Wavepacket dynamics in locally periodic media

Focus: effects of Bloch band degeneracies

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October 2, 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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  $\Longrightarrow$ Call this a *locally periodic* medium.
- Model of *electron* propagation in crystalline media with *defects* and of *light* propagation through photonic variants.

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- Focus: effects of *eigenvalue degeneracies* on wave dynamics.
  2×2 matrix example:

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

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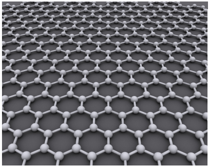
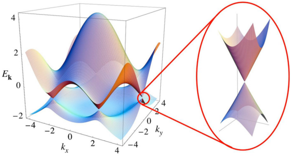
- Example: *honeycomb lattice symmetry* of graphene, gives rise to 'Dirac points' in band structure, *transport properties*:





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I will then discuss future directions of this work.

Models

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

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

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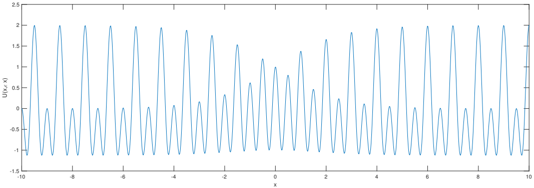
- Example ($d = 1$): $U(x, \epsilon x) = \cos(4\pi x) + \tanh(\epsilon x)\cos(2\pi x)$



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- Maxwell's equations in dimension $d = 3$:

$$\partial_t \boldsymbol{D}^\delta(\boldsymbol{x}, t) = \nabla \times \boldsymbol{H}^\delta(\boldsymbol{x}, t) \qquad \nabla \cdot \boldsymbol{D}^\delta(\boldsymbol{x}, t) = 0$$
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- Assume matrix to be *positive-definite* and *Hermitian* for all $\boldsymbol{x}$.
- 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*:

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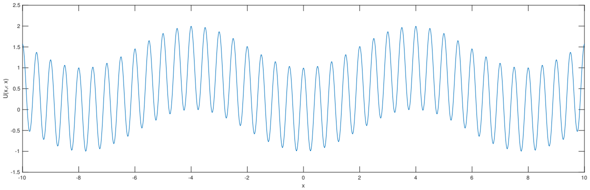

- Re-scale: $\boldsymbol{x}' := \epsilon \boldsymbol{x}, t' := \epsilon t, \psi^{\epsilon\prime}(\boldsymbol{x}', t') := \psi^{\epsilon}(\boldsymbol{x}, t)$.

$$\begin{aligned} &i\epsilon\partial_t \psi^\epsilon = -\epsilon^2 \frac{1}{2} \Delta_{\boldsymbol{x}} \psi^\epsilon + V\left(\frac{\boldsymbol{x}}{\epsilon}\right)\psi^\epsilon + W(\boldsymbol{x})\psi^\epsilon \\ &\forall \boldsymbol{v} \in \Lambda, V(\boldsymbol{z}+\boldsymbol{v}) = V(\boldsymbol{z}). \end{aligned} \qquad (\star)$$

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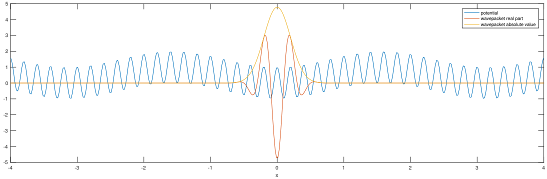

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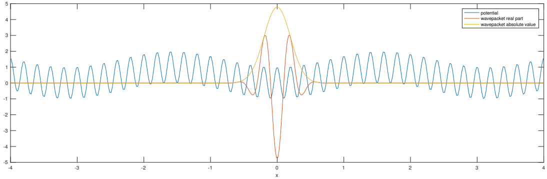

- Limit $\epsilon \downarrow 0$ a 'non-standard' *geometric optics/WKB* limit:

$$\epsilon := \frac{\text{wavelength} \approx \text{scale of variation of } V \text{ (periodic)}}{\text{scale of variation of } W \text{ (perturbation)}} \ll 1.$$

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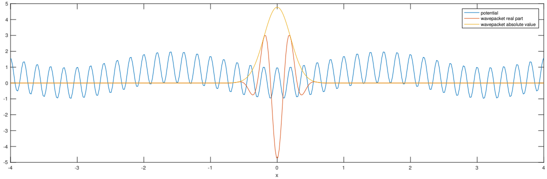

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NB *multi-scale* WKB ansatz *breaks down* near degeneracies.

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$$\mathcal{G}(\boldsymbol{y}, t) := \frac{1}{(1+it)^{d/2}} \exp\left(\frac{-|y|^2}{2(1+it)}\right)$$

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

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- Galilean invariance of (F) $\implies$ travelling Gaussian solutions with center at $\boldsymbol{q}(t) := \boldsymbol{q}_0 + \boldsymbol{p}_0 t$:

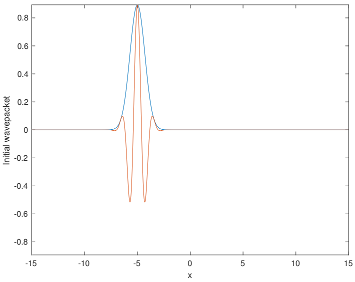
$$\psi^\epsilon(\boldsymbol{x}, t) = \epsilon^{-d/4}e^{iS(t)/\epsilon}e^{i\boldsymbol{p}_0\cdot(\boldsymbol{x}-\boldsymbol{q}(t))/\epsilon}\mathcal{G}\left(\frac{\boldsymbol{x}-\boldsymbol{q}(t)}{\epsilon^{1/2}}, t\right)$$

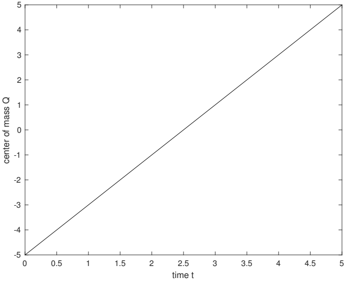
for any $(\boldsymbol{q}_0, \boldsymbol{p}_0) \in \mathbb{R}^d \times \mathbb{R}^d$. $S(t) := \frac{1}{2}|p_0|^2 t$.

Gaussian exact solution of free Schrödinger, $d = 1$:

$$\psi^\epsilon(x,t) = \epsilon^{-d/4} e^{iS(t)/\epsilon} e^{ip(t)(x-q(t))/\epsilon} \mathcal{G}\left(\frac{x-q(t)}{\epsilon^{1/2}}, t\right).$$

$q(t), p(t)$ satisfy Hamiltonian dynamics with $\mathcal{H} = p^2$:





Theorem (Hagedorn 1980, Heller 1976)

For any trajectory $(\boldsymbol{q}(t), \boldsymbol{p}(t))$ generated by the classical Hamiltonian $\mathcal{H} := \frac{|p|^2}{2} + W(\boldsymbol{q})$, 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 $\boldsymbol{q}(t)$*:*

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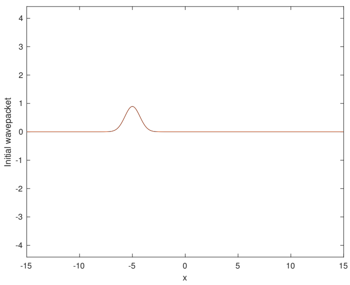
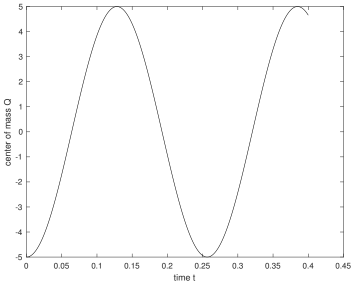
When W *quadratic, solution exact! Error* $\propto \|\partial_q^3 W(q)\|_{L^\infty}$*. Can improve error bound:* $O_{L^2_x(\mathbb{R}^d)}(\epsilon^{n/2}e^{Ct})$*, any positive integer* n*.*

Gaussian exact solution of Schrödinger's equation with harmonic oscillator potential $W \propto q^2$, $d = 1$:

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

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





Theorem $\implies$ Schrödinger's equation with an anharmonic oscillator potential $W \propto q^4$, $d = 1$ has an *approximate* Gaussian solution:

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

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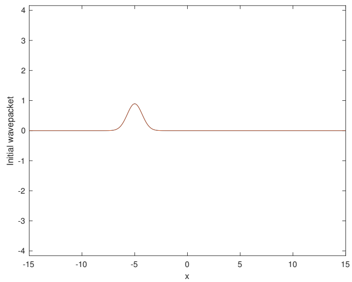

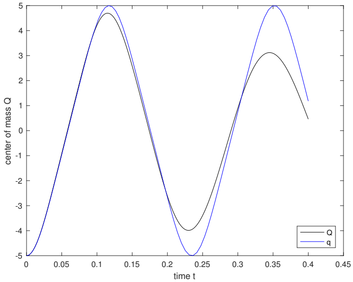

Wavepacket ansatz does not capture dynamics of PDE for t large.

Wavepacket dynamics in locally periodic media

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

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\begin{aligned}
& 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 \\
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\end{aligned} \qquad (\star)
$$

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

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

and *spectral localization* of the wavepacket in phase space.

Spectral theory of periodic operators

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

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

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$$H\,\Phi(\boldsymbol{z};\boldsymbol{p}) = E(\boldsymbol{p})\Phi(\boldsymbol{z};\boldsymbol{p})$$
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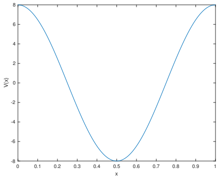
  symmetry of BC $\implies$ restrict $\boldsymbol{p}$ to a primitive cell of the reciprocal lattice: first Brillouin zone $\mathcal{B}$

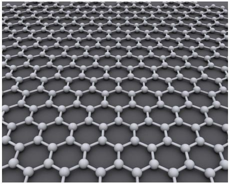
- Fixed quasi-momentum $\boldsymbol{p}$, self-adjoint elliptic eigenvalue problem $\implies$ discrete real spectrum:

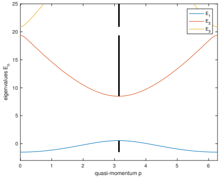
$$E_1(\boldsymbol{p}) \leq E_2(\boldsymbol{p}) \leq ... \leq E_n(\boldsymbol{p}) \leq ...$$

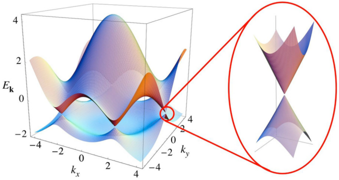
Spectral theory of periodic operators

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









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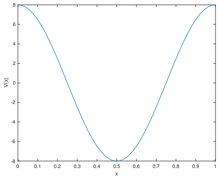

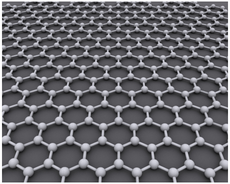

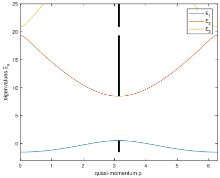

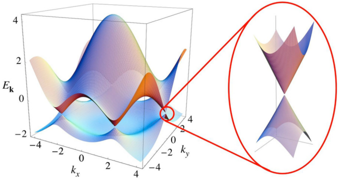

- Spectrum of $H = -\frac{1}{2}\Delta_{\boldsymbol{z}} + V(\boldsymbol{z})$ is then the union of real intervals swept out by $E_n(\boldsymbol{p})$.

Spectral theory of periodic operators

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

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- The set of associated eigenfunctions (Bloch waves) $\{\Phi_n(\boldsymbol{z};\boldsymbol{p}) : n \in \mathbb{N}, \boldsymbol{p} \in \mathcal{B}\}$ 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:

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

(P) is the *reduced Bloch eigenvalue problem*.

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

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

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

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

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

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

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.
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Hamiltonian system for dynamics away from degeneracies

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

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

$$\mathcal{F}_n(\boldsymbol{p}) = \mathrm{Im} \sum_{m \neq n} \frac{\langle \psi_n(\boldsymbol{p}) | \nabla_{\boldsymbol{p}} H(\boldsymbol{p}) \psi_m(\boldsymbol{p}) \rangle \times (n \leftrightarrow m)}{(E_m(\boldsymbol{p}) - E_n(\boldsymbol{p}))^2}$$

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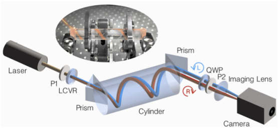
- Experimentally measured in photonics, where polarization condition $\boldsymbol{p} \cdot \boldsymbol{e}(\boldsymbol{p}) = 0$ degenerate at $\boldsymbol{p} = 0$:

$\Longrightarrow$

spin Hall effect of light



[a]

[a] **Bliokh et al., Nature Photonics, 2008.**

Strategy of proof

- Recall form of the asymptotic solution:

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

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

$$\mathcal{Q}^\epsilon(t) = \boldsymbol{q}(t) + \epsilon^{1/2} \int_{\mathbb{R}^d} \boldsymbol{y} |a(\boldsymbol{y}, t)|^2 \, \mathrm{d}\boldsymbol{y} + O(\epsilon)$$

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Dynamics of $\mathcal{Q}^\epsilon, \mathcal{P}^\epsilon$ couples to evolution of $\boldsymbol{q}, \boldsymbol{p}, a$ (complicated) as well as the Bloch functions $\chi_n(\boldsymbol{z}; \boldsymbol{p})$.

Theorem (Watson-Weinstein-Lu 2016)

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

$$(\boldsymbol{q}, \boldsymbol{p}, a) \mapsto (\mathcal{Q}^\epsilon, \mathcal{P}^\epsilon, a^\epsilon)$$

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

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the observables $\mathcal{Q}^\epsilon(t)$ and $\mathcal{P}^\epsilon(t)$ satisfy:

$$\dot{\mathcal{Q}}^\epsilon(t) = \nabla_{\mathcal{P}^\epsilon} E_n(\mathcal{P}^\epsilon(t)) - \underbrace{\epsilon\dot{\mathcal{P}}^\epsilon(t) \times \mathcal{F}_n(\mathcal{P}^\epsilon(t))}_{\text{Anomalous velocity}} + \epsilon \boldsymbol{C}_1[a^\epsilon](t) + O(\epsilon^{3/2})$$

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

where $\mathcal{F}_n(\mathcal{P}^\epsilon)$ denotes the Berry curvature of the Bloch band.

Theorem (Watson-Weinstein-Lu 2016 continued)

2) 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:

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

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

$$\dot{\mathcal{Q}}^\epsilon = \nabla_{\mathcal{P}^\epsilon} \mathcal{H}^\epsilon \qquad i\partial_t a^\epsilon = \frac{\delta \mathcal{H}}{\delta \overline{a^\epsilon}} \qquad \text{(S)}$$
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[1] **Chang et al. Phys. Rev. B 1996; Xiao et al. Rev. Mod. Phys. 2010.**

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

[1] **Chang et al. Phys. Rev. B 1996; Xiao et al. Rev. Mod. Phys. 2010.**

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

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

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

$$\dot{\mathcal{P}}^\epsilon(t) = -\nabla_{\mathcal{Q}^\epsilon} W(\mathcal{Q}^\epsilon(t)) \quad \underbrace{-\epsilon \frac{1}{2} \partial^3_{\mathcal{Q}^\epsilon} W(\mathcal{Q}^\epsilon) \left\langle a^\epsilon(y,t) | y^2 a^\epsilon(y,t) \right\rangle_{L^2_y}}_{\textit{coupling of discrete degrees of freedom to wave-field}}$$

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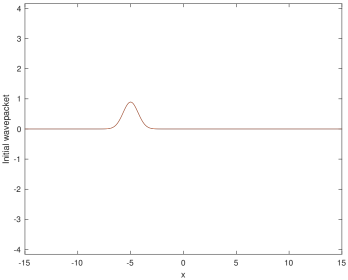
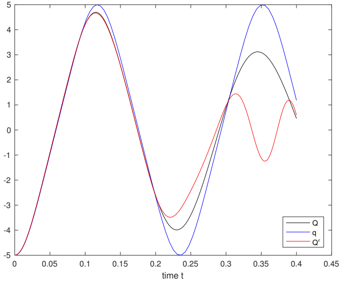
- Center of mass dynamics when potential $W \propto q^4$:





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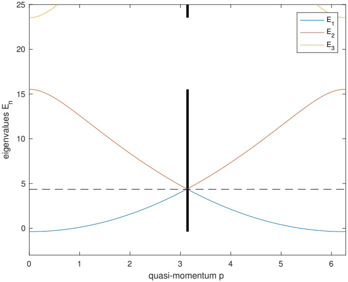
- Degeneracies, where $E_n(\boldsymbol{p}^*) = E_{n+1}(\boldsymbol{p}^*)$, usually associated with *symmetries* of periodic structure. In $d = 1$, rich set of examples: *Jacobi elliptic functions*.



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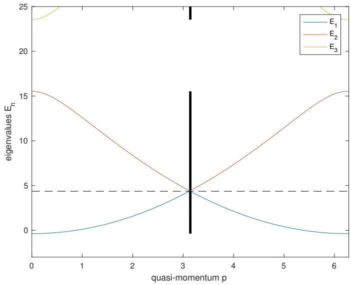
- Degeneracies, where $E_n(\boldsymbol{p}^*) = E_{n+1}(\boldsymbol{p}^*)$, usually associated with *symmetries* of periodic structure. In $d = 1$, rich set of examples: *Jacobi elliptic functions*.



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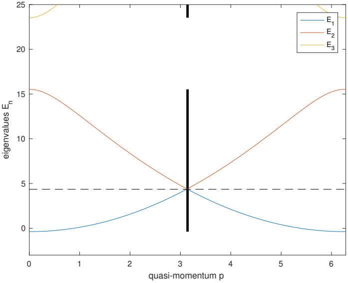
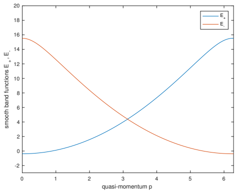


- New degree of freedom: *coupling* between degenerate states
- At crossings, Bloch band functions: $\boldsymbol{p} \to E_n(\boldsymbol{p})$ *not smooth*

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* $d = 1$*).*



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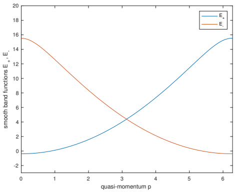

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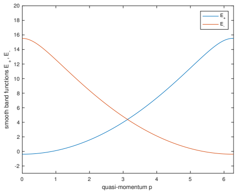

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- *As $t \uparrow t^*$, error in single band approximation blows up:*

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

$\implies$ *emergent time-scale:* $s \sim \frac{t - t^*}{\sqrt{\epsilon}}$.

Theorem (Watson-Weinstein 2016 continued)

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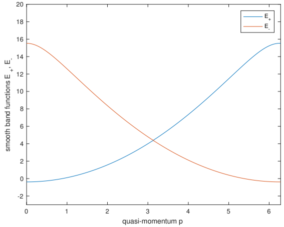

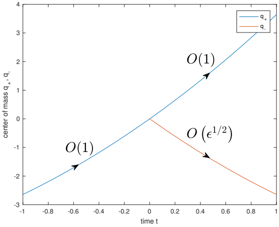

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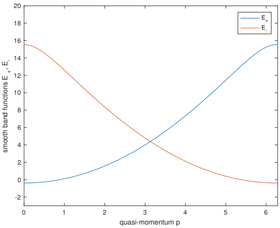

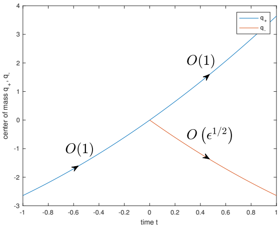

Result is an analog of those obtained by Hagedorn (B-O approx.)

Consistency with Landau-Zener theory

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

$$i\epsilon\partial_t\psi^\epsilon = H(t)\psi^\epsilon$$

with $\mathrm{Spec}[H(t)] = E_+(t) \cup E_-(t)$, linear crossing at $t = t^*$.

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

$$\|c_-(t)\|^2 = \frac{2\pi|\,\langle\chi_-(t^*)|\dot{\chi}_+(t^*)\rangle\,|^2}{|\dot{E}_+(t^*) - \dot{E}_-(t^*)|}\sqrt{\epsilon} + o(\sqrt{\epsilon}).$$

Ongoing work/future directions

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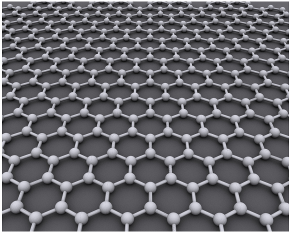

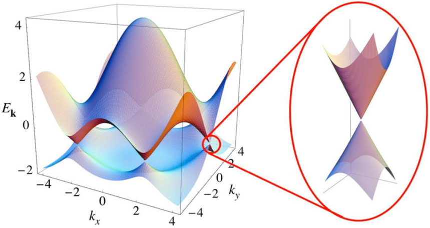

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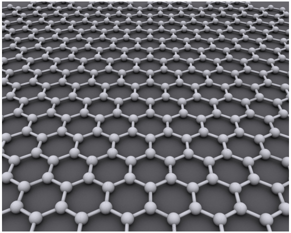

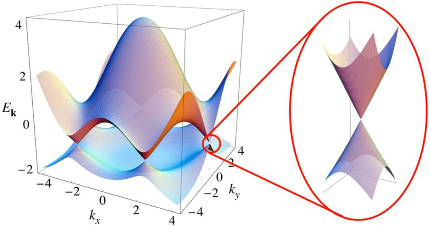

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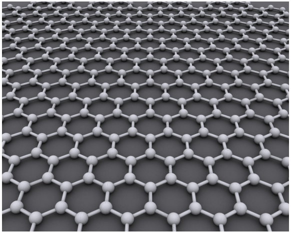

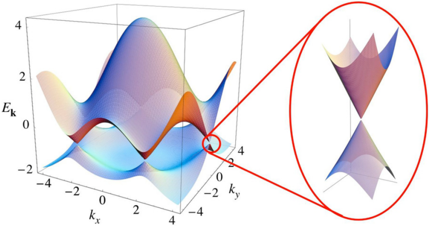

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Expect <u>$O(1)$ coupling between bands</u> in these cases; proved by Hagedorn (B-O approximation).

Thanks for listening!