DIFFRACTION OF BLOCH WAVES

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Outline

Part I. The (long) pretalk.

1. Short wave asymptotics in $\mathbb{R}^{1+N}$.

2. Exactly periodic media.

3. Important consequences for physics/technology.

Part II. The (short) talk.

4. Not quite periodic media.

5. The ray average hypothesis.

6. A general result.

Short Wavelength Wave Packets

This talk is about the propagation of wave of short wavelength,

$$u^\epsilon \;\sim\; e^{2\pi i(\tau(\xi)t + x.\xi)/\epsilon}\, a(t,x)\,, \qquad := \text{wave packets}$$

Example. D'Alembert's wave equation,

$$\Box\, u(t,x) \sim 0\,, \qquad \Box := \partial_t^2 - \sum_{j=1}^{N} \partial_j^2\,,$$

$$\partial_j := \partial/\partial x_j\,, \qquad \tau(\xi)^2 = |\xi|^2, \quad \tau = \pm|\xi|.$$

Question. Why short wavelength?

Answer #1. Oscillation determines a velocity, For $\Box$,

group velocity $= -\nabla_\xi \tau = \mathcal{V} = \mp\xi/|\xi|\,, \quad \big(\partial_t + \mathcal{V}.\partial_x\big)a \;=\; 0\,.$

Answer #2. Rectilinear propagation. A solution which is not short wavelength will bend around an obstacle. Short wavelength solutions will, to leading order, propagate on straight lines leading to a shadow. Figure at blackboard.

Geometric Optics in Physics and Mathematics

The law of rectilinear propagation is an approximation in the limit of small wavelength.

Similarly for the laws of reflection and refraction of geometric optics.

The physical theory of geometric optics is a short wavelength approximation to the Maxwell's equations.

We use the word geometric optics to be synonymous with short wavelength asymptotics for partial differential equations.

Derivation of Rectilinear Propagation

Solutions which are superpositions of plane waves with wave number ξ/ϵ satisfying $\xi/\epsilon - \underline{\xi}/\epsilon = O(1)$,

$$u^\epsilon(t,x) = \int e^{2\pi i(\tau(\xi)t + x.\xi)/\epsilon}\, \alpha\Big(\frac{\xi - \underline{\xi}}{\epsilon}\Big)\, d\xi, \quad \alpha \in C_0^\infty(\mathbb{R}^N).$$

Change variable,

$$\frac{\xi - \underline{\xi}}{\epsilon} := \zeta, \qquad \xi = \underline{\xi} + \epsilon\zeta, \qquad d\xi = \epsilon^N d\zeta.$$

$$\int e^{2\pi i(\tau(\underline{\xi}+\epsilon\zeta)t + x.(\underline{\xi}+\epsilon\zeta))/\epsilon}\, \alpha(\zeta)\, \epsilon^N\, d\zeta$$

Taylor approximation to order 1. Divide by ϵ^N,

$$e^{2\pi i(\tau(\underline{\xi})t + \underline{\xi}.x)/\epsilon} \int e^{2\pi i(x - \mathcal{V}t).\zeta}\, \alpha(\zeta)\, d\zeta = e^{2\pi i S/\epsilon}\, a(x - \mathcal{V}t),$$

$$S := \tau(\underline{\xi})t + \underline{\xi}.x, \qquad a(x) := \int e^{2\pi i x.\zeta}\, \alpha(\zeta)\, d\zeta\,.$$

Derivation of Diffractive Geometric Optics

$$e^{2\pi i S/\epsilon} \int e^{2\pi i((\tau(\underline{\xi}+\epsilon\zeta)-\tau(\underline{\xi}))t/\epsilon + x.\zeta)}\ \alpha(\zeta)\ d\zeta$$

Taylor to order 2. $e^{2\pi i S/\epsilon}$ times

$$\int e^{2\pi i(x-\mathcal{V}t).\zeta}\ e^{2\pi i \nabla_\xi^2 \tau(\underline{\xi})(\zeta,\zeta)\epsilon t}\ \alpha(\zeta)\ d\zeta = a(x-\mathcal{V}t, \epsilon t),$$

$$a(\mathcal{T}, x) \ = \ \int e^{2\pi i x.\zeta}\ e^{2\pi i \nabla_\xi^2 \tau(\underline{\xi})(\zeta,\zeta)\mathcal{T}}\ \alpha(\zeta)\ d\zeta$$

$$\partial_{\mathcal{T}} a \ = \ 2\,\pi\, i\, \nabla_\xi^2 \tau(\underline{\xi})(\partial_x, \partial_x) a\,.$$

Schrödinger in slow time $\mathcal{T}$. Accurate to $t \sim 1/\epsilon$.

Captures decay and spreading. Diffractive geometric optics.

The (nonlinear) Schrödinger equation for lasers is diffractive geometric optics for a (nonlinear) Maxwell equation.

Purely Periodic Media

$$u_{tt} \ - \ \operatorname{div} A(x) \operatorname{grad} u \ = \ 0$$

$\partial_x^\beta A \in L^\infty$, $A_{ij}(x)$ positive definite, 1-periodic in x.

$$\text{"any"} \quad u(x) \ = \ \int e^{2\pi i x\xi} \ a(\xi) \ d\xi \qquad \big(\text{Fourier}\big)$$

Identify ξ modulo $\mathbb{Z}^N$,

$$\xi = \theta + n, \qquad n \in \mathbb{Z}^N, \quad \theta \in [0,1[^N$$

$$\begin{aligned} u \ &= \ \int_{[0,1[^N} \sum_n a(\theta + n) \ e^{2\pi i x(\theta+n)} \ d\theta \\ &= \ \int_{[0,1[^N} e^{2\pi i \theta . x} g(x,\theta) \ d\theta, \quad g \text{ periodic in } x, \ \ (\text{pd.} = 1) \end{aligned}$$

Def. *g is θ-periodic iff $e^{-2\pi i\theta . x} g$ is periodic.*

Bloch Spectral Theory

Every u is a sum over $\theta \in [0,1[^N$ of θ-periodic functions.

$$g \text{ is } \theta\text{−periodic} \quad \Rightarrow \quad \partial_x g \text{ is } \theta\text{−periodic.}$$

$$g \text{ is } \theta\text{−periodic and } a \text{ is periodic} \quad \Rightarrow \quad a\, g \text{ is } \theta\text{−periodic}$$

$$-\mathrm{div}\, A(x)\, \mathrm{grad} \Big\{\theta\text{−periodic}\Big\} \subset \Big\{\theta\text{−periodic}\Big\}$$

Selfadjoint. Compact resolvent (ellipticity). For $\theta \neq 0$,

Eigenvalues and normalized eigenfunctions,

$$0 < \lambda_1(\theta) \le \lambda_2(\theta) \le \cdots \le \lambda_n(\theta) \le \quad \cdots \quad \to \quad +\infty.$$

$e^{2\pi i\theta.x}\,\psi_n(x,\theta)$, ψ_n periodique.

$$-\mathrm{div}\, A(x)\, \mathrm{grad}\Big(e^{2\pi i\theta.x}\,\psi_n(x,\theta)\Big) = \lambda_n(\theta)\Big(e^{2\pi i\theta.x}\,\psi_n(x,\theta)\Big).$$

Spectrum is $\cup_n \lambda_n\big([0,1]^N\big)$. Closed intervals called *bands*. Separated by open *gaps* (which may be absent).

Solutions of $v_{tt} - \mathrm{div}\, A\, \mathrm{grad}\, v = 0$ are superpositions in θ, n of the **Bloch plane waves**

$$e^{2\pi i(\omega t+\theta.x)}\,\psi_n(x,\theta), \qquad 4\pi^2\omega^2 = \lambda_n(\theta) \quad (\textbf{Bloch disp rel})$$

Three Regimes for Waves in Periodic Media

Consider a periodic medium with period $\epsilon << 1$. Waves with wavelength ℓ.

For long waves $\ell >> \epsilon$, the medium is approximated by a homogenized medium which does not vary on the small scale. The effective coefficients are computed as in the static (elliptic) case.

The dispersion relation and group velocities are those of the homogenized equations. For a second order scalar equation, the dispersion relation is quadratic in frequency and wave number.

If $\ell << \epsilon$, then from the point of view of the wave, the medium is slowly varying and the approximations of standard geometric optics are appropriate. The group velocities vary on the short scale ϵ.

We discuss the resonant case, $\ell \sim \epsilon$. A principal interest is that the dispersion relation can be very different from the preceding regimes.

Bloch Wave Packets

Fix $\underline{\theta}$, and $\lambda_n(\underline{\theta}) \neq 0$ a **simple** eigenvalue, and ω satisfying the Bloch dispersion relation. ω and ψ_n are analytic in θ on a neighborhood of $\underline{\theta}$.

For an ϵ-periodic medium, have exact plane waves of wavelength ϵ,

$$e^{2\pi i(\omega(\theta)t+\theta.x)/\epsilon}\ \psi_n(x/\epsilon,\theta).$$

Superposition yields wave packets,

$$\int_{[0,1[^N} e^{2\pi i(\omega(\theta)t+\theta.x)/\epsilon}\ \psi_n(x/\epsilon,\theta)\ \alpha\Big(\frac{\theta-\underline{\theta}}{\epsilon}\Big)\,d\theta, \quad \alpha\in C_0^\infty$$

Introduce $\zeta := (\theta-\underline{\theta})/\epsilon$. Change variable. Taylor of order 1 yields,

$$e^{2\pi i(\omega(\underline{\theta})t+\underline{\theta}.x)/\epsilon}\ \psi_n(x/\epsilon,\underline{\theta})\ \int_{[0,1[^N} e^{2\pi\zeta.(x-\mathcal{V}t)}\ \alpha(\zeta)\,d\zeta + O(\epsilon),$$

$$\mathcal{V} := -\nabla_\theta\omega(\underline{\theta})\,.$$

The leading term is

$$e^{2\pi i(\omega(\underline{\theta})t+\underline{\theta}.x)/\epsilon}\ \psi_n(x/\epsilon,\underline{\theta})\ a(x-\mathcal{V}t)\,.$$

A Bloch plane wave times a slowly varying envelope which is transported at the group velocity $\mathcal{V}$. This is a **Bloch wave packet**. *N.B. resonant scaling.*

Five Important Conseqeuces

1. Designer materials. Wave packets of wavelength $\sim \epsilon$ in an ϵ-periodic medium have a dispersion relation $4\pi\omega^2 = \lambda_n(\theta)$ which does not resemble the dispersion relation of the original problem.

Can engineer periodic materials with properties **radically** different than those of the constituent materials.

The is **not** the case for the standard situation $\lambda >> \epsilon$ which leads to homogenization and properties which are different but not radically so.

2. Slow light For the original equations, group velocities are bounded below by a strictly positive quantity.

For Bloch wave packets, one can have $\mathcal{V} = 0$.

For example if $\lambda_n(\underline{\theta})$ is a value at the edge of a band. Then λ_n has a max or min so $\mathcal{V} = \nabla_\theta \lambda_n$ vanishes.

Can construct photonic materials which radically slow light. Challenge: completely optical computers.

3. Forbidden temporal frequencies. Suppose that the interval I is in a *gap* in the spectrum of $-\mathrm{div}\, A(x)\, \mathrm{grad}$.

If $u(t,x)$ solves the ϵ-periodic wave equation. Then

$$\int_{-\infty}^{\infty} e^{-2\pi i\tau t/\epsilon}\; u(t,x)\; dt$$

vanishes for $\tau \in I$. This is a forbidden region for the temporal Fourier transform.

If a wave packet from outside a large piece of ϵ-periodic medium arrives with temporal frequency in the forbidden region, it is totally reflected (to leading order).

4. Photonic crystal fibers. Using periodic materials, large and therefore large capacity monomode optical fibers have been constructed. This is important for the high energy laser projects.

5. Enhanced dispersion. The propagation for times $t \sim 1/\epsilon$ of wavelength $\sim \epsilon$ wave packets in perfectly ϵ-periodic media is to leading order,

$$e^{2\pi i(\omega(\underline{\theta})+\underline{\theta}.x)/\epsilon}\ \psi_n(x/\epsilon, \underline{\theta})\ a(\epsilon t, x - \mathcal{V}t)$$

with $a(\mathcal{T}, x)$ determined from its initial data by

$$c\, i\, \partial_{\mathcal{T}} a \ = \ \nabla^2_\theta \omega(\underline{\theta})(\partial_x, \partial_x) a\,.$$

The rank of $\nabla^2_\theta \omega(\underline{\theta})$ is generically equal to N. The decay of wave packets is more rapid, $\sim t^{-N/2}$.

For constant coefficient div A grad , waves decay at the slower rate $t^{(1-N)/2}$.

From the fact that the hessian of the dispersion relation has rank $N-1$.

End of Pretalk

Some Harder Problems

It is **very** hard to make perfectly or even nearly so, periodic materials.

It is important to understand slightly nonperiodic materials. In particular the impact of the ”impurities”.

Fourier and Bloch transforms are no help.

It is important to understand weak random perturbations of periodic media.

For fibers and other applications, it is important to understand propagations over long time intervals.

Here is the main result in that vein that we have proved.

$$P^\epsilon(t,x,\partial_{t,x})\, u^\epsilon \;:=\; \frac{\partial^2 u^\epsilon}{\partial t^2} \;-\; \operatorname{div}\,(A^\epsilon\, \operatorname{grad}\, u^\epsilon) = 0$$

where A^ϵ are oscillating coefficients of the form

$$A^\epsilon(x) \;=\; A_0\,(x/\epsilon) + \epsilon^2 A_1\,(t,x,x/\epsilon)\,,$$

The functions $A_0(y)$ and $A_1(t,x,y)$ are smooth symmetric matrix valued functions on $\mathbb{T}^N_y$ and $\mathbb{R}^{1+N}\times\mathbb{T}^N_y$ respectively. For each α, j,

$$\big\{\partial^\alpha_{t,x,y}\rho_j\,,\,\partial^\alpha_{t,x,y}A_j\big\} \;\in\; L^\infty(\mathbb{R}^{1+N}_{t,x}\times\mathbb{T}^N_y)\,.$$

There is a constant $\delta>0$ so that for all y,

$$A_0(y) \;\geq\; \delta\, I \;>\; 0\,.$$

The $O(\epsilon^2)$ perturbations affect the leading term of the approximate solutions for $t=O(1/\epsilon)$.

The Ray Average Hypothesis

Define

$$\gamma(t,x) \ := \ \int_{\mathbb{T}^N_y} \overline{\psi}_n(y) \Big(-\operatorname{div}_y A_1\,(t,x,y)\operatorname{grad}_y \Big)\,\psi_n(y)\ dy\,.$$

First assume that the ray averages

$$\tilde{\gamma}(x) \ := \ \lim_{T\to+\infty} \frac{1}{T}\int_0^T \gamma(t, x+\mathcal{V}t)\ dt$$

exist. This existence is equivalent to the fact that the solution of the transport equation

$$(\partial_t \ + \ \mathcal{V}.\partial_x)g \ = \ \gamma(t,x) - \tilde{\gamma}(x-\mathcal{V}t),$$

is sublinear in time.

We make the following "ray average hypothesis". For all α, the solution $g_\alpha(t,x)$ of

$$\Big(\partial_t \ + \ \mathcal{V}.\partial_x\Big)g_\alpha \ = \ \partial^\alpha_{t,x}\big(\gamma(t,x) - \tilde{\gamma}(x-\mathcal{V}t)\big), \quad g_\alpha\big|_{t=0} \ = \ 0,$$

satisfies $g_\alpha \in L^\infty([0,\infty[\times\mathbb{R}^N)$.

This hypothesis is satisfied: **i.** If g is periodic with arbitrary period. **ii.** For almost all quasiperiodic γ and group velocities $\mathcal{V}$ (small divisors).

Bloch wave packet initial data,

$$u^\epsilon(0,x) \;=\; b(x)\; e^{2\pi i x.\underline{\theta}/\epsilon}\; \psi_n(x/\epsilon, \underline{\theta}),$$

$$\partial_t u^\epsilon(0,x) \;=\; \frac{c(x)}{\epsilon}\, e^{2\pi i x.\underline{\theta}/\epsilon}\; \psi_n(x/\epsilon, \underline{\theta}).$$

$\omega^\pm :=$ the roots of the dispersion relation. $S^\pm := \omega^\pm t + \underline{\theta} x$.

$$\tilde{w}_0^\pm(\mathcal{T}, x, y) := a^\pm(\mathcal{T}, x)\; \psi_n(y, \underline{\theta})$$

$$\left(4\pi i \partial_{\mathcal{T}} \;\mp\; \nabla_\theta^2 \omega^\pm(\partial_x, \partial_x) + \frac{\tilde{\gamma}(x)}{\omega^\pm}\right) a^\pm \;=\; 0$$

$$a^+|_{\mathcal{T}=0} \;=\; \frac{b(x)}{2} + \frac{c(x)}{4\pi i \omega^+}\,, \qquad a^-|_{\mathcal{T}=0} \;=\; \frac{b(x)}{2} - \frac{c(x)}{4\pi i \omega^-}\,,$$

Theorem. *Assume the ray average hypothesis for both group velocities* $\pm\mathcal{V}$, *and,* $b, c \in H^\infty(\mathbb{R}^N)$. *Let*

$$v^\epsilon(t,x) \;:=\; \sum_\pm\; e^{2\pi i S^\pm(t,x)/\epsilon}\; \tilde{w}_0^\pm(\epsilon t, x \pm \mathcal{V}t, x/\epsilon).$$

Then v^ϵ *is an approximate solution with relative error* $O(\epsilon)$. *Precisely, for any* $T > 0$ *the derivatives of order* ≤ 1 *satisfy,*

$$\sup_{0 \leq t \leq T/\epsilon}\; \sup_{|\alpha| \leq 1}\; \left\| (\epsilon\, \partial_{t,x})^\alpha \big(u^\epsilon(t) \;-\; v^\epsilon(t)\big) \right\|_{L^2(\mathbb{R}^N)} \;\leq\; C\,\epsilon\,.$$

Four Remarks on the Proof

1. (WKB) A three term three scale approximate solution is constructed,

$$v^\epsilon(t,x) \;:=\; e^{2\pi i S/\epsilon}\, W^\epsilon(\epsilon t, x - \mathcal{V}t, x/\epsilon)\,,$$

$$W^\epsilon(\mathcal{T},x,y) \;:= \\ w_0(\mathcal{T},x,y) + \epsilon\, w_1(\mathcal{T},x,y) + \epsilon^2\, w_2(\mathcal{T},x,y)\,,$$

Apply differential operator and set coefficients of powers of ϵ equal to zero.

2. (JMR). An operator neither injective nor surjective appears. The kernel and range are complementary. Each equation is projected on the kernel and range.

The projection methods are new for this Bloch spectral context.

The "algebraic lemmas of gemetric optics" are particularly interesting.

3. The construction of the first corrector in the proof fails badly when the ray average hypothesis is not satisfied. This may signal an interesting instability. Or it may mean that there is a better *ansatz*. A voir.

4. The gradient estimate is easy. The L^2 estimate is not.

Ideas to Remember

Physical geometric optics is a two scale asymptotic limit Mawell's equations.

The derivation of rectilinear propagation is surprisingly easy.

For two scale problems it takes at least two term approximate solution to get a small residual.

For three scale problems it takes at least three term approximate solution to get a small residual.

The (nonlinear) Schrödinger equations of laser physics are a three scale limit of Maxwell.

Spectral gaps and total reflection for periodic media.

In the resonant regime $\ell \sim \epsilon$ anormal dispersion relations occur (slow light).

The asymptotic theory in that regime is in good shape for $t \sim 1$. It is OK by still has challenges for the scale $t \sim 1/\epsilon$ of diffractive geometric optics.