Dynamics of wavepackets in crystals by multiscale analysis

Alexander Watson$^1$

Michael Weinstein$^{12}$, Jianfeng Lu$^3$

$^1$Applied Physics and Applied Mathematics, Columbia University
$^2$Mathematics, Columbia University $^3$Mathematics, Duke University

November 28, 2016
Motivation: dynamics of electrons in crystals

- **Idea:** Electron in a crystal moving under the influence of an applied electric field can be modeled as a *wavepacket* (localized, propagating) solution of Schrödinger’s equation

- **Seek an effective (simplified) description of the dynamics** (PDE → ODEs)

- **Assumption:** Potential *slowly-varying* relative to lattice constant; treat wavepacket as *localized* with respect to variation of potential, *spread* over a few lattice periods

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1 Solid State Physics, Ashcroft and Mermin (1976).
First: wavepacket dynamics under the influence of a slowly-varying potential without periodic background

Model:

\[ i \partial_t \psi^\epsilon = -\frac{1}{2} \Delta_x \psi^\epsilon + W(\epsilon x), \]

assume \( \epsilon \ll 1 \).

Re-scale:

\[ x' := \epsilon x, \quad t' := \epsilon t, \quad \psi^{\epsilon'}(x', t') := \psi^\epsilon(x, t) \]

dropping primes we obtain equivalent form:

\[ i \epsilon \partial_t \psi^\epsilon = -\epsilon^2 \frac{1}{2} \Delta_x \psi^\epsilon + W(x) \psi^\epsilon \]
WKB method

Model:
\[ i\epsilon \partial_t \psi^\epsilon = -\epsilon^2 \frac{1}{2} \Delta_x \psi^\epsilon + W(x) \psi^\epsilon. \]

Make the WKB ansatz:
\[ \psi^\epsilon(x, t) = e^{i\phi(x,t)/\epsilon} a^\epsilon(x, t) \]

Expanding \( a^\epsilon \) in powers of the small parameter:
\[ a^\epsilon(x, t) = a^0(x, t) + \epsilon a^1(x, t) + \ldots \]

Construct an approximate solution by collecting terms \( \propto \epsilon^0, \epsilon^1 \ldots \) \( \implies \) equations for \( \phi, a^j \)
Analysis of terms $\propto \epsilon^0$

Equating terms in the expansion $\propto \epsilon^0$:

$$\left[ \partial_t \phi + \frac{1}{2} (\nabla_x \phi)^2 + W(x) \right] a^0(x, t) = 0$$ (1)

For a non-trivial solution $a^0 \neq 0 \implies$ equation for phase $\phi(x, t)$:

$$\partial_t \phi + \frac{1}{2} (\nabla_x \phi)^2 + W(x) = 0$$

Known as the *eikonal*, Hamilton-Jacobi type.
Solution of eikonal equation

Fully nonlinear equation for $\phi(x, t)$:

$$\partial_t \phi + \frac{1}{2} (\nabla_x \phi)^2 + W(x) = 0$$

Solve by method of characteristics:

$$\dot{q}(t) = p(t), \quad \dot{p}(t) = -\nabla_q W(q(t))$$

$$q(0) = x, \quad p(0) = \nabla_x \phi(x, 0)$$

$\uparrow$ equations of motion of Hamiltonian $\frac{1}{2} p^2 + W(q)$

$$\phi(q(t), t) = \int_0^t \frac{1}{2} p(t')^2 - W(q(t')) \, dt'$$

$\implies \phi(q(t), t)$ is the action along $q(t)$. Solution $\phi(x, t)$ explicit as long as flow map $x \mapsto q(t; x)$ invertible, if not: caustic.
Analysis of terms $\propto \epsilon$

Equating terms $\propto \epsilon \implies$ *transport equation* for $a^0(x, t)$:

$$\partial_t a^0 + \nabla_x \phi \cdot \nabla_x a^0 + \frac{1}{2} (\nabla^2_x \phi) a^0 = 0.$$  

Again, solution explicit while $x \mapsto q(t; x)$ invertible (no caustics):

$$a^0(q(t; x), t) = \frac{1}{\sqrt{\text{Jacobian}(x \mapsto q(t; x))}} a^0(x, 0). \quad (3)$$

$\implies$ initial data *transported along solutions of the characteristic equations* generated by $\mathcal{H} = \frac{1}{2} p^2 + W(q)$. 


Rigorous error bound

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

So far (formal analysis): 
\[ \psi^\epsilon(x, t) = e^{i\phi(x, t)/\epsilon} a^0(x, t) + O(\epsilon) \]
\( \phi, a^0 \) explicit (solve ODEs) up to time of first caustic \( T_C > 0 \).

How to make \( O(\epsilon) \) rigorous?

Define \( \eta^\epsilon(x, t) := \psi^\epsilon(x, t) - e^{i\phi(x, t)/\epsilon} a^0(x, t) \), assume \( \eta^\epsilon(x, 0) = 0 \). Then \( \eta^\epsilon \) satisfies:

\[ i\epsilon \partial_t \eta^\epsilon = -\frac{1}{2} \epsilon^2 \Delta_x \eta^\epsilon + W(x) \eta^\epsilon + r^\epsilon, \quad (4) \]

Let \( T < T_C \). Standard \( L^2 \) estimate for solutions of (4):

\[ \| \eta^\epsilon(\cdot, t) \|_{L^2} \leq \frac{1}{\epsilon} \int_0^t \| r^\epsilon(\cdot, t') \|_{L^2} \, dt' \quad (5) \]

Forms of \( \phi, a^0 \) \( \implies \) \( \sup_{t \in [0, T]} \| r^\epsilon(\cdot; t) \|_{L^2} \leq C_1 \epsilon^2 \),

\( L^2 \) estimate (5) \( \implies \) \( \sup_{t \in [0, T]} \| \eta^\epsilon(\cdot, t) \|_{L^2} \leq C_2 \epsilon \).
Motivation: dynamics of electrons in crystals

Seek *generalization* of WKB theory (geometric optics):

wavelength $\ll$ scale of medium features

$\rightarrow$ slowly varying *periodic* media:

wavelength $\approx$ scale of periodicity of medium

$\ll$ scale of *variation of periodic structure*

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2 *Solid State Physics, Ashcroft and Mermin (1976).*
Outline of talk

- Generalization of WKB theory to slowly-varying periodic media by a *multi-scale* WKB ansatz
- Extensions of this description:
  - First-order corrections to dynamics
  - Dynamics at band crossings

Key tool: multi-scale *semiclassical wavepacket* ansatz

- Ongoing work/future directions
Model: Schrödinger’s equation

Non-dimensionalized Schrödinger equation:

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

\( U \) periodic with respect to a \( d \)-dimensional lattice \( \Lambda \) in its first argument:

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

In this talk:

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

\[ \forall \mathbf{v} \in \Lambda, \: V(x + \mathbf{v}) = V(x) \]

recover standard WKB setting when \( V = 0 \).
Recap: spectral theory of periodic operators

- Recall the spectral theory of the operator with periodic potential ($\epsilon = 0$ case):

\[
h := -\frac{1}{2} \Delta z + V(z)
\]
\[
\forall \mathbf{v} \in \Lambda, \quad V(z + \mathbf{v}) = V(z)
\]

- Bloch’s theorem: bounded eigenfunctions of $h$ satisfy the $p$-quasi-periodic boundary condition:

\[
h \Phi(z; p) = E(p) \Phi(z; p)
\]
\[
\forall \mathbf{v} \in \Lambda, \quad \Phi(z + \mathbf{v}) = e^{i p \cdot \mathbf{v}} \Phi(z; p)
\]

symmetry of BC $\implies$ restrict $p$ to a primitive cell of the reciprocal lattice: first Brillouin zone $\mathcal{B}$

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

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

- Maps $p \in \mathcal{B} \rightarrow E_n(p) \in \mathbb{R}$ are the Bloch band dispersion surfaces

- The spectrum of $h = -\frac{1}{2} \Delta_z + V(z)$ is then the union of real intervals swept out by the Bloch band dispersion functions $E_n(p)$

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$^3$Fefferman, Lee-Thorp, Weinstein; PNAS 2014.
The set of Bloch waves (eigenfunctions) \( \{ \Phi_n(z; p) : n \in \mathbb{N}, p \in B \} \) 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:

\[
h(p) \chi(z; p) = E(p) \chi(z; p)
\]
\[
\forall \mathbf{v} \in \Lambda, \chi(z + \mathbf{v}) = \chi(z; p)
\]

(6) is the reduced Bloch eigenvalue problem.
Re-scaling

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

Again, re-scale:
\[ x' := \epsilon x, \ t' := \epsilon t, \ \psi'^\epsilon(x', t') := \psi^\epsilon(x, t) \]

Dropping the primes gives the equivalent formulation:
\[ i \epsilon \partial_t \psi^\epsilon = -\epsilon^2 \frac{1}{2} \Delta_x \psi^\epsilon + V \left( \frac{x}{\epsilon} \right) \psi^\epsilon + W(x) \psi^\epsilon \]
Multiscale WKB method

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

Make the *multiscale WKB ansatz*:

\[ \psi^\epsilon(x, t) = e^{i \phi(x, t)/\epsilon} f^\epsilon(z, x, t)|_{z=x/\epsilon} \]

Expanding \( f^\epsilon \) in powers of the small parameter:

\[ f^\epsilon(z, x, t) = f^0(z, x, t) + \epsilon f^1(z, x, t) + \ldots \]

Impose that \( f^j \) have the periodicity of the lattice \( \Lambda \) in \( z \):

\[ \forall v \in \Lambda, f^j(z + v, x, t) = f^j(z, x, t) \]

Equating terms of like order, we obtain equations for \( \phi, f^j \)
Analysis of terms $\propto \epsilon^0$

Equating terms in the expansion $\propto \epsilon^0$ obtain self-adjoint elliptic eigenvalue problem in $z$ for $f^0$ which depends on $x, t$ as parameters:

$$\left[\frac{1}{2}(\nabla_x \phi - i \nabla_z)^2 + V(z)\right]f^0(z, x, t) = \left[-\partial_t \phi - W(x)\right]f^0(z, x, t)$$

$\forall v \in \Lambda, f^0(z + v, x, t) = f^0(z, x, t)$.  \hspace{1cm} (7)

Let $E_n$ be an isolated Bloch band (non-degenerate eigenvalue):

$$\forall p \in B, E_{n-1}(p) < E_n(p) < E_{n+1}(p)$$

Then we can solve (7) by taking:

$$f^0(z, x, t) = a^0(x, t)\chi_n(z; \nabla_x \phi)$$

$$\partial_t \phi + E_n(\nabla_x \phi) + W(x) = 0$$
Eikonal equation

Again, *Eikonal* equation for $\phi(x, t)$:

$$\partial_t \phi + E_n(\nabla_x \phi) + W(x) = 0$$

Fully nonlinear, solve by *method of characteristics*:

$$\dot{q}(t) = \nabla_p E_n(p(t)), \quad \dot{p}(t) = -\nabla_q W(q(t))$$

$$q(0) = x, \quad p(0) = \nabla_x \phi(x, 0)$$

(8)

↑ equations of motion of Hamiltonian $E_n(p) + W(q)$

$$\phi(q(t), t) = \int_0^t \dot{q}(t') \cdot p(t') - E_n(p(t')) - W(q(t')) \, dt'$$

$\implies \phi(q(t), t)$ is the *action* along $q(t)$. Again, solution $\phi(x, t)$ explicit as long as $x \mapsto q(t; x)$ invertible, if not: *caustics.*
First order analysis

Equating terms proportional to $\epsilon +$ imposing periodic BCs obtain \textit{inhomogeneous} self-adjoint elliptic equation in $z$ for $f^1$:

$$
\left[ \frac{1}{2} (\nabla_x \phi - i \nabla_z)^2 + V(z) - E_n(\nabla_x \phi) \right] f^1(z, x, t)
$$

$$
= \left[ i \partial_t + i (\nabla_x \phi - i \nabla_z) \cdot \nabla_x + i \frac{1}{2} \nabla^2_x \phi \right] f^0(z, x, t)
$$

Fredholm alternative $\implies$ solvability equivalent to vanishing projection of RHS onto null-space of LHS operator $\implies$ transport equation for $a^0$:

$$
\partial_t a^0 + \nabla_p E_n(\nabla_x \phi) \cdot \nabla_x a^0 + \frac{1}{2} \nabla_x \cdot \nabla_p E_n(\nabla_x \phi)
$$

$$
+ i \nabla_x W(x) \cdot \langle \chi_n(\cdot; \nabla_x \phi) | i \nabla_p \chi_n(\cdot; \nabla_x \phi) \rangle_{L^2(\mathbb{R}^d/\Lambda)} = 0
$$

$\implies$ initial conditions are \textit{transported along solutions of the characteristic equations} generated by $\mathcal{H} = E_n(p) + W(q)$
Outline of talk

- Generalization of WKB theory to slowly-varying periodic media by a *multi-scale* WKB ansatz
- Extensions of this description:
  - First-order corrections to dynamics ($\propto \epsilon$)
  - Dynamics at band crossings (eigenvalue degeneracies)

**Key tool:** multi-scale *semiclassical wavepacket* ansatz

- First-order corrections $\implies$ *spin Hall effect of light*:

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4 [Bliokh, Niv, Kleiner, Hasman; Nature Photonics 2008.](#)

Let \((q(t), p(t))\) denote a classical trajectory generated by the Bloch band Hamiltonian \(H = E_n(p) + W(q)\) such that the band \(E_n\) is isolated at each \(p(t)\):

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

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

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

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

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

Writing the solution in terms of the multiscale variables:

\[
\psi^\epsilon(x, t) = \tilde{\psi}^\epsilon(y, z, t) \bigg|_{y = \frac{x - q(t)}{\epsilon^{1/2}}, z = \frac{x}{\epsilon}} + O_{L^2_x(\mathbb{R}^d)}(\epsilon^{1/2})
\]

\(q(t), p(t)\) the center of mass and average quasi-momentum of the wavepacket, to leading order in \(\epsilon^{1/2}\):

\[
Q^\epsilon(t) := \int_{\mathbb{R}^d} x |\tilde{\psi}^\epsilon(y, z, t)|^2 \bigg|_{y = \frac{x - q(t)}{\epsilon^{1/2}}, z = \frac{x}{\epsilon}} \, dx
\]

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

\[
P^\epsilon(t) := \int_{\mathbb{R}^d} \overline{\tilde{\psi}^\epsilon(y, z, t)}(-i\epsilon^{1/2}\nabla_y)\tilde{\psi}^\epsilon(y, z, t) \bigg|_{y = \frac{x - q(t)}{\epsilon^{1/2}}, z = \frac{x}{\epsilon}} \, dx
\]

\[
= p(t) + \epsilon^{1/2} \int_{\mathbb{R}^d} a(y, t)(-i\nabla_y) a(y, t) \, dy + O(\epsilon)
\]
Theorem (Watson-Weinstein-Lu 2016)

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

$$
\dot{Q}^\epsilon(t) = \nabla P^\epsilon E_n(P^\epsilon(t)) + \epsilon C_1[a^\epsilon](t)
$$

$$
- \epsilon \dot{P}^\epsilon(t) \times F_n(P^\epsilon(t)) + O(\epsilon^{3/2})
$$

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

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

$$
i \partial_t a^\epsilon = -\frac{1}{2} \nabla_y \cdot D_{P^\epsilon}^2 E_n(P^\epsilon(t)) \nabla_y a^\epsilon + \frac{1}{2} y \cdot D_{Q^\epsilon}^2 W(Q^\epsilon(t)) y a^\epsilon
$$
Theorem (Watson-Weinstein-Lu 2016 continued)

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

$$
\mathcal{H}^\epsilon := E_n(P^\epsilon) + W(Q^\epsilon) + \epsilon \nabla Q^\epsilon W(Q^\epsilon) \cdot A_n(P^\epsilon) \\
+ \epsilon \frac{1}{2} \int_{\mathbb{R}^d} \nabla_y a^\epsilon \cdot D^2_{P^\epsilon} E_n(P^\epsilon) \nabla_y a^\epsilon \, dy + \epsilon \frac{1}{2} \int_{\mathbb{R}^d} y a^\epsilon \cdot D^2_{Q^\epsilon} W(Q^\epsilon) y a^\epsilon \, dy
$$

where $A_n(P^\epsilon)$ is the $n$-th band Berry connection.

$$
\dot{Q}^\epsilon = \nabla_{P^\epsilon} \mathcal{H}^\epsilon, \quad \dot{P}^\epsilon = -\nabla_{Q^\epsilon} \mathcal{H}^\epsilon, \quad \imath \partial_t a^\epsilon = \frac{\delta \mathcal{H}}{\delta a^\epsilon}
$$
Gaussian reduction of envelope equation

The equation satisfied by the wavepacket envelope:

\[ i \partial_t a^\epsilon = -\frac{1}{2} \nabla_y \cdot D_{\mathcal{P}^\epsilon}^2 E_n(\mathcal{P}^\epsilon(t)) \nabla_y a^\epsilon + \frac{1}{2} y \cdot D_{\mathcal{Q}^\epsilon}^2 W(\mathcal{Q}^\epsilon(t)) y a^\epsilon \]

has family of exact solutions which form a basis e.g. time-dependent Gaussians\(^5\):

\[
a^\epsilon(y, t) = \frac{1}{[\det A^\epsilon(t)]^{1/2}} \exp \left(-\frac{1}{2} y \cdot B^\epsilon(t) A^\epsilon(t)^{-1} y \right)
\]

\[
\dot{A}^\epsilon(t) = i D_{\mathcal{P}^\epsilon}^2 E_n(\mathcal{P}^\epsilon) B^\epsilon(t), \quad \dot{B}^\epsilon(t) = i D_{\mathcal{Q}^\epsilon}^2 W(\mathcal{Q}^\epsilon) A^\epsilon(t) \quad (9)
\]

appropriate initial data \( \implies (\mathcal{Q}^\epsilon, \mathcal{P}^\epsilon, a^\epsilon) \) system reduces to ODEs

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\(^5\)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
- Applied potential $W(Q) = \frac{1}{6} Q^3 + \frac{1}{2} Q^2$
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 $Q^c = -\infty$
Dynamics at band crossings

- Would like to relax the ‘isolated band’ assumption:

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

- Crossings usually associated with symmetries

- At crossings Bloch band functions: \( p \rightarrow (E_n(p), \chi_n(z; p)) \) not smooth in general, e.g. conical degeneracies (Dirac points) \( \Rightarrow \) restrict to \( d = 1 \)
Theorem (Watson-Weinstein 2016)

\( p^* \) denote a crossing point in \( d = 1 \)

\( E_+(p), E_-(p) \) denote smooth band functions at \( p^* \)

\( (p_+(t), q_+(t)) \) denote a classical trajectory of the \(+\)-band Hamiltonian \( E_+(p) + W(q) \) s.t. \( p_+(0) = p^*, \dot{p}_+(0) \neq 0 \)

Then the solution of the PDE on a small interval \( t \in [-T, T] \), with initial data at \( t = -T \) a wavepacket associated with the \(+\)-band localized about \( (p_+(-T), q_+(-T)) \), remains to leading order a wavepacket associated with the \(+\)-band localized about the classical trajectory \( (p_+(t), q_+(t)) \ \forall t \in [-T, T] \).
Theorem (Watson-Weinstein 2016 ctd.)

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

$$
q_-(0) = q_+(0) \\
p_-(0) = p_+(0) = p^*.
$$

This correction is of order $\epsilon^{1/2}$ (in $L^2_\times(\mathbb{R})$) and is explicitly characterized.
Remarks on band crossing result

- Proof is by matched asymptotic expansion: error in single-band approximation blows up as $t \uparrow 0$, resolution by more general ansatz which includes contributions from the band $E_-$ $\Rightarrow$ excited wave

- Since $\partial_p E_+(p^*) = -\partial_p E_-(p^*)$, 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 Hagedorn\(^6\) in the context of Born-Oppenheimer approximation of molecular dynamics

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Recap of talk

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- Extensions of this description:
  - First-order corrections to dynamics
  - Dynamics at band crossings

Key tool: multi-scale *semiclassical wavepacket* ansatz

- **Ongoing work/future directions**
Ongoing work/future directions

- Schrödinger → Maxwell: spin Hall effect of light:

- Conical band crossings:

  e.g. *anisotropic* Maxwell’s equations, *honeycomb lattice potentials*