Wavepacket dynamics in locally periodic media
Focus: effects of Bloch band degeneracies

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September 12, 2017

Research supported in part by NSF Grants DMS-1412560 (AW & MIW) and DMS-1454939 (JL) and Simons Foundation Math + X Investigator Award #376319 (AW & MIW)
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Model of electron propagation in crystalline media with defects and of light propagation through photonic variants.
Focus: effects of eigenvalue degeneracies on wave dynamics.

2 × 2 matrix example:

\[ H(p_1, p_2) := \begin{pmatrix} 0 & p_1 + p_2 i \\ p_1 - p_2 i & 0 \end{pmatrix}, \quad E_{\pm}(p_1, p_2) = \pm \sqrt{p_1^2 + p_2^2}. \]

Eigenvalues degenerate at \( p_1 = p_2 = 0. \)
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Eigenvalues \textit{degenerate} at $p_1 = p_2 = 0$.

In periodic media wave dynamics controlled by \textit{Bloch band dispersion surfaces}. Symmetries of periodic structure \implies \textit{Bloch band degeneracies}

Example: \textit{honeycomb lattice symmetry} of graphene, gives rise to ‘Dirac points’ in band structure, \textit{transport properties}:
After introducing the model PDEs we study, I will describe in detail the following results:

1. A new Hamiltonian system controlling the dynamics of wavepackets in locally periodic media which are spectrally localized away from Bloch band degeneracies. Rich dynamics! Anomalous locality due to Berry curvature of the Bloch band and (new) 'particle-field' coupling.

2. The dynamics of a wavepacket incident on a Bloch band degeneracy in one dimension. Consistency with 'Landau-Zener' theory for the probability of an inter-band transition.

I will then discuss future directions of this work.
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Models

>Schrödinger’s equation with a real ‘two-scale’ (assume $\epsilon \ll 1$) potential $U$:

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

$x \in \mathbb{R}^d$, $d$ positive integer.
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- Assume $U$ is *locally periodic* in the sense that for each fixed $X \in \mathbb{R}^d$, $U(x, X)$ is periodic in $x$:

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

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- Example ($d = 1$): $U(x, \epsilon x) = \cos(4\pi x) + \tanh(\epsilon x) \cos(2\pi x)$
Maxwell’s equations in dimension $d = 3$:

\[
\begin{align*}
\partial_t D^\delta(x, t) &= \nabla \times H^\delta(x, t) \quad \nabla \cdot D^\delta(x, t) = 0 \\
\partial_t B^\delta(x, t) &= -\nabla \times E^\delta(x, t) \quad \nabla \cdot B^\delta(x, t) = 0,
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\]

with a ‘two-scale’ (assume $\delta \ll 1$) matrix of constitutive relations:

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\begin{pmatrix}
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▶ Vector equations $\implies$ degeneracies when periodicity trivial!
Wavepacket dynamics in locally periodic structures

- Simplest case. Schrödinger’s equation with a ‘two-scale’
  (assume $\epsilon \ll 1$) potential which may be written as a sum:

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

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

- Model of an electron in a crystal under the influence of an
  external electric field generated by $W$.

- Example ($d = 1$):
  $$U(x, \epsilon x) = 1 + \cos(4\pi x) - \cos(\epsilon x)^2$$
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Re-scale: \( x' := \epsilon x, t' := \epsilon t, \psi^{\epsilon'}(x', t') := \psi^{\epsilon}(x, t) \).

\[
i \epsilon \partial_t \psi^{\epsilon} = -\epsilon^2 \frac{1}{2} \Delta_x \psi^{\epsilon} + V\left(\frac{x}{\epsilon}\right) \psi^{\epsilon} + W(x) \psi^{\epsilon}
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\[\forall \mathbf{v} \in \Lambda, V(z + \mathbf{v}) = V(z).\]
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Seek wavepacket solutions, wavelength \( \propto \epsilon \), width \( \propto \sqrt{\epsilon} \)

\( \implies \) extended with respect to scale of periodic variation \( (\propto \epsilon) \), localized with respect to slow modulation \( (\propto 1) \):
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Seek wavepacket solutions, wavelength $\propto \epsilon$, width $\propto \sqrt{\epsilon}$

$\implies$ extended with respect to scale of periodic variation ($\propto \epsilon$), localized with respect to slow modulation ($\propto 1$):

Limit $\epsilon \downarrow 0$ a ‘non-standard’ geometric optics/WKB limit:

\[ \epsilon := \frac{\text{wavelength} \approx \text{scale of variation of } V \text{ (periodic)}}{\text{scale of variation of } W \text{ (perturbation)}} \ll 1. \]
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\( \forall \mathbf{v} \in \Lambda, \ V(\mathbf{z} + \mathbf{v}) = V(\mathbf{z}). \) (\star)

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NB multi-scale WKB ansatz breaks down near degeneracies.
Wavepacket dynamics without periodicity

► ‘Free’ case \( V = W = 0 \):

\[
i \epsilon \partial_t \psi^\epsilon = -\frac{1}{2} \epsilon^2 \Delta x \psi^\epsilon
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(F)
Wavepacket dynamics without periodicity

- ‘Free’ case $V = W = 0$:
  
  $$i\epsilon \partial_t \psi^\epsilon = -\frac{1}{2}\epsilon^2 \Delta_x \psi^\epsilon \quad \text{(F)}$$

- Has (appropriately scaled) stationary, spreading Gaussian exact solutions. Define:
  
  $$G(y, t) := \frac{1}{(1 + it)^{d/2}} \exp \left( \frac{-|y|^2}{2(1 + it)} \right)$$

  Then: $\psi^\epsilon(x, t) = \epsilon^{-d/4} G \left( \frac{x}{\epsilon^{1/2}}, t \right)$ satisfies (F).

  Pre-factor ensures $L^2$ norm preserved in the limit $\epsilon \downarrow 0$. 
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- Galilean invariance of (F) $\implies$ travelling Gaussian solutions with center at $q(t) := q_0 + p_0 t$:

\[ \psi^\epsilon(x, t) = \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{ip_0 \cdot (x - q(t))/\epsilon} G \left( \frac{x - q(t)}{\epsilon^{1/2}}, t \right) \]

for any $(q_0, p_0) \in \mathbb{R}^d \times \mathbb{R}^d$. $S(t) := \frac{1}{2} |p_0|^2 t$. 
Theorem (Hagedorn 1980, Heller 1976)

For any trajectory \((q(t), p(t))\) generated by the classical Hamiltonian \(\mathcal{H} := \frac{|p|^2}{2} + W(q)\), there exists a solution of the PDE:

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asymptotic as \(\epsilon \downarrow 0\) to a semiclassical wavepacket up to ‘Ehrenfest time’ \(t \sim \ln 1/\epsilon\):

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Envelope satisfies Schrödinger’s equation with harmonic oscillator Hamiltonian driven by \(q(t)\):

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When \(W\) quadratic, solution exact! Error \(\propto \|\partial^3_q W(q)\|_{L^\infty}\).
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When \(W\) quadratic, solution exact! Error \(\propto \|\partial_q^3 W(q)\|_{L^\infty}\). Can improve error bound: \(O_{L^2_x(\mathbb{R}^d)}(\epsilon^n e^{Ct})\), any positive integer \(n\).
Theorem \implies \text{Schrödinger’s equation with an anharmonic oscillator potential \( W \propto q^4 \), \( d = 1 \) has an approximate Gaussian solution:}

\[
\psi^\epsilon(x, t) = \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{ip(t)(x-q(t))/\epsilon} \mathcal{G}
\left(\frac{x-q(t)}{\epsilon^{1/2}}, t\right) + O_L^2(\epsilon^{1/2} e^{Ct})
\]

\( q(t), p(t) \) satisfy Hamiltonian dynamics: \( \mathcal{H} = p^2 + q^4 \).

\[
\begin{align*}
\text{Initial wavepacket} & \\
\text{center of mass } Q & 
\end{align*}
\]

\[
\begin{align*}
\text{Wavepacket ansatz does not capture dynamics of PDE for } t \text{ large.}
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\]
Wavepacket dynamics in locally periodic media

\[ i\epsilon \partial_t \psi^\epsilon = -\epsilon^2 \frac{1}{2} \Delta_x \psi^\epsilon + V \left( \frac{x}{\epsilon} \right) \psi^\epsilon + W(x) \psi^\epsilon \tag{\star} \]

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- When \( V \neq 0 \), dynamics depends crucially on Bloch band structure (spectral theory) of periodic operator obtained by taking \( W = 0 \) in \((\star)\):

\[ H := -\frac{1}{2} \Delta_z + V(z) \]

and spectral localization of the wavepacket in phase space.
Spectral theory of periodic operators

- Recall the spectral theory of the operator with periodic potential:

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- Bloch’s theorem: bounded eigenfunctions of \( H \) satisfy the \( p \)-quasi-periodic boundary condition:

\[ H \Phi(z; p) = E(p)\Phi(z; p) \]

\[ \forall v \in \Lambda, \Phi(z + v) = e^{ip \cdot v} \Phi(z; p) \]

symmetry of BC \( \implies \) restrict \( p \) to a primitive cell of the reciprocal lattice: first Brillouin zone \( B \)
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Symmetry of BC \( \implies \) restrict \( p \) to a primitive cell of the reciprocal lattice: first Brillouin zone \( B \)

Fixed quasi-momentum \( p \), self-adjoint elliptic eigenvalue problem \( \implies \) discrete real spectrum:

\[ E_1(p) \leq E_2(p) \leq \ldots \leq E_n(p) \leq \ldots \]
Spectral theory of periodic operators

- Maps \( p \in \mathcal{B} \rightarrow E_n(p) \in \mathbb{R} \) are the Bloch band dispersion functions (surfaces).
Spectral theory of periodic operators

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- Spectrum of \( H = -\frac{1}{2} \Delta z + V(z) \) is then the union of real intervals swept out by \( E_n(p) \).
Spectral theory of periodic operators

- The set of associated eigenfunctions (Bloch waves) \( \{ \Phi_n(z; p) : n \in \mathbb{N}, p \in B \} \) is complete in \( L^2(\mathbb{R}^d) \).
Spectral theory of periodic operators

- The set of associated eigenfunctions (Bloch waves) 
  \( \{ \Phi_n(z; p) : n \in \mathbb{N}, p \in \mathcal{B} \} \) is complete in \( L^2(\mathbb{R}^d) \).
- Can decompose \( \Phi_n(z; p) = e^{ip \cdot z} \chi_n(z; p) \) where \( \chi_n(z; p) \) satisfies another self-adjoint elliptic eigenvalue problem with periodic boundary conditions:

  \[
  H(p) \chi(z; p) = E(p) \chi(z; p)
  \]

  \( \forall \mathbf{v} \in \Lambda, \chi(z + \mathbf{v}) = \chi(z; p) \) \hspace{1cm} (P)

  \[ H(p) := \frac{1}{2} (p - i \nabla z)^2 + V(z), \]

  (P) is the reduced Bloch eigenvalue problem.

Let \((q(t), p(t))\) denote any classical trajectory generated by the Bloch band Hamiltonian \(\mathcal{H} = E_n(p) + W(q)\) such that the band \(E_n\) is non-degenerate at each \(p(t)\):

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

Then there exists a solution \(\psi(\mathbf{x}, t)\) which is asymptotic as \(\epsilon \downarrow 0\) to a semiclassical wavepacket up to ‘Ehrenfest time’ \(t \sim \ln 1/\epsilon\):

\[
\psi(\mathbf{x}, t) = \epsilon^{-d/4} e^{i S(t)/\epsilon} e^{ip(t) \cdot (\mathbf{x} - q(t))/\epsilon} a \left( \frac{\mathbf{x} - q(t)}{\epsilon^{1/2}}, t \right) \chi_n \left( \frac{\mathbf{x}}{\epsilon}; p(t) \right)
+ O_{L^2_{\mathbf{x}}(\mathbb{R}^d)}(\epsilon^{1/2} e^{Ct}).
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Then there exists a solution \(\psi^\epsilon(x,t)\) which is asymptotic as \(\epsilon \downarrow 0\) to a semiclassical wavepacket up to ‘Ehrenfest time’ \(t \sim \ln 1/\epsilon\):

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

Wavepacket envelope \(a(y,t)\) satisfies a Schrödinger equation with harmonic oscillator Hamiltonian, driven by \(q(t), p(t)\):

\[
i \partial_t a = -\frac{1}{2} \nabla_y \cdot D^2_p E_n(p(t)) \nabla_y a + \frac{1}{2} y \cdot D^2_q W(q(t)) y a
\]
Wavepacket dynamics in locally periodic structures

Results:

1. A new Hamiltonian system controlling the dynamics of wavepackets which are spectrally localized away from Bloch band degeneracies.
2. The dynamics of a wavepacket incident on a Bloch band degeneracy.
Hamiltonian system for dynamics away from degeneracies

- We derive the equations of motion of the center of mass $Q^\epsilon(t)$ and expected (quasi-)momentum $P^\epsilon(t)$ of the wavepacket with corrections $\propto \epsilon$. 

- Experimentally measured in photonics, where polarization condition $p \cdot e(p) = 0$ degenerate at $p = 0$:

$$= \Rightarrow$$

Hamiltonian system for dynamics away from degeneracies

- We derive the equations of motion of the *center of mass* $Q^\epsilon(t)$ and *expected (quasi-)momentum* $P^\epsilon(t)$ of the wavepacket with corrections $\propto \epsilon$.

- Of particular interest, a correction due to Berry curvature $\mathcal{F}_n$ which takes the form of a *monopole* at degeneracies:

$$\mathcal{F}_n(p) = \text{Im} \sum_{m \neq n} \frac{\langle \psi_n(p) | \nabla_p H(p) \psi_m(p) \rangle \times (n \leftrightarrow m)}{(E_m(p) - E_n(p))^2}$$
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- Experimentally measured in photonics, where polarization condition $p \cdot e(p) = 0$ degenerate at $p = 0$: 

\[ \implies \text{spin Hall effect of light} \]

\[^a\text{Bliokh et al., Nature Photonics, 2008.}\]
Strategy of proof

- Recall form of the asymptotic solution:

\[ \psi^\varepsilon(x, t) = \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{i\p(t) \cdot (x - q(t))/\epsilon} a \left( \frac{x - q(t)}{\epsilon^{1/2}}, t \right) \chi_n \left( \frac{x}{\epsilon}; p(t) \right) \]

\[ + \, O_{L^2_x(\mathbb{R}^d)}(\epsilon^{1/2} e^{Ct}). \]  

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(AS)

Using (AS), we obtain expansions of the center of mass \( Q^\epsilon \) and average quasi-momentum \( P^\epsilon \) in powers of \( \epsilon^{1/2} \):

\[ Q^\epsilon(t) = q(t) + \epsilon^{1/2} \int_{\mathbb{R}^d} y |a(y, t)|^2 \, dy + O(\epsilon) \]

\[ P^\epsilon(t) = p(t) + \epsilon^{1/2} \int_{\mathbb{R}^d} \overline{a(y, t)(-i\nabla_y) a(y, t)} \, dy + O(\epsilon) \]
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\]

Dynamics of \( Q^\epsilon, P^\epsilon \) couples to evolution of \( q, p, a \) (complicated) as well as the Bloch functions \( \chi_n(z; p) \).
Theorem (Watson-Weinstein-Lu 2016)

1) Let $Q^\epsilon, P^\epsilon$ denote the center of mass and averaged quasi-momentum of the wavepacket asymptotic solution. Then, after making the near-identity change of variables:

$$(q, p, a) \mapsto (Q^\epsilon, P^\epsilon, a^\epsilon)$$

where $a^\epsilon(y, t)$ satisfies:

$$i\partial_t a^\epsilon = -\frac{1}{2} \nabla_y \cdot D_{P^\epsilon}^2 E_n(P^\epsilon(t)) \nabla_y a^\epsilon + \frac{1}{2} y \cdot D_{Q^\epsilon}^2 W(Q^\epsilon(t)) y a^\epsilon \quad (E)$$
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the observables $Q^\epsilon(t)$ and $P^\epsilon(t)$ satisfy:

$$\dot{Q}^\epsilon(t) = \nabla P^\epsilon E_n(P^\epsilon(t)) - \epsilon P^\epsilon(t) \times \mathcal{F}_n(P^\epsilon(t)) + \epsilon C_1[a^\epsilon](t) + O(\epsilon^{3/2})$$

$\text{Anomalous velocity}$

$$\dot{P}^\epsilon(t) = -\nabla Q^\epsilon W(Q^\epsilon(t)) + \epsilon C_2[a^\epsilon](t) + O(\epsilon^{3/2}) \quad (O)$$

where $\mathcal{F}_n(P^\epsilon)$ denotes the Berry curvature of the Bloch band.
Theorem (Watson-Weinstein-Lu 2016 continued)

2) The coupled dynamics of \( Q^\epsilon(t), P^\epsilon(t), a^\epsilon(y, t) \) can be derived from the \( \epsilon \)-dependent Hamiltonian:

\[
\mathcal{H}^\epsilon := E_n(P^\epsilon) + W(Q^\epsilon) + \epsilon \nabla Q^\epsilon W(Q^\epsilon) \cdot \mathcal{A}_n(P^\epsilon) \\
+ \frac{1}{2} \int_{\mathbb{R}^d} \nabla y \overline{a^\epsilon} \cdot D^2_{Q^\epsilon} E_n(P^\epsilon) \nabla y a^\epsilon \, dy \\
+ \frac{1}{2} \int_{\mathbb{R}^d} y \overline{a^\epsilon} \cdot D^2_{Q^\epsilon} W(Q^\epsilon) y a^\epsilon \, dy
\]

where \( \mathcal{A}_n(P^\epsilon) \) is the \( n \)-th band Berry connection.

\[
\dot{Q}^\epsilon = \nabla P^\epsilon \mathcal{H}^\epsilon \\
\dot{P}^\epsilon = -\nabla Q^\epsilon \mathcal{H}^\epsilon \\
i \partial_t a^\epsilon = \frac{\delta \mathcal{H}}{\delta a^\epsilon} \quad \text{(S)}
\]

Theorem (Watson-Weinstein-Lu 2016 continued)

2) The coupled dynamics of $Q^\epsilon(t), P^\epsilon(t), a^\epsilon(y, t)$ can be derived from the $\epsilon$-dependent Hamiltonian:

$$
\mathcal{H}^\epsilon := E_n(P^\epsilon) + W(Q^\epsilon) + \epsilon \nabla Q^\epsilon W(Q^\epsilon) \cdot A_n(P^\epsilon)
$$

$$
+ \epsilon \frac{1}{2} \int_{\mathbb{R}^d} \nabla y \overline{a^\epsilon} \cdot D_{P^\epsilon}^2 E_n(P^\epsilon) \nabla y a^\epsilon \, dy
+ \epsilon \frac{1}{2} \int_{\mathbb{R}^d} y \overline{a^\epsilon} \cdot D_{Q^\epsilon}^2 W(Q^\epsilon) y a^\epsilon \, dy
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$$

$$
i \partial_t a^\epsilon = \frac{\delta \mathcal{H}}{\delta a^\epsilon} \quad (S)
$$

- The system (S) contains terms which do not appear in the works of Niu et al.$^1$

---

Aside: dynamics of a particle coupled to a wave-field

When $V = 0$, system reduces to:

$$
\dot{Q}^\epsilon(t) = \mathcal{P}^\epsilon(t)
$$

$$
\dot{P}^\epsilon(t) = -\nabla_{Q^\epsilon} W(Q^\epsilon(t)) - \epsilon \frac{1}{2} \partial^3_{Q^\epsilon} W(Q^\epsilon) \left\langle a^\epsilon(y, t) | y^2 a^\epsilon(y, t) \right\rangle_{L^2_y}
$$

Coupling of discrete degrees of freedom to wave-field

$$
i \partial_t a^\epsilon = -\frac{1}{2} \partial^2_{P^\epsilon} E_n(P^\epsilon(t)) \partial^2_y a^\epsilon + \frac{1}{2} \partial^2_{Q^\epsilon} W(Q^\epsilon(t)) y^2 a^\epsilon
$$
Aside: dynamics of a particle coupled to a wave-field

- When $V = 0$, system reduces to:

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\]

- Center of mass dynamics when potential $W \propto q^4$:

\[
i \partial_t a^\epsilon = -\frac{1}{2} \partial^2 \mathcal{P}^\epsilon E_n(\mathcal{P}^\epsilon(t)) \partial_y^2 a^\epsilon + \frac{1}{2} \partial^2 Q^\epsilon W(Q^\epsilon(t)) y^2 a^\epsilon
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Results:

1. A new Hamiltonian system controlling the dynamics of wavepackets which are spectrally localized away from Bloch band degeneracies.

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Dynamics at Bloch band degeneracies

- So far, assumed that the wavepacket avoids degeneracies:

\[ \forall t \geq 0, E_{n-1}(p(t)) < E_n(p(t)) < E_{n+1}(p(t)) \]
Dynamics at Bloch band degeneracies

So far, assumed that the wavepacket avoids degeneracies:

∀t ≥ 0, En−1(p(t)) < En(p(t)) < En+1(p(t))

Degeneracies, where En(p*) = En+1(p*), usually associated with symmetries of periodic structure. In d = 1, rich set of examples: Jacobi elliptic functions.
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- New degree of freedom: coupling between degenerate states
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- New degree of freedom: coupling between degenerate states
- At crossings, Bloch band functions: \( p \rightarrow E_n(p) \) not smooth
Theorem (Watson-Weinstein 2016)

- $p^*$ a degenerate point in $d = 1$. $E_+(p), E_-(p)$ smooth band functions in a neighborhood of $p^*$ (always exist in $d = 1$).

![Graph showing smooth band functions $E_+, E_-$ vs. quasi-momentum $p$.]
Theorem (Watson-Weinstein 2016)

- $p^*$ a degenerate point in $d = 1$. $E_+(p), E_-(p)$ smooth band functions in a neighborhood of $p^*$ (always exist in $d = 1$).

- Consider a wavepacket associated with the band $E_+$ with quasi-momentum $p_+(t)$ that is driven towards the degeneracy i.e. there exists $t^*$ such that: $\lim_{t \uparrow t^*} p_+(t) = p^*$. 
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- As $t \uparrow t^*$, error in single band approximation blows up:

$$\|\psi^\epsilon(\cdot, t) - WP(\cdot, t)\|_{L^2} \sim \frac{\sqrt{\epsilon}}{|t - t^*|} + \frac{\epsilon}{|t - t^*|^2}$$

\[\implies \text{ emergent time-scale: } s \sim \frac{t-t^*}{\sqrt{\epsilon}}.\]
Theorem (Watson-Weinstein 2016 continued)

By studying in detail the dynamics of the PDE on the emergent time-scale $s = \frac{t-t^*}{\sqrt{\epsilon}}$, we find that the blow-up may be resolved by allowing coupling between degenerate states.
Theorem (Watson-Weinstein 2016 continued)

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  \[ \implies \text{at } t = t^* \text{ a second wavepacket associated with the band } E_- \text{ is excited.} \]
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  \[ \Rightarrow \] at \( t = t^* \) a second wavepacket associated with the band \( E_- \) is excited.

- ‘Excited’ wavepacket has size \( \propto \sqrt{\epsilon} \) (in \( L^2 \)), may be explicitly characterized. Group velocity opposite sign: ‘reflected’ wave.
By studying in detail the dynamics of the PDE on the emergent time-scale $s = \frac{t - t^*}{\sqrt{\epsilon}}$, we find that the blow-up may be resolved by allowing coupling between degenerate states.

$\implies$ at $t = t^*$ a second wavepacket associated with the band $E_-$ is excited.

‘Excited’ wavepacket has size $\propto \sqrt{\epsilon}$ (in $L^2$), may be explicitly characterized. Group velocity opposite sign: ‘reflected’ wave.
Theorem (Watson-Weinstein 2016 continued)

- By studying in detail the dynamics of the PDE on the emergent time-scale \( s = \frac{t - t^*}{\sqrt{\epsilon}} \), we find that the blow-up may be resolved by allowing coupling between degenerate states.

\[ \Rightarrow \text{ at } t = t^* \text{ a second wavepacket associated with the band } E_\text{–} \text{ is excited.} \]

- ‘Excited’ wavepacket has size \( \propto \sqrt{\epsilon} \) (in \( L^2 \)), may be explicitly characterized. Group velocity opposite sign: ‘reflected’ wave.

Result is an analog of those obtained by Hagedorn (B-O approx.)
Consistency with Landau-Zener theory

- Schrödinger’s equation with a time-dependent Hamiltonian:

\[ i\epsilon \partial_t \psi^\epsilon = H(t) \psi^\epsilon \]

with \( \text{Spec}[H(t)] = E_+(t) \cup E_-(t) \), linear crossing at \( t = t^* \).
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- Seek a solution: \( \psi^\epsilon(t) = \sum_{\sigma = \pm} c_\sigma(t) \chi_\sigma(t) e^{-i \int_{t^*}^t E_\sigma(\tau) d\tau} \).
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  obtain system for co-efficients:

\[
\begin{align*}
\dot{c}_+(t) &= \langle \chi_+(t) | \dot{\chi}_-(t) \rangle e^{\frac{i \int_{t^*}^{t} E_+(\tau) - E_-(\tau) d\tau}{\epsilon}} c_-(t) \\
\dot{c}_-(t) &= \langle \chi_-(t) | \dot{\chi}_+(t) \rangle e^{\frac{i \int_{t^*}^{t} E_-(\tau) - E_+(\tau) d\tau}{\epsilon}} c_+(t).
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\dot{c}_-(t) &= \langle \chi_-(t) | \dot{\chi}_+(t) \rangle \frac{\displaystyle i \int_{t^*}^t (E_-(\tau) - E_+(\tau)) \, d\tau}{\epsilon} c_+(t).
\end{align*}
\]

- Suppose \( c_+(0) = 1, c_-(0) = 0 \). Integrating in time, using oscillations \( \implies \)

\[
\| c_-(t) \|^2 = \frac{2\pi | \langle \chi_-(t^*) | \dot{\chi}_+(t^*) \rangle |^2}{| \dot{E}_+(t^*) - \dot{E}_-(t^*) |} \sqrt{\epsilon} + o(\sqrt{\epsilon}).
\]
Ongoing work/future directions

▶ What are the Berry curvature-induced dynamics at and after the Ehrenfest timescale of validity of the semiclassical wavepacket ansatz $t \sim \ln 1/\epsilon$?

▶ Extension of band crossing theory to conical band crossings, which appear in dispersion surfaces of honeycomb lattice potentials, anisotropic photonic media: and to avoided crossings, gap $\propto \sqrt{\epsilon}$.

Expect $O(1)$ coupling between bands in these cases; proved by Hagedorn (B-O approximation).
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![Image of honeycomb lattice and dispersion surface]
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Thanks for listening!