Dynamics of wavepackets in crystals by multiscale analysis

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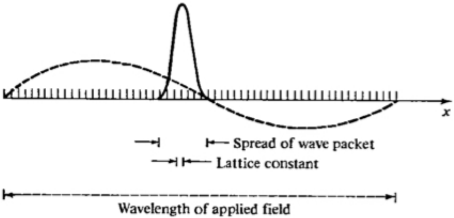
Motivation: dynamics of electrons in crystals

- 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 $\rightarrow$ 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:

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

assume $\epsilon \ll 1$.

Re-scale:

$$\boldsymbol{x}' := \epsilon \boldsymbol{x}, t' := \epsilon t, \psi^{\epsilon\prime}(\boldsymbol{x}', t') := \psi^\epsilon(\boldsymbol{x}, t)$$

dropping primes we obtain equivalent form:

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

WKB method

Model:

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

Make the *WKB ansatz*:

$$\psi^\epsilon(\boldsymbol{x},t) = e^{i\phi(\boldsymbol{x},t)/\epsilon}a^\epsilon(\boldsymbol{x},t)$$

Expanding a^ϵ in powers of the small parameter:

$$a^\epsilon(\boldsymbol{x},t) = a^0(\boldsymbol{x},t) + \epsilon a^1(\boldsymbol{x},t) + \dots$$

Construct an approximate solution by collecting terms $\propto \epsilon^0, \epsilon^1 \dots \implies$ equations for ϕ, a^j

Analysis of terms $\propto \epsilon^0$

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

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

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

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

Known as the *eikonal*, Hamilton-Jacobi type.

Solution of eikonal equation

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

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

Solve by *method of characteristics*:

$$\begin{aligned} \dot{\boldsymbol{q}}(t) = \boldsymbol{p}(t), \dot{\boldsymbol{p}}(t) = -\nabla_{\boldsymbol{q}} W(\boldsymbol{q}(t)) \\ \boldsymbol{q}(0) = \boldsymbol{x}, \boldsymbol{p}(0) = \nabla_{\boldsymbol{x}} \phi(\boldsymbol{x}, 0) \end{aligned} \tag{2}$$

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

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

$\implies$ $\phi(\boldsymbol{q}(t), t)$ is the *action* along $\boldsymbol{q}(t)$. Solution $\phi(\boldsymbol{x}, t)$ explicit as long as flow map $\boldsymbol{x} \mapsto \boldsymbol{q}(t; \boldsymbol{x})$ invertible, if not: *caustic*.

Analysis of terms $\propto \epsilon$

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

$$\partial_t a^0 + \nabla_{\boldsymbol{x}}\phi \cdot \nabla_{\boldsymbol{x}} a^0 + \frac{1}{2}(\nabla_{\boldsymbol{x}}^2 \phi) a^0 = 0.$$

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

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

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

Rigorous error bound

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

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

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

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

$$i\epsilon\partial_t\eta^\epsilon = -\frac{1}{2}\epsilon^2\Delta_{\boldsymbol{x}}\eta^\epsilon + W(\boldsymbol{x})\eta^\epsilon + r^\epsilon, \tag{4}$$

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

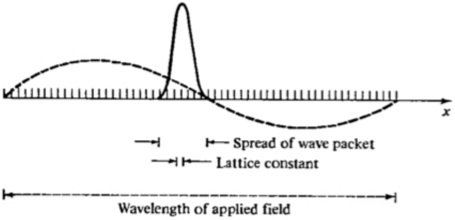
$$\|\eta^\epsilon(\cdot,t)\|_{L^2} \leq \frac{1}{\epsilon}\int_0^t \|r^\epsilon(\cdot,t')\|_{L^2}\,\mathrm{d}t' \tag{5}$$

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:

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

U periodic with respect to a d-dimensional lattice Λ in its first argument:

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

In this talk:

$$i\partial_t \psi^\epsilon = -\frac{1}{2}\Delta_{\boldsymbol{x}}\psi^\epsilon + V(\boldsymbol{x})\psi^\epsilon + W(\epsilon\boldsymbol{x})\psi^\epsilon$$
$$\forall \boldsymbol{v} \in \Lambda, V(\boldsymbol{x} + \boldsymbol{v}) = V(\boldsymbol{x})$$

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):

$$h := -\frac{1}{2}\Delta_{\boldsymbol{z}} + V(\boldsymbol{z})$$
$$\forall \boldsymbol{v} \in \Lambda, V(\boldsymbol{z} + \boldsymbol{v}) = V(\boldsymbol{z})$$

- Bloch's theorem: bounded eigenfunctions of h satisfy the $\boldsymbol{p}$-quasi-periodic boundary condition:

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

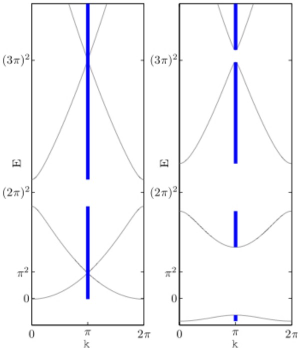
  symmetry of BC $\implies$ restrict $\boldsymbol{p}$ to a primitive cell of the reciprocal lattice: first Brillouin zone $\mathcal{B}$

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

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

Spectral theory of periodic operators

- Maps $\boldsymbol{p} \in \mathcal{B} \to E_n(\boldsymbol{p}) \in \mathbb{R}$ are the Bloch band dispersion surfaces
- The spectrum of $h = -\frac{1}{2}\Delta_{\boldsymbol{z}} + V(\boldsymbol{z})$ is then the union of real intervals swept out by the Bloch band dispersion functions $E_n(\boldsymbol{p})$



[3]

[3] **Fefferman, Lee-Thorp, Weinstein; PNAS 2014.**

Spectral theory of periodic operators

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

$$\begin{aligned} & h(\boldsymbol{p})\chi(\boldsymbol{z};\boldsymbol{p}) = E(\boldsymbol{p})\chi(\boldsymbol{z};\boldsymbol{p}) \\ & \forall \boldsymbol{v} \in \Lambda, \chi(\boldsymbol{z}+\boldsymbol{v}) = \chi(\boldsymbol{z};\boldsymbol{p}) \\ & h(\boldsymbol{p}) := \frac{1}{2}(\boldsymbol{p} - i\nabla_{\boldsymbol{z}})^2 + V(\boldsymbol{z}) \end{aligned} \tag{6}$$

(6) is the *reduced Bloch eigenvalue problem*

Re-scaling

Model:

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

Again, re-scale:

$$\boldsymbol{x}' := \epsilon\boldsymbol{x}, t' := \epsilon t, \psi^{\epsilon\prime}(\boldsymbol{x}', t') := \psi^\epsilon(\boldsymbol{x}, t)$$

Dropping the primes gives the equivalent formulation:

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

Multiscale WKB method

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

Make the *multiscale WKB ansatz*:

$$\psi^\epsilon(\boldsymbol{x}, t) = e^{i\phi(\boldsymbol{x},t)/\epsilon} \left. f^\epsilon(\boldsymbol{z}, \boldsymbol{x}, t)\right|_{\boldsymbol{z}=\frac{\boldsymbol{x}}{\epsilon}}$$

Expanding f^ϵ in powers of the small parameter:

$$f^\epsilon(\boldsymbol{z}, \boldsymbol{x}, t) = f^0(\boldsymbol{z}, \boldsymbol{x}, t) + \epsilon f^1(\boldsymbol{z}, \boldsymbol{x}, t) + \ldots$$

Impose that f^j have the periodicity of the lattice Λ in $\boldsymbol{z}$:

$$\forall \boldsymbol{v} \in \Lambda, f^j(\boldsymbol{z} + \boldsymbol{v}, \boldsymbol{x}, t) = f^j(\boldsymbol{z}, \boldsymbol{x}, t)$$

Equating terms of like order, we obtain equations for ϕ, f^j

Analysis of terms $\propto \epsilon^0$

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

$$\left[\frac{1}{2}(\nabla_{\boldsymbol{x}}\phi - i\nabla_{\boldsymbol{z}})^2 + V(\boldsymbol{z})\right] f^0(\boldsymbol{z},\boldsymbol{x},t) = [-\partial_t\phi - W(\boldsymbol{x})]\, f^0(\boldsymbol{z},\boldsymbol{x},t)$$
$$\forall \boldsymbol{v} \in \Lambda, f^0(\boldsymbol{z}+\boldsymbol{v},\boldsymbol{x},t) = f^0(\boldsymbol{z},\boldsymbol{x},t). \tag{7}$$

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

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

Then we can solve (7) by taking:

$$f^0(\boldsymbol{z},\boldsymbol{x},t) = a^0(\boldsymbol{x},t)\chi_n(\boldsymbol{z};\nabla_{\boldsymbol{x}}\phi)$$
$$\partial_t\phi + E_n(\nabla_{\boldsymbol{x}}\phi) + W(\boldsymbol{x}) = 0$$

Eikonal equation

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

$$\partial_t \phi + E_n(\nabla_{\boldsymbol{x}} \phi) + W(\boldsymbol{x}) = 0$$

Fully nonlinear, solve by *method of characteristics*:

$$\begin{aligned} &\dot{\boldsymbol{q}}(t) = \nabla_{\boldsymbol{p}} E_n(\boldsymbol{p}(t)), \dot{\boldsymbol{p}}(t) = -\nabla_{\boldsymbol{q}} W(\boldsymbol{q}(t)) \\ &\boldsymbol{q}(0) = \boldsymbol{x}, \boldsymbol{p}(0) = \nabla_{\boldsymbol{x}} \phi(\boldsymbol{x}, 0) \end{aligned} \tag{8}$$

$\uparrow$ equations of motion of Hamiltonian $E_n(\boldsymbol{p}) + W(\boldsymbol{q})$

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

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

First order analysis

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

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

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

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

$$\partial_t a^0 + \nabla_{\boldsymbol{p}} E_n(\nabla_{\boldsymbol{x}}\phi) \cdot \nabla_{\boldsymbol{x}} a^0 + \frac{1}{2}\nabla_{\boldsymbol{x}} \cdot \nabla_{\boldsymbol{p}} E_n(\nabla_{\boldsymbol{x}}\phi)$$

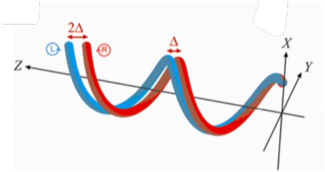
$$+ i\nabla_{\boldsymbol{x}} W(\boldsymbol{x}) \cdot \langle \chi_n(\cdot; \nabla_{\boldsymbol{x}}\phi) | i\nabla_{\boldsymbol{p}} \chi_n(\cdot; \nabla_{\boldsymbol{x}}\phi)\rangle_{L^2(\mathbb{R}^d/\Lambda)} = 0$$

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

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*:

4 

[4] **Bliokh, Niv, Kleiner, Hasman; Nature Photonics 2008.**

Theorem (Carles-Sparber 2008, Hagedorn 1980, Heller 1976)

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

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

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

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

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

$$\psi^\epsilon(\boldsymbol{x}, t) =$$

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

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

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

Writing the solution in terms of the multiscale variables:

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

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

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

Theorem (Watson-Weinstein-Lu 2016)

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

$$\dot{\mathcal{Q}}^\epsilon(t) = \nabla_{\mathcal{P}^\epsilon} E_n(\mathcal{P}^\epsilon(t)) + \epsilon \boldsymbol{C}_1[a^\epsilon](t)$$

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

$$\dot{\mathcal{P}}^\epsilon(t) = -\nabla_{\mathcal{Q}^\epsilon} W(\mathcal{Q}^\epsilon(t)) + \epsilon \boldsymbol{C}_2[a^\epsilon](t) + O(\epsilon^{3/2})$$

where $\mathcal{F}_n(\mathcal{P}^\epsilon)$ *is the Berry curvature of the Bloch band.* $\boldsymbol{C}_1[a^\epsilon](t), \boldsymbol{C}_2[a^\epsilon](t)$ *describe coupling to the wavepacket envelope* $a^\epsilon(\boldsymbol{y}, t)$, *which satisfies:*

$$i\partial_t a^\epsilon = -\frac{1}{2}\nabla_{\boldsymbol{y}} \cdot D^2_{\mathcal{P}^\epsilon} E_n(\mathcal{P}^\epsilon(t))\nabla_{\boldsymbol{y}} a^\epsilon + \frac{1}{2}\boldsymbol{y} \cdot D^2_{\mathcal{Q}^\epsilon} W(\mathcal{Q}^\epsilon(t))\boldsymbol{y} a^\epsilon$$

Theorem (Watson-Weinstein-Lu 2016 continued)

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

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

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

$$\dot{\mathcal{Q}}^\epsilon = \nabla_{\mathcal{P}^\epsilon} \mathcal{H}^\epsilon \qquad i\partial_t a^\epsilon = \frac{\delta \mathcal{H}}{\delta \overline{a^\epsilon}}$$
$$\dot{\mathcal{P}}^\epsilon = -\nabla_{\mathcal{Q}^\epsilon} \mathcal{H}^\epsilon$$

Gaussian reduction of envelope equation

The equation satisfied by the wavepacket envelope:

$$i\partial_t a^\epsilon = -\frac{1}{2}\nabla_{\boldsymbol{y}} \cdot D^2_{\mathcal{P}^\epsilon} E_n(\mathcal{P}^\epsilon(t))\nabla_{\boldsymbol{y}} a^\epsilon + \frac{1}{2}\boldsymbol{y} \cdot D^2_{\mathcal{Q}^\epsilon} W(\mathcal{Q}^\epsilon(t))\boldsymbol{y} a^\epsilon$$

has family of exact solutions which form a basis
e.g. time-dependent Gaussians[5]:

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

$$\dot{A}^\epsilon(t) = iD^2_{\mathcal{P}^\epsilon} E_n(\mathcal{P}^\epsilon) B^\epsilon(t), \quad \dot{B}^\epsilon(t) = iD^2_{\mathcal{Q}^\epsilon} W(\mathcal{Q}^\epsilon) A^\epsilon(t) \qquad (9)$$

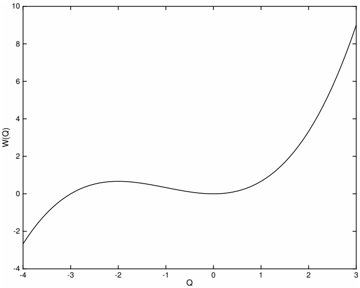
appropriate initial data $\implies$ $(\mathcal{Q}^\epsilon, \mathcal{P}^\epsilon, a^\epsilon)$ system reduces to ODEs

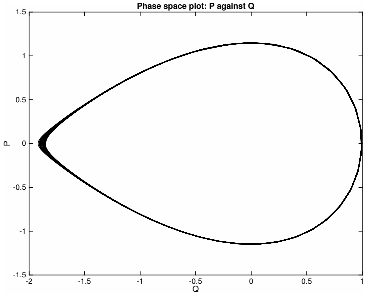
[5] **Hagedorn; Annals of Physics 1998**.

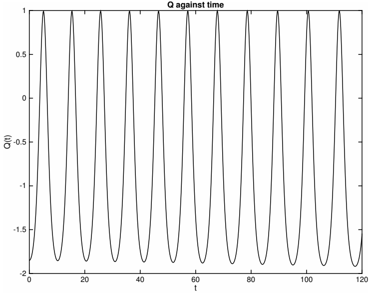
Numerical simulation: $\epsilon = 0$, decoupled system

Study coupling of observables to wave-field:

- One-dimensional: $d = 1$
- Uniform background: $V\left(\frac{x}{\epsilon}\right) = 0$
- Gaussian envelope
- Applied potential $W(\mathcal{Q}) = \frac{1}{6}\mathcal{Q}^3 + \frac{1}{2}\mathcal{Q}^2$



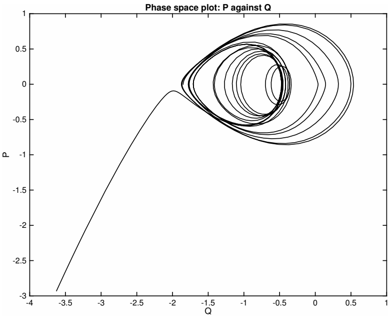


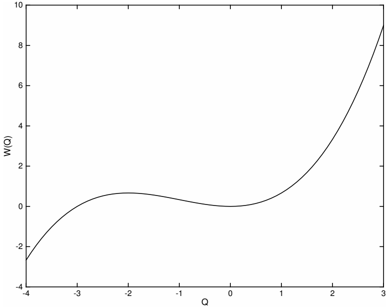


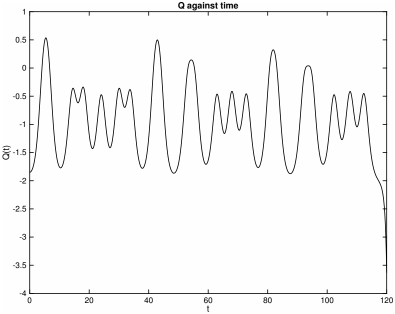
Numerical simulation: $\epsilon \neq 0$, coupled system

Simulation of full coupled system:

- Wave-field coupling has destabilizing effect on periodic orbits
- Wavepacket may escape potential well to $\mathcal{Q}^{\epsilon} = -\infty$





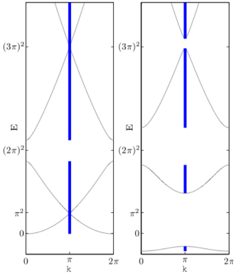


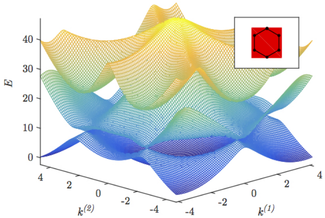
Dynamics at band crossings

- Would like to relax the 'isolated band' assumption:

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

- Crossings usually associated with *symmetries*





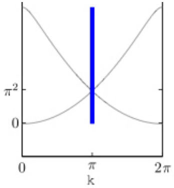
- At crossings Bloch band functions: $\boldsymbol{p} \to (E_n(\boldsymbol{p}), \chi_n(\boldsymbol{z}; \boldsymbol{p}))$ *not smooth* in general, e.g. conical degeneracies (Dirac points) $\implies$ restrict to $d = 1$

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 $L^2_x(\mathbb{R})$) 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 $E_- \implies$ 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

[6] **Molecular propagation through electron energy level crossings**, **Hagedorn G.**, **Memoirs of the American Mathematical Society (1994)**.

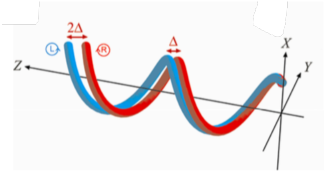
Recap of talk

- 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

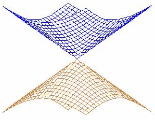
  Key tool: multi-scale *semiclassical wavepacket* ansatz
- Ongoing work/future directions

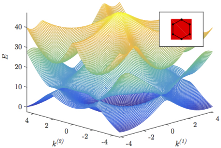
Ongoing work/future directions

- Schrödinger $\to$ Maxwell: spin Hall effect of light:



- Conical band crossings:





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