Dynamics of wavepackets in crystals by multiscale analysis

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Motivation: the spin Hall effect of light

Causes a linearly polarized beam of light (wavelength λ) in a gradient index medium (smoothly varying refractive index n(x), λ ≪ scale of variation of the medium) to split into its constituent circularly polarized parts:



- Splitting $\Delta \propto$ light wavelength λ
- Experimental verification: K. Bliokh et al. 'Geometrodynamics of spinning light' Nature Photonics 2008

Ray optics doesn't explain spin Hall effect of light

- \blacktriangleright Effect appears in the regime: wavelength $\lambda\ll$ scale of variation of the medium
- Ray optics for a beam: center of mass q(t) and averaged wavevector p(t) of a beam satisfy classical equations:

$$\dot{\boldsymbol{q}}(t) = \hat{\boldsymbol{p}}(t)$$

 $\dot{\boldsymbol{p}}(t) = \nabla n(\boldsymbol{q}(t))$

 Polarization independent, cannot explain spin Hall effect of light

Corrected ray optics equations

Resolution: corrected ray equations, include an *anomalous* velocity proportional to λ:

$$egin{aligned} \dot{m{q}}(t) &= \hat{m{p}}(t) + \lambda \dot{m{p}}(t) imes \mathcal{F}_{\sigma}(m{p}(t)) \ \dot{m{p}}(t) &=
abla n(m{q}(t)) \end{aligned}$$

where $\sigma = \pm$ denotes the handedness of the polarization.

$$egin{aligned} \mathcal{F}_{\sigma}(oldsymbol{p}) &:=
abla_{oldsymbol{p}} imes \langle oldsymbol{e}_{\sigma}(oldsymbol{p}) | i
abla_{oldsymbol{p}} oldsymbol{e}_{\sigma}(oldsymbol{p})
angle \ &= \sigma rac{oldsymbol{p}}{|oldsymbol{p}|^3} \end{aligned}$$

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is the *Berry curvature* associated with each circular polarization state e_{σ} .

Ray optics limit analogous to the semiclassical limit of quantum mechanics

- Semiclassical limit of Schrödinger's equation with potential W(q):
 - \blacktriangleright seek wavepacket solutions, wavelength \ll scale of variation of potential
 - ► center of mass and average wavevector of a wavepacket follow classical trajectories of $\mathcal{H} = \frac{1}{2} |\mathbf{p}|^2 + W(\mathbf{q})$
 - justify by 'WKB ansatz':

$$\psi(\mathbf{x},t) = e^{i\phi(\mathbf{x},t)/\hbar} a(\mathbf{x},t) + O(\hbar)$$

- Ray optics limit of Maxwell's equations in isotropic gradient-index media:
 - wavelength \ll scale of variation of refractive index n(q)
 - ► center of mass and average wavevector of a beam follow classical trajectories of H = |p| - n(q)
 - justify by 'ray optics ansatz':

$$\boldsymbol{E}(\boldsymbol{x},t) = e^{i\phi(\boldsymbol{x},t)/\lambda} \sum_{\sigma \in \pm} a_{\sigma}(\boldsymbol{x},t) \boldsymbol{e}_{\sigma}(\nabla \phi) + O(\lambda)$$

Ray optics with polarization analogous to semiclassical quantum mechanics in a crystal

- Beam polarization vector e(p) must be transverse to the wavevector: p · e(p) = 0.
- Analogous to semiclassical quantum mechanics with a periodic background V(x):

$$-rac{1}{2}\Delta_{\mathbf{x}}
ightarrow -rac{1}{2}\Delta_{\mathbf{x}} + V(\mathbf{x}),$$

 $orall \mathbf{v} \in \Lambda : V(\mathbf{x} + \mathbf{v}) = V(\mathbf{x})$

Wavepacket solutions modulated *Bloch waves* associated with a Bloch band $E_n(\mathbf{p})$, with role of wavevector played by pseudo-momentum.

- ► 3-fold degeneracy of polarization condition at *p* = 0 ⇒ Berry curvature ⇒ spin Hall effect of light.
- ► Bloch bands $E_n(\mathbf{p})$ may be degenerate \implies Berry curvature \implies anomalous velocity

Outline of talk

- 'Semiclassical wavepacket' asymptotic solutions of Schrödinger's equation with a periodic background and describe range of validity of the asymptotics
- Corrections to the asymptotics which describe anomalous velocity due to Berry curvature (analogous to the spin Hall effect of light)

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- Landau-Zener Bloch band crossing interactions
- Ongoing work/future directions

Model: electron dynamics in crystals

Electrons in solids under the influence of an external potential which is *slowly-varying* relative to the lattice constant can be modelled as *wavepackets* which are localized relative to the varying potential but also spread over a few lattice periods



¹Solid State Physics, Ashcroft and Mermin (1976). < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) < (□) <

Model: electron dynamics in crystals

Non-dimensionalized model Schrödinger equation:

$$i\partial_t\psi^\epsilon = -\frac{1}{2}\Delta_{\mathbf{x}}\psi^\epsilon + U(\mathbf{x},\epsilon\mathbf{x})\psi^\epsilon$$

where two-scale potential U is periodic with respect to the lattice of ions Λ in its first argument:

$$\forall \mathbf{v} \in \Lambda, U(\mathbf{x} + \mathbf{v}, \mathbf{X}) = U(\mathbf{x}, \mathbf{X})$$

Focus on simpler case:

$$U(\mathbf{x}, \epsilon \mathbf{x}) = V(\mathbf{x}) + W(\epsilon \mathbf{x})$$

We consider the limit e ≪ 1: the external potential W(ex) slowly varying on the scale of the lattice period

Recap: spectral theory of periodic operators

Recall the spectral theory of the operator with periodic potential obtained by taking \(\epsilon = 0\) (no applied field):

$$h := -\frac{1}{2}\Delta_{\boldsymbol{x}} + V(\boldsymbol{x})$$

 $\forall \boldsymbol{v} \in \Lambda, V(\boldsymbol{x} + \boldsymbol{v}) = V(\boldsymbol{x})$

Bloch's theorem: suffices to study the eigenvalue problem on a single cell with *p*-pseudo-periodic boundary conditions:

$$h \Phi(\mathbf{x}; \mathbf{p}) = E(\mathbf{p}) \Phi(\mathbf{x}; \mathbf{p})$$
$$\forall \mathbf{v} \in \Lambda, \Phi(\mathbf{x} + \mathbf{v}) = e^{i\mathbf{p} \cdot \mathbf{v}} \Phi(\mathbf{x}; \mathbf{p})$$

symmetry of boundary condition \implies we may restrict p to a primitive cell of the reciprocal lattice: first Brillouin zone ${\cal B}$

 Fixed *p*, known as pseudo-momentum, self-adjoint elliptic eigenvalue problem ⇒ discrete real spectrum:

$$E_1(\boldsymbol{p}) \leq E_2(\boldsymbol{p}) \leq \ldots \leq E_n(\boldsymbol{p}) \leq \ldots$$

Spectral theory of periodic operators

- Maps p ∈ B → E_n(p) ∈ ℝ are the Bloch band dispersion functions
- ► The set of 'Bloch waves' are a basis (in L²(ℝ^d)) of eigenfunctions of h = -¹/₂Δ_x + V(x):

$$\left\{\Phi_n(\boldsymbol{x};\boldsymbol{p}):=e^{i\boldsymbol{p}\cdot\boldsymbol{x}}\chi_n(\boldsymbol{x};\boldsymbol{p}),n\in\mathbb{N},\boldsymbol{p}\in\mathcal{B}
ight\}$$

 $\chi_n(\mathbf{x}; \mathbf{p})$ satisfies another self-adjoint elliptic eigenvalue problem with periodic boundary conditions on a single cell

► The spectrum of *h* is then the union of real intervals swept out by the Bloch band dispersion functions E_n(**p**)

Semiclassical re-scaling

Our model is:

$$i\partial_t\psi^\epsilon = -\frac{1}{2}\Delta_{\mathbf{x}}\psi^\epsilon + V(\mathbf{x})\psi^\epsilon + W(\epsilon\mathbf{x})\psi^\epsilon$$

It will be convenient to work with the 'semiclassical re-scaling':

$$\begin{aligned} \mathbf{x}' &:= \epsilon \mathbf{x}, t' := \epsilon t, \\ \psi^{\epsilon'}(\mathbf{x}', t') &:= \psi^{\epsilon}(\mathbf{x}, t). \end{aligned}$$

After dropping the primes we obtain:

$$i\epsilon\partial_t\psi^\epsilon = -\epsilon^2 \frac{1}{2}\Delta_{\mathbf{x}}\psi^\epsilon + V\left(\frac{\mathbf{x}}{\epsilon}\right)\psi^\epsilon + W(\mathbf{x})\psi^\epsilon$$

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Theorem (Carles-Sparber 2008, Hagedorn 1980)

Let $(\mathbf{p}(t), \mathbf{q}(t))$ denote classical trajectories generated by the Bloch band Hamiltonian $\mathcal{H} = E_n(\mathbf{p}) + W(\mathbf{q})$, and assume the band E_n is isolated at each $\mathbf{p}(t)$:

$$\forall t \geq 0, E_{n-1}(\boldsymbol{p}(t)) < E_n(\boldsymbol{p}(t)) < E_{n+1}(\boldsymbol{p}(t)).$$

Then there exists a solution $\psi^{\epsilon}(\mathbf{x}, t)$ of the PDE:

$$i\epsilon\partial_t\psi^\epsilon = -\epsilon^2 \frac{1}{2}\Delta_{\mathbf{x}}\psi^\epsilon + V\left(\frac{\mathbf{x}}{\epsilon}\right)\psi^\epsilon + W(\mathbf{x})\psi^\epsilon$$

which is asymptotic as $\epsilon \downarrow 0$ to a 'semiclassical wavepacket' up to 'Ehrenfest time' $t \sim \ln 1/\epsilon$:

$$\begin{split} \psi^{\epsilon}(\mathbf{x},t) &= \\ \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{-i\mathbf{p}(t)\cdot\mathbf{q}(t)/\epsilon} a\left(\frac{\mathbf{x}-\mathbf{q}(t)}{\epsilon^{1/2}},t\right) e^{i\mathbf{p}(t)\cdot\mathbf{x}/\epsilon} \chi_n\left(\frac{\mathbf{x}}{\epsilon};\mathbf{p}(t)\right) \\ &+ O_{L^2(\mathbb{R}^d)}(\epsilon^{1/2} e^{Ct}). \end{split}$$

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Precise interpretation of functions $(\boldsymbol{q}(t), \boldsymbol{p}(t))$

Writing the solution in terms of the multiscale variables:

$$\psi^{\epsilon}(\mathbf{x},t) = \left. \tilde{\psi}^{\epsilon}(\mathbf{y},\mathbf{z},t) \right|_{\mathbf{y} = \frac{\mathbf{x} - \mathbf{q}(t)}{\epsilon^{1/2}}, \mathbf{z} = \frac{x}{\epsilon}} + O_{L_{\mathbf{x}}^{2}(\mathbb{R}^{d})}(\epsilon^{1/2})$$

q(t), p(t) nothing but the center of mass and expected pseudo-momentum of the wavepacket, to leading order in $\epsilon^{1/2}$:

$$\begin{aligned} \boldsymbol{\mathcal{Q}}^{\epsilon}(t) &:= \int_{\mathbb{R}^d} \boldsymbol{x} |\tilde{\psi}^{\epsilon}(\boldsymbol{y}, \boldsymbol{z}, t)|_{\boldsymbol{y}=\frac{\boldsymbol{x}-\boldsymbol{q}(t)}{\epsilon^{1/2}}, \boldsymbol{z}=\frac{\boldsymbol{x}}{\epsilon}}^2 \, \mathrm{d}\boldsymbol{x} \\ &= \boldsymbol{q}(t) + O(\epsilon^{1/2}) \\ \boldsymbol{\mathcal{P}}^{\epsilon}(t) &:= \int_{\mathbb{R}^d} \overline{\tilde{\psi}^{\epsilon}(\boldsymbol{y}, \boldsymbol{z}, t)} (-i\epsilon^{1/2} \nabla_{\boldsymbol{y}}) \tilde{\psi}^{\epsilon}(\boldsymbol{y}, \boldsymbol{z}, t) \Big|_{\boldsymbol{y}=\frac{\boldsymbol{x}-\boldsymbol{q}(t)}{\epsilon^{1/2}}, \boldsymbol{z}=\frac{\boldsymbol{x}}{\epsilon}}^2 \, \mathrm{d}\boldsymbol{x} \\ &= \boldsymbol{p}(t) + O(\epsilon^{1/2}) \end{aligned}$$

$O(\epsilon)$ corrections to dynamics of observables

Expect correction to equations of motion of center of mass and expected pseudo-momentum due to Berry curvature of Bloch band ∝ wavelength *ϵ*, analogous to the spin Hall effect of light²

²M. C. Chang and Q. Niu, 'Berry phase, hyperorbits, and the Hofstader's Spectrum' Phys. Rev. Lett. 199 Phys. Rev. Lett. 1995

Theorem (Watson-Weinstein-Lu 2016)

1) The observables $Q^{\epsilon}(t)$ and $\mathcal{P}^{\epsilon}(t)$, the center of mass and average pseudo-momentum, satisfy the equations of motion:

$$\begin{split} \dot{\boldsymbol{\mathcal{Q}}}^{\epsilon}(t) &= \nabla_{\boldsymbol{\mathcal{P}}^{\epsilon}} E_n(\boldsymbol{\mathcal{P}}^{\epsilon}(t)) + \epsilon \boldsymbol{\mathcal{C}}_1[\boldsymbol{a}^{\epsilon}](t) \\ &- \epsilon \dot{\boldsymbol{\mathcal{P}}}^{\epsilon}(t) \times \boldsymbol{\mathcal{F}}_n(\boldsymbol{\mathcal{P}}^{\epsilon}(t)) + O(\epsilon^{3/2}) \\ \dot{\boldsymbol{\mathcal{P}}}^{\epsilon}(t) &= - \nabla_{\boldsymbol{\mathcal{Q}}^{\epsilon}} W(\boldsymbol{\mathcal{Q}}^{\epsilon}(t)) + \epsilon \boldsymbol{\mathcal{C}}_2[\boldsymbol{a}^{\epsilon}](t) + O(\epsilon^{3/2}) \end{split}$$

where $\mathcal{F}_n(\mathcal{P}^{\epsilon})$ is the Berry curvature of the Bloch band. $C_1[a^{\epsilon}](t), C_2[a^{\epsilon}](t)$ describe coupling to the wavepacket envelope $a^{\epsilon}(\mathbf{y}, t)$, which satisfies:

$$i\partial_{t}\boldsymbol{a}^{\epsilon}(\boldsymbol{y},t) = -\frac{1}{2}\nabla_{\boldsymbol{y}}\cdot\nabla_{\boldsymbol{\mathcal{P}}^{\epsilon}}\nabla_{\boldsymbol{\mathcal{P}}^{\epsilon}}E_{n}(\boldsymbol{\mathcal{P}}^{\epsilon}(t))\cdot\nabla_{\boldsymbol{y}}\boldsymbol{a}^{\epsilon}(\boldsymbol{y},t) \\ +\frac{1}{2}\boldsymbol{y}\cdot\nabla_{\boldsymbol{\mathcal{Q}}^{\epsilon}}\nabla_{\boldsymbol{\mathcal{Q}}^{\epsilon}}W(\boldsymbol{\mathcal{Q}}^{\epsilon}(t))\cdot\boldsymbol{y}\boldsymbol{a}^{\epsilon}(\boldsymbol{y},t) + O_{L^{2}_{\boldsymbol{y}}(\mathbb{R}^{d})}(\epsilon^{1/2})$$

Theorem (Watson-Weinstein-Lu 2016 continued)

2) After an appropriate change of variables, the coupled dynamics of $\mathcal{Q}^{\epsilon}(t), \mathcal{P}^{\epsilon}(t), a^{\epsilon}(\mathbf{y}, t)$ can be derived from the ϵ -dependent Hamiltonian:

$$\begin{aligned} \mathcal{H}^{\epsilon} &:= E_{n}(\mathcal{P}^{\epsilon}) + W(\mathcal{Q}^{\epsilon}) + \epsilon \nabla_{\mathcal{Q}^{\epsilon}} W(\mathcal{Q}^{\epsilon}) \mathcal{A}_{n}(\mathcal{P}^{\epsilon}) \\ &+ \epsilon \frac{1}{2} \int_{\mathbb{R}^{d}} \nabla_{\mathbf{y}} \overline{a^{\epsilon}(\mathbf{y}, t)} \cdot \nabla_{\mathcal{P}^{\epsilon}} \nabla_{\mathcal{P}^{\epsilon}} E_{n}(\mathcal{P}^{\epsilon}) \cdot \nabla_{\mathbf{y}} a^{\epsilon}(\mathbf{y}, t) \, d\mathbf{y} \\ &+ \epsilon \frac{1}{2} \int_{\mathbb{R}^{d}} \mathbf{y} \overline{a^{\epsilon}(\mathbf{y}, t)} \cdot \nabla_{\mathcal{Q}^{\epsilon}} \nabla_{\mathcal{Q}^{\epsilon}} W(\mathcal{Q}^{\epsilon}) \cdot \mathbf{y} a^{\epsilon}(\mathbf{y}, t) \, d\mathbf{y} + O(\epsilon^{3/2}) \end{aligned}$$

where $\mathcal{A}_n(\mathcal{P}^{\epsilon})$ is the n-th band Berry connection. The equations of motion can then be written:

$$\begin{aligned} \dot{\mathcal{Q}}^{\epsilon} &= \nabla_{\mathcal{P}^{\epsilon}} \mathcal{H}^{\epsilon} \\ \dot{\mathcal{P}}^{\epsilon} &= -\nabla_{\mathcal{Q}^{\epsilon}} \mathcal{H}^{\epsilon} \end{aligned} \qquad i\partial_{t} \mathbf{a}^{\epsilon} = \frac{\delta \mathcal{H}}{\delta \overline{\mathbf{a}^{\epsilon}}} \end{aligned}$$

Gaussian reduction of envelope equation

The equation satisfied by the wavepacket envelope:

$$\begin{split} i\partial_t a^{\epsilon}(\boldsymbol{y},t) &= -\frac{1}{2} \nabla_{\boldsymbol{y}} \cdot \nabla_{\boldsymbol{\mathcal{P}}^{\epsilon}} \nabla_{\boldsymbol{\mathcal{P}}^{\epsilon}} E_n(\boldsymbol{\mathcal{P}}^{\epsilon}(t)) \cdot \nabla_{\boldsymbol{y}} a^{\epsilon}(\boldsymbol{y},t) \\ &+ \frac{1}{2} \boldsymbol{y} \cdot \nabla_{\boldsymbol{\mathcal{Q}}^{\epsilon}} \nabla_{\boldsymbol{\mathcal{Q}}^{\epsilon}} W(\boldsymbol{\mathcal{Q}}^{\epsilon}(t)) \cdot \boldsymbol{y} a^{\epsilon}(\boldsymbol{y},t) \end{split}$$

has basis of exact solutions: e.g. time-dependent Gaussians³:

$$\begin{aligned} \mathbf{a}^{\epsilon}(\mathbf{y},t) &= \frac{1}{[\det A^{\epsilon}(t)]^{1/2}} \exp\left(-\frac{1}{2}\mathbf{y} \cdot B^{\epsilon}(t)A^{\epsilon-1}(t)\mathbf{y}\right) \\ \dot{A}^{\epsilon}(t) &= i\nabla_{\boldsymbol{\mathcal{P}}^{\epsilon}} \nabla_{\boldsymbol{\mathcal{P}}^{\epsilon}} E_{n}(\boldsymbol{\mathcal{P}}^{\epsilon})B^{\epsilon}(t) \\ \dot{B}^{\epsilon}(t) &= i\nabla_{\boldsymbol{\mathcal{Q}}^{\epsilon}} \nabla_{\boldsymbol{\mathcal{Q}}^{\epsilon}} W(\boldsymbol{\mathcal{Q}}^{\epsilon})A^{\epsilon}(t) \end{aligned}$$

³Raising and lowering operators for semiclassical wave packets, G. A. Hagedorn, Annals of Physics 1998.

Numerical simulation: $\epsilon = 0$, decoupled system

Study coupling of observables to wave-field:

- One-dimensional: d = 1
- Uniform background: $V\left(\frac{x}{\epsilon}\right) = 0$
- Gaussian envelope





Numerical simulation: $\epsilon \neq 0$, coupled system

Simulation of full coupled system:

- Wave-field coupling has destabilizing effect on periodic orbits
- ► Wavepacket may escape potential well to Q^ϵ = -∞





Band crossing dynamics in d = 1

Would like to relax the 'isolated band' assumption:

$$\forall t \geq 0, E_{n-1}(\boldsymbol{p}(t)) < E_n(\boldsymbol{p}(t)) < E_{n+1}(\boldsymbol{p}(t))$$



At crossings the Bloch band functions: *p* → *E_n(p)* are not smooth in general. In *d* = 1 there exists a 'smooth choice' of bands in a neighborhood of the crossing: *E₊(p)*, *E₋(p)*.

Theorem (Watson-Weinstein 2016)

Let $E_+(p)$, $E_-(p)$ denote smooth band functions in a neighborhood of a crossing point p^* . Let $(q_+(t), p_+(t))$ denote a classical trajectory of the +-band Hamiltonian $E_+(p) + W(q)$ which passes through the crossing point at t = 0: $p_+(0) = p^*$, $\partial_q W(q_+(0)) \neq 0$. Then, if $\psi^{\epsilon}(x, t)$ solves the PDE on the interval $t \in [-T, T]$ and is associated with the +-band at t = -T:

$$\psi^{\epsilon}(x, -T) = \epsilon^{-1/4} e^{ip_{+}(-T)(x-q_{+}(-T))/\epsilon} a_{+} \left(\frac{x-q_{+}(-T)}{\epsilon^{1/2}}, -T\right) \chi_{+} \left(\frac{x}{\epsilon}; p_{+}(-T)\right)$$

then at t = T, the wavepacket remains to leading order associated with the +-band:

 $\psi^{\epsilon}(x,T) = \epsilon^{-1/4} e^{iS(T)/\epsilon} e^{ip_{+}(T)(x-q_{+}(T))/\epsilon} a_{+} \left(\frac{x-q_{+}(T)}{\epsilon^{1/2}},T\right) \chi_{+} \left(\frac{x}{\epsilon};p_{+}(T)\right) + O_{L^{2}_{x}(\mathbb{R})}(\epsilon^{1/2})$

Theorem (Watson-Weinstein 2016 continued)

At the crossing time t = 0, a wavepacket associated with E_{-} is excited whose observables $(q_{-}(t), p_{-}(t))$ follow a classical trajectory of the band Hamiltonian $E_{-}(p) + W(q)$ with initial data:

$$egin{aligned} q_{-}(0) &= q_{+}(0) \ p_{-}(0) &= p_{+}(0) &= p^{*} \end{aligned}$$

This wavepacket has magnitude (in $L^2_x(\mathbb{R})$) proportional to $\epsilon^{1/2}$.

Remarks on band crossing result

- ► Proof is by matched asymptotic expansion: error in single-band approximation blows up as t → 0, resolution by making more general ansatz for asymptotic solution which includes contributions from the band E₋ ⇒ excited wave
- Since ∂_pE₊(p^{*}) = −∂_pE_−(p^{*}), the wavepacket 'excited' at the crossing has opposite group velocity. Call this a 'reflected wave'
- Our result can be seen as an analog of those obtained by Hagedorn⁵ in the context of Born-Oppenheimer approximation of molecular dynamics

Recap of talk

- 'Semiclassical wavepacket' asymptotic solutions of Schrödinger's equation with a periodic background
- Corrections to the asymptotics which describe anomalous velocity due to Berry curvature (analogous to the spin Hall effect of light) and particle-field coupling between physical observables and the shape of the wavepacket envelope

- Landau-Zener Bloch band crossing interactions
- Ongoing work/future directions



 Rigorous derivation of spin Hall effect for circularly polarized 'ray optics wavepackets'



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Ongoing work

• Important *non-separable* example in d = 2:

$$U(\mathbf{x}, \epsilon \mathbf{x}) = V_{h,e}(\mathbf{x}) + \kappa(\mathbf{k} \cdot \epsilon \mathbf{x}) V_{h,o}(\mathbf{x})$$

where $V_{h,e}(\mathbf{x})$, $V_{h,o}(\mathbf{x})$ have symmetry of a honeycomb lattice Λ_h , and satisfy:

$$V_{h,e}(-\mathbf{x}) = V_{h,e}(\mathbf{x}), V_{h,o}(-\mathbf{x}) = -V_{h,o}(\mathbf{x})$$

and $\kappa(\zeta)$ models a domain wall along the line $\boldsymbol{k} \cdot \boldsymbol{x} = 0$:

$$\lim_{\zeta \to -\infty} \kappa(\zeta) = -\kappa_{\infty} < 0, \\ \kappa(0) = 0, \\ \lim_{\zeta \to \infty} \kappa(\zeta) = \kappa_{\infty} > 0$$





 System shown to support robust edge states by Fefferman, Lee-Thorp and Weinstein 'Edge states in honeycomb structures', Arxiv 1506:06111



 Study semiclassical wavepackets localized near to the edge: anomalous velocity due to Berry curvature along the edge

Future directions

 Spin Hall effect in anisotropic media, biaxial crystals: dispersion surfaces conically degenerate along optic axis



- Crossing result in higher dimensions: 'smooth bands'
 E₊(p), E₋(p) in a neighborhood of the crossing may not exist
- Metamaterials: how can we generalize results when features vary over scale of the wavelength?⁶



⁶X. Yin, Z. Ye, Y. Wang,

X. Zhang 'Photonic spin Hall effect at metasurfaces' Science 2013.

Thanks for listening!

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