial_\eta f + \cos\theta\,\partial_\theta\partial_\eta f\right)\big|_{\eta=0}. \tag{224}$$

This formula can be extended to functions f which are not differentiable in Cartesian coordinates, but are twice differentiable in polar coordinates, as the dispersion relations are at band-crossing points. Note that in the latter case the gradient $\nabla f(\boldsymbol{k}_\otimes)$ depends on the polar angle θ, thus producing a one-parameter family of vectors. The simplest example of such a function is

$$f = \sqrt{(k_1 - k_{*1})^2 + (k_2 - k_{*2})^2} = \eta.$$

A rather laborious analysis of the integral (221) with the amplitude $\tilde{\boldsymbol{U}}_n(\boldsymbol{r}, \boldsymbol{k}, \varrho t)$, which is centred near a band-crossing point $\boldsymbol{k}_\otimes$, shows that the maximal order of contribution occurs under the same condition $\boldsymbol{m} = t\nabla\omega_n(\boldsymbol{k}_\otimes)$. In the latter case, the magnitude of the integral contribution is of the order of $\mathrm{O}(\varrho^{4/3})$ for $d = 2$ which is different from the factor $\mathrm{O}(\varrho^{d/2})$ for a simple non-degenerate critical point of the dispersion relation. For a band-crossing point $\boldsymbol{k}_\otimes$ the gradient $\nabla\omega_n(\boldsymbol{k}_\otimes)$ is evaluated with the help of the formula (224). One can see from the formula (224) that there is a family of group velocities parametrized by the angle θ. This observation suggests that a band-crossing point $\boldsymbol{k}_\otimes$ is similar to a point scatterer which scatters a wavepacket in different directions with different group velocities.

In the case $d = 3$ band-crossing points $\boldsymbol{k}_\otimes$ form smooth curves (see section 5.4). The function $\omega_n(\boldsymbol{k})$ is differentiable in the direction $\boldsymbol{\xi}$ tangent to the curve, and the tangential component $\partial_{\boldsymbol{\xi}}\omega_n(\boldsymbol{k}_\otimes)$ is well defined. To evaluate derivatives $\omega_n(\boldsymbol{k}_\otimes)$ in directions orthogonal to the curve one has to introduce the polar coordinates in the direction orthogonal to the $\boldsymbol{\xi}$ plane, and, then, to use (224). Thus, the family of vectors $\nabla\omega_n(\boldsymbol{k}_\otimes)$ depending on one parameter θ describes all possible group velocities. As before, $\boldsymbol{m} = t\nabla\omega_n(\boldsymbol{k}_\otimes)$ produces the maximal order $\mathrm{O}(\varrho^{11/6})$ of (221).

5.4. Analyticity and singularity of dispersion relations

The analytical properties of the eigenvalues $\omega_n(\boldsymbol{k})$ and the Bloch eigenmodes $\hat{\boldsymbol{g}}_n(\boldsymbol{r}, \boldsymbol{k})$ for the Maxwell operator $\mathcal{M}(\boldsymbol{k}) = \widehat{\mathcal{M}}(\boldsymbol{k})$ are very important for our analysis of the oscillatory integrals. It must be noted that the issue of differentiability of eigenvalues is far from trivial [49, sections II.5 and II.7], especially in the case of several parameters. All the difficulties are related to multiple eigenvalues. The multiplicity of eigenvalues of differential operators and their dependence on parameters are subjects of extensive studies (see, for instance, [48, 49, 74, 76] and [4, appendix 10, p 425], for detailed discussions of the dependence of eigenvalues on parameters). It turns out, that in our problems for the space dimensions $d = 1, 2, 3$ in a generic situation it is sufficient to consider only the multiplicity two.

Recall first, that $\boldsymbol{k} = (k_1, \ldots, k_d)$. We assume that the eigenvalues are naturally ordered

$$\omega_1(\boldsymbol{k}) \leqslant \omega_2(\boldsymbol{k}) \leqslant \cdots. \tag{225}$$

If for a given $\boldsymbol{k}_0$ the eigenvalue $\omega_n(\boldsymbol{k}_0)$ is simple, i.e. of multiplicity one, then both $\omega_n(\boldsymbol{k})$ and $\hat{\boldsymbol{g}}_n(\boldsymbol{r}, \boldsymbol{k})$ (as well as $\tilde{\boldsymbol{g}}_n(\boldsymbol{r}, \boldsymbol{k})$) depend analytically on $\boldsymbol{k}$ in a vicinity of the point $\boldsymbol{k}_0$. In the case when $\boldsymbol{k}_0$ is not a simple point the situation becomes more intricate and depends on the dimension of $\boldsymbol{k}$.

If a point $\boldsymbol{k}$ is not simple we call it a *band-crossing point*. For a band-crossing point $\boldsymbol{k}_\otimes$ two eigenvalues from different bands for the same value of quasimomentum coincide, that is there exists at least one n such that $\omega_n(\boldsymbol{k}_\otimes) = \omega_{n+1}(\boldsymbol{k}_\otimes)$.

Let us pick a band-crossing point $\boldsymbol{k}_\otimes$ and consider the related group of the equal eigenfrequencies

$$\omega_\otimes = \omega_n(\boldsymbol{k}_\otimes) = \cdots = \omega_{n+s-1}(\boldsymbol{k}_\otimes)$$

where s is the multiplicity of $\omega_\otimes$. Following [49] we call this the $\omega_\otimes$-group. Note that s is finite since the resolvent of $\mathcal{M}(\boldsymbol{k})$ is compact. We need to study the analytic properties of the eigenvalues and eigenmodes as functions $\boldsymbol{k}$ in a small vicinity $\Omega(\boldsymbol{k}_\otimes)$ of the band-crossing point $\boldsymbol{k}_\otimes$. We use the well known formula for the orthogonal projector on the subspace spanned by eigenvectors related to the $\omega_\otimes$-group [49, section 4, (3.11)],

$$\Pi_{\omega_\otimes}(\boldsymbol{k}) = -\frac{1}{2\pi\mathrm{i}} \int_{|\zeta-\omega_\otimes|=\delta} [\mathcal{M}(\boldsymbol{k}) - \zeta I]^{-1}\,\mathrm{d}\zeta. \tag{226}$$

This projector acts in the Hilbert space $\mathcal{H}$ with the scalar product defined by (174) where $\sigma(\boldsymbol{r})$ is defined in (191). In formula (226) δ is chosen small enough to isolate all the eigenvalues of the $\omega_\otimes$-group from the rest of the spectrum for all values $\boldsymbol{k}$ from the small vicinity $\Omega(\boldsymbol{k}_\otimes)$. In particular, formula (226) implies readily the analytical dependence of the projection $\Pi_{\omega_\otimes}(\boldsymbol{k})$ on $\boldsymbol{k}$ in $\Omega(\boldsymbol{k}_\otimes)$.

Using (226) one can reduce the analysis of the infinite-dimensional operator $\mathcal{M}(\boldsymbol{k})$ to the analysis of an $s \times s$ matrix $M(\boldsymbol{k})$ where s is the multiplicity of $\omega_\otimes$ [49, section 7.3]. This reduction is done as follows. First one constructs a unitary operator $U(\boldsymbol{k})$ which depends on $\boldsymbol{k}$ analytically in $\Omega(\boldsymbol{k}_\otimes)$, and such that

$$\Pi_{\omega_\otimes}(\boldsymbol{k}) = U(\boldsymbol{k})\Pi_{\omega_\otimes}(\boldsymbol{k}_{\omega_\otimes}). \tag{227}$$

Then we introduce the invariant subspace $E_{\omega_\otimes}(\boldsymbol{k})$ of the $\omega_\otimes$-group:

$$E_{\omega_\otimes}(\boldsymbol{k}) = \Pi_{\omega_\otimes}(\boldsymbol{k})\mathcal{H} \tag{228}$$

and define

$$\bar{M}(\boldsymbol{k}) = \text{restriction of } U^{-1}(\boldsymbol{k})\Pi_{\omega_\otimes}(\boldsymbol{k})\mathcal{M}(\boldsymbol{k})U(\boldsymbol{k}) \text{ to } E_{\omega_\otimes}(\boldsymbol{k}_{\omega_\otimes}). \tag{229}$$

Finally, the matrix $M(\boldsymbol{k})$ is obtain from the linear operator $\bar{M}(\boldsymbol{k})$ by choosing any orthonormal basis in the space $E_{\omega_\otimes}(\boldsymbol{k}_{\omega_\otimes})$. Observe, that the $s \times s$ matrix $M(\boldsymbol{k})$ (a) has the same eigenvalues as $\omega_\otimes$-group of the original infinitely dimensional operator $\mathcal{M}(\boldsymbol{k})$ and (b) depends on $\boldsymbol{k}$ analytically in $\Omega(\boldsymbol{k}_\otimes)$.

Since we are interested just in the analyticity of the eigenvalues and eigenmodes we may deal with the following normalized modification of $M(\boldsymbol{k})$:

$$M_1(\boldsymbol{k}) = M(\boldsymbol{k}) - \frac{1}{s}\,\mathrm{Trace}\,\{M(\boldsymbol{k})\} \tag{230}$$

for which

$$M_1(\boldsymbol{k}_{\omega_\otimes}) = 0 \qquad \mathrm{Trace}\,\{M_1(\boldsymbol{k})\} = 0. \tag{231}$$

Let us look at the $s \times s$ matrix $M_1(\boldsymbol{k})$ and its entries as functions of $\boldsymbol{k}$. Note first of all that since $M_1(\boldsymbol{k})$ is Hermitian and has zero trace the matrix has $S = s(s+1)/2 - 1$ entries which depend on the operator $\mathcal{M}(\boldsymbol{k})$ and can be chosen independently for a general operator. If the spectrum of $M_1(\boldsymbol{k}_{\omega_\otimes})$ consists of exactly one point (that is zero), the zero eigenvalue has multiplicity s, and, consequently, $M_1(\boldsymbol{k}_{\omega_\otimes}) = 0$ and, hence, all the entries of the matrix at $\boldsymbol{k} = \boldsymbol{k}_{\omega_\otimes}$ are zero. Vanishing of the entries analytically depending on $\boldsymbol{k}$ produces $s \times (s+1)/2$ equations on the variables $\boldsymbol{k}$. One of these equation is satisfied since $M_1(\boldsymbol{k})$ has zero trace. If the number $s \times (s+1)/2 - 1$ of non-trivial equations is greater than the number d of parameters, in a generic situation the equations should not have a solution at all, so for a generic operator which depends on d parameters $\boldsymbol{k}$ the multiplicity s does not occur when $s \times (s+1)/2 - 1 > d$. We consider only generic cases when $s \times (s+1)/2 - 1 \leqslant d$. *Observe, that for* $d = 1$ *the highest typical multiplicity* s *is* 1*, that is multiple points are absent and for* $d = 2, 3$ *and even* $d = 4$ *the highest typical multiplicity* s *is 2! Hence, remarkably, in the generic situations for the dimensions* $d = 2, 3, 4$ *we need to study only the matrices* $M(\boldsymbol{k})$ *with size* 2×2.

Remark. The general relation between the number of parameters and the multiplicity of the eigenvalues is given in [4, p 425]. This phenomenon is described as a repelling of eigenvalues. Multiplicity of eigenvalues of generic differential operators is studied, for example in [48, 74, 76].

Remark. In the one-dimensional case $d = 1$ it can be shown (see [72], section 17.1), that for any operator (which may be non-generic) and any band-crossing point $\boldsymbol{k}_{\otimes}$ one can renumerate the eigenvalues (destroying the order (225)) so that the eigenvalues will be analytic in a small vicinity of $\boldsymbol{k}_{\otimes}$.

From now on we consider only generic situations.

One-dimensional case $d = 1$. In this case for generic operators band-crossing points are absent. A special band-crossing point $\boldsymbol{k}_0 = 0$ corresponding to $\omega = 0$ which corresponds to constant eigenfunctions persists (it relates to the symmetry $\omega \to -\omega$) and has to be considered separately; we do not discuss it here since we consider carriers with high frequencies.

Two-dimensional case $d = 2$. In the generic case $s = 2$ and at a given band-crossing point $\boldsymbol{k}_{\omega_{\otimes}}$ there are exactly two coinciding $\omega_n(\boldsymbol{k}_{\omega_{\otimes}}) = \omega_{n+1}(\boldsymbol{k}_{\omega_{\otimes}})$, and

$$M(\boldsymbol{k}) = \begin{bmatrix} z_1 & z_2 \\ z_2 & -z_1 \end{bmatrix} + \begin{bmatrix} \omega_0 & 0 \\ 0 & \omega_0 \end{bmatrix} \tag{232}$$

where z_1, z_2 and ω_0 are real analytic in $\boldsymbol{k}$. We study now the dependence of eigenvectors and eigenvalues on $\boldsymbol{k}$. Since ω_0 is analytic in $\boldsymbol{k}$ we set $\omega_0 = 0$ for simplicity without impacting on the analyticity of the eigenvalues and the eigenvectors. Then the eigenvalues $\omega_{\pm}$ and the eigenvectors $G_{\pm}$ of $M(\boldsymbol{k})$ become

$$\omega_{\pm} = \pm\sqrt{z_1^2 + z_2^2} \tag{233}$$

$$G_{\pm} = \left(z_2, \pm\sqrt{z_1^2 + z_2^2} - z_1\right) = (z_2, \omega_{\pm} - z_1). \tag{234}$$

In addition to that, evidently,

$$z_1(\mathbf{0}) = 0 \qquad z_2(\mathbf{0}) = 0. \tag{235}$$

In a generic case the Jacobian matrix $\frac{\mathrm{d}z}{\mathrm{d}\boldsymbol{k}}$ at $\boldsymbol{k}_{\omega_{\otimes}}$ has rank two and, hence,

$$\det \begin{bmatrix} \dfrac{\partial z_1}{\partial k_1} & \dfrac{\partial z_1}{\partial k_2} \\ \dfrac{\partial z_2}{\partial k_1} & \dfrac{\partial z_2}{\partial k_2} \end{bmatrix} \neq 0. \tag{236}$$

In view of (236) we can make a non-degenerate analytic change of variables (k_1, k_2) to (z_1, z_2). So it suffices to study the analytic properties of $M(\boldsymbol{k})$ defined by (232) as a function of z_1 and

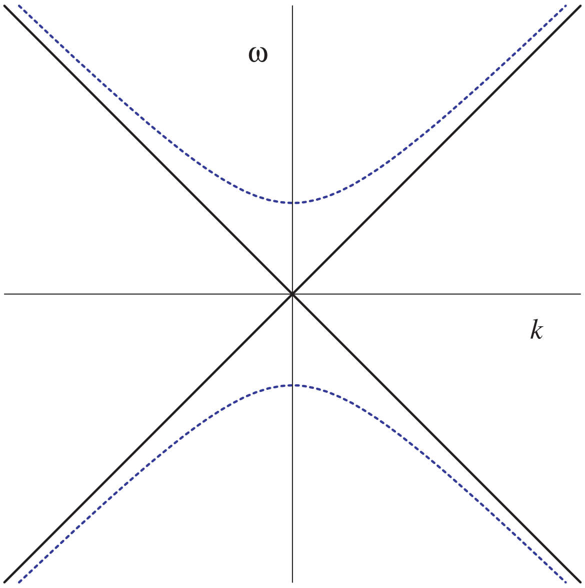

Figure 2. In the one-dimensional case, $d = 1$, the two eigenvalue branches intersecting as $\omega_{12}(k) = \pm|k|$ are shown as a full line. They separate under a generic small perturbation of related operators into two curves similar to those shown by the broken curve. This fact indicates that the alternative to $\pm|k|$ analytic parametrization $\pm k$ is not robust.

z_2. Note that when (236) holds the system (235) with perturbed $z_1(\boldsymbol{k}), z_2(\boldsymbol{k})$ again has a solution, so a band-crossing point is robust.

It is convenient to introduce the polar coordinates ρ, θ in the (z_1, z_2)-plane. In these coordinates the eigenvalues $\omega_\pm$ and eigenvectors $G_\pm$ of $M(\boldsymbol{k})$ after normalization take the form

$$\omega_\pm = \pm\rho \qquad G_+(\theta) = \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{bmatrix} \qquad G_-(\theta) = \begin{bmatrix} \sin(\theta/2) \\ -\cos(\theta/2) \end{bmatrix}. \tag{237}$$

Evidently, the eigenvalues and the eigenvectors are analytic functions of ϱ and θ, respectively. Formula (237) shows that vectors $G_+(\theta), G_-(\theta)$ make one full turn in the plane when θ varies over $[0, 4\pi]$ and therefore cannot be parametrized by a one-valued continuous 2π periodic function of the polar angle. We also compute the projectors on $G_\pm(\theta)$:

$$\Pi_+(\theta) = \begin{bmatrix} \cos^2(\theta/2) & \cos(\theta/2)\sin(\theta/2) \\ \cos(\theta/2)\sin(\theta/2) & \sin^2(\theta/2) \end{bmatrix} = \frac{1}{2}\left\{ I + \begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix} \right\}$$
$$\Pi_-(\theta) = \begin{bmatrix} \sin^2(\theta/2) & -\cos(\theta/2)\sin(\theta/2) \\ -\cos(\theta/2)\sin(\theta/2) & \cos^2(\theta/2) \end{bmatrix} = \frac{1}{2}\left\{ I - \begin{bmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{bmatrix} \right\} \tag{238}$$

which are one-valued 2π periodic analytic functions of the polar angle. To refer to the described properties of the band-crossing points $k_\otimes$ we sometimes call them *conical*.

Remark. The equalities $\omega_\pm = \pm\rho$ imply $\omega_- \leqslant \omega_+$ in compliance with (225). The eigenfrequencies ω_+ and ω_- can be viewed as two branches of an analytic function which have a common point (band-crossing point) $\boldsymbol{k}_\otimes$. Note that for any curve in the $\boldsymbol{k}$-plane not

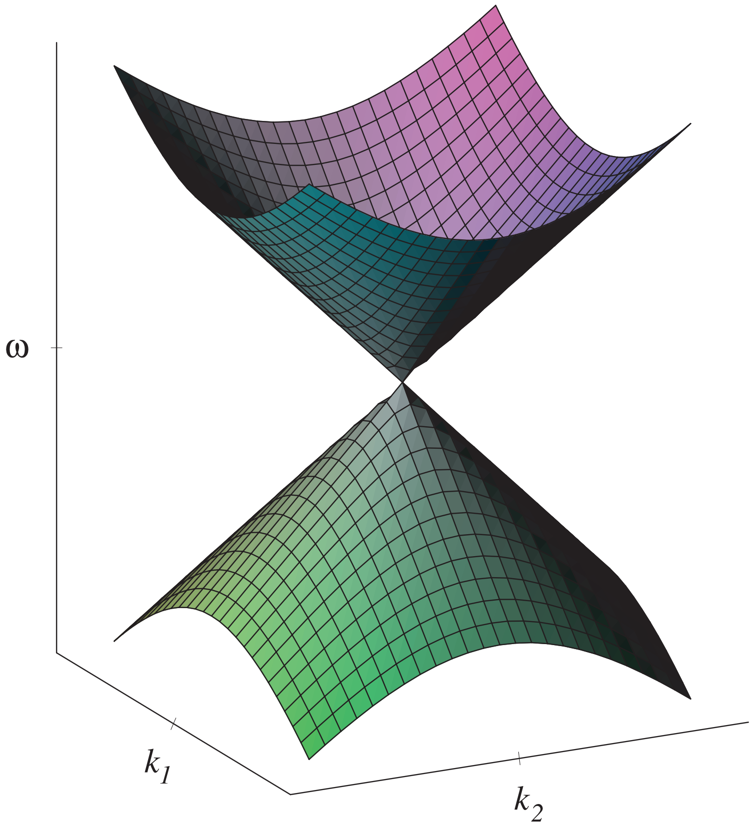

Figure 3. In the two-dimensional case, $d = 2$, two branches of eigenvalues at a band-crossing point typically form a conical surface as shown in the figure. Remarkably, the intersection is a point, and not a curve! Another remarkable phenomenon is that the conical intersection for two eigenvalue surfaces is robust and it continues to hold under small self-adjoint perturbations of the related operators.

passing through $\boldsymbol{k}_\otimes$ the function $\omega_+(\boldsymbol{k})$ is analytic. However, if a curve passes through the band-crossing point $\boldsymbol{k}_\otimes$ one can obtain an analytic branch only by switching from $\omega_+(\boldsymbol{k})$ to $\omega_-(\boldsymbol{k})$ at $\boldsymbol{k}_\otimes$. This observation indicates that in the case of two parameters k_1 and k_2, unlike the case of just one parameter, *there is no way to 'renumerate' the branches of the eigenvalues to achieve analyticity in* (k_1, k_2) *in a vicinity of the band-crossing point.*

Remark. The vectors $G_\pm(\theta)$ defined by (237) branch near the band-crossing point and cannot be presented by a continuous function of the parameters (k_1, k_2), whereas the projectors and eigenvalues are well defined continuous functions of (k_1, k_2).

Note that if we do not use z-variables as in (232) but, instead, directly use the polar variables

$$k_1 = k_{\otimes 1} + \eta \cos\theta \qquad k_2 = k_{\otimes 2} + \eta \sin\theta$$

then the frequency $\omega(\boldsymbol{k})$ will still be an analytic function of η, θ if (236) holds. Though the expressions for $\omega_\pm$ and $\Pi_\pm$ will not be that simple anymore, still we can use the polar coordinates for the asymptotic analysis of the oscillatory integrals.

Three-dimensional case $d = 3$. The functions $z_1(k_1, k_2, k_3)$, $z_2(k_1, k_2, k_3)$ are analytic in a neighbourhood of $\boldsymbol{k}_\otimes$. Let us assume that

$$z_1(\boldsymbol{k}_\otimes) = 0 \qquad z_2(\boldsymbol{k}_\otimes) = 0.$$

In a generic case the vectors $\nabla z_1(\boldsymbol{k}_\otimes)$ and $\nabla z_2(\boldsymbol{k}_\otimes)$ are not parallel, that is

$$\boldsymbol{a}(\boldsymbol{k}_\otimes) = \nabla z_1(\boldsymbol{k}_\otimes) \times \nabla z_2(\boldsymbol{k}_\otimes) \neq 0.$$

The equations

$$z_1(\boldsymbol{k}) = 0 \qquad z_2(\boldsymbol{k}) = 0 \tag{239}$$

determine a smooth curve Γ in the 3D torus that passes through $\boldsymbol{k}_\otimes$. The tangent line to the curve at $\boldsymbol{k}_\otimes$ is parallel to $\boldsymbol{a}(\boldsymbol{k}_\otimes)$. One of the three components of $\boldsymbol{a}(\boldsymbol{k}_\otimes)$ is not zero. For instance, let it be

$$a_3 = \det \begin{bmatrix} \partial_1 z_1(\boldsymbol{k}_\otimes) & \partial_2 z_1(\boldsymbol{k}_\otimes) \\ \partial_1 z_2(\boldsymbol{k}_\otimes) & \partial_2 z_2(\boldsymbol{k}_\otimes) \end{bmatrix} \neq 0. \tag{240}$$

Now if we introduce new variables (z_1, z_2, k_3), then the curve Γ in these coordinates turns into an interval of the straight line: $z_1 = 0$, $z_2 = 0$, $|k_3| < \delta_0$.

Introducing the cylindrical coordinates ρ, θ, k_3 in (z_1, z_1, k_3)-space as in the two-dimensional case we find that the eigenvalues $\omega_\pm$ and the eigenvectors $G_\pm$ are defined by the same equalities (237) and, hence, are analytic functions of ρ and θ, respectively. In addition to that, the projections $\Pi_\pm(\theta)$ onto the subspaces corresponding to $G_\pm$ are globally one-valued analytic functions of the cylindrical coordinates in the vicinity of Γ.

The above considerations (237) and (238) show, in particular, that though the eigenfunctions $\boldsymbol{G}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}) = \boldsymbol{G}_{\pm,n}(\boldsymbol{r}, \boldsymbol{k})$ with a fixed sign $\pm$ are branching (two-valued) functions of $\boldsymbol{k}$ in a vicinity of a conical point $\boldsymbol{k}_\otimes$ the Bloch components $\tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k})$ defined by (219) are one-valued regular functions, and, hence, the integrals of the form

$$\int \boldsymbol{A}(\boldsymbol{k}, \boldsymbol{k}')\, \boldsymbol{Q} \,\dot{:}\, \tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{k}') \tilde{\boldsymbol{U}}_{\bar{n}'}(\boldsymbol{k} - \boldsymbol{k}')\, \mathrm{d}\boldsymbol{k}' \tag{241}$$

are well defined.

We assume from now on that in the sense clarified above all the band-crossing points are generic. In particular, the Bloch eigenmodes possess the following properties.

(a) For $d = 2$ every $\omega_n(\boldsymbol{k})$ is analytic for all but a finite number of band-crossing points $\boldsymbol{k}_{\otimes l}$. For every such point there exists its vicinity in which the eigenvalues, the eigenvectors and the corresponding projections are analytical in the corresponding polar coordinates.
(b) For $d = 3$ every $\omega_n(\boldsymbol{k})$ is analytic for all but a finite number of band-crossing curves $\Gamma_{\otimes l}$. For every point on every one of those curves there exists its vicinity in which the eigenvalues, the eigenvectors and the corresponding projections are analytical in the corresponding cylindrical coordinates.

Remark. Note that the dependence on the parameter $\boldsymbol{k}$ does not affect the form of singularity in $\boldsymbol{k}'$ since it is very special: $\omega_{n''}(\boldsymbol{k} - \boldsymbol{k}')$ for different $\boldsymbol{k}$ has the same singularity but located at different points. Albeit such a dependence may cause overlapping of the singularities for different phases at the same point. We intend to address these issues in detail in another paper.

6. Nonlinear Maxwell equations

In this section we relate the constitutive relations written in terms of $\boldsymbol{E}$, which is a common way to do it, with the same relations written in terms of the field $\boldsymbol{D}$ as we do in this paper. We also discuss in this section the frequency representations of the quantities of interest.

We remind the reader that the dielectric medium nonlinearity comes into the theory through the nonlinear constitutive relation

$$\boldsymbol{D}(\boldsymbol{r},t) = \boldsymbol{E}(\boldsymbol{r},t) + 4\pi \boldsymbol{P}(\boldsymbol{r},t;\boldsymbol{E}(\cdot)) \tag{242}$$

between the electric inductance $\boldsymbol{D}$ and the electric field $\boldsymbol{E}$ where the electric polarization $\boldsymbol{P}(\boldsymbol{r},t;\boldsymbol{E}(\cdot))$ is a nonlinear function of $\boldsymbol{E}(\boldsymbol{r},t)$. It is customary in nonlinear optics to express $\boldsymbol{P}$ in the form of the series [15],

$$\begin{aligned} \boldsymbol{P}(\boldsymbol{r},t;\boldsymbol{E}(\cdot)) &= \boldsymbol{P}^{(1)}(\boldsymbol{r},t;\boldsymbol{E}(\cdot)) + \alpha \boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{r},t;\boldsymbol{E}(\cdot)) \\ \boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{r},t;\boldsymbol{E}(\cdot)) &= \boldsymbol{P}^{(2)}(\boldsymbol{r},t;\boldsymbol{E}(\cdot)) + \boldsymbol{P}^{(3)}(\boldsymbol{r},t;\boldsymbol{E}(\cdot)) + \cdots \end{aligned} \tag{243}$$

where $\boldsymbol{P}^{(1)}$ is linear in the field $\boldsymbol{E}$, $\boldsymbol{P}^{(2)}$ is quadratic and so on. Usually, in nonlinear optics only the first term in the expansion of $\boldsymbol{P}_{\mathrm{NL}}$ is kept. Depending on the symmetry of the media $\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{r},t;\boldsymbol{E}(\cdot))$ it is either quadratic or cubic. Since we study the case of periodic media the position dependence of the polarization term is assumed to be periodic.

We also assume the linear term in (243) to be of the form

$$\boldsymbol{P}^{(1)}(\boldsymbol{r},t) = \chi^{(1)}(\boldsymbol{r})\boldsymbol{E}(\boldsymbol{r},t) \tag{244}$$

where the linear susceptibility $\chi_1^{(1)}(\boldsymbol{r})$ is a periodic tensor function of the position vector $\boldsymbol{r}$, i.e.

$$\chi^{(1)}(\boldsymbol{r}+\boldsymbol{m}) = \chi^{(1)}(\boldsymbol{r}). \tag{245}$$

We also assume that $\chi^{(1)}$ is a symmetric non-negative tensor with real-valued entries, i.e.

$$\chi^{(1)}_{jj'} = \chi^{(1)}_{j'j} \qquad \operatorname{Im}\chi^{(1)}_{jj'} = 0 \qquad j, j' = 1,2,3 \qquad \left(\chi^{(1)}\boldsymbol{E},\boldsymbol{E}\right) \geqslant 0. \tag{246}$$

As to the nonlinear terms $\boldsymbol{P}^{(h)}(\boldsymbol{r},t;\boldsymbol{E}(\cdot))$, following to [15] we assume that for $h \geqslant 1$ the polarization $\boldsymbol{P}^{(h)}(\boldsymbol{r},t;\boldsymbol{E}(\cdot))$ has the following canonical form:

$$\boldsymbol{P}^{(h)}(\boldsymbol{r},t;\boldsymbol{E}(\cdot)) = \int_{-\infty}^{t}\cdots\int_{-\infty}^{t} \mathbb{R}^{(h)}(\boldsymbol{r};t-t_1,\ldots,t-t_h) \,\vdots\, \prod_{j=1}^{h} \boldsymbol{E}\left(\boldsymbol{r},t_j\right)\mathrm{d}t_j. \tag{247}$$

Similarly to (181), in coordinates (247) reads

$$P^{(h)}_{(\xi_0)}(\boldsymbol{r},t;\boldsymbol{E}) = \int_{-\infty}^{t}\cdots\int_{-\infty}^{t} R^{(h)}_{(\xi_0\xi_1\ldots\xi_h)}(\boldsymbol{r};t-t_1,\ldots,t-t_h)\prod_{j=1}^{h} E_{(\xi_j)}\left(\boldsymbol{r},t_j\right)\mathrm{d}t_j \tag{248}$$

with the summation convention over repeated suffices.

The general form of $P^{(h)}$ stems from a fundamental physical principle: time-invariance [15]. As to the time dependence of the functions $\mathbb{R}^{(h)}(\boldsymbol{r};t_1,\ldots,t_h)$ we assume that they are smooth and satisfy the following relations:

$$\mathbb{R}^{(h)}(\boldsymbol{r};t_1,\ldots,t_h) = 0 \qquad \text{if at least one } t_j \text{ is negative} \tag{249}$$

$$\left|\mathbb{R}^{(h)}(\boldsymbol{r};t_1,\ldots,t_h)\right| \leqslant C_h' \exp\left(-C_h\sum_{j=1}^{h} t_j\right) \tag{250}$$

where C'_h and C'_h are positive constants. *The condition (249) states that the field at instant t may depend only on the values of the field at earlier times. The condition (250) requires the dependence of the field at instant t on its values at earlier times to decay exponentially.*

An alternative description of the polarization, which is used more often, is provided by frequency response tensors $\boldsymbol{\chi}^{(h)}$, known as the susceptibilities [15],

$$\boldsymbol{\chi}^{(h)}(\boldsymbol{r};\omega_1,\ldots,\omega_h)=\int_0^\infty\cdots\int_0^\infty\exp\left(\mathrm{i}\sum_{j=1}^h\omega_j t_j\right)\mathbb{R}^{(h)}(\boldsymbol{r};t_1,\ldots,t_h)\prod_{j=1}^h\mathrm{d}t_j \tag{251}$$

which are the Fourier transform of $\mathbb{R}^{(h)}$ and may be considered as a response to monochromatic waves with frequencies $\omega_1,\ldots,\omega_h$. Naturally, for a periodic medium the susceptibilities are periodic:

$$\boldsymbol{\chi}^{(h)}(\boldsymbol{r}+\boldsymbol{m};\boldsymbol{\omega})=\boldsymbol{\chi}^{(h)}(\boldsymbol{r};\boldsymbol{\omega})\qquad \boldsymbol{m}\text{ in }\mathbb{Z}^3\quad h\geqslant 1\quad \boldsymbol{\omega}=(\omega_1,\ldots,\omega_h). \tag{252}$$

6.1. Recasting constitutive relations

Having selected the field $\boldsymbol{D}$ rather than $\boldsymbol{E}$ to be the main field variable we have to recast the nonlinear constitutive relations (242) and (243) to express $\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{r},t;\boldsymbol{E}(\cdot))=\boldsymbol{P}^{(h)}(\boldsymbol{r},t;\boldsymbol{E}(\cdot))$ as a function of $\boldsymbol{D}(\cdot)$. To do that we first rewrite (242) using (243):

$$\boldsymbol{E}(\boldsymbol{r},t)=\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\boldsymbol{D}(\boldsymbol{r},t)-4\pi\alpha\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\boldsymbol{P}^{(h)}(\boldsymbol{r},t;\boldsymbol{E}(\cdot)) \tag{253}$$

where $\boldsymbol{\eta}^{(1)}(\boldsymbol{r})=\left(\mathbf{1}+4\pi\boldsymbol{\chi}^{(1)}(\boldsymbol{r})\right)^{-1}$ is the impermeability, $h\geqslant 2$. The nonlinear part $\boldsymbol{P}_{\mathrm{NL}}$ of this representation for the field $\boldsymbol{E}$ depends on $\boldsymbol{E}$, whereas we would like to have a representation depending only on $\boldsymbol{D}$.

We consider the operator $\boldsymbol{P}_{\mathrm{NL}}$ on the space of functions of t defined on $(-\infty,T]$ which take values in an appropriate Sobolev space W closed with respect to multiplication. Under natural restrictions this operator is differentiable in the norm

$$\sup_{t\leqslant T}\|\boldsymbol{D}(t)\|_W. \tag{254}$$

Since $\boldsymbol{P}_{\mathrm{NL}}(\boldsymbol{r},t;\boldsymbol{E}(\cdot))$ has homogeneity h at least two, its differential is zero at $\boldsymbol{E}(\cdot)=0$. By the implicit function theorem we represent $\boldsymbol{E}(\cdot)$ as a function of $\boldsymbol{D}(\cdot)$ for bounded $\boldsymbol{D}$ and small α which is analytic in $\boldsymbol{D}$ and α and we can write

$$\boldsymbol{E}(\boldsymbol{r},t)=\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\boldsymbol{D}(\boldsymbol{r},t)-\alpha\boldsymbol{S}^{(h)}(\boldsymbol{r},t;\boldsymbol{D})+\mathrm{O}(\alpha^2) \tag{255}$$

where

$$\boldsymbol{S}^{(h)}(\boldsymbol{r},t;\boldsymbol{D})=4\pi\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\boldsymbol{P}^{(h)}\left(\boldsymbol{r},t;\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\boldsymbol{D}\right). \tag{256}$$

This dependence is analytic in $\boldsymbol{D}$ and α.

Hence, we have the same type of dependence as for the original $\boldsymbol{P}^{(h)}$. The only difference is that we have in place of (247)

$$\boldsymbol{S}^{(h)}(\boldsymbol{r},t;\boldsymbol{D})=\int_{-\infty}^t\cdots\int_{-\infty}^t\mathbb{R}_D^{(h)}(\boldsymbol{r};t-t_1,\ldots,t-t_h)\,\vdots\,\prod_{j=1}^h\boldsymbol{D}\left(\boldsymbol{r},t_j\right)\mathrm{d}t_j \tag{257}$$

where

$$\begin{aligned}\mathbb{R}_D^{(h)}(\boldsymbol{r};t-t_1,\ldots,t-t_h)\,\vdots\,\prod_{j=1}^h\boldsymbol{D}\left(\boldsymbol{r},t_j\right)\\ =4\pi\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\mathbb{R}^{(h)}(\boldsymbol{r};t-t_1,\ldots,t-t_h)\,\vdots\,\prod_{j=1}^h\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\boldsymbol{D}\left(\boldsymbol{r},t_j\right).\end{aligned} \tag{258}$$

We denote as in (251)

$$\chi_D^{(h)}(\boldsymbol{r};\omega_1,\ldots,\omega_h)=\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\mathbb{R}_D^{(h)}(\boldsymbol{r};t_1,\ldots,t_h)\exp\left\{\mathrm{i}\sum\omega_j t_j\right\}\prod_{j=1}^{h}\mathrm{d}t_j. \tag{259}$$

In particular, for the quadratic and cubic nonlinearities of the form (258) we obtain the following expressions for the susceptibilities $\chi_D^{(h)}(\boldsymbol{r};\boldsymbol{\omega})$ in terms of $\chi^{(h)}(\boldsymbol{r};\boldsymbol{\omega})$, for $h=2$:

$$\chi_D^{(2)}(\boldsymbol{r};\boldsymbol{\omega})\,\vdots\,\boldsymbol{V}\boldsymbol{V}'=4\pi\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\chi^{(2)}(\boldsymbol{r};\boldsymbol{\omega})\,\vdots\,\left[\left(\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\boldsymbol{D}\right)\left(\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\boldsymbol{D}'\right)\right] \tag{260}$$

where on the right-hand side $\boldsymbol{D}$ is the first component of $\boldsymbol{V}=(\boldsymbol{D},\boldsymbol{B})$. Similarly, for $h=3$:

$$\chi_D^{(3)}(\boldsymbol{r};\boldsymbol{\omega})\,\vdots\,\prod_{j=1}^{3}\boldsymbol{V}^{(j)}=4\pi\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\chi^{(3)}(\boldsymbol{r};\boldsymbol{\omega})\,\vdots\,\prod_{j=1}^{3}\left[\boldsymbol{\eta}^{(1)}(\boldsymbol{r})\boldsymbol{D}\right]^{(j)}. \tag{261}$$

As was mentioned, susceptibilities are most widely used in nonlinear optics for the description of nonlinear, frequency-dependent media. The susceptibility $\chi_D^{(h)}(\boldsymbol{r};\omega_1,\ldots,\omega_h)$ describes the nonlinear response to monochromatic waves with frequencies $\omega_1,\ldots,\omega_h$. Naturally, $\chi_D^{(h)}(\boldsymbol{r};\omega_1,\ldots,\omega_h)$ can also be used to describe wavepackets with monochromatic carriers with frequencies $\omega_1,\ldots,\omega_h$. This allows one to define $\boldsymbol{S}^{(h)}(\boldsymbol{r},t;\boldsymbol{D})$ on wavepacket solutions to the nonlinear Maxwell equations in terms of the susceptibilities. Namely, for a wavepacket of the form

$$\tilde{\boldsymbol{U}}(\boldsymbol{r},\boldsymbol{k},t,\tau)=\sum_{\bar{n}}\exp\{-\mathrm{i}\omega_{\bar{n}}(\boldsymbol{k})t\}\,\tilde{\boldsymbol{V}}_{\bar{n}}(\boldsymbol{r},\boldsymbol{k},t,\tau)\qquad\tau=\varrho t \tag{262}$$

we have

$$\boldsymbol{S}_D^{(h)}(\boldsymbol{r},t;\boldsymbol{U})=\boldsymbol{S}_D^{(h)}(\boldsymbol{r},t;\boldsymbol{D})=\frac{1}{(2\pi)^{hd}}\sum_{\bar{n}^1,\ldots,\bar{n}^{(h)}}\int\cdots\int\exp\left\{-\mathrm{i}\sum\omega_{\bar{n}^{(l)}}\left(\boldsymbol{k}^{(l)}\right)\right\}t\chi_D^{(h)}$$
$$\times\left(\boldsymbol{r};\omega_{\bar{n}^{(1)}}\left(\boldsymbol{k}^{(1)}\right),\ldots,\omega_{\bar{n}^{(h)}}\left(\boldsymbol{k}^{(h)}\right)\right)\vdots\prod_{j=1}^{h}\tilde{\boldsymbol{V}}_{\bar{n}^{(j)}}(\boldsymbol{r},\boldsymbol{k}^{(j)},\varrho t)\,\mathrm{d}\boldsymbol{k}'\ldots\mathrm{d}\boldsymbol{k}^{(h)}. \tag{263}$$

In particular, in the quadratic case $h=2$

$$\boldsymbol{S}_D^{(2)}(\boldsymbol{r},t;\boldsymbol{U})=\boldsymbol{S}_D^{(2)}(\boldsymbol{r},t;\boldsymbol{D})$$
$$=\frac{1}{(2\pi)^{2d}}\sum_{\bar{n}',\bar{n}''}\int\int\mathrm{e}^{\left\{-\mathrm{i}\left(\omega_{\bar{n}'}(\boldsymbol{k}')+\omega_{\bar{n}'}(\boldsymbol{k}-\boldsymbol{k}')\right)t\right\}}\chi_D^{(2)}\left(\boldsymbol{r};\omega_{\bar{n}'}(\boldsymbol{k}'),\omega_{\bar{n}''}(\boldsymbol{k}-\boldsymbol{k}')\right)$$
$$\vdots\,\tilde{\boldsymbol{V}}_{\bar{n}'}(\boldsymbol{r},\boldsymbol{k}',\varrho t)\tilde{\boldsymbol{V}}_{\bar{n}''}(\boldsymbol{r},\boldsymbol{k}-\boldsymbol{k}',\varrho t)\,\mathrm{d}\boldsymbol{k}'\,\mathrm{d}\boldsymbol{k}. \tag{264}$$

Note that $\boldsymbol{S}_D^{(h)}(\boldsymbol{r},t;\boldsymbol{U})$ depends only on $\boldsymbol{D}$ since $\chi_D^{(h)}$ in (260) and (261) depend only on the $\boldsymbol{D}$-component of $\boldsymbol{U}$. We now introduce the Floquet–Bloch representation

$$\tilde{\boldsymbol{S}}_D^{(2)}(\boldsymbol{r},\boldsymbol{k},t;\boldsymbol{U})=\tilde{\boldsymbol{S}}_D^{(2)}(\boldsymbol{r},t;\boldsymbol{D})$$
$$=\frac{1}{(2\pi)^{d}}\sum_{\bar{n}',\bar{n}''}\int\mathrm{e}^{\left\{-\mathrm{i}\left(\omega_{\bar{n}'}(\boldsymbol{k}')+\omega_{\bar{n}'}(\boldsymbol{k}-\boldsymbol{k}')\right)t\right\}}\chi_D^{(2)}\left(\boldsymbol{r};\omega_{\bar{n}'}(\boldsymbol{k}'),\omega_{\bar{n}''}\left(\boldsymbol{k}-\boldsymbol{k}'\right)\right)$$
$$\vdots\,\tilde{\boldsymbol{V}}_{\bar{n}'}\left(\boldsymbol{r},\boldsymbol{k}',\varrho t\right)\tilde{\boldsymbol{V}}_{\bar{n}''}(\boldsymbol{r},\boldsymbol{k}-\boldsymbol{k}',\varrho t)\,\mathrm{d}\boldsymbol{k}'. \tag{265}$$

Substituting $\boldsymbol{E}(\boldsymbol{r},t) = \boldsymbol{\eta}^{(1)}(\boldsymbol{r})\boldsymbol{D}(\boldsymbol{r},t) - \alpha \boldsymbol{S}_D^2(\boldsymbol{r},t;\boldsymbol{D})$ into the Maxwell equations (3) in the form of dimensionless variables and the velocity of light $c = 1$, we obtain equations (15) and (16) which for the reader's convenience we write here again:

$$\partial_t \boldsymbol{U} = -\mathrm{i}\mathcal{M}\boldsymbol{U} + \alpha \boldsymbol{F}_{\mathrm{NL}}(\boldsymbol{U}) - \boldsymbol{J} \qquad \boldsymbol{U}(t) = 0 \quad t \leqslant 0 \tag{266}$$

$$\boldsymbol{U}(\boldsymbol{r},t) = \begin{bmatrix} \boldsymbol{D} \\ \boldsymbol{B} \end{bmatrix} = \begin{bmatrix} \boldsymbol{U}_D \\ \boldsymbol{U}_B \end{bmatrix}$$
$$\mathcal{M}\boldsymbol{U} = \mathrm{i} \begin{bmatrix} \mu^{-1}\nabla \times \boldsymbol{B} \\ -\nabla \times \left(\eta^{(1)}(\boldsymbol{r})\boldsymbol{D}\right) \end{bmatrix} \tag{267}$$
$$\boldsymbol{J} = \boldsymbol{J}(\boldsymbol{r},t) = 4\pi \begin{bmatrix} \boldsymbol{J}_E \\ \boldsymbol{J}_M \end{bmatrix} \qquad \boldsymbol{F}_{\mathrm{NL}}(\boldsymbol{U}) = \begin{bmatrix} \boldsymbol{0} \\ \nabla \times \boldsymbol{S}_D^{(h)}(\boldsymbol{r},t;\boldsymbol{D}) \end{bmatrix}.$$

For a more detailed discussion of the relations between $\boldsymbol{S}^{(h)}(\boldsymbol{r},t;\boldsymbol{D})$ given by (257) and $\boldsymbol{S}^{(h)}(\boldsymbol{r},t;\boldsymbol{D})$ given by (257) see section 6.2.

Following the strategy described in section 4 we will use the general set-up from section 3.1 combined with Floquet–Bloch decompositions studied in detail in section 5. According to the method we take the solution $\boldsymbol{V}^{(0)}$ to the linear problem and we seek the solution $\boldsymbol{U}(\boldsymbol{r},t)$ in the form

$$\boldsymbol{U}(t) = \mathrm{e}^{-\mathrm{i}\mathcal{M}t}\boldsymbol{V}(\tau) = \mathrm{e}^{-\mathrm{i}\mathcal{M}t}\left[\boldsymbol{W}(\tau) + \boldsymbol{V}^{(0)}(\tau)\right] \tag{268}$$

$$\boldsymbol{U}(\boldsymbol{r},\tau,t) = \sum_{\vec{n}} \frac{1}{(2\pi)^3} \int_{[-\pi,\pi]^3} \mathrm{e}^{-\mathrm{i}\omega_{\vec{n}}(\boldsymbol{k})t}\left[\tilde{\boldsymbol{W}}_{\vec{n}}(\boldsymbol{k},\tau) + \tilde{\boldsymbol{V}}_{\vec{n}}^{(0)}(\boldsymbol{k},\tau)\right]\mathrm{d}\boldsymbol{k} \tag{269}$$

where $\tau = \varrho t$ and ϱ is a small positive constant. It is customary to refer to the parameter τ as the *slow time*. Plugging in the field $\boldsymbol{U}$ defined by (268) and (269) in (266) we obtain the equations equivalent to (266)

$$\partial_\tau \tilde{\boldsymbol{W}}_{\vec{n}}(\boldsymbol{k},\tau) = \frac{\alpha}{\varrho}\exp\{\mathrm{i}\omega_{\vec{n}}(\boldsymbol{k})t\}\left\{\boldsymbol{F}_{\mathrm{NL}}\left[\mathrm{e}^{-\mathrm{i}\mathcal{M}t}\left(\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)}\right)\right]\right\}_{\vec{n}}(\boldsymbol{k}). \tag{270}$$

We expand $\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)}$ in the Floquet–Bloch series similar to (269) and obtain

$$\tilde{\boldsymbol{W}}_{\vec{n}}(\boldsymbol{r},\boldsymbol{k},\tau) = \frac{\alpha}{\varrho}\sum_{\vec{n}',\vec{n}''}\int_0^\tau \int_{[-\pi,\pi]^3} \mathrm{e}^{\mathrm{i}\phi_{\vec{n}}(\boldsymbol{k},\boldsymbol{k}')\tau_1/\varrho}\tilde{Q}_{\vec{n}}\left[\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)} | \,\boldsymbol{r},\boldsymbol{k},\boldsymbol{k}',\tau_1\right]\mathrm{d}\boldsymbol{k}'\,\mathrm{d}\tau_1 \tag{271}$$

where $\phi_{\vec{n}}(\boldsymbol{k},\boldsymbol{k}')$ is given by (145) and

$$\tilde{Q}_{\vec{n}}\left[\boldsymbol{U}|\,\boldsymbol{r},\boldsymbol{k},\boldsymbol{k}',\tau_1\right]$$
$$= \frac{1}{(2\pi)^d}\tilde{\Pi}_{\vec{n}}(\boldsymbol{k})\begin{bmatrix} \boldsymbol{0} \\ \nabla \times \boldsymbol{\chi}_D^{(2)}\left(\boldsymbol{r};\omega_{\vec{n}'}(\boldsymbol{k}'),\omega_{\vec{n}''}(\boldsymbol{k}'')\right) \vdots \tilde{\boldsymbol{U}}_{\vec{n}'}(\boldsymbol{k}')\tilde{\boldsymbol{U}}_{\vec{n}''}(\boldsymbol{k}-\boldsymbol{k}') \end{bmatrix} \tag{272}$$

where $\boldsymbol{\chi}_D^{(2)}$ is defined in terms of $\boldsymbol{\chi}^{(2)}$ by (260). We consider the right-hand side of (271) as an oscillatory integral with the indicated integrand. In the sections 7 and 4 it is shown that for small ϱ the leading terms in the integral (271) are determined by critical points of the phase which satisfy the equation $\nabla_{\boldsymbol{k}'}\phi_{\vec{n}}(\boldsymbol{k},\boldsymbol{k}') = 0$.

6.2. Nonlinear polarization operators

In this subsection we justify the definition of the operator $\boldsymbol{S}^{(h)}$ in terms of susceptibilities given in (263). Applying (169) to (256) we express $\boldsymbol{S}^{(h)}(\boldsymbol{r}, t; \boldsymbol{V})$ in terms of its Floquet–Bloch transformation and substituting (262) we obtain as in (182),

$$\begin{aligned}\boldsymbol{S}^{(h)}(\boldsymbol{r}, t; \boldsymbol{U}) &= \boldsymbol{S}^{(h)}(\boldsymbol{r}, t; \boldsymbol{D}) \\ &= (2\pi)^{-hd} \sum_{\bar{n}^1,\ldots,\bar{n}^{(h)}} \int \cdots \int \exp\left\{-\mathrm{i} \sum \omega_{\bar{n}^{(j)}}\left(\boldsymbol{k}^{(j)}\right) t_j\right\} \mathbb{R}_D^{(h)}(\boldsymbol{r}; t-t_1, \ldots, t-t_h) \\ &\quad \vdots \prod_{j=1}^{h} \tilde{\boldsymbol{V}}_{D\bar{n}^{(j)}}\left(\boldsymbol{k}^{(j)}, \varrho t_j\right) \mathrm{d}t_1 \ldots \mathrm{d}t_h \, \mathrm{d}\boldsymbol{k} \, \mathrm{d}\boldsymbol{k}' \ldots \mathrm{d}\boldsymbol{k}^{(h-1)} \qquad \boldsymbol{V} = \begin{pmatrix} \boldsymbol{V}_D \\ \boldsymbol{V}_B \end{pmatrix}\end{aligned}$$

where we use the same notation for tensors as in (183), (247) and (248). Note that the time derivative of the slow amplitude

$$\partial_t \boldsymbol{V}(\boldsymbol{k}, \varrho t) = \mathrm{O}(\varrho)$$

is small, and, hence,

$$\boldsymbol{V}_{\bar{n}^{(j)}}\left(\boldsymbol{k}^{(j)}, \tau_j\right) = \boldsymbol{V}_{\bar{n}^{(j)}}\left(\boldsymbol{k}^{(j)}, \varrho t_j\right) = \boldsymbol{V}_{\bar{n}^{(j)}}\left(\boldsymbol{k}^{(j)}, \varrho t\right) + \mathrm{O}\left(\varrho \left|t - t_j\right| |\partial_\tau \boldsymbol{v}|\right).$$

By (250) the function

$$\left|\mathbb{R}_D^{(h)}(\boldsymbol{r}; t-t_1, \ldots, t-t_h)\right| \sum \left|t - t_j\right|$$

is integrable. Consider now

$$\begin{aligned}&\int \cdots \int \mathbb{R}_D^{(h)}(\boldsymbol{r}; t-t_1, \ldots, t-t_h) \\ &\qquad \vdots \exp\left\{-\mathrm{i} \sum \omega_{\bar{n}^{(j)}}\left(\boldsymbol{k}^{(j)}\right) t_j\right\} \prod_{j=1}^{h} \boldsymbol{V}_{D\bar{n}^{(j)}}\left(\boldsymbol{k}^{(j)}, \varrho t\right) \mathrm{d}t_1 \ldots \mathrm{d}t_h \\ &= \exp\left\{-\mathrm{i} \sum \omega_{\bar{n}^{(j)}}\left(\boldsymbol{k}^{(j)}\right) t\right\} \int \cdots \int \mathbb{R}_D^{(h)}(\boldsymbol{r}; t-t_1, \ldots, t-t_h) \\ &\qquad \vdots \exp\left\{-\mathrm{i} \sum \omega_{\bar{n}^{(j)}}(\boldsymbol{k}^{(j)}) \left(t_j - t\right)\right\} \prod_{j=1}^{h} \boldsymbol{V}_{D\bar{n}^{(j)}}\left(\boldsymbol{k}^{(j)}, \varrho t\right) \mathrm{d}t_1 \ldots \mathrm{d}t_h + \mathrm{O}(\varrho) \\ &= \exp\left\{-\mathrm{i} \sum \omega_{\bar{n}^{(j)}}(\boldsymbol{k}^{(j)}) t\right\} \\ &\qquad \times \boldsymbol{\chi}_D^{(h)}\left(\boldsymbol{r}; \omega_{\bar{n}'}(\boldsymbol{k}'), \ldots, \omega_{\bar{n}^{(h)}}(\boldsymbol{k}^{(h)})\right) \vdots \prod_{j=1}^{h} \boldsymbol{V}_{D\bar{n}^{(j)}}\left(\boldsymbol{k}^{(j)}, \varrho t\right) + \mathrm{O}(\varrho).\end{aligned}$$

Neglecting

$$R = \int \cdots \int \mathrm{O}(\varrho) \, \mathrm{d}\boldsymbol{k} \, \mathrm{d}\boldsymbol{k}' \ldots \mathrm{d}\boldsymbol{k}^{(h-1)}$$

we obtain (263). Note that if we do not neglect R and would define $\boldsymbol{F}_{\mathrm{NL}}$ in terms of $\boldsymbol{S}^{(h)}(\boldsymbol{r}, t; \boldsymbol{D})$ given by (257), we would obtain results similar to those given in section 4.1. Asymptotic expansions in that case would include additional terms resulting from R, which usually have higher order, but sometimes would intervene with instantaneous terms complicating the final expressions. These observations are another confirmation of the advantages of the frequency representation we preferred to use in this paper.

7. Oscillatory integrals for nonlinear interactions

In this section we discuss: (a) the classical results on the non-degenerate simple critical points and (b) results related to degenerate critical points. There is a quite evident analogy between the geometrical (ray) optics approximation within the classical wave theory, on one hand, and the theory of weakly nonlinear periodic medium developed here, on the other hand. In both theories the quantities of interest can be represented by oscillatory integrals with a large parameter in the phase function of the integrand. Then by the stationary phase method the dominant contributions to the integrals are given by small vicinities of a few critical points, and these vicinities are naturally related to wavepackets. In both theories wavepackets are the elementary waves used to express and explain the basic phenomena. The similarities between the theories, however, are complemented by some important differences.

7.1. Asymptotics of oscillatory integrals

In this section we consider the oscillatory integrals of the form

$$I(\eta) = \int_{\mathbb{R}^d} \exp\{\mathrm{i}\eta\Phi(\boldsymbol{x})\} A(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \qquad \eta \to \infty \tag{273}$$

where the phase function $\Phi(\boldsymbol{x})$ and the amplitude function $A(\boldsymbol{x})$ are infinitely smooth (the integration parameter $\boldsymbol{x}$ arises as $\boldsymbol{k}'$ in previous sections). We will also consider separately the case when singular (band-crossing) points are present, and assume that the singularities can be resolved using appropriate polar coordinates. In our studies such integrals appear in (138) and (142), where $\boldsymbol{x} = \boldsymbol{k}'$ and the phase and the amplitude functions, and hence the oscillatory integral, depend on the parameter $\boldsymbol{k}$:

$$I(\boldsymbol{k}, \eta) = \int_{\mathbb{R}^d} \exp\{\mathrm{i}\eta\Phi(\boldsymbol{k}, \boldsymbol{x})\} A(\boldsymbol{k}, \boldsymbol{x})\,\mathrm{d}\boldsymbol{x} \qquad \eta \to \infty \tag{274}$$

where $\boldsymbol{k}$ is the quasimomentum taking values in the torus $[-\pi, \pi]^d$. Recall that a point $\boldsymbol{x}_0$ is called a *critical point* of a function $\Phi(\boldsymbol{x})$ if

$$\nabla_x \Phi(\boldsymbol{x}_0) = \mathbf{0}. \tag{275}$$

As we discussed in the introduction the analysis of *the phase critical points becomes the central mathematical problem in the study of the wavepacket propagation in weakly nonlinear media.* The first step in the classification of critical points is based on the Hessian quadratic form

$$\Phi''(\boldsymbol{x}_0) = \left\{\partial^2_{jj'}\Phi(\boldsymbol{x}_0) : 1 \leqslant j, j' \leqslant d\right\}.$$

The critical point is called a *non-degenerate critical point* if, in addition to (275), the Hessian Φ'' of Φ at $\boldsymbol{x}_0$ does not have zero eigenvalues, i.e.

$$\det \Phi''(\boldsymbol{x}_0) \neq 0. \tag{276}$$

The asymptotic behaviour of the oscillatory integrals $I(\eta)$ can be found based on the *stationary phase* method, according to which the main contribution to the integral $I(\eta)$ as $\eta \to \infty$ is given by integrals over small neighbourhoods of the critical points of its phase function $\Phi(\boldsymbol{x})$. The statement below shows that the contribution of non-critical points is insignificant [71, section 8, section 2.1, proposition 4].

Proposition 1. *Suppose that $A(\boldsymbol{x})$ is infinitely differentiable and its support (the set of points where $A(\boldsymbol{x}) \neq 0$) is bounded. Suppose also that the phase function $\Phi(\boldsymbol{x})$ is a smooth real-valued function that has no critical points in the support of $A(\boldsymbol{x})$. Then for every $N \geqslant 0$*

$$I(\eta) = \mathrm{O}(\eta^{-N}) \qquad \eta \to \infty. \tag{277}$$

Using this proposition and partition of unity one reduces the analysis of oscillatory integrals to small neighbourhoods of critical points. The contribution of non-degenerate critical points is evaluated with the aid of the Morse lemma [71, section 8, section 2.3.2] and is described by the following statement ([6], theorem 6.2, [23, 24], [71], section 8, section 2.3 proposition 6).

Proposition 2. *Suppose that the phase function $\Phi(\boldsymbol{x})$ is a smooth real-valued function, and $\boldsymbol{x}_0$ is a non-degenerate critical point of $\Phi(\boldsymbol{x})$. Suppose also that the amplitude function $A(\boldsymbol{x})$ is smooth and is zero away from a sufficiently small neighbourhood of $\boldsymbol{x}_0$. Then*

$$I(\eta) = \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\eta\Phi(\boldsymbol{x})} A(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = a_0\eta^{-d/2} + \eta^{-d/2}\sum_{j=1}^{\infty} a_j\eta^{-j} \qquad \eta \to \infty \tag{278}$$

where $a_0 = b_0 A(\boldsymbol{x}_0)$

$$b_0 = \frac{(2\pi)^{d/2}}{\sqrt{|\det \Phi''(\boldsymbol{x}_0)|}} \exp\left\{\mathrm{i}\eta\Phi(\boldsymbol{x}_0) + \frac{\mathrm{i}\pi}{4}\,\mathrm{sign}\left[\Phi''(\boldsymbol{x}_0)\right]\right\} \tag{279}$$

and $\mathrm{sign}\left[\Phi''(\boldsymbol{x}_0)\right]$ *is the signature of the matrix $\Phi''(\boldsymbol{x}_0)$ (the algebraic sum of the signs of the matrix eigenvalues) and the series is understood to be an asymptotic one.*

In the case when the critical point is degenerate, i.e.

$$\nabla\Phi(\boldsymbol{x}_0) = \mathbf{0} \qquad \det \Phi''(\boldsymbol{x}_0) = 0 \tag{280}$$

the computation of the asymptotic of the integral becomes more complicated. It involves as the first step the analysis of the *type* $\mathcal{T}$ of the point $\boldsymbol{x}_0$ related to a relevant portion of the Taylor series for Φ at $\boldsymbol{x}_0$ and then the computation of the asymptotic behaviour of the oscillatory integral. In the case of the dependence of Φ on $\boldsymbol{k}$ the condition of degeneracy (280) becomes

$$\nabla\Phi(\boldsymbol{k}, \boldsymbol{x}_0) = \mathbf{0} \qquad \det \Phi''(\boldsymbol{k}, \boldsymbol{x}_0) = 0. \tag{281}$$

The set of all the values of parameters $\boldsymbol{k}$ for which the phase $\Phi(\boldsymbol{k}, \boldsymbol{x})$ has degenerate critical points form a hypersurface in the space of the parameters $\boldsymbol{k}$. This hypersurface is called the *caustic* [6, section 6.1.4]. We make an effort here to cover all the values of the quasimomentum $\boldsymbol{k}$ including the caustic ones.

A general qualitative result describing the asymptotics of oscillatory integrals in $\mathbb{R}^d$ for the case of degenerate critical points is as follows ([6], theorem 6.3, [71], section 8, section 5.5).

Proposition 3. *Suppose that the phase function $\Phi(\boldsymbol{x})$ is a smooth real-valued function, and $\boldsymbol{x}_0$ is a critical (possibly degenerate) point of $\Phi(\boldsymbol{x})$. Suppose also that the amplitude function $A(\boldsymbol{x})$ is smooth and is zero away from a sufficiently small neighbourhood of $\boldsymbol{x}_0$. Then*

$$\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\eta\Phi(\boldsymbol{x})} A(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \exp\{\mathrm{i}\eta\Phi(\boldsymbol{x}_0)\}\sum_{\alpha}\sum_{s=0}^{d-1} a_{\alpha s}\eta^{-\alpha}(\ln\eta)^s \qquad \eta \to \infty \tag{282}$$

where α ranges over a sequence of negative rationals lying in an arithmetic progression, and the series is understood as an asymptotic one.

Propositions 1–3 provide a sufficient base for the asymptotic analysis of the oscillatory integrals in the case of a smooth or analytical phase and amplitude. For a generic phase $\Phi(\boldsymbol{x})$ which occurs in three-parameter families, the principal term of formula (282) takes a simpler form, namely the logarithms do not enter (multiplicities of the singular indices are zero),

$$\int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\eta\Phi(\boldsymbol{x})} A(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = \mathrm{e}^{\mathrm{i}\eta\Phi(\boldsymbol{x}_0)} a_0\eta^{-q_0} + \mathrm{O}(\eta^{-q_1}) \qquad \eta \to \infty \quad q_1 > q_0. \tag{283}$$

We can also estimate q_1 in generic cases. For non-degenerate points $q_1 = q_0 + 1$. When we have a simplest degeneracy of class $\mathcal{T} = A_p$ with $p > 1$, we have $q_1 = q_0 + \frac{1}{p+1}$ (the critical points A_p are described in (287)). Note that only the degeneracies A_p with $p \leqslant 5$ happen for cumulative integrals in the cases $d = 1, 2, 3$.

When studying the asymptotic behaviour of the oscillatory integrals, we also have to consider the points where the phase $\Phi(\boldsymbol{x})$ or the amplitude $A(\boldsymbol{x})$ are not differentiable (band-crossing points). We call the critical points *simple* when $\Phi(\boldsymbol{x})$ is smooth and (275) holds. Points where the differentiability of the phase and/or the amplitude is violated in a special way (which is described in section 5.4) are called *band-crossing critical points* (BC points, see section 5.4). Fortunately, one can find an appropriate change of variables (polar or cylindric coordinates are sufficient in the generic case) after which the phase at the BC point becomes differentiable and even analytic; one has to consider integrals in a half-space after such a change of variables (since the polar radius is positive) and the functions have a special structure (for example, smooth functions are constant when the polar radius vanishes). Fortunately, the leading terms of the asymptotics of the integrals arising from the band-crossing points can also be found. The resulting expressions though are involved, and we describe them in a forthcoming paper; corresponding values of oscillatory indices are given in table 2.

As to the simple critical points, it turns out that in the generic cases of d-parametric families of dispersion relations, $d \leqslant 3$, the following asymptotic formula always holds:

$$I(\eta) = \sum_{\boldsymbol{x}_0 \text{ in } \mathcal{C}_0} a_0(\boldsymbol{x}_0)\eta^{-q_0(\boldsymbol{x}_0)}\,(1 + \mathrm{o}(1)) \qquad \eta \to \infty \tag{284}$$

where $\boldsymbol{x}_0$ runs the set $\mathcal{C}_0$ of all the critical points of the phase Φ in the integration domain, and the index $q_0 = q_0(\boldsymbol{x}_0)$ is called the *oscillatory index of the critical point* $\boldsymbol{x}_0$. Taking into account the dependence of our oscillatory integrals on the parameter $\boldsymbol{k}$ we arrive at

$$I(\boldsymbol{k}, \eta) = \sum_{\boldsymbol{x}_0 \text{ in } \mathcal{C}_0(\boldsymbol{k})} a_0\,(\boldsymbol{k}, \boldsymbol{x}_0)\,\eta^{-q_0(\boldsymbol{k},\boldsymbol{x}_0)}\,(1 + \mathrm{o}(1)) \qquad \eta \to \infty. \tag{285}$$

It turns out that *in a generic case there are only finitely many critical points* for every given $\boldsymbol{k}$ and, hence, the set $\mathcal{C}_0(\boldsymbol{k})$ is finite. So, keeping the principal terms only, we can rewrite (285)

$$I(\boldsymbol{k}, \eta) = \eta^{-q_0(\boldsymbol{k})} \sum_{\boldsymbol{x}_0 \text{ in } \mathcal{C}_0'(\boldsymbol{k})} a_0\,(\boldsymbol{k}, \boldsymbol{x}_0)\,(1 + \mathrm{o}(1)) \tag{286}$$

$$\eta \to \infty \quad q_0(\boldsymbol{k}) = \min_{\boldsymbol{x}_0} q_0\,(\boldsymbol{k}, \boldsymbol{x}_0).$$

The simplest critical points $\boldsymbol{x}_0$ are points of class $\mathcal{T} = A_p$ when the phase $\Phi(\boldsymbol{x})$ can be written after a non-degenerate change of variables $\boldsymbol{x} \to \tilde{\boldsymbol{x}}$ in a neighbourhood of $\boldsymbol{x}_0$ with unit Jacobian determinant at $\boldsymbol{x}_0$ in the form

$$\Phi = \pm_1\mu_1\widetilde{x}_1^2 \pm_2 \cdots \pm_{d-1} \mu_{d-1}\widetilde{x}_{d-1}^2 \pm_d \mu_d\widetilde{x}_d^{p+1} \tag{287}$$

where

$$\mu_j > 0 \qquad j = 1, \ldots, d \text{ and } \pm_j \mu_j \text{ are the eigenvalues of } \Phi''(\boldsymbol{x}_0).$$

If the Hessian is non-degenerate, then $p = 1$ and μ_d is the eigenvalue too. When $p > 1$ we denote

$$\left|\det \Phi''_{d-1}(\boldsymbol{x}_0)\right| = \mu_1 \cdots \mu_{d-1}.$$

The above-mentioned change of variables always exists according to the generalized Morse lemma if the rank of the Hessian of the analytic function Φ at the critical point $\boldsymbol{x}_0$ is $d - 1$, therefore such points are of type A_p. For a critical point of class $\mathcal{T} = A_p$ the leading term of the asymptotics takes the form (see, for example, [11, section 6.1]):

$$I(\eta) = \int_{\mathbb{R}^d} e^{i\eta\Phi(\boldsymbol{x})} A(\boldsymbol{x})\, d\boldsymbol{x}$$
$$= \eta^{-(d-1)/2-1/(p+1)} b_{\mathcal{T}} A(\boldsymbol{x}_0)\, e^{i\eta\Phi(\boldsymbol{x}_0)} + O\left(\eta^{-(d-1)/2-2/(p+1)}\right) \qquad \eta \to \infty \tag{288}$$

where the coefficient $b_{\mathcal{T}} = b_{A_p}$ is determined by the phase Φ at $\boldsymbol{x}_0$:

$$b_{A_p} = \frac{2(2\pi)^{(n-1)/2}\Gamma\,(1/(p+1))}{(p+1)\mu_d^{1/(p+1)}\sqrt{\left|\det \Phi''_{d-1}(\boldsymbol{x}_0)\right|}} \exp\left\{\frac{i\pi}{4}\,\mathrm{sign}\left[\Phi''_{d-1}(\boldsymbol{x}_0)\right] \pm_d \frac{i\pi}{2p+2}\right\} \tag{289}$$
$$\mathrm{sign}\left[\Phi''_{d-1}(\boldsymbol{x}_0)\right] = \pm_1 1 \pm_2 \cdots \pm_{d-1} 1$$

and the oscillatory index is

$$q_{\mathcal{T}} = q_{A_p} = \frac{d-1}{2} + \frac{1}{p+1}.$$

It is important to note that our analysis shows that cumulative terms for generic phase functions can only be associated with points of the types $\mathcal{T} = A_p$. In contrast, instantaneous terms for $d = 3$ can also be associated with points of more complicated types $D_4^{\pm}$ (see [5, 6]). We do not discuss such points here, but simply collect in the table 2 all the values of indices q_0 of the related powers ϱ^{q_0}, $\varrho = \eta^{-1}$. In the instantaneous case $q_{\mathcal{T}} = q_0 - 1$.

In all our studies we consider only degeneracies which are robust, that is *persist under small perturbations* $\delta\omega_n(\boldsymbol{k})$ *of the dispersion relations* $\omega_n(\boldsymbol{k}), \omega_{n'}(\boldsymbol{k}'), \ldots$. We would like to note that robust functions $\omega_n(\boldsymbol{k}), \omega_{n'}(\boldsymbol{k}'), \ldots$ are generic in the sense that they form an open dense set in a suitable functional space.

Note that the assumption that the dispersion relations are generic excludes extremely degenerate cases, and it is a common assumption in the literature on nonlinear waves (see, for example, [64, section 2e], [78, section 11.1]).

We consider here asymptotic approximations for every given $\boldsymbol{k}$, and, hence, it is sufficient to use for every $\boldsymbol{k}$ power expansions in η. Though such expansions are suitable for every fixed $\boldsymbol{k}$, they are not uniform. That can be seen from variations of the order of the asymptotic approximation as the type of critical point varies. The uniform dependence is clearly a more complicated phenomenon. For example, if two non-degenerate critical points $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ collide at $\boldsymbol{k} = \boldsymbol{k}_0$ forming one degenerate point of class A_2, to get a uniform in $\boldsymbol{k}$ asymptotic approximation at $\boldsymbol{k}_0$ one has to use Airy functions (see, for example, [22, section 6.2], [33, section 4.2]). In this paper we do not consider uniform asymptotic approximations.

7.2. Cumulative and instantaneous response

In this subsection we show that when the FMC condition does not hold, the τ_1 integrals in (271) can be reduced to instantaneous terms with the factor ϱ. Formula (271) includes expressions of the form

$$\tilde{I}\left(\boldsymbol{k}, \frac{\tau}{\varrho}\right) = \int_0^{\tau} \int_{[-\pi,\pi]^3} e^{i\phi_{\vec{n}}(\boldsymbol{k},\boldsymbol{k}')\tau_1/\varrho}\, \tilde{Q}_{\vec{n}}\left[\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)} | \, \boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}', \tau_1\right] d\boldsymbol{k}'\, d\tau_1. \tag{290}$$

Let us consider points $\boldsymbol{k}'$ close to a given point $\boldsymbol{k}'_*$ for which the FMC does not hold:

$$\phi_{\vec{n}}\left(\boldsymbol{k}, \boldsymbol{k}'_*\right) \neq 0. \tag{291}$$

To evaluate the contribution to the integral by a neighbourhood of $\boldsymbol{x}_*$ we introduce a smooth cut-off function $\beta(\boldsymbol{k}')$, $\beta(\boldsymbol{k}'_*) = 1$, $0 \leqslant \beta(\boldsymbol{k}') \leqslant 1$, which is non-zero only for $\boldsymbol{k}'$ close to the point $\boldsymbol{k}'_*$. Then we use the identity $\beta(\boldsymbol{k}') + \left(1 - \beta(\boldsymbol{k}')\right) = 1$ and introduce

$$A(\boldsymbol{k}, \boldsymbol{k}', \tau) = \beta(\boldsymbol{k}')\tilde{Q}_{\vec{n}}\left[\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)} | \boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}', \tau_1\right]. \tag{292}$$

Then integrating by parts we obtain

$$\tilde{I}_1\left(\boldsymbol{k}, \tau, \frac{\tau}{\varrho}\right) = \int_0^\tau \int_{[-\pi,\pi]^d} \mathrm{e}^{\mathrm{i}\phi_{\vec{n}}(\boldsymbol{k},\boldsymbol{k}')\tau_1/\varrho} A(\boldsymbol{k}, \boldsymbol{k}', \tau)\,\mathrm{d}\boldsymbol{k}'\,\mathrm{d}\tau_1 = \varrho I^{\mathrm{in}}\left(\boldsymbol{k}, \tau, \frac{\tau}{\varrho}\right) \tag{293}$$

$$-\varrho \int_0^\tau \int_{[-\pi,\pi]^d} \mathrm{e}^{\mathrm{i}\phi_{\vec{n}}(\boldsymbol{k},\boldsymbol{k}')\tau_1/\varrho}\, \partial_{\tau_1} \frac{A\left(\boldsymbol{k}, \boldsymbol{k}', \tau_1\right)}{\mathrm{i}\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}')\tau_1}\,\mathrm{d}\boldsymbol{k}'\,\mathrm{d}\tau_1 \tag{294}$$

where

$$I^{\mathrm{in}}\left(\boldsymbol{k}, \tau, \frac{\tau}{\varrho}\right) = \int_{[-\pi,\pi]^d} \frac{A\left(\boldsymbol{k}, \boldsymbol{k}'\boldsymbol{x}, \tau\right)}{\mathrm{i}\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}')\tau} \mathrm{e}^{\mathrm{i}\phi_{\vec{n}}(\boldsymbol{k},\boldsymbol{k}')\tau/\varrho}\,\mathrm{d}\boldsymbol{k}'. \tag{295}$$

The first term $I^{\mathrm{in}}\,(\boldsymbol{k}, \tau, \tau/\varrho)$ gives the *instantaneous* contribution at $\tau_1 = \tau$ with a modified tensor

$$\tilde{Q}^{\mathrm{in}}_{\vec{n}}\left[\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)} | \boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}', \tau\right] = \frac{1}{\mathrm{i}\phi_{\vec{n}}(\boldsymbol{k}, \boldsymbol{k}')\tau} \tilde{Q}_{\vec{n}}\left[\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)} | \boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}', \tau\right]. \tag{296}$$

Note that $\tilde{Q}_{\vec{n}}\left[\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)} | \boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}', \tau\right]$ and $A\,(\boldsymbol{k}, \boldsymbol{x}, \tau)$ vanish at $\tau = 0$ with power at least $\mathrm{O}\left(\tau^2\right)$, since $\tilde{Q}_{\vec{n}}$ is quadratic and $\tilde{\boldsymbol{W}}(\tau) = \tilde{\boldsymbol{V}}^{(0)} = 0$ as $\tau \leqslant 0$ and (28) holds with bounded $\boldsymbol{j}$. Note also that we consider the limit of integration $\tau \geqslant \tau_0 > 0$. Further analysis of the oscillatory integral $I^{\mathrm{in}}\,(\boldsymbol{k}, \tau, \tau/\varrho)$ from (295) based on methods of section 7 yields integrals I_{IGV} in (153) and (154).

Now let us estimate the time integral in (294). Note that (292) implies

$$\partial_\tau A(\boldsymbol{k}, \boldsymbol{k}', \tau) = \beta(\boldsymbol{k}')\partial_\tau \tilde{Q}_{\vec{n}}\left[\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)} | \boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}', \tau_1\right] = \beta(\boldsymbol{k}')\,[B_1 + B_2]$$

$$B_1 = \tilde{Q}_{\vec{n}}\left[\left(\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)}\right)\left(\partial_\tau \tilde{\boldsymbol{W}} + \partial_\tau \tilde{\boldsymbol{V}}^{(0)}\right) | \boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}', \tau\right]$$

$$B_2 = \tilde{Q}_{\vec{n}}\left[\left(\partial_\tau \tilde{\boldsymbol{W}} + \partial_\tau \tilde{\boldsymbol{V}}^{(0)}\right)\left(\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)}\right) | \boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}', \tau\right].$$

Using (270) and (28) we obtain

$$B_1 = \left[\tilde{Q}_{\vec{n}}\left(\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)}\right)B | \boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}', \tau\right] \tag{297}$$

where components of B are given by

$$(B)_{\vec{n}''} = \left\{\mathrm{e}^{\mathrm{i}\omega_{\vec{n}''}(\boldsymbol{k}-\boldsymbol{k}')\tau/\varrho} \frac{\alpha}{\varrho} \boldsymbol{F}_{\mathrm{NL}}\left[\mathrm{e}^{-\mathrm{i}\mathcal{M}t}\left(\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)}\right)\right] + \boldsymbol{j}\right\}_{\vec{n}''}. \tag{298}$$

A similar expression can be derived for B_2. Expanding bilinear operator $\boldsymbol{F}_{\mathrm{NL}}$ we get several oscillatory integrals of different magnitude.

Our analysis shows that $\tilde{\boldsymbol{W}} = \frac{\alpha}{\varrho}\mathrm{O}(\varrho^{q_0})$, $q_0 > 0$ compared with $\tilde{\boldsymbol{V}}^{(0)} = \mathrm{O}(1)$; we assume $\alpha\varrho^{q_0-1} \ll 1$. Furthermore,

$$\frac{\alpha}{\varrho}\boldsymbol{F}_{\mathrm{NL}}\left[\mathrm{e}^{-\mathrm{i}\mathcal{M}t}\left(\tilde{\boldsymbol{W}} + \tilde{\boldsymbol{V}}^{(0)}\right)\right] = \frac{\alpha}{\varrho}\mathrm{O}(\varrho^{q_0}).$$

The remaining part of B_1 can be estimated in terms of expressions

$$\tilde{Q}_{\vec{n}}\left[\left(\tilde{\boldsymbol{V}}^{(0)}\right)(\boldsymbol{j})_{\vec{n}''} | \boldsymbol{r}, \boldsymbol{k}, \boldsymbol{k}', \tau\right] \tag{299}$$

which do not have τ-oscillating terms. Integrating by parts the integral

$$-\varrho \int_0^{\tau} \int_{\mathbb{R}^d} \mathrm{e}^{\mathrm{i}\phi_{\bar{n}}(\boldsymbol{k},\boldsymbol{k}')\tau_1/\varrho} \frac{\tilde{Q}_{\bar{n}}\big[\tilde{\boldsymbol{V}}_{\bar{n}'}^{(0)}(\boldsymbol{k}')\cdot \boldsymbol{j}_{\bar{n}''}\big(\boldsymbol{k}-\boldsymbol{k}'\big)\big]}{\mathrm{i}\phi_{\bar{n}}(\boldsymbol{k},\boldsymbol{k}')\tau_1} \beta(\boldsymbol{k}')\,\mathrm{d}\boldsymbol{k}'\,\mathrm{d}\tau_1 \tag{300}$$

we obtain the factor ϱ^2. Hence, all the components of the time integral in (293) produce oscillatory integrals similar to the instantaneous term I^{in}, but with smaller indices ϱ^{1+q}, $q > 0$. A more detailed analysis, which we skip, supports this conclusion. Therefore, if the FMC does not hold, the principal part of the integral (293) is given by the instantaneous term I^{in}.

If $\phi_{\bar{n}}(\boldsymbol{k}, \boldsymbol{x}_*) = 0$ we cannot reduce the τ_1-integral $\tilde{I}_1(\boldsymbol{k}, \tau/\varrho)$ to the value the integrand at $\tau_1 = \tau$, and, hence, we have to keep the τ_1-integral and obtain the cumulative terms. Note that both the cumulative and the instantaneous integrals include oscillatory integrals in $\boldsymbol{k}'$ which are estimated based on the stationary phase principle (see section 7).

7.3. Classification of critical points of the phase

In the quadratic case the phase function can be written as

$$\begin{aligned}\phi_{\bar{n}}(\boldsymbol{k},\boldsymbol{k}') &= \omega_{\bar{n}}(\boldsymbol{k}) - \omega_{\bar{n}'}(\boldsymbol{k}') - \omega_{\bar{n}''}(\boldsymbol{k}-\boldsymbol{k}') \\ &= \pm\omega_n(\boldsymbol{k}) \mp_1 \big[\omega_{n'}(\boldsymbol{k}') \pm_2 \omega_{n''}(\boldsymbol{k}-\boldsymbol{k}')\big].\end{aligned} \tag{301}$$

When a critical point $\boldsymbol{k}'_*$ is such that $\boldsymbol{k}-\boldsymbol{k}'_* \neq \boldsymbol{k}'_*$, or when $n' \neq n''$, the function $\omega_{n'}(\boldsymbol{k}')$ near $\boldsymbol{k}'_*$ and $\omega_{n''}(\boldsymbol{k}-\boldsymbol{k}')$ near $\boldsymbol{k}-\boldsymbol{k}'_*$ may be perturbed independently, which implies that the quantity

$$\big[\omega_{n'}(\boldsymbol{k}') \pm_2 \omega_{n''}(\boldsymbol{k}-\boldsymbol{k}')\big]$$

can be considered as a general function of $\boldsymbol{k}'$. Such a situation we call *non-symmetric*. When, on the other hand, $\boldsymbol{k}-\boldsymbol{k}'_* = \boldsymbol{k}'_*$, $n' = n''$ we have a special case, which we call *symmetric*. The analysis of singularities in both cases should be done separately. In the non-symmetric case we can use classification of singularities of parametric families of phase functions (see [5, 6]). In the symmetric case we have to do an extra analysis.

Now we discuss band-crossing points. Recall that there are simple critical points where the phase is smooth, and the band-crossing points where the differentiability of the phase and/or the amplitude is violated. As was shown in section 5.4, the generic singularities are of conical type (see figure 3). In the case $d = 2$ the functions $\omega_{\bar{n}'}(\boldsymbol{k}')$ can have isolated conical points of two types. The first type of conical point occurs when only one of the points $\boldsymbol{k}'$ and $\boldsymbol{k}'' = \boldsymbol{k}-\boldsymbol{k}'$ is conical. For almost all $\boldsymbol{k}$ the conical points, if they are present, are of the first type. The second type, which we call double conical, occurs when the both $\boldsymbol{k}'_{\otimes}$ and $\boldsymbol{k}''_{\otimes} = \boldsymbol{k}-\boldsymbol{k}'_{\otimes}$ are conical points of $\omega_{n'}(\boldsymbol{k}')$ and $\omega_{n''}(\boldsymbol{k}'')$, respectively. Double conical points exist for some $\boldsymbol{k}$ since one always can choose $\boldsymbol{k} = \boldsymbol{k}''_{\otimes} + \boldsymbol{k}'_{\otimes}$ to obtain them. Clearly, the set of corresponding $\boldsymbol{k}$ is discrete since $\boldsymbol{k}'_{\otimes}$, $\boldsymbol{k}''_{\otimes}$ form discrete sets. The double conical property, in general, is not consistent with the frequency matching condition, and, hence, the double conical points contributions are of instantaneous type. Single conical points may give the cumulative contribution. By introducing the polar coordinates at a conical point (see section 5.4, η, θ are the polar radius and angle, respectively) we can show that the single conical point contribution is $\mathrm{O}(\varrho^2)$ when the generalized GVC does not hold.

In the case $d = 3$ the function $\omega_{\bar{n}'}(\boldsymbol{k}')$, in general, has a smooth curve(s) of conical points. Computations in cylindrical coordinates show that when GVC does not hold and the critical point in the tangential to the curve direction is non-degenerate, the contribution is $\mathrm{O}(\varrho^{5/2})$. The order of contribution when other possibilities are realized is presented in table 2. The values of $\boldsymbol{k} = \boldsymbol{k}''_{\otimes} + \boldsymbol{k}'_{\otimes}$ for which both $\boldsymbol{k}'_{\otimes}, \boldsymbol{k}''_{\otimes}$ are conical for given n', n'' in the three-dimensional case form a surface(s) Γ in the three-dimensional $\boldsymbol{k}$ parameter space, and for every $\boldsymbol{k}$ from this surface we have a discrete set of $\boldsymbol{k}'_{\otimes}$ and $\boldsymbol{k}''_{\otimes}$. Since the phase function may change the sign on Γ, the surface may contain a curve of points where FMC holds. Therefore, a cumulative integral related to double BC points may appear.

There is one special band-crossing point $\boldsymbol{k}'_{\otimes} = 0$ which corresponds to constant eigenfunctions of the Maxwell operator with the zero eigenvalue $\omega = 0$. This case should also be considered separately since $\omega = 0$ is a special point for the intrinsic symmetry $\pm\omega_n(\boldsymbol{k})$ of the dispersion relations; this case is related to *optical rectification*. All the described cases ought to be studied separately, and their analysis will be provided in a forthcoming paper.

7.4. Justification of the first nonlinear response approximation

Here we show that the first nonlinear response gives the leading term of asymptotics on large time intervals and analyse conditions of its applicability. The Maxwell system (266) after substitution $t = \tau\varrho$ takes the form

$$\begin{aligned} &\partial_\tau \boldsymbol{U} = -\mathrm{i}\mathcal{M}\boldsymbol{U} + \frac{\alpha}{\varrho}\boldsymbol{F}_{\mathrm{NL}}(\boldsymbol{U}) - \boldsymbol{J} \qquad \nabla\cdot\boldsymbol{U} = 0 \qquad \nabla\cdot\boldsymbol{J} = 0 \\ &\boldsymbol{U}(t) = 0 \qquad t \leqslant 0 \qquad \boldsymbol{J}(t) = 0 \qquad t \leqslant 0 \end{aligned} \tag{302}$$

where $\boldsymbol{F}_{\mathrm{NL}}(\boldsymbol{U})$ is a quadratic nonlinearity, $\boldsymbol{J}(\tau) = \mathrm{e}^{-\mathrm{i}\mathcal{M}\tau/\varrho}\boldsymbol{j}(\tau)$. Since $\boldsymbol{F}_{\mathrm{NL}}(\boldsymbol{U})$ is quadratic we have the bilinear property

$$\boldsymbol{F}_{\mathrm{NL}}(\boldsymbol{U}) = \boldsymbol{F}_{\mathrm{NL}}(\boldsymbol{U}, \boldsymbol{U}) \tag{303}$$

$$\boldsymbol{F}_{\mathrm{NL}}(\boldsymbol{U} + \boldsymbol{V}, \boldsymbol{W}) = \boldsymbol{F}_{\mathrm{NL}}(\boldsymbol{U}, \boldsymbol{W}) + \boldsymbol{F}_{\mathrm{NL}}(\boldsymbol{V}, \boldsymbol{W}). \tag{304}$$

We consider functions $\boldsymbol{U}(t)$ defined for $-\infty < t \leqslant T$, with a fixed $T > 0$. Using substitution

$$\boldsymbol{U}(\tau) = \mathrm{e}^{-\mathrm{i}\mathcal{M}\tau/\varrho}\boldsymbol{V}(\tau) \qquad t = \tau\varrho \tag{305}$$

and solving the linear equation

$$\partial_t \boldsymbol{V}^{(0)} = \boldsymbol{j} \qquad \boldsymbol{V}^{(0)}(\tau) = 0 \qquad \tau \leqslant 0 \tag{306}$$

we rewrite the Maxwell equation in the Floquet–Bloch form

$$\partial_\tau \tilde{\boldsymbol{W}} = \frac{\alpha}{\varrho}\boldsymbol{F}^{(1)}_{\mathrm{NL}}\big(\tilde{\boldsymbol{V}}^{(0)} + \tilde{\boldsymbol{W}}\big). \tag{307}$$

Integrating this equation with respect to time yields

$$\tilde{\boldsymbol{W}}(\tau) = \int_0^\tau \frac{\alpha}{\varrho}\boldsymbol{F}^{(1)}_{\mathrm{NL}}\big(\tilde{\boldsymbol{V}}^{(0)} + \tilde{\boldsymbol{W}}\big)\,\mathrm{d}\tau_1 = \frac{\alpha}{\varrho}\boldsymbol{F}^{(2)}_{\mathrm{NL}}\big(\tilde{\boldsymbol{V}}^{(0)} + \tilde{\boldsymbol{W}}\big). \tag{308}$$

Our analysis of oscillatory integrals allows one to *split the nonlinear interaction term* $\boldsymbol{F}^{(2)}_{\mathrm{NL}}$ into two parts: the part $\bar{\boldsymbol{F}}_{\mathrm{NL}}$ with restricted interactions determined by selection rules (FMC and GV) and the remainder $\boldsymbol{F}^{(3)}_{\mathrm{NL}}$:

$$\boldsymbol{F}^{(2)}_{\mathrm{NL}}(\boldsymbol{U}) = \bar{\boldsymbol{F}}_{\mathrm{NL}}(\boldsymbol{U}) + \boldsymbol{F}^{(3)}_{\mathrm{NL}}(\boldsymbol{U}). \tag{309}$$

Therefore, we obtain formula (37) which has the form

$$\tilde{\boldsymbol{W}}(\boldsymbol{k}, \tau) = \frac{\alpha}{\varrho}\bar{\boldsymbol{F}}_{\mathrm{NL}}\big(\tilde{\boldsymbol{V}}^{(0)} + \tilde{\boldsymbol{W}}\big)(\boldsymbol{k}, \tau) + \frac{\alpha}{\varrho}\boldsymbol{F}^{(3)}_{\mathrm{NL}}\big(\tilde{\boldsymbol{V}}^{(0)} + \tilde{\boldsymbol{W}}\big)(\boldsymbol{k}, \tau). \tag{310}$$

The stationary phase method implies that if $\boldsymbol{U} = \mathrm{O}(1)$, for $\tau \geqslant \tau_0 > 0$, then

$$\begin{aligned} \boldsymbol{F}_{\mathrm{NL}}^{(3)}(\boldsymbol{U})(\boldsymbol{k}) &= \mathrm{O}\left(\tau\left(\frac{\varrho}{\tau}\right)^{q_1(\boldsymbol{k})}\right) \\ \bar{\boldsymbol{F}}_{\mathrm{NL}}(\boldsymbol{U})(\boldsymbol{k}) &= \mathrm{O}\left(\tau\left(\frac{\varrho}{\tau}\right)^{q_0(\boldsymbol{k})}\right) \qquad q_1(\boldsymbol{k}) > q_0(\boldsymbol{k}) > 0. \end{aligned} \tag{311}$$

This results in the smallness of $\tilde{\boldsymbol{W}}(\boldsymbol{k}, \tau)$, namely

$$\tilde{\boldsymbol{W}}(\boldsymbol{k}, \tau) = \boldsymbol{F}_{\mathrm{NL}}^{(2)}\big(\tilde{\boldsymbol{V}}^{(0)} + \tilde{\boldsymbol{W}}\big)(\boldsymbol{k}, \tau) = \frac{\alpha}{\varrho}\mathrm{O}\left(\tau\left(\frac{\varrho}{\tau}\right)^{q_0(\boldsymbol{k})}\right) \tag{312}$$

provided that

$$\tilde{\boldsymbol{W}} = \mathrm{O}(1) \qquad \tilde{\boldsymbol{V}}^{(0)} = \mathrm{O}(1) \tag{313}$$

and provided that the stationary phase method is applicable. Since $\boldsymbol{F}_{\mathrm{NL}}^{(2)}$ contains integration in τ we have to also assume that $q_0(\boldsymbol{k}) + 1 > 0$. The case $q_0(\boldsymbol{k}) + 1 = 0$ implies a logarithmic time dependence. If $q_0(\boldsymbol{k}) + 1 < 0$ the integral in τ_1 in (308) converges, and we have to replace τ by 1 in (312). Under these conditions we obtain

$$\tilde{\boldsymbol{V}}^{(1)}(\tau) = \frac{\alpha}{\varrho}\mathrm{O}\left(\tau\left(\frac{\varrho}{\tau}\right)^{q_0}\right) \qquad \tilde{\boldsymbol{W}}(\tau) = \frac{\alpha}{\varrho}\mathrm{O}\left(\tau\left(\frac{\varrho}{\tau}\right)^{q_0}\right) \qquad q_0 = \inf_{\boldsymbol{k}} q_0(\boldsymbol{k}) \tag{314}$$

if $1 - q_0 > 0$ and similarly

$$\tilde{\boldsymbol{V}}^{(1)}(\tau) = \frac{\alpha}{\varrho}\mathrm{O}(\varrho^{q_0}) \qquad \tilde{\boldsymbol{W}}(\tau) = \frac{\alpha}{\varrho}\mathrm{O}(\varrho^{q_0}) \tag{315}$$

if $1 - q_0 < 0$. Using table 2 where all possible values of $q_0(\boldsymbol{k})$ are given we obtain

$$\begin{aligned} q_0 &\geqslant \tfrac{1}{2} && \text{for} \quad d = 1 \\ q_0 &\geqslant \tfrac{2}{3} && \text{for} \quad d = 2 \\ q_0 &\geqslant \tfrac{7}{6} && \text{for} \quad d = 3. \end{aligned} \tag{316}$$

Using that $\boldsymbol{F}_{\mathrm{NL}}^{(2)}$ is a quadratic operator we expand

$$\begin{aligned} \boldsymbol{F}_{\mathrm{NL}}^{(2)}\big(\tilde{\boldsymbol{V}}^{(0)} + \tilde{\boldsymbol{W}}\big) &= \boldsymbol{F}_{\mathrm{NL}}^{(2)}\big(\tilde{\boldsymbol{V}}^{(0)} + \tilde{\boldsymbol{W}}, \tilde{\boldsymbol{V}}^{(0)} + \tilde{\boldsymbol{W}}\big) = \boldsymbol{F}_{\mathrm{NL}}^{(2)}\big(\tilde{\boldsymbol{V}}^{(0)}, \tilde{\boldsymbol{V}}^{(0)}\big) \\ &\quad + \boldsymbol{F}_{\mathrm{NL}}^{(2)}\big(\tilde{\boldsymbol{W}}, \tilde{\boldsymbol{W}}\big) + \boldsymbol{F}_{\mathrm{NL}}^{(2)}\big(\tilde{\boldsymbol{V}}^{(0)}, \tilde{\boldsymbol{W}}\big) + \boldsymbol{F}_{\mathrm{NL}}^{(2)}\big(\tilde{\boldsymbol{W}}, \tilde{\boldsymbol{V}}^{(0)}\big). \end{aligned} \tag{317}$$

A similar expansion can be used for $\bar{\boldsymbol{F}}_{\mathrm{NL}}$ and $\boldsymbol{F}_{\mathrm{NL}}^{(3)}$. Note that in view of (313), (314) and (316) the linear wave $\tilde{\boldsymbol{V}}^{(0)}$ and the nonlinear response $\tilde{\boldsymbol{W}}$ are of different order. Therefore,

$$\boldsymbol{F}_{\mathrm{NL}}^{(2)}\big(\tilde{\boldsymbol{V}}^{(0)} + \tilde{\boldsymbol{W}}\big)(\boldsymbol{k}) = \boldsymbol{F}_{\mathrm{NL}}^{(2)}\big(\tilde{\boldsymbol{V}}^{(0)}, \tilde{\boldsymbol{V}}^{(0)}\big)(\boldsymbol{k}) + \frac{\alpha}{\varrho}\mathrm{O}\left(\tau\left(\frac{\varrho}{\tau}\right)\varrho^{q_0(\boldsymbol{k})+q_0}\right). \tag{318}$$

At the same time, since

$$\boldsymbol{F}_{\mathrm{NL}}^{(2)}\big(\tilde{\boldsymbol{V}}^{(0)}, \tilde{\boldsymbol{V}}^{(0)}\big)(\boldsymbol{k}) = \bar{\boldsymbol{F}}_{\mathrm{NL}}\big(\tilde{\boldsymbol{V}}^{(0)}, \tilde{\boldsymbol{V}}^{(0)}\big)(\boldsymbol{k}) + \mathrm{O}\left(\tau\left(\frac{\varrho}{\tau}\right)^{q_1(\boldsymbol{k})}\right) = \mathrm{O}\left(\tau\left(\frac{\varrho}{\tau}\right)^{q_0(\boldsymbol{k})}\right) \tag{319}$$

we obtain from (309), (318) and (308)

$$\tilde{\boldsymbol{W}}(\tau)(\boldsymbol{k}) = \frac{\alpha}{\varrho}\boldsymbol{F}_{\mathrm{NL}}^{(2)}\big(\tilde{\boldsymbol{V}}^{(0)} + \tilde{\boldsymbol{W}}\big)(\boldsymbol{k}) = \frac{\alpha}{\varrho}\bar{\boldsymbol{F}}_{\mathrm{NL}}\big(\tilde{\boldsymbol{V}}^{(0)}, \tilde{\boldsymbol{V}}^{(0)}\big)(\boldsymbol{k}) + \frac{\alpha}{\varrho}\boldsymbol{F}^{(4)} \tag{320}$$

where $\boldsymbol{F}^{(4)}$ is of higher order in ϱ than $\bar{\boldsymbol{F}}_{\mathrm{NL}}$; therefore (144) holds. So we obtain that *the leading term is given by the first nonlinear response*

$$\boldsymbol{V}^{(1)}(\boldsymbol{k},\tau)=\frac{\alpha}{\varrho}\bar{\boldsymbol{F}}_{\mathrm{NL}}\big(\tilde{\boldsymbol{V}}^{(0)},\tilde{\boldsymbol{V}}^{(0)}\big)(\boldsymbol{k}) \tag{321}$$

which is of the lowest order $\mathrm{O}\left(\alpha\,(\varrho/\tau)^{q_0(\boldsymbol{k})-1}\right)$ when $q_0(\boldsymbol{k})-1<0$; we obtain $\mathrm{O}\left(\alpha\varrho^{q_0(\boldsymbol{k})-1}\right)$ when $q_0(\boldsymbol{k})-1>0$ and $\alpha\mathrm{O}\,(\ln(1/\tau))$ when $q_0(\boldsymbol{k})-1=0$. Note that deriving this estimate we use only (313) and the stationary phase estimates (312) and (319). Since $\tilde{\boldsymbol{V}}^{(0)}$ is given explicitly and has good smoothness properties, we can apply the stationary phase method in its strong form and find explicitly asymptotic approximations of $\boldsymbol{F}_{\mathrm{NL}}^{(2)}\big(\tilde{\boldsymbol{V}}^{(0)},\tilde{\boldsymbol{V}}^{(0)}\big)(\boldsymbol{k})$ using the results of section 7. In particular, we obtain the formulae in section 4.1. Therefore, the validity of (319) can be proven rigorously. Since $\tilde{\boldsymbol{W}}$ is an unknown solution, we cannot assume the uniform smoothness condition for it. It is also not clear whether one can apply the stationary phase method in its standard classical form which relies heavily on the uniform smoothness of amplitudes. Therefore, we have to discuss (312) in more detail in the following section.

Remark. One can apply a simplified approach to justify the first nonlinear response approximation. One may from the very beginning take the first nonlinear response $\boldsymbol{V}^{(1)}$ in (321) as an approximation to a solution of (307). The solution $\boldsymbol{V}^{(1)}$ is $\mathrm{O}(\varrho^{q_0})$. Solving (307) for $\tilde{\boldsymbol{W}}-\boldsymbol{V}^{(1)}$ we obtain an equation with a small right-hand side which is $\mathrm{O}\left(\varrho^{2q_0}\right)$, but the linearized part of the equation may be *unstable.* Therefore, thanks to the instability, this simplified approach works only when the slow time $\tau=t\varrho$ varies on intervals of length of the order of $\ln(1/\varrho)$. The approach described in this subsection is not sensitive to the instability and it works on longer time intervals at least of the order of ϱ^{-2} (see section 7.6 for a discussion). At the same time the simplified approach on intervals for τ of the order of $\ln(1/\varrho)$ can be made mathematically rigorous up to every detail. To justify the approach we applied above for longer time intervals, which is physically more reasonable, one has to use methods from the following subsection. Complete mathematical proofs justifying the developed approach on slow time τ intervals of the order of one are given in a forthcoming paper. In particular, we have proved that the first nonlinear response gives the leading term of asymptotics of the exact solution.

7.5. Consistency of the stationary phase method

The use of the classical stationary phase method is fundamentally based on certain smoothness assumptions on the phase and the amplitude functions in the oscillatory integrals under consideration (see [71], section 8). In our case the phase $\Phi=\phi_{\vec{n}}(\boldsymbol{k},\boldsymbol{k}')$ defined by (145) is expressed explicitly in terms of the dispersion relations of the underlying linear medium and, hence, does not depend on the final solution to the nonlinear problem. Therefore, assuming we know everything about the linear medium we have control over the smoothness of the phase.

Unlike the phase, the amplitude $A(\boldsymbol{k},\boldsymbol{k}',\tau)$ defined by (292) does depend on the solution $\tilde{\boldsymbol{W}}(\boldsymbol{k}')$ to the nonlinear problem and, hence, the smoothness properties of $A(\boldsymbol{k},\boldsymbol{k}',\tau)$ in $\boldsymbol{k}'$ are not that easy to verify. According to (140) the integral (290) contains an amplitude which includes products of components of $\tilde{\boldsymbol{V}}_{\vec{n}'}(\boldsymbol{r},\boldsymbol{k}',\tau_1)$ and $\tilde{\boldsymbol{V}}_{\vec{n}''}(\boldsymbol{r},\boldsymbol{k}-\boldsymbol{k}',\tau_1)$. Recall that $\tilde{\boldsymbol{V}}=\tilde{\boldsymbol{V}}^{(0)}+\tilde{\boldsymbol{W}}$ and the leading part of $\tilde{\boldsymbol{W}}$ is given by $\tilde{\boldsymbol{V}}^{(1)}$; recall that $\tilde{\boldsymbol{V}}^{(0)}$ is uniformly smooth. Addressing this problem, it is important to note that for small ϱ the uniform smoothness of $\tilde{\boldsymbol{W}}(\boldsymbol{k})$ with respect to $\boldsymbol{k}$, and, hence, the uniform smoothness of $A(\boldsymbol{k},\boldsymbol{k}',\tau)$ with respect to $\boldsymbol{k}'$ cannot be assumed. Indeed, the leading term

$$\tilde{\boldsymbol{V}}^{(1)}(\boldsymbol{k})=\frac{\alpha}{\varrho}\bar{\boldsymbol{F}}_{\mathrm{NL}}\big(\tilde{\boldsymbol{V}}^{(0)},\tilde{\boldsymbol{V}}^{(0)}\big)(\boldsymbol{k})$$

has a different order $\varrho^{q_0(\boldsymbol{k})}$ of asymptotic approximations in ϱ for different $\boldsymbol{k}$. The strongest singularity in $\boldsymbol{k}$ occurs on the $(d-1)$-dimensional 'surface' $\Gamma_{\mathrm{FMC}}\left(\tilde{\boldsymbol{V}}^{(1)}(\boldsymbol{k})\right)$ where the FMC holds; the order $q_0(\boldsymbol{k})$ increases by 1 if $\boldsymbol{k}$ moves from Γ_{FMC} and FMC breaks. Fortunately, the lack of uniform smoothness does not prohibit an estimate of the form (312). Observe that the amplitude $A(\boldsymbol{k}, \boldsymbol{k}', \tau)$ is smooth in $\boldsymbol{k}'$ for every $\varrho > 0$, but the estimates of its derivatives worsen as ϱ becomes smaller; therefore we call points of $\Gamma_{\mathrm{FMC}}\left(\tilde{\boldsymbol{V}}^{(1)}(\boldsymbol{k})\right)$ *asymptotically singular.* Note also that (312) is a weaker form of the stationary phase method, and it is more robust than the exact formulae for the asymptotic approximation produced by the stationary phase method (see, in particular, the corollary in [71], section 8.1.2). Let us show now that the lack of uniform smoothness does not compromise the applicability of the stationary phase method in its weaker form. Here we discuss only the most generic asymptotically singular points $\boldsymbol{k}'$ of $A(\boldsymbol{k}, \boldsymbol{k}', \tau)$. We assume $\boldsymbol{k}$ to be fixed and discuss only the cases related to a typical $\boldsymbol{k}$.

First we consider the points when only for one (say, $\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{k}')$) of the two factors $\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{r}, \boldsymbol{k}', \tau_1)$ and $\tilde{\boldsymbol{V}}_{\bar{n}''}^{(1)}(\boldsymbol{r}, \boldsymbol{k}-\boldsymbol{k}', \tau_1)$ the point $\boldsymbol{k}'$ is asymptotically singular (similarly one may consider a product of $\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{r}, \boldsymbol{k}', \tau_1)$ and $\tilde{\boldsymbol{V}}_{\bar{n}''}^{(0)}(\boldsymbol{r}, \boldsymbol{k}-\boldsymbol{k}', \tau_1)$). We take into account only the main singularity resulting from breaking of FMC, that is $\boldsymbol{k}'$ lies on $\Gamma_{\mathrm{FMC}}\left(\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{k}')\right)$. First we discuss the situation of proposition 1 that is $\nabla_{\boldsymbol{k}'}\phi(\boldsymbol{k}') \neq 0$. Since critical points of ϕ form a discrete set typically they do not get onto Γ_{FMC}, so we assume $\nabla_{\boldsymbol{k}'}\phi(\boldsymbol{k}') \neq 0$ on all Γ_{FMC}. When $\nabla\phi(\boldsymbol{k}')$ is not orthogonal to Γ_{FMC}, we can use a classical proof of proposition 1, but we have to differentiate only in the directions tangent to Γ_{FMC}. Since the amplitude is smooth in the tangential directions the classical argument based on the smoothness of the amplitude works and we obtain an analogue of proposition 1. There may exist a subset Γ_0 (typically discrete) of Γ_{FMC} where $\nabla\phi(\boldsymbol{k}')$ is orthogonal to Γ_{FMC}. Near this subset we need to use the derivative in the normal direction to Γ_{FMC}. Therefore, the behaviour of the amplitude in the normal direction k to the Γ_{FMC} is of importance. In this case we cannot obtain an arbitrary high power ϱ^N as in proposition 1, but still we obtain $\varrho^{\frac{1}{2}+d}$ as we show below. On this discrete set $\Gamma_0\left(\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{k}')\right)$ we assume that $\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{k}')$ is a response to non-degenerate points only.

Now we consider the behaviour of $\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{k})$ at such a point. Namely, we consider the case when $\boldsymbol{k} = \boldsymbol{k}_0$ lies on $\Gamma_0\left(\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{k})\right)$. We use for $\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{k})$ the same type of expression (290) with a phase $\phi_1(\boldsymbol{k}, \boldsymbol{k}')$ which has a simple non-degenerate critical point $\boldsymbol{k}'_*$ when $\boldsymbol{k} = \boldsymbol{k}_0$. To illustrate the effect of breaking of the FMC condition for a non-degenerate critical point we consider the integral

$$\int_0^\tau \int \tau_1^p \exp\left\{\mathrm{i}\frac{\tau_1\left(\boldsymbol{k}'-\boldsymbol{k}'_*\right)^2}{\varrho} + \mathrm{i}\delta k\frac{\tau_1}{\varrho}\right\} \mathrm{d}\boldsymbol{k}'\,\mathrm{d}\tau_1. \tag{322}$$

This integral models the leading part of amplitude $\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{k}, \tau)$ at the non-degenerate critical point $\boldsymbol{k}'_*$ where $\tau \leqslant 1$. Here $\left(\boldsymbol{k}'-\boldsymbol{k}'_*\right)^2 + \delta k$ models the phase function $\phi_1(\boldsymbol{k}, \boldsymbol{k}')$ with a non-degenerate critical point at $\boldsymbol{k}' = \boldsymbol{k}'_*$; $|\delta| = |\nabla_{\boldsymbol{k}}\phi(\boldsymbol{k}, \boldsymbol{k}'_*)|$; the variable k is a coordinate in the normal direction to $\Gamma_{\mathrm{FMC}}\left(\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{k})\right)$. Clearly, FMC holds for $k = 0$, $\boldsymbol{k}' = \boldsymbol{k}'_*$. We take $p \geqslant 2$ since $\tilde{\boldsymbol{V}}(\tau)$ vanishes at $\tau = 0$ and $\tilde{\boldsymbol{V}}^{(1)}$ is quadratic in $\tilde{\boldsymbol{V}}$. Integrating in $\boldsymbol{k}'$ we obtain

$$\varrho^{d/2}\pi^{d/2}\mathrm{e}^{\mathrm{i}d\pi/4}\int_0^\tau \tau_1^{p-d/2}\exp\left\{\mathrm{i}\delta k\frac{\tau_1}{\varrho}\right\}\mathrm{d}\tau_1 = \varrho^{d/2}\tau^{1+p-d/2}\psi\left(\frac{k\tau\delta}{\varrho}\right) \tag{323}$$

where

$$\psi(s) = s^{-1-p+d/2}\pi^{d/2}\mathrm{e}^{\mathrm{i}d\pi/4}\int_0^s \tau_1^{p-d/2}\exp\{\mathrm{i}\tau_1\}\,\mathrm{d}\tau_1. \tag{324}$$

The function $\psi(s)$, $s = k/\varrho$, is analytic in $s \geqslant 0$, $\psi(0) \neq 0$. The function $\psi(s)$ is bounded and for large s we have $\psi(s) = c_0 s^{-1} \mathrm{e}^{\mathrm{i}s} + \mathrm{O}\left(s^{-2}\right)$, $c_0 \neq 0$. Hence, the violation of FMC increases the index of the factor ϱ of the amplitude from $\varrho^{d/2}$ to $\varrho^{d/2-1}$.

Now we substitute the obtained expression into the oscillating integral of form (290). Let us use $\varrho^{d/2}\tau^{1+p-d/2}\psi(k/\varrho)$ as an integrand which models $\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{k}')$ with asymptotic singularity at the point $\boldsymbol{k}' = \boldsymbol{k}_0$ on $\Gamma_{\mathrm{FMC}}\big(\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{k}')\big)$. Note that $k = 0$ is the equation of $\Gamma_{\mathrm{FMC}}\big(\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{k}')\big)$. Let us consider the integral in the direction normal to Γ_{FMC} with the phase modelled by mk, $|\nabla_{\boldsymbol{k}}\phi(\boldsymbol{k}_0)| = |m|$, assuming that $m \neq 0$ and $m + \delta \neq 0$. Then, for a smooth function $a(k)$ supported near zero we have

$$\int a(k)\tau_1^{1+p-d/2}\varrho^{d/2}\psi\left(\frac{k\tau_1\delta}{\varrho}\right)\mathrm{e}^{\mathrm{i}mk\tau_1/\varrho}\,\mathrm{d}k$$
$$= \tau_1^{p-d/2}\left(\frac{\varrho}{k}\right)\varrho^{1+d/2}\int a\left(\frac{\varrho k}{\tau_1}\right)\psi\,(k\delta)\,\mathrm{e}^{\mathrm{i}mk}\,\mathrm{d}k = \mathrm{O}(\varrho^{1+d/2}). \tag{325}$$

We suppose that the phase ϕ is non-degenerate critical in tangential directions to Γ_{FMC}, and, hence, the integration in the tangential directions yields $\varrho^{(d-1)/2}$. Consequently, the oscillatory integral is estimated by $\mathrm{O}\big(\varrho^{\frac{1}{2}+d}\big)$ with the index which is higher than all possible values of the index $q_0(\boldsymbol{k})$. Therefore, we can conclude that an estimate of the type (312) still holds.

There is another typical situation, namely when two factors have the same asymptotically singular point $\boldsymbol{k}'$. In that case $\Gamma_{\mathrm{FMC}}\big(\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{k}')\big)$ intersects $\Gamma_{\mathrm{FMC}}\big(\tilde{\boldsymbol{V}}_{\bar{n}''}^{(1)}(\boldsymbol{k} - \boldsymbol{k}')\big)$ at $\boldsymbol{k}'$. The intersection Γ' can be non-empty only when $d = 2, 3$ and consists of discrete points when $d = 2$ and smooth curves when $d = 3$. When $d = 3$ and $\nabla\phi(\boldsymbol{k}')$ is not orthogonal to Γ', we can differentiate in the tangent to the Γ' direction and still obtain proposition 1, so we have to consider only discrete set of points of Γ' at which $\nabla\phi(\boldsymbol{k}')$ is orthogonal to Γ'. Considerations in this situation are similar in cases $d = 2$ and 3. We consider $d = 2$. We assume that the normals γ_1 and γ_2 to $\Gamma_{\mathrm{FMC}}\big(\tilde{\boldsymbol{V}}_{\bar{n}'}^{(1)}(\boldsymbol{k}')\big)$ and $\Gamma_{\mathrm{FMC}}\big(\tilde{\boldsymbol{V}}_{\bar{n}''}^{(1)}(\boldsymbol{k} - \boldsymbol{k}')\big)$, respectively, at Γ' are not parallel (it is a generic case). So we can write $\nabla\phi(\boldsymbol{k}') = k_1\gamma_1 + k_2\gamma_2$. Then the integral (290) is similar to

$$\iint a(k_1, k_2)\varrho^d\psi_1\left(\frac{k_1}{\varrho}\right)\psi_2\left(\frac{k_2}{\varrho}\right)\exp\left[\mathrm{i}\frac{m}{\varrho}\,(k_1\gamma_1 + k_2\gamma_2)\right]\mathrm{d}k_1\,\mathrm{d}k_2 = \mathrm{O}\big(\varrho^{2+d}\big). \tag{326}$$

The index here is again higher than all possible values of the index $q_0(\boldsymbol{k})$. Therefore, an estimate of the type (312) holds in this case too.

We do not consider non-typical cases which may occur for special values of $\boldsymbol{k}$, when possible degeneracies of the phase function may interfere with the effect of non-uniform smoothness of the amplitude on the surface Γ_{FMC}. Singularities which are weaker than on Γ_{FMC} discussed above are also not considered here. The complete analysis would require the study of all possible combinations of different types of degeneracies and seems to be beyond our reach right now. We also would like to point out that combinations of different types of singularities at the same point may happen only for very special pairs of $\boldsymbol{k}$, $\boldsymbol{k}'$, and, hence, we expect that they will give only small contributions if any to the energy transfer even if the weak form of the stationary phase method could fail at those points.

Hence, in all the considered cases the use of the stationary phase method in its weaker form is *self-consistent*: the asymptotic singularities of $\tilde{\boldsymbol{W}}(\boldsymbol{k})$ in $\boldsymbol{k}$ predicted by our analysis *do not alter the ultimate estimates* of the form (312) used in the process of derivation.

7.6. Time intervals for adequate approximations

As was mentioned in the final remark of section 7.4 one can give a rigorous mathematical proof which shows that all of our results hold for τ at least of the order of $\ln(1/\varrho)$. This estimate can be improved if we assume applicability of the stationary phase method discussed in the previous subsection. Let us consider larger slow time intervals $\tau \gg 1$. The first condition for applicability of our analysis is that (313) holds on the considered time interval; this ensures that linear and nonlinear terms are of the same order, which is a criterion of applicability of the quadratic approximation of the nonlinearity [16]. Note that conditions (313) always hold for small $\tau \geqslant \tau_0 > 0$ for small ϱ. Here we discuss the following question: for how long a time will these conditions still hold? We use a so-called bootstrapping argument. As long as (313) holds, that is $\tilde{\boldsymbol{W}}$, $\tilde{\boldsymbol{V}}^{(0)}$ are bounded by a constant, we can apply consequences of (313). If these consequences formally imply boundedness of $\tilde{\boldsymbol{W}}$, $\tilde{\boldsymbol{V}}^{(0)}$ on a larger interval with the same (or smaller) constant, one can extend applicability of all results from smaller time interval to this larger interval using continuity of time. Here we give only formal estimates which give physically reasonable intervals of applicability. If (313) holds, then using the stationary phase method we obtain (314) and (315). This condition implies (313) if $1 - q_0 > 0$ and

$$\frac{\alpha\tau}{\varrho}\mathrm{O}\left(\frac{\varrho}{\tau}\right)^{q_0} \ll 1. \tag{327}$$

Recall that $q_0(\boldsymbol{k}) \geqslant q_0 \geqslant \frac{1}{2}$ for $d = 1$ and $q_0 \geqslant \frac{2}{3}$ for $d = 2$. Therefore, for $d = 1$ (327) takes the form $\frac{\alpha}{\varrho}\tau(\varrho/\tau)^{1/2} \ll 1$ which is equivalent to

$$t \ll \alpha^{-2} \qquad \text{for} \quad d = 1. \tag{328}$$

For $d = 2$ the condition (327) is

$$\tau\left(\frac{\alpha}{\varrho}\right)\left(\frac{\varrho}{\tau}\right)^{2/3} \ll 1 \tag{329}$$

that is

$$t \ll \alpha^{-3} \qquad \text{for} \quad d = 2. \tag{330}$$

When $d = 3$ we have $q_0 \geqslant \frac{7}{6}$ and $1 - \frac{7}{6} < 0$ so we use (315). This condition implies (313) if

$$\alpha\varrho^{q_0 - 1} \ll 1. \tag{331}$$

Since $q_0 \geqslant \frac{7}{6}$ for $d = 3$ we obtain

$$\alpha\varrho^{1/6} \ll 1. \tag{332}$$

The latter is always true for $\varrho \ll 1$ and bounded α, and, hence, under that condition we do not have restrictions on t in terms of α. Therefore, our approach is applicable on time intervals which are large compared with α^{-1}, as long as condition (313) on the boundedness of the first nonlinear response holds. Note also that we assume that $\tilde{\boldsymbol{V}}^{(0)}(\tau)$ is bounded, which is an additional condition that can be verified based on (28).

8. Notation

Here we collect the notation for the quantities often used in the paper:

$\boldsymbol{r} = (x_1, x_2, x_3)$	Position vector in the space
$\mathbb{R}^d$	d-dimensional Euclidean space, $d = 1, 2, 3$
$\mathbb{Z}^d$	d-dimensional cubic lattice, i.e. the set of integer-valued vectors $\boldsymbol{n}$ from $\mathbb{R}^d$
$t, \tau = \varrho t$	Time and 'slow' time

$\boldsymbol{k}$	Wavevector (quasimomentum)
ω	Angular frequency
$\omega(\boldsymbol{k})$, $\omega_n(\boldsymbol{k})$	Dispersion relations
c	Speed of light
ε, $\boldsymbol{\varepsilon}$	Dielectric constant tensor
$\eta = \boldsymbol{\varepsilon}^{-1}$	Electric impermeability
χ, $\chi^{(h)}$	Susceptibilities of homogeneity h
ζ	A quantity which takes two values ± 1
$\bar{n} = (\zeta, n)$	Extended index n
$\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k})$	Eigenfunction of the Maxwell operator with Floquet–Bloch boundary condition with eigenvalue $\zeta\omega_n(\boldsymbol{k})$ from nth band with the quasimomentum $\boldsymbol{k}$
$\tilde{U}_{\bar{n}}(\boldsymbol{k})$	Coefficient in the Floquet–Bloch expansion of a function $\boldsymbol{U}(\boldsymbol{r})$ in the basis $\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k})$
$\vec{n} = (\bar{n}_1, \bar{n}_2, \ldots, \bar{n}_{h+1})$	Vector of extended indices
$\int = \int_{\mathbb{R}^d}$	Where the value of d depends on the context
z^*	The conjugate to complex number z.

$\boldsymbol{E}(\boldsymbol{r}, t)$, $\boldsymbol{D}(\boldsymbol{r}, t)$, $\boldsymbol{H}(\boldsymbol{r}, t)$, $\boldsymbol{B}(\boldsymbol{r}, t)$, $\boldsymbol{P}(\boldsymbol{r}, t)$ are, respectively, the electric field, electric inductance, magnetic field, magnetic inductance and electric polarization. To shorten the notation we often drop the symbols $\boldsymbol{r}$ and t depending on the situation,

$$\boldsymbol{U}(t) = \boldsymbol{U}(\boldsymbol{r}, t) = \begin{bmatrix} \boldsymbol{D}(\boldsymbol{r}, t) \\ \boldsymbol{B}(\boldsymbol{r}, t) \end{bmatrix}.$$

The $\tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{k}) = \tilde{\boldsymbol{U}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k}) = \tilde{U}_{\bar{n}}(\boldsymbol{k})\tilde{\boldsymbol{G}}_{\bar{n}}(\boldsymbol{r}, \boldsymbol{k})$ component of $\boldsymbol{U}(\boldsymbol{r})$ in the Floquet–Bloch expansion

$\mathrm{O}(f)$ to denote a quantity which depends on another non-negative quantity f and such that

$$|\mathrm{O}(f)| \leqslant Cf \qquad \text{where} \quad C \text{ is a constant.} \tag{333}$$

In particular, O(1) is simplify a bounded quantity, i.e.

$$|\mathrm{O}(1)| \leqslant \text{constant} \tag{334}$$

$\mathrm{o}(f)$ means that $\mathrm{o}(f)/f \to 0$.

To abbreviate tensor expressions we will use the following notation:

$$\boldsymbol{f}\left(\boldsymbol{U}^{(1)}, \ldots, \boldsymbol{U}^{(h)}\right) = \boldsymbol{f} \vdots \prod_{i=1}^{h} \boldsymbol{U}^{(i)} \qquad \boldsymbol{f}(\boldsymbol{U}, \boldsymbol{U}) = \boldsymbol{f} \vdots \boldsymbol{U}^2 \tag{335}$$

with the understanding that the tensor is symmetrized. For instance, for a bilinear tensor $\boldsymbol{f}$ when $h = 2$ we have

$$\boldsymbol{f} \vdots \boldsymbol{u}\boldsymbol{v} = \boldsymbol{f} \vdots \boldsymbol{v}\boldsymbol{u}$$

FM, FMC	Frequency matching condition
PhM, PhMC	Phase matching condition
GV, GVC	Group velocity matching condition
SHG	Second-harmonic generation
BC points	Band-crossing points

Acknowledgments

AB and AF are sponsored by the Air Force Office of Scientific Research, Air Force Materials Command, USAF, under grant no F49620-99-1-0203.

References

[1] Agrawal G 1995 *Nonlinear Fiber Optics* (New York: Academic)
[2] Ashcroft N and Mermin N 1976 *Solid State Physics* (New York: Holt, Rinehart and Winston)
[3] Agrawal G and Boyd R 1992 *Contemporary Nonlinear Optics* (New York: Academic)
[4] Arnold V I 1989 *Methods of Classical Mechanics (Graduate Texts in Mathematics, vol 60)* (New York: Springer)
[5] Arnold V I, Gusein-Zade S M and Varchenko A N 1985 *Singularities of Differentiable Mappings vol 1 (Monographs in Mathematics vol 82)* (Boston, MA: Birkhäuser)
[6] Arnold V I, Gusein-Zade S M and Varchenko A N 1988 *Singularities of Differentiable Mappings vol 2 (Monographs in Mathematics vol 83)* (Boston, MA: Birkhäuser)
[7] Aközbek N and John S 1998 Optical solitary waves in two- and three-dimensional nonlinear photonic band-gap structures *Phys. Rev.* E **57** 2287–319
[8] Axmann W and Kuchment P 1999 An efficient finite element method for computing spectra of photonic and acoustic band-gap materials *J. Comput. Phys.* **150** 468–81
[9] Bulgakov A, Bulgakov S and Vazquez L 1998 Second-harmonic resonant excitation in optical periodic structures with nonlinear anisotropic layers *Phys. Rev.* E **58** 7887–98
[10] Berger V 1999 Nonlinear photonic crystals *Phys. Rev. Lett.* **81** 4136–9
[11] Bleistein N and Handelsman R A 1986 *Asymptotic Expansions of Integrals* (New York: Dover)
[12] Bogoliubov N N and Mitropolsky Y A 1961 *Asymptotic Methods in the Theory of Non-Linear Oscillations* (Delhi: Hindustan)
[13] Babin A, Mahalov A and Nicolaenko B 1997 Regularity and integrability of 3D Euler and Navier–Stokes equations for rotating fluids *Asymptotic Anal.* **15** 103–50
[14] Belyakov V 1992 *Diffraction Optics of Complex-Structured Periodic Medium* (Berlin: Springer)
[15] Butcher P and Cotter D 1990 *The Elements of Nonlinear Optics* (Cambridge: Cambridge University Press)
[16] Boyd R 1992 *Nonlinear Optics* (New York: Academic)
[17] Broderick N, Mongo T, Bennett P and Richardson D 1999 Nonlinearity in holey optical fibers: measurements and future opportunities *Opt. Lett.* **24** 1395–7
[18] Bennink R, Yoon Y, Boyd R and Sipe J 1999 Accessing the optical nonlinearity of metals with metal–dielectric photonic bandgap structures *Opt. Lett.* **24** 1416–8
[19] Centini M *et al* 1999 Despersive properties of finite, one-dimensional photonic bandgap structures: applications to nonlinear quadratic interactions *Phys. Rev.* E **60** 4891–8
[20] Dobson D 1999 An efficient method for band structure calcuations in 2D photonic crystals *J. Comput. Phys.* **149** 363–76
[21] Estrada R and Kanwal R 1994 *Asymptotic Analysis: a Distributional Approach* (Boston, MA: Birkhäuser)
[22] Fedorjuk M V 1987 *Asimptotika Integraly i Rjady* (Moscow: Nauka)
[23] Fedorjuk M V 1962 The method of stationary phase for multiple integrals *J. Commun. Math. Math. Phys.* **2** 145–50
[24] Fedorjuk M V 1977 *The Saddle-Point Method* (Moscow: Nauka)
[25] Figotin A 1999 High-contrast photonic crystals *Diffusive Waves in Complex Media* ed J P Fouque (Dordrecht: Kluwer) pp 109–36
[26] Figotin A and Godin Yu 1997 The computation of spectra of some 2D photonic crystals *J. Comput. Phys.* **136** 585–98
[27] Figotin A, Godin Yu and Vitebsky I 1998 2D tunable photonic crystals *Phys. Rev.* B **57** 2841–8
[28] Figotin A and Klein A 1997 Localization of classical waves II. Electromagnetic waves *Commun. Math. Phys.* **184** 411–41
[29] Figotin A and Klein A 1996 Localization of classical waves I. Acoustic waves *Commun. Math. Phys.* **180** 439–82
[30] Figotin A and Klein A 1998 Localization of light in lossless inhomogeneous dielectrics *J. Opt. Soc. Am.* A **15** 1423–35
[31] Figotin A and Kuchment P 1996 Band-gap structure of the spectrum of periodic dielectric and acoustic media. II. 2D photonic crystals *SIAM J. Appl. Math.* **56** 1561–620
[32] Figotin A and Kuchment P 1998 Spectral properties of classical waves in high contrast periodic media *SIAM J. Appl. Math.* **58** 683–702

[33] Felsen L and Marcuvits N 1994 *Radiation and Scattering of Waves* (Oxford: Oxford University Press, Piscataway, NJ: IEEE)
[34] Fogel I *et al* 1998 Spontaneous emission and nonlinear effects in photonic bandgap materials *Pure Appl. Opt.* **7** 393–407
[35] Jackson J 1975 *Classical Electrodynamics* (New York: Wiley)
[36] John S 1991 Localization of light *Phys. Today* (May)
[37] Joly J-L, Metivier G and Rauch J 1998 Diffractive nonlinear geometric optics with rectification *Indiana Univ. Math. J.* **47** 1167–241
[38] Donnat P, Joly J-L, Metivier G and Rauch J 1996 Diffractive nonlinear geometric optics *Séminaire sur les Équations aux Dérivées Partielles 1995–6* (Palaiseau: École Polytechnique) Exp. no XVII, 25 pp
[39] Donnat P and Rauch J 1997 Dispersive nonlinear geometric optics *J. Math. Phys.* **38** 1484–523
[40] Georgieva A, Richerbauer K T and Venakides S 1999 Wave propagation and resonance in one-dimesional nonlinear discrete periodic medium *SIAM J. Appl. Math.* **60** 272–94
[41] Fejer M M, Magel G A, Jundt D H and Byer R L 1992 Quasi-phase-matched second harmonic generation: tuning and tolerances *IEEE J. Quantum Electron.* **28** 2631
[42] Harrington R 1961 *Time-Harmonic Electromagnetic Fields* (New York: McGraw-Hill)
[43] Hattori T, Tsurumachi N and Nakatsuka H 1997 Analysis of optical nonlinearity by defect states in one-dimensional photonic crystals *J. Opt. Soc. Am.* B **14** 348–55
[44] Haus J, Viswanathan, Scalora M, Kalocsai A, Cole J and Theimer J 1998 Enhanced second-harmonic generation in media with a weak periodicity *Phys. Rev.* A **57** 2120–8
[45] Hunter J K and Keller J B 1983 Weakly nonlinear high frequency waves *Commun. Pure Appl. Math.* **36** 547–69
[46] Joly J-L, Métivier G and Rauch J 1996 Nonlinear oscillations beyond caustics *Commun. Pure Appl. Math.* **49** 443–527
[47] Joannopoulos J, Meade R and Winn J 1995 *Photonic Crystals* (Princeton, NJ: Princeton University Press)
[48] Kappeler T 1988 Multiplicities of the eigenvalues of the Schrödinger equation in any dimension *J. Funct. Anal.* **77** 346–51
[49] Kato T 1995 *Perturbation Theory for Linear Operators* (Berlin: Springer)
[50] Kevorkian J and Bosley D 1998 Multiple-scale homogenization for weakly nonlinear conservation laws with rapid spatial fluctuations *Stud. Appl. Math.* **101** 127–83
[51] Kevorkian J and Cole J 1966 *Multiple Scale and Singular Perturbation Methods* (Berlin: Springer)
[52] Kuchment P 1993 *Floquet Theory for Partial Differential Operators* (Basel: Birkhäuser)
[53] Kuchment P 1999 The mathematics of photonic crystals *Mathematical Modeling in Optical Sciences* (Philadelphia, PA: SIAM)
[54] Klein A 1999 Localization of light in randomized periodic media *Diffusive Waves in Complex Media* ed J P Fouque (Dordrecht: Kluwer) pp 73–92
[55] Koroteev N, Magnitskii S, Tarasishin A and Zheltikov A 1999 Compression of ultrashort light pulses in photonic crystals: when envelopes cease to be slow *Opt. Commun.* **159** 191–202
[56] Kryloff N and Bogoliuboff N 1947 *Introduction to Nonlinear Mechanics* (Princeton, NJ: Princeton University Press) (a free translation by Solomon Lefschetz of excerpts from two Russian monographs)
[57] Kuchment P and Kunyansky L 1999 Spectral properties of high contrast band-gap materials and operators on graphs *Exp. Math.* **8** 1–28
[58] Mills D 1991 *Nonlinear Optics* (Berlin: Springer)
[59] Mitropolskii Yu A and Nguen Van Dao 1997 *Applied Asymptotic Methods in Nonlinear Oscillations* (Dordrecht: Kluwer)
[60] Martorell J, Vilaceca R and Corbalan R 1997 Second harmonic generation in a photonic crystal *Appl. Phys. Lett.* **70** 702–4
[61] Nayfeh A 1973 *Perturbation Methods* (New York: Wiley)
[62] Nelson R and Boyd R 1999 Enhanced third-order nonlinear optical response of photonic bandgap materials *J. Mod. Opt.* **46** 1061–9
[63] Nayfeh A H and Mook D T 1976 *Nonlinear Oscillations* (New York: Wiley)
[64] Newell A C and Moloney J V 1992 *Nonlinear Optics* (Reading, MA: Addison-Wesley)
[65] Rarity J and Weisbuch C 1996 *Microcavities and Photonic Bandgaps: Physics and Applications (NATO ASI Series E, vol 324)* (Dordrecht: Kluwer)
[66] Reed M and Simon B 1978 *Analysis of Operators* vol 4 (New York: Academic)
[67] Scalora M *et al* 1997 Pulsed second-harmonic generation in nonlinear, one-dimensional, periodic structures *Phys. Rev.* A **56** 3166–74
[68] Soukoulis C 1996 *Photonic B and Gap Materials (NATO ASI Series E, vol 315)* (Dordrecht: Kluwer)
[69] Saleh B and Teich M 1991 *Fundamentals of Photonics* (New York: Wiley)

[70] Sauter E G 1996 *Nonlinear Optics* (New York: Wiley)
[71] Stein E 1993 *Harmonic Analysis. Real-Variable Methods, Orthogonality and Oscillatory Integrals* (Princeton, NJ: Princeton University Press)
[72] Shubin M 1994 *Partial Differential Equations, VII. Spectral Theory of Differential Operators* (Berlin: Springer)
[73] Tarasishin A, Zheltikov A and Magnitskii S 1999 Matched second-harmonic generation of ultrasoft laser pulses in photonic crystals *JETP Lett.* **70** 819–25
[74] Teytel M 1999 How rare are multiple eigenvalues? *Commun. Pure Appl. Math.* **52** 917–34
[75] Tran P 1997 Optical limiting and switching of short pulses by use of a nonlinear photonic bandgap structures with a defect *J. Opt. Soc. Soc.* B **14** 2589–95
[76] Uhlenbeck K 1976 Generic properties of eigenfunctions *Am. J. Math.* **98** 1059–78
[77] Villeneuve P and Piché M 1994 Photonic B and gaps in periodic dielectric structures *Prog. Quantum Electron.* **18** 153–200
[78] Whitham G 1974 *Linear and Nonlinear Waves* (New York: Wiley)
[79] Winn J, Fan S and Joannopoulos J 1999 Interband transitions in photonic crystals *Phys. Rev.* B **59** 1551–4
[80] Wang Z *et al* 1997 Nonlinear transmission resonance in a two-dimensional periodic structure with photonic B and gap *Phys. Rev.* B **56** 9185–8
[81] Yariv A and Yeh P 1984 *Optical Waves in Crystals* (New York: Wiley)
[82] Zhu Y and Ming N 1999 Dielectric superlattices for nonlinear optical effects *Opt. Quantum Electron.* **31** 1093–128