Evolution of Gaussian wave packets generated by a non-Hermitian Hamiltonian in the semiclassical limit

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QM3 = Quantum Matter meets Maths
April 2020

Quantum and classical dynamics

Sir William Rowan Hamilton
1805 - 1865

★ Classical Hamiltonian dynamics:
Position q and momentum p

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}$$

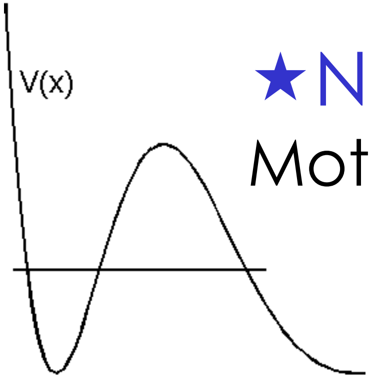
★ Quantum dynamics:
Schrödinger equation

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = \hat{H}\psi(x,t)$$

Erwin Schrödinger
Nobel Prize 1933

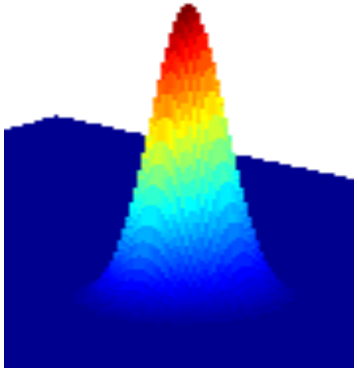
★ Connection? ⟶ For example, via "wave packets"

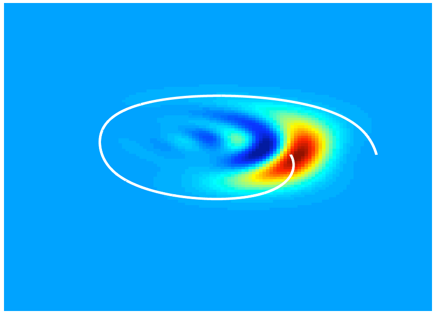
Outline



★Non-Hermitian quantum mechanics:
Motivation, dynamical aspects, open questions

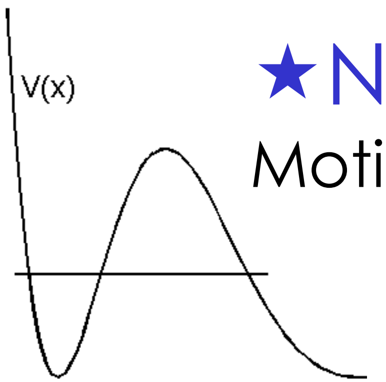
★The classical approximation:
Gaussian states and their geometry, wave packet dynamics in the semiclassical limit





★Non-Hermitian classical limit:
Classical dissipative motion, a generalised canonical structure, applications

Outline



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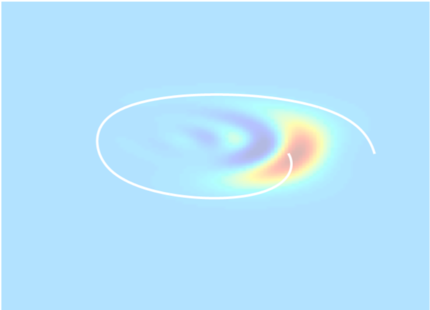

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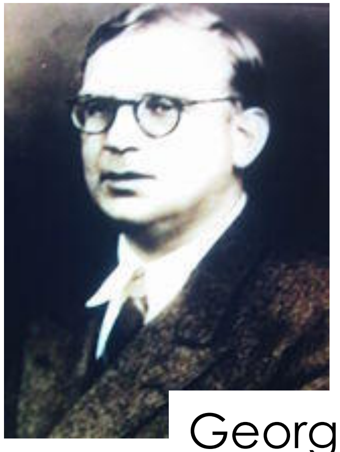
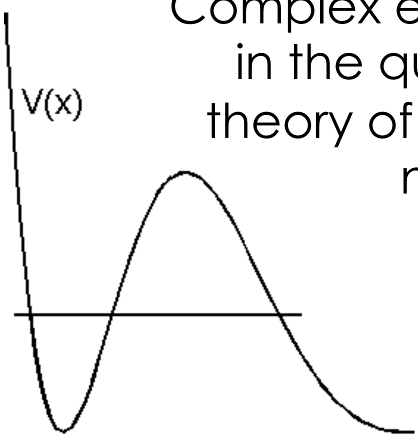
Non-Hermitian quantum systems?



George Gamow



Complex energies in the quantum theory of atomic nuclei in 1928

★Non-Hermitian Hamiltonians: complex energy, probability (and energy) not conserved ⇒ **open/decaying systems**

★Non-Hermitian Hamiltonians with purely real spectrum can be used to define consistent quantum theory for closed systems

⇒ **PT symmetric quantum theory**

Bender et al 1998

★Here: $$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi = (\hat{H} - \mathrm{i}\hat{\Gamma})\psi$$

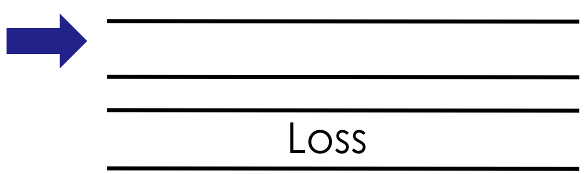
Non-Hermitian QM in coupled optical wave guides

★ Two-level model:

$$H = \begin{pmatrix} 0 & v \\ v & -2\mathrm{i}\gamma \end{pmatrix}$$

$$\lambda_{\pm} = -\mathrm{i}\gamma \pm \sqrt{v^2 - \gamma^2}$$

Coupled optical wave guides:



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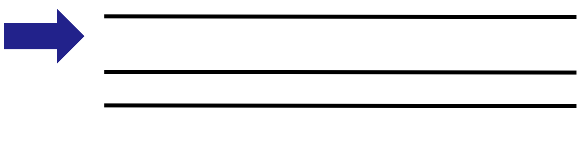

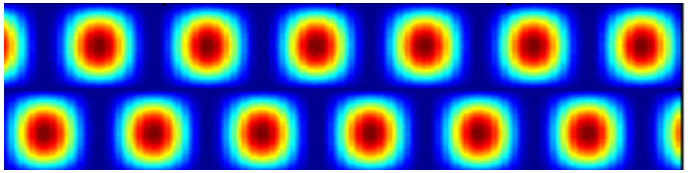

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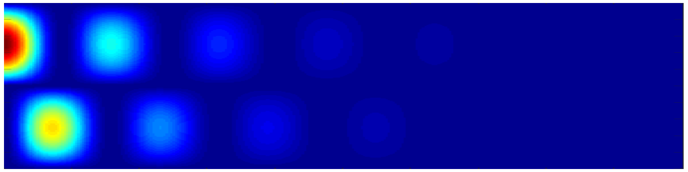

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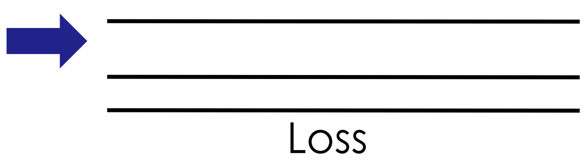

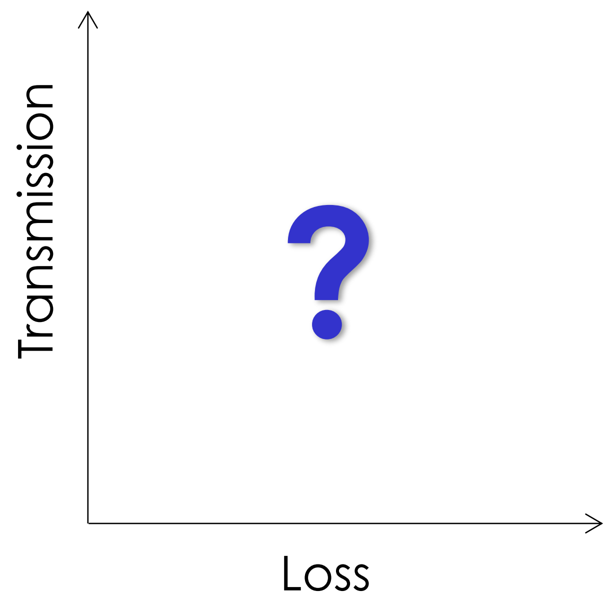

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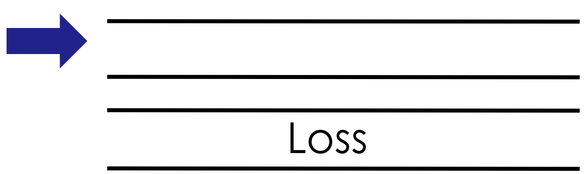
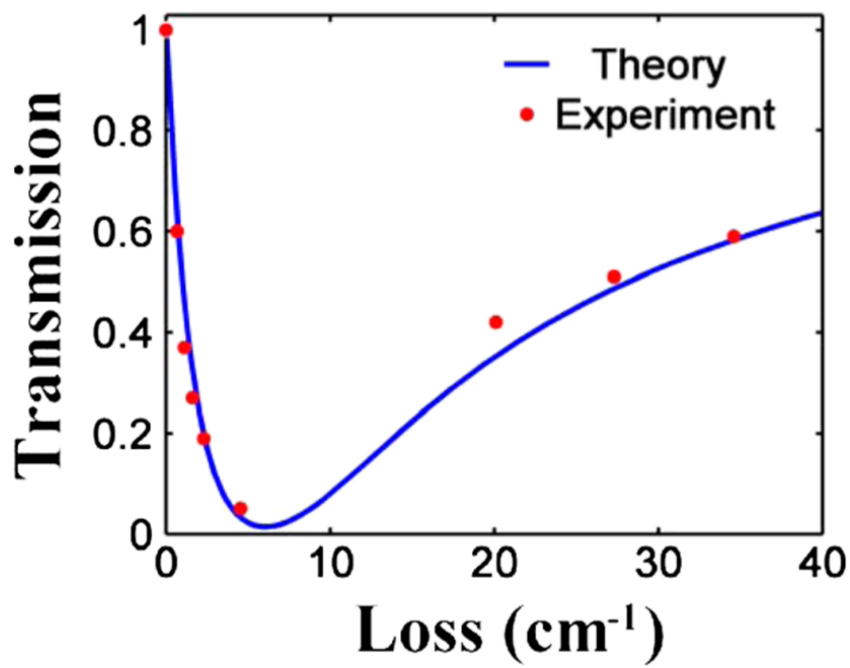




A. Guo *et al.*, Phys. Rev. Lett. 103, 093902 (2009)

Non-Hermitian quantum dynamics

★ New and interesting dynamical features

★ Only few model systems investigated

★ Numerical simulation of realistic quantum dynamics hard

★ Hermitian systems: useful semiclassical methods

★ Non-Hermitian systems: Little known about classical counterparts

Non-Hermitian classical analogue?

★Hermitian classical approximation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\Psi|\hat{F}|\Psi\rangle = \mathrm{i}\langle\Psi|[\hat{H},\hat{F}]|\Psi\rangle \longrightarrow \frac{\mathrm{d}}{\mathrm{d}t}F = \{H,F\}$$

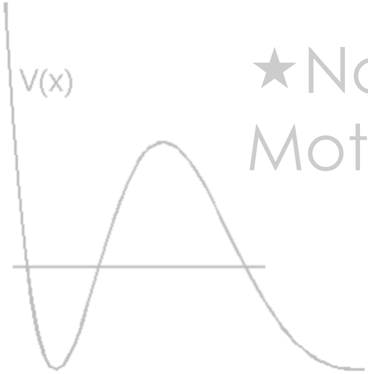
★Generalised Heisenberg equations of motion:

$$\frac{d}{dt}\langle\Psi|\hat{F}|\Psi\rangle = \mathrm{i}\langle\Psi|\hat{H}^{\dagger}\hat{F} - \hat{F}\hat{H}|\Psi\rangle$$

★And for the expectation values $\langle\hat{F}\rangle = \dfrac{\langle\Psi|\hat{F}|\Psi\rangle}{\langle\Psi|\Psi\rangle}$:

$$\frac{d}{dt}\langle\hat{F}\rangle = \mathrm{i}\langle\hat{H}^{\dagger}\hat{F} - \hat{F}\hat{H}\rangle + \mathrm{i}\langle\hat{F}\rangle\langle\hat{H}^{\dagger} - \hat{H}\rangle$$

Outline



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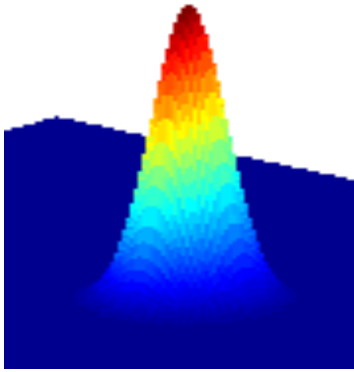
★The classical approximation:
Gaussian states and their geometry, wave packet dynamics in the semiclassical limit



★Non-Hermitian classical limit:
Classical dissipative motion, a generalised canonical structure, applications

Gaussian states and their geometry

★ Gaussian wave packets:

$$\psi_Z^B(x) = \left(\frac{\mathrm{Im}B}{\pi\hbar}\right)^{1/4} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}[P(x-Q)+\frac{1}{2}B(x-Q)^2]}$$

★ With $Z=(P,Q)\in\mathbb{R}^2$, $B\in\mathbb{C}$ with $\mathrm{Im}B>0$

★ Expectation values and uncertainties:

$$\langle\hat{q}\rangle = Q, \quad \langle\hat{p}\rangle = P$$

$$(\Delta\hat{q})^2 = \frac{\hbar}{2\mathrm{Im}B} \quad (\Delta\hat{p})^2 = \frac{\hbar|B|^2}{2\mathrm{Im}B}$$

Gaussian states and semiclassical limit

$$\psi_z^B(x) = \left(\frac{\mathrm{Im}(B)}{\pi}\right)^{\frac{1}{4}} \mathrm{e}^{\mathrm{i}\left(\frac{B}{2}(x-q)^2 + p(x-q)\right)}$$

★ Expectation values and uncertainties:

$$\langle \hat{A} \rangle = A(z) + O(\hbar)$$
$$(\Delta A)^2 = \nabla A(z) \cdot \Sigma \nabla A(z) + O(\hbar^2)$$

★ With covariance matrix

$$\Sigma = \frac{\hbar}{2\mathrm{Im}(B)} \begin{pmatrix} \mathrm{Re}(B)^2 + \mathrm{Im}(B)^2 & \mathrm{Re}(B) \\ \mathrm{Re}(B) & 1 \end{pmatrix}$$

The semiclassical limit with Gaussian states

★Gaussian states stay Gaussian under evolution with quadratic Hamiltonian!

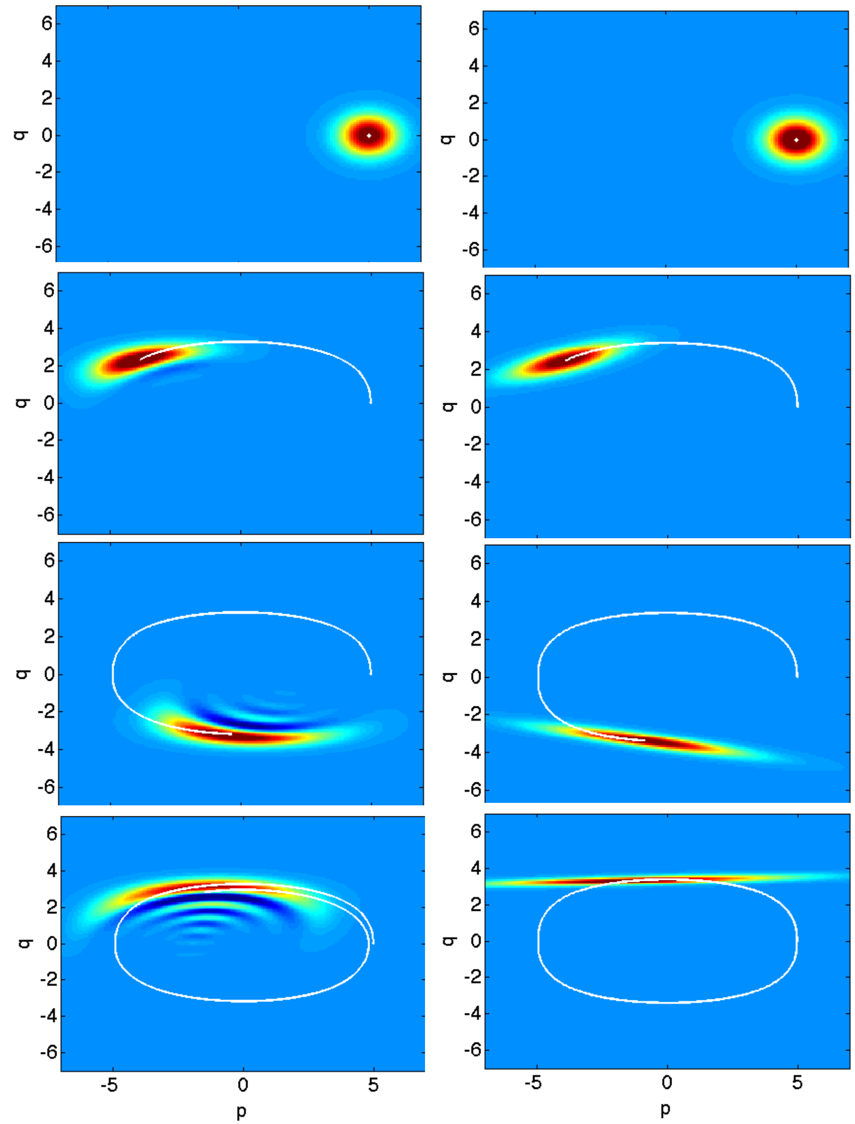
★Gaussian ansatz for time evolved Wigner function!

★Quadratic Taylor expansion around the central trajectory z(t)

★Yields semiclassical evolution:

$$\dot{p} = -\frac{\partial H}{\partial q}\ , \ \dot{q} = \frac{\partial H}{\partial p}$$

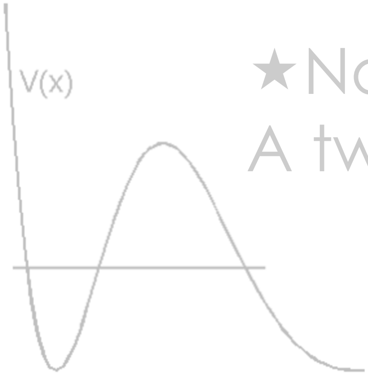
$$\dot{\Sigma} = \Omega H'' \Sigma - \Sigma H'' \Omega$$



anharmonic oscillator

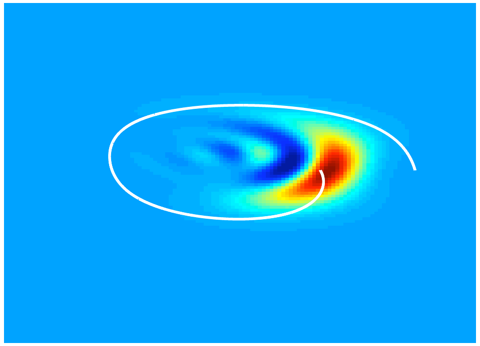
Hepp, Heller, Littlejohn 1970's

Outline



★Non-Hermitian quantum mechanics:
A two-level syste, exceptional points, PT-symmetry

★The classical approximation:
Gaussian states and their geometry, wave packet dynamics in the semiclassical limit



★Non-Hermitian classical limit:
Classical dissipative motion, a generalised canonical structure, applications

Non-Hermitian Semiclassical limit

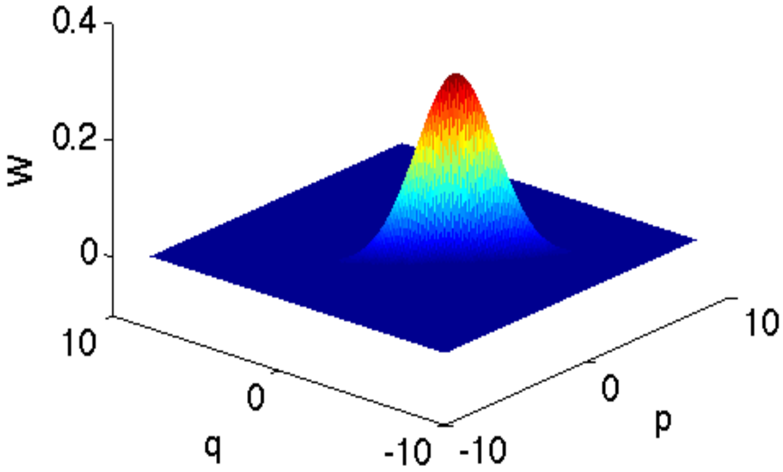
★Time evolution of Gaussian wave packets

$$\psi(x,t) = \frac{\mathrm{Im}B(t)^{1/4}}{(\pi\hbar)^{1/4}} \mathrm{e}^{\frac{\mathrm{i}}{\hbar}\left[p(t)(x-q(t))+\frac{1}{2}B(t)(x-q(t))^2+\alpha(t)\right]}$$

in the semiclassical limit $\hbar \to 0$

★ Still: Gaussian states stay Gaussian under evolution with quadratic Hamiltonian!

★Quadratic Taylor expansion of Hamiltonian around central trajectory z(t)=(p(t),q(t))



Non-Hermitian "semiclassical" dynamics

★ Time evolution with general non-Hermitian Hamiltonian: $H = H_R - \mathrm{i}H_I$

★ Ansatz for time-evolved state:

$$\psi(x,t) = N(t)\left(\frac{\mathrm{Im}(B(t))}{\pi}\right)^{\frac{1}{4}} \mathrm{e}^{\mathrm{i}\left(\frac{B(t)}{2}(x-q(t))^2 + p(t)(x-q(t)) + \alpha(t)\right)}$$

★ Taylor expansion of H around centre of wave packet up to second order

★ Coupled dynamical equations for phase-space coordinates and (co)variances

Semiclassical limit for non-Hermitian systems

$$H = H_R - \mathrm{i}H_I$$

$$\dot{p} = -\frac{\partial H_R}{\partial q} - \Sigma_{pp}\frac{\partial H_I}{\partial p} - \Sigma_{pq}\frac{\partial H_I}{\partial q}$$

$$\dot{q} = \frac{\partial H_R}{\partial p} - \Sigma_{pq}\frac{\partial H_I}{\partial p} - \Sigma_{qq}\frac{\partial H_I}{\partial q}$$

★ With covariance matrix Σ

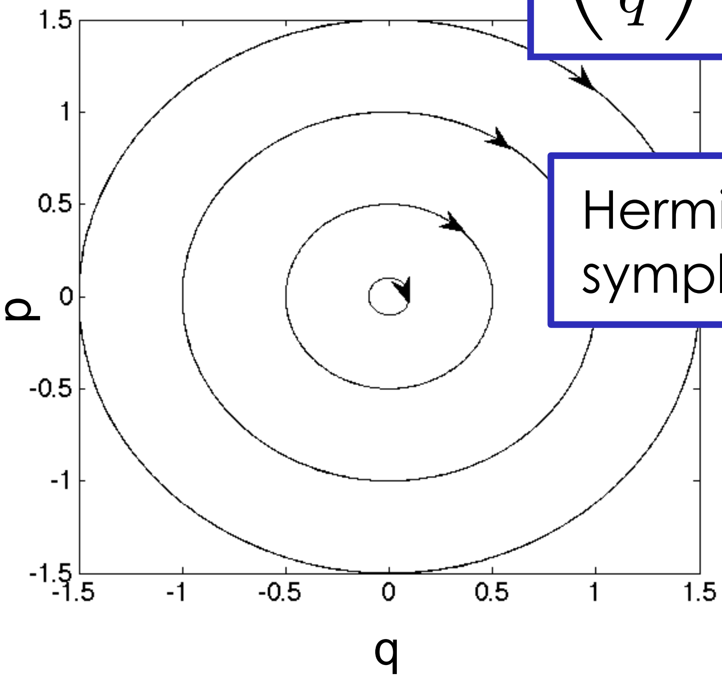
$$\Sigma_{pp} = \tfrac{2}{\hbar}(\Delta p)^2, \quad \Sigma_{qq} = \tfrac{2}{\hbar}(\Delta q)^2, \quad \Sigma_{pq} = \Sigma_{qp} = \tfrac{2}{\hbar}\Delta_{pq}$$

$$\dot{\Sigma} = \Omega H_R''\Sigma - \Sigma H_R''\Omega - \Omega H_I''\Omega - \Sigma H_I''\Sigma$$

EMG, H.J. Korsch, and A. Rush, New J. Phys. 18 (2016) 075009

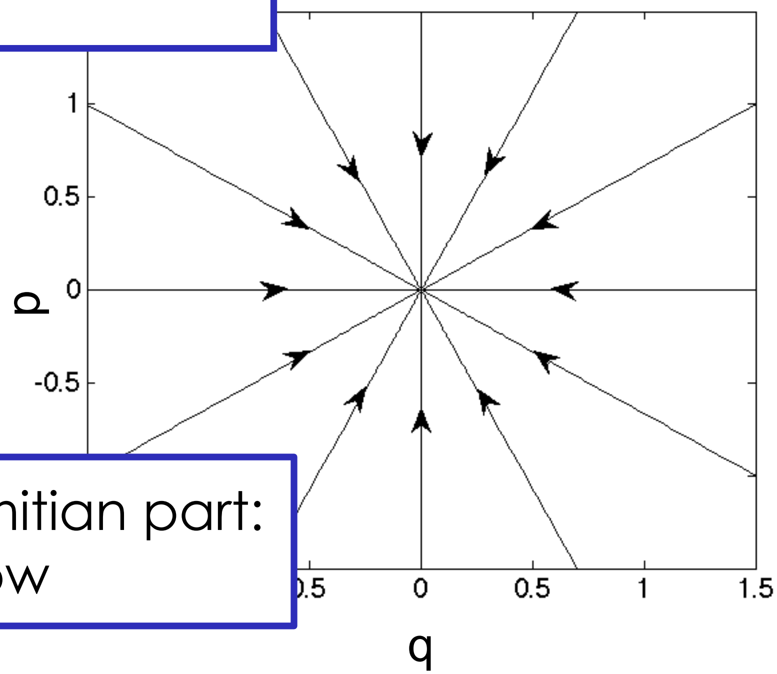
The generalised canonical equations

$$\begin{pmatrix} \dot{p} \\ \dot{q} \end{pmatrix} = \Omega \nabla H_R - \Sigma \nabla H_I$$



Hermitian part: symplectic flow

Hamiltonian (conservative) dynamics



Anti-Hermitian part: metric flow

Aims to drive the dynamics on the “direct” way towards a minimum of H_I .

Non-Hermitian semiclassical dynamics

★ Dynamics of position and momentum

$$\dot{p} = -\frac{\partial H_R}{\partial q} - \Sigma_{pp}\frac{\partial H_I}{\partial p} - \Sigma_{pq}\frac{\partial H_I}{\partial q}$$

$$\dot{q} = \frac{\partial H_R}{\partial p} - \Sigma_{pq}\frac{\partial H_I}{\partial p} - \Sigma_{qq}\frac{\partial H_I}{\partial q}$$

★ Coupled to covariance dynamics

$$\dot{\Sigma} = \Omega H_R''\Sigma - \Sigma H_R''\Omega - \Omega H_I''\Omega - \Sigma H_I''\Sigma$$

★ Resulting dynamics of squared norm/total power:

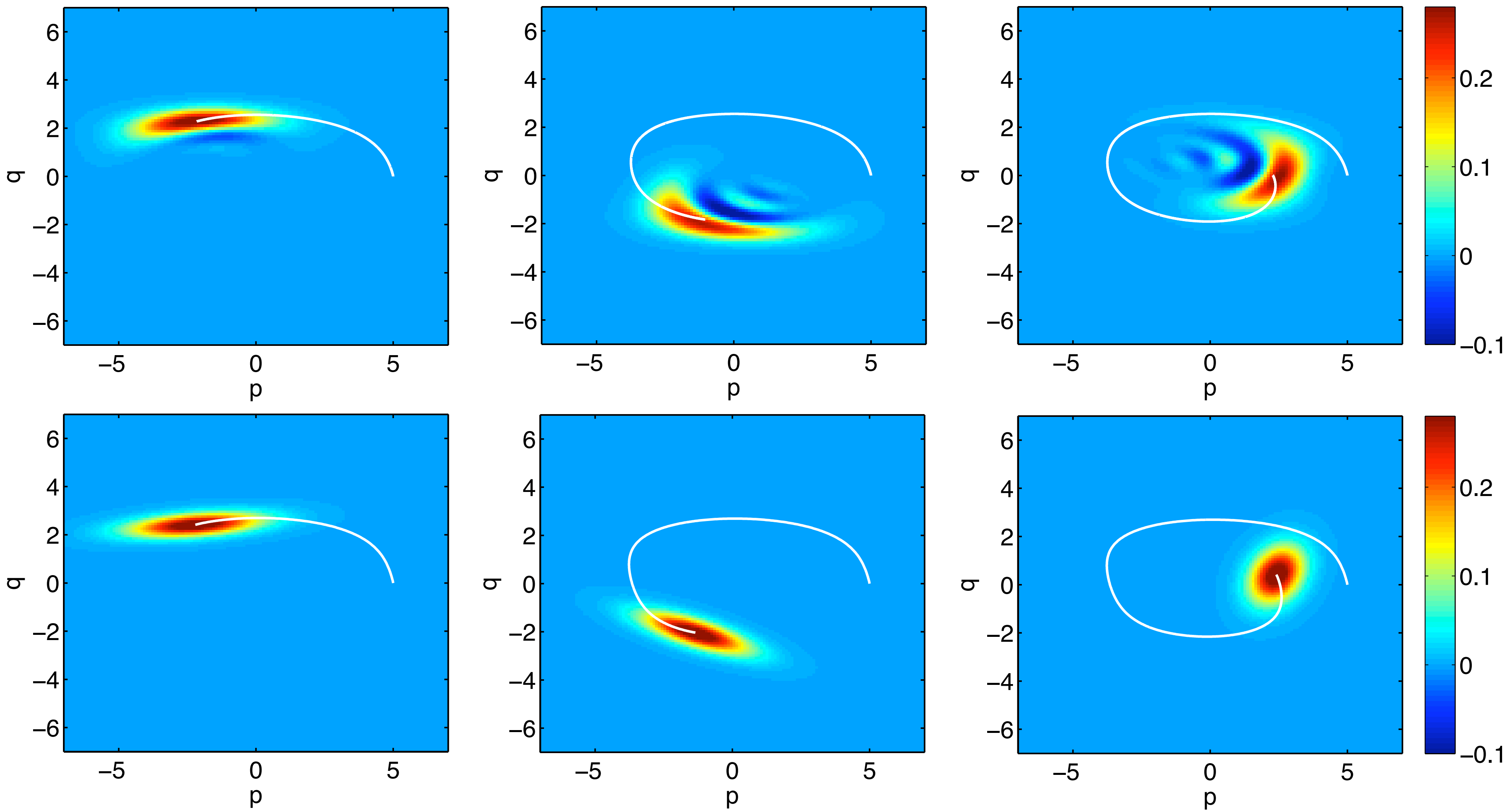
$$\dot{P} = -\big(2H_I - \tfrac{1}{2}\mathrm{Tr}(\Omega H_I''\Omega\Sigma^{-1})\big)P$$

EMG, H.J. Korsch, and A. Rush, New J. Phys. 18 (2016) 075009

The non-Hermitian anharmonic oscillator

$$\hat{H} = \frac{\omega}{2}(\hat{p}^2 + \hat{q}^2) + \frac{\beta}{4}\hat{q}^4, \quad \hat{\Gamma} = \frac{\gamma}{2}(\hat{p}^2 + \hat{q}^2)$$

$\omega = 1,\ \gamma = 0.2,\ \beta = 0.5$



Beam propagation in optical waveguides

★Propagation of electric field amplitude ψ in paraxial approximation in direction z:

$$i\hbar\frac{\partial\psi}{\partial z} = -\frac{\hbar^2}{2n_0}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

Effective $\hbar = \dfrac{\lambda}{2\pi}$

Reference refractive index

Refractive index modulation in x direction:

$$V(x) = \frac{n_0^2 - n^2(x)}{2n_0} \approx n_0 - n(x)$$

★Gaussian approximation yields "geometric optics" beam dynamics

Geometric optics in the presence of loss and gain

★Complex refractive index models absorption and amplification

★Gaussian approximation yields:

$$\dot{p} = -V_R'(q) + \frac{\mathrm{Re}(B)}{\mathrm{Im}(B)} V_I'(q),$$

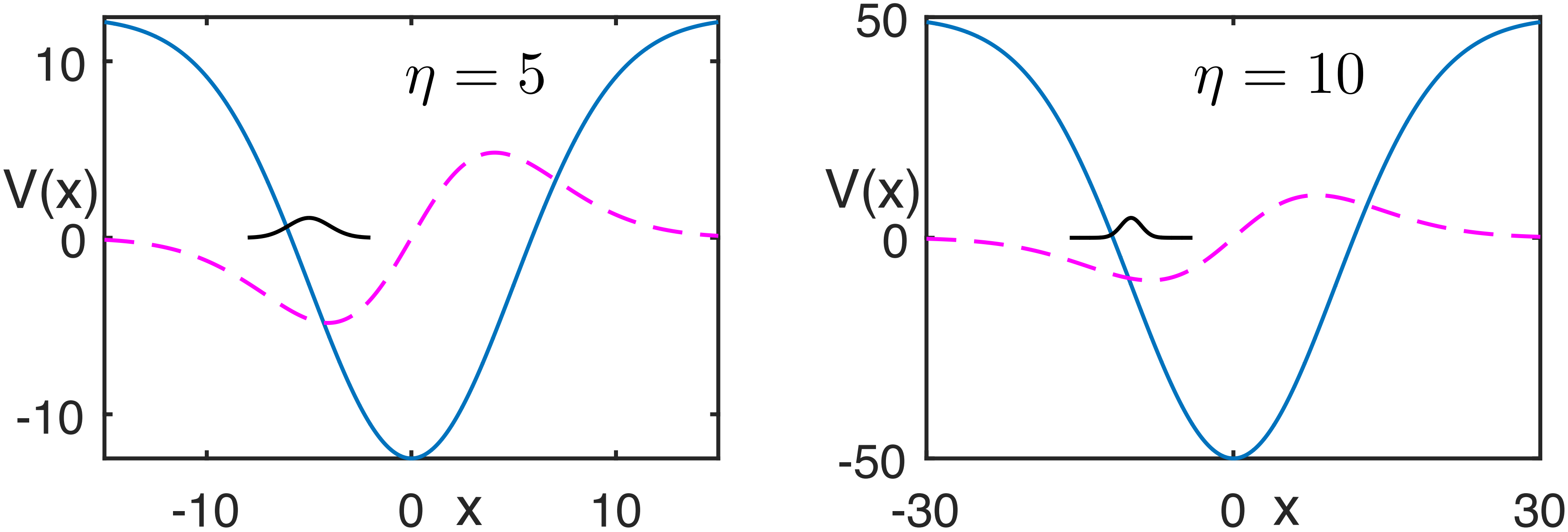
$$\dot{q} = p + \frac{1}{\mathrm{Im}(B)} V_I'(q),$$

$$\dot{B} = -B^2 - V_R''(q) - \mathrm{i} V_I''(q),$$

$$\dot{N} = \left(\frac{1}{\hbar} V_I(q) + \frac{1}{4\mathrm{Im}(B)} V_I''(q) \right) N$$

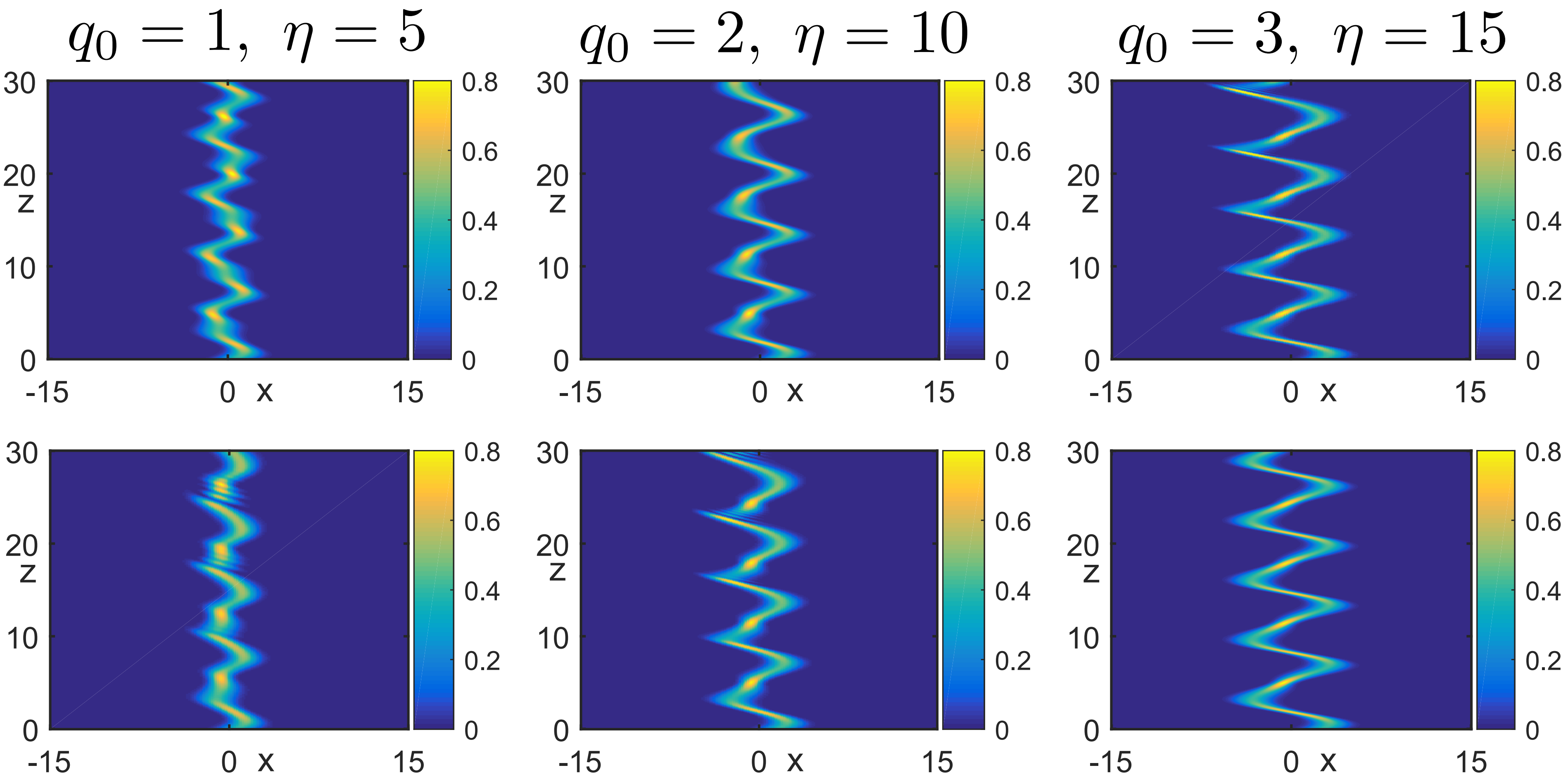
Example: PT-symmetric wave guide

$$V(x) = -\left(1 - \mathrm{i}\frac{\gamma}{\eta}\tanh\left(\frac{x}{\eta}\right)\right)\eta^2 \mathrm{e}^{-\frac{\omega^2 x^2}{2\eta^2}}$$



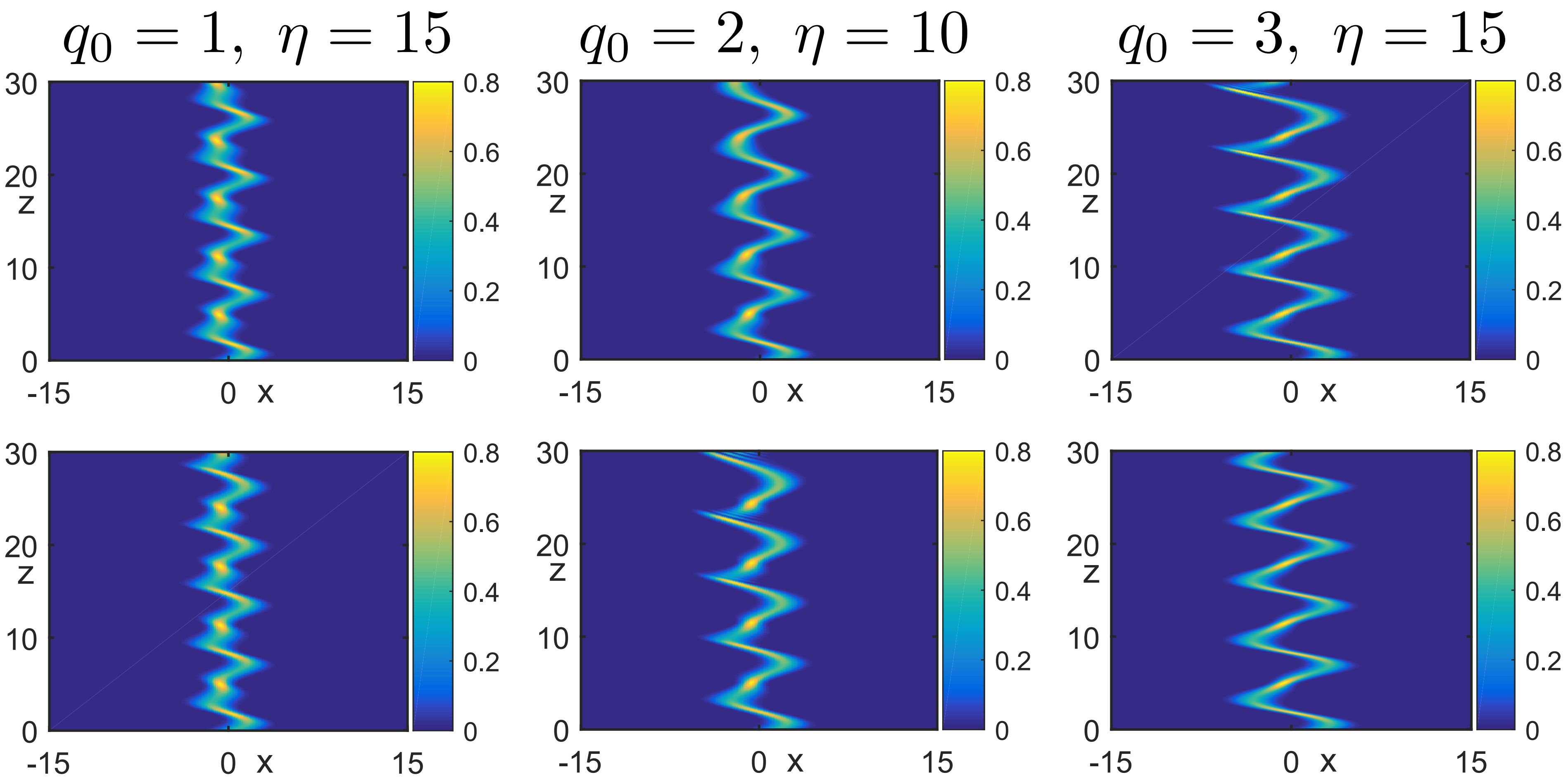
Gaussian approximation expected to be good for large η

Example: PT-symmetric wave guide



Guassian approximation (top) and exact numerical propagation (bottom), $B_0 = \frac{\mathrm{i}}{2}$

Example: PT-symmetric wave guide



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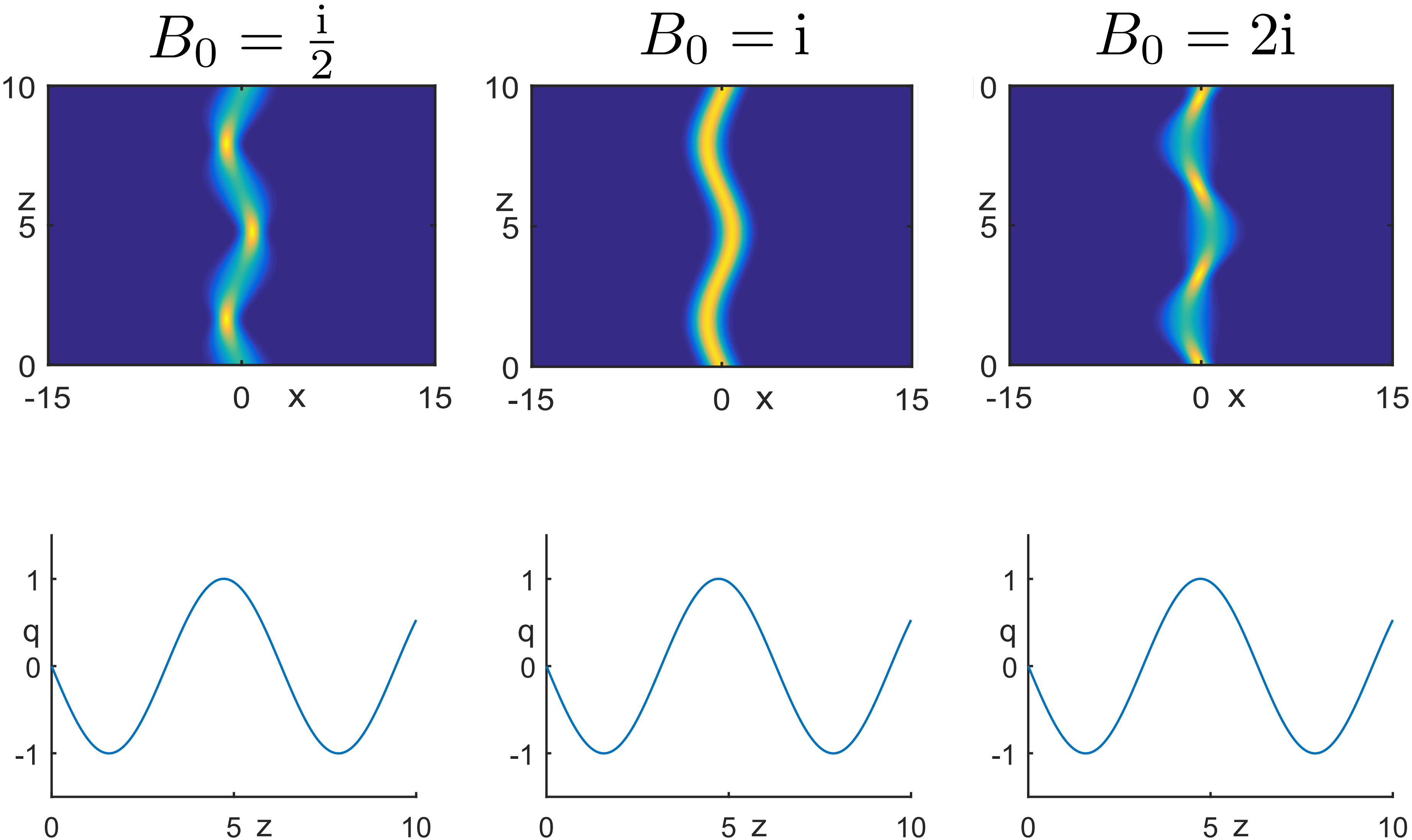
Geometric optics without absorption



EMG, Rush, Schubert, IEEE JSTQE 22 (2016) 5000906

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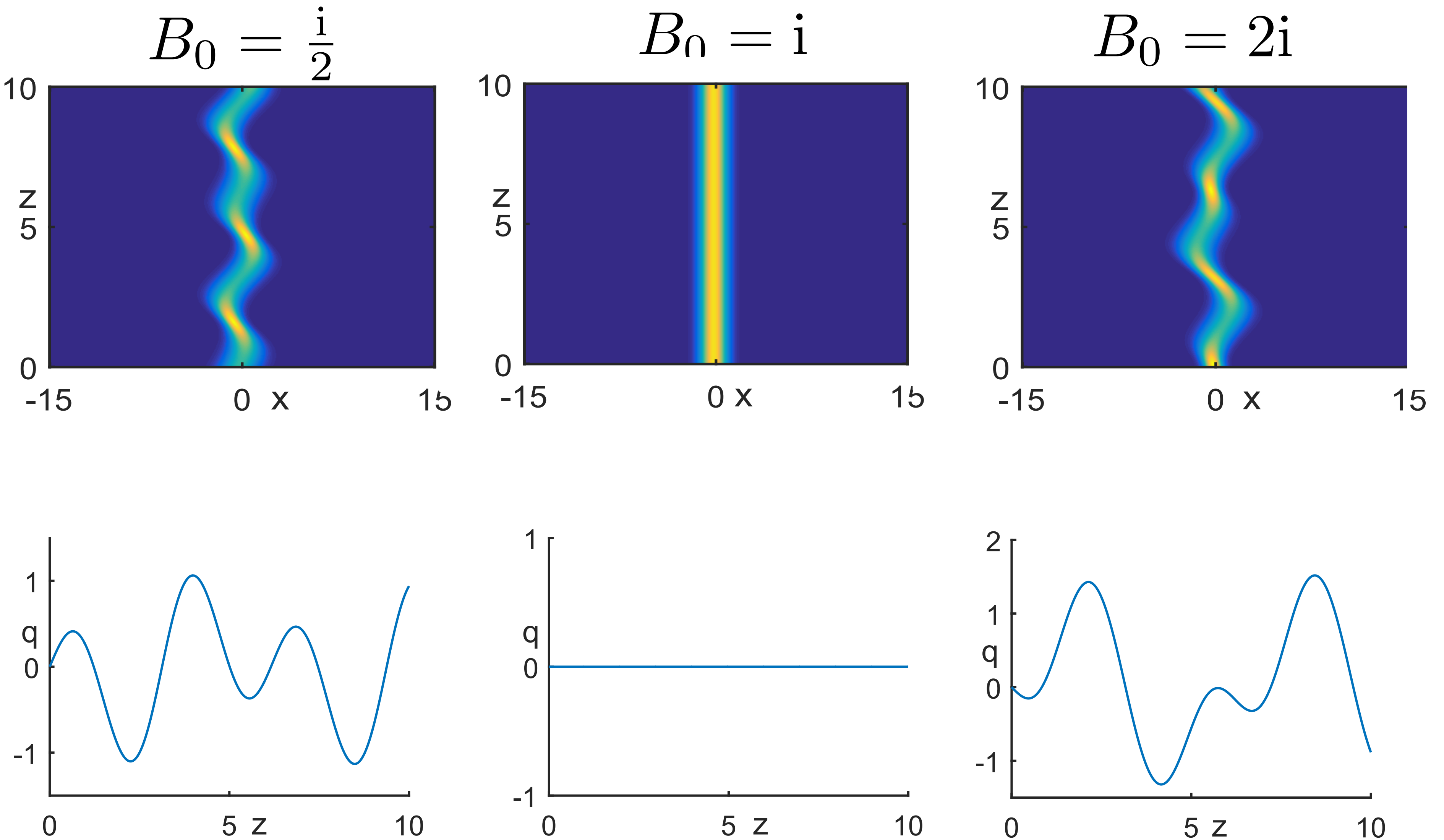
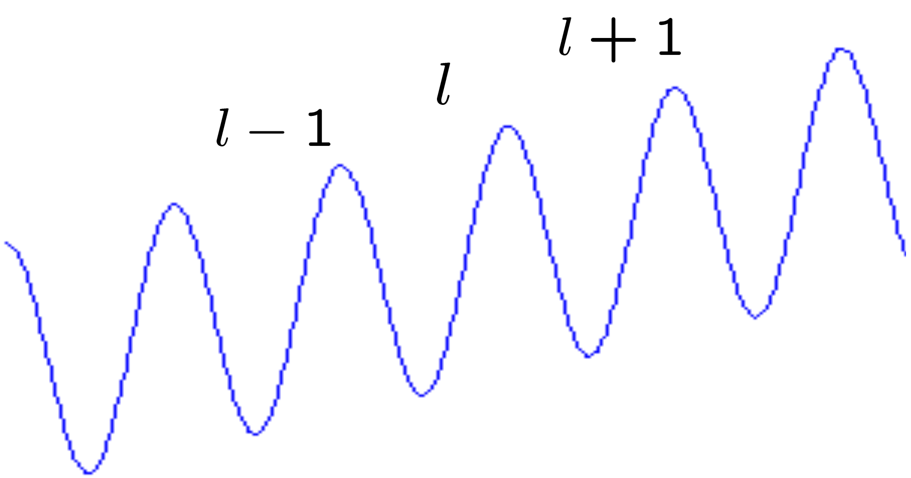


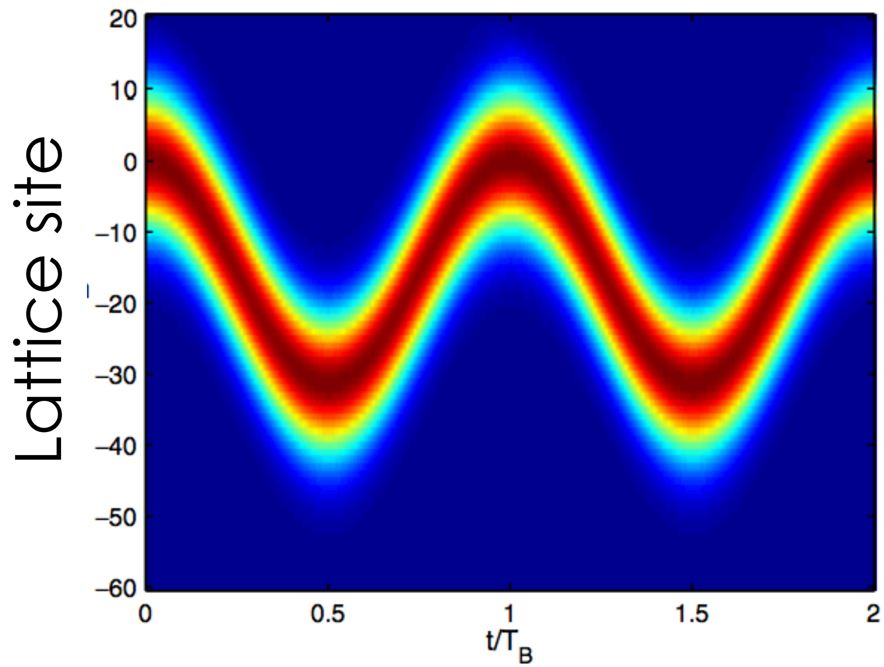
EMG, Rush, Schubert, IEEE JSTQE 22 (2016) 5000906

Bloch oscillations - single-band tight-binding Hamiltonian

$$\hat{H} = Fd\sum_l l|l\rangle\langle l| - \frac{J}{2}\sum_l \left(|l+1\rangle\langle l| + |l\rangle\langle l+1|\right)$$

On-site energy   Tunneling/hopping between sites





T. Hartmann, F. Keck, S. Mossmann, and H.J. Korsch, New J. Phys. 6 (2004) 2

Algebraic formulation

$$\hat{H} = Fd\hat{N} - \frac{J}{2}\left(\hat{K} + \hat{K}^\dagger\right)$$

★ With the shift algebra

$$\hat{K} = \sum_n |n\rangle\langle n+1|\,, \quad \hat{K}^\dagger = \sum_n |n+1\rangle\langle n|, \quad \text{and} \quad \hat{N} = \sum_n n|n\rangle\langle n|$$

$$[\hat{K},\hat{N}] = \hat{K}\,, \quad [\hat{K}^\dagger,\hat{N}] = -\hat{K}^\dagger\,, \quad [\hat{K},\hat{K}^\dagger] = 0$$

★ Define quasimomentum operator $\hat{\kappa}$ via $\hat{K} = \mathrm{e}^{\mathrm{i}\hat{\kappa}}$

★ "Conjugate" of the discrete position operator:

$$[\hat{N},\hat{\kappa}] = \mathrm{i}$$

Bloch oscillations – quasiclassical explanation

$$\hat{H} = E(\hat{\kappa}) + Fd\hat{N}, \quad \text{with} \quad E(\hat{\kappa}) = -\frac{J}{2}\cos(\hat{\kappa})$$

★ Heisenberg equations of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\kappa}\rangle = -Fd \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{N}\rangle = \left\langle \frac{\partial E(\hat{\kappa})}{\partial\hat{\kappa}} \right\rangle$$

★ Acceleration theorem: $\langle\hat{\kappa}\rangle(t) = -Fdt + \langle\hat{\kappa}\rangle(0)$

★ Ehrenfest theorem:

$$N(t) \approx N_0 + \frac{E(\kappa_0) - E(\kappa(t))}{Fd}$$

Non-Hermitian tight-binding lattice

$$\hat{H} = \sum_{n=-\infty}^{+\infty} \left(g_1 |n\rangle\langle n+1| + g_2 |n+1\rangle\langle n| + 2Fn|n\rangle\langle n| \right)$$

$$g_{1,2} \in \mathbb{C}, \quad F \in \mathbb{R}$$

★ Quasiclassical dynamics?

★ Modified Heisenberg equations of motion

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} \langle \hat{A} \rangle = \langle [\hat{A}, \hat{H}_R] \rangle - \mathrm{i} \Big(\langle [\hat{A}, \hat{H}_I]_+ \rangle - 2 \langle \hat{A} \rangle \langle \hat{H}_I \rangle \Big)$$

$H = H_R - \mathrm{i}H_I$ not directly useful...

Non-Hermitian semiclassical dynamics

★ Dynamics of position and momentum

$$\dot{p} = -\frac{\partial H_R}{\partial q} - \Sigma_{pp}\frac{\partial H_I}{\partial p} - \Sigma_{pq}\frac{\partial H_I}{\partial q}$$
$$\dot{q} = \frac{\partial H_R}{\partial p} - \Sigma_{pq}\frac{\partial H_I}{\partial p} - \Sigma_{qq}\frac{\partial H_I}{\partial q}$$

★ Coupled to covariance dynamics

$$\dot{\Sigma} = \Omega H_R''\Sigma - \Sigma H_R''\Omega - \Omega H_I''\Omega - \Sigma H_I''\Sigma$$

★ Resulting dynamics of squared norm/total power:

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$$g_{1,2} \in \mathbb{C}, \quad F \in \mathbb{R}$$

★ Classical dynamics:

$$H = g_1 \mathrm{e}^{\mathrm{i}p} + g_2 \mathrm{e}^{-\mathrm{i}p} + 2Fq,$$

$$\dot{p} = -\frac{\partial H_R}{\partial q} - \Sigma_{pp} \frac{\partial H_I}{\partial p} - \Sigma_{pq} \frac{\partial H_I}{\partial q}$$

$$\dot{q} = \frac{\partial H_R}{\partial p} - \Sigma_{pq} \frac{\partial H_I}{\partial p} - \Sigma_{qq} \frac{\partial H_I}{\partial q}$$

Quasiclassical dynamics

$$\dot{p} = -\frac{\partial H_R}{\partial q} - \Sigma_{pp}\frac{\partial H_I}{\partial p}$$
$$\dot{q} = \frac{\partial H_R}{\partial p} - \Sigma_{pq}\frac{\partial H_I}{\partial p}$$

With $$H_R = \mathrm{Re}g_+ \cos p - \mathrm{Im}g_- \sin p + 2Fq,$$
$$H_I = -\mathrm{Im}g_+ \cos p - \mathrm{Re}g_- \sin p.$$

And $$\dot{\Sigma} = \Omega H_R''\Sigma - \Sigma H_R''\Omega - \Omega H_I''\Omega - \Sigma H_I''\Sigma$$

Good approximation for small Σ_{pp}

Limit of narrow momentum packets

- ★ Can be analytically solved to yield:
  - ★ Acceleration theorem: $p(t) = p_0 - 2Ft$
  - ★ Dynamics of centre:

Constant covariance

$$\dot{q} = \frac{\partial \mathrm{Re}(E(p))}{\partial p} + \frac{\partial \mathrm{Im}(E(p))}{\partial p} \Sigma_{pq}$$

★ Exact for zero momentum uncertainty

★ Vanishing covariance: Centre still traces real part of field-free dispersion relation / band structure!

Example: Hatano-Nelson lattice

$$\hat{H} = \sum_{n=-\infty}^{+\infty} \left(g e^{+\mu} |n\rangle\langle n+1| + g e^{-\mu} |n+1\rangle\langle n| + 2Fn|n\rangle\langle n| \right)$$

★ Simple mapping to Hermitian Hamiltonian and analytical solution

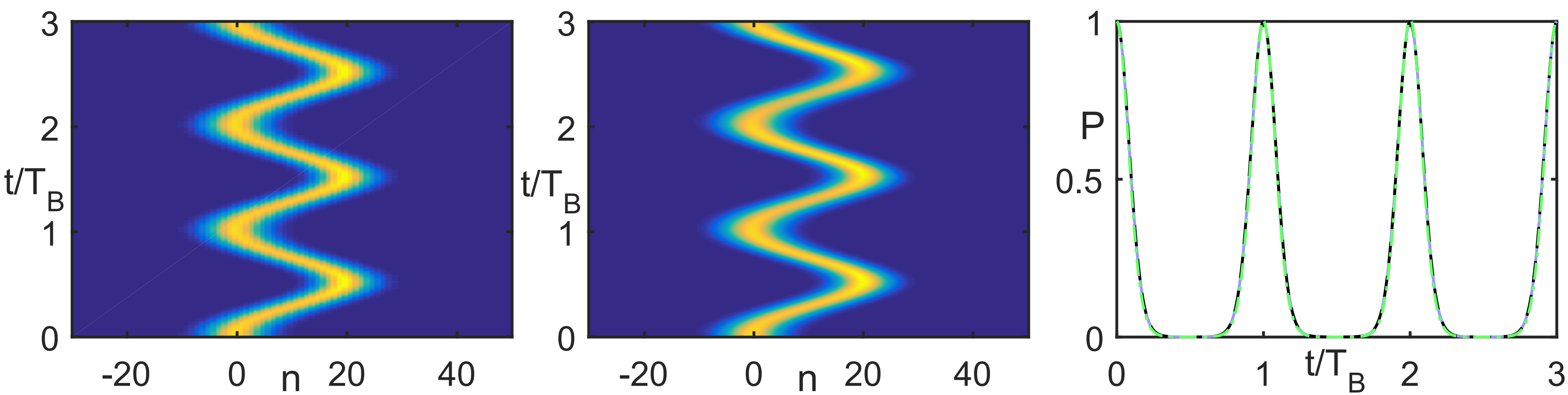
★ Experimental realisation in optical resonator structures proposed by Longhi et al (Sci. Rep. 5, 13376)

★ Classical Hamiltonian:

$$H = 2g \cosh\mu \cos p + 2\mathrm{i}g \sinh\mu \sin p + 2Fq$$

Example: Hatano-Nelson lattice

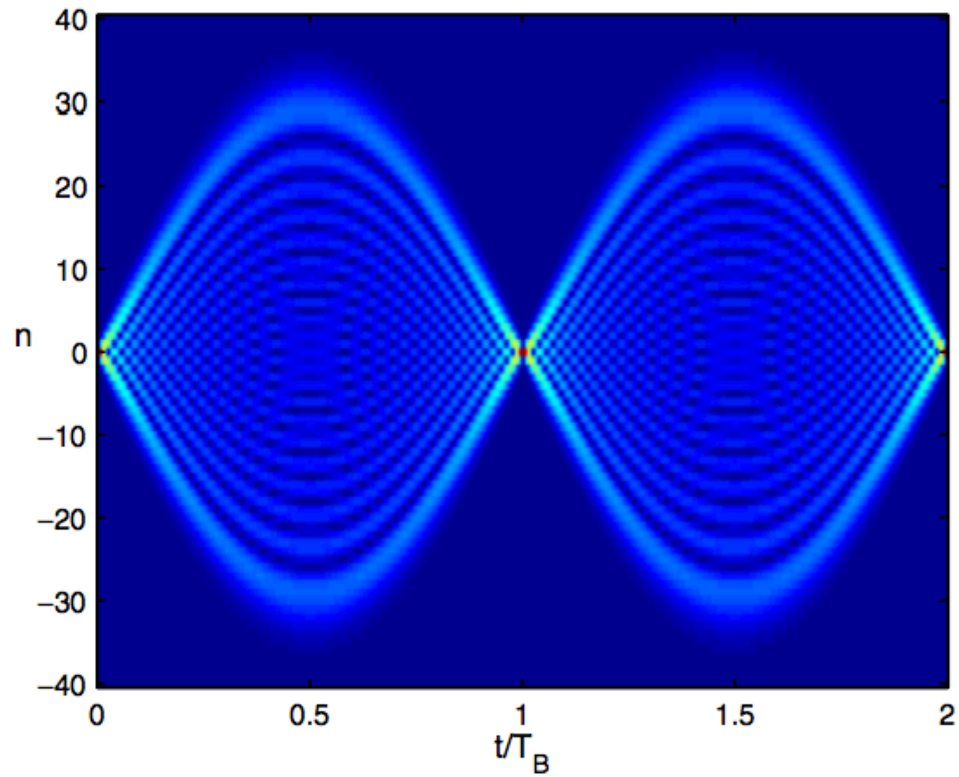
Propagation of (wide) Gaussian beam



$$F = 0.1, \;\; g = 1, \;\; \mu = 0.2$$

Breathing modes

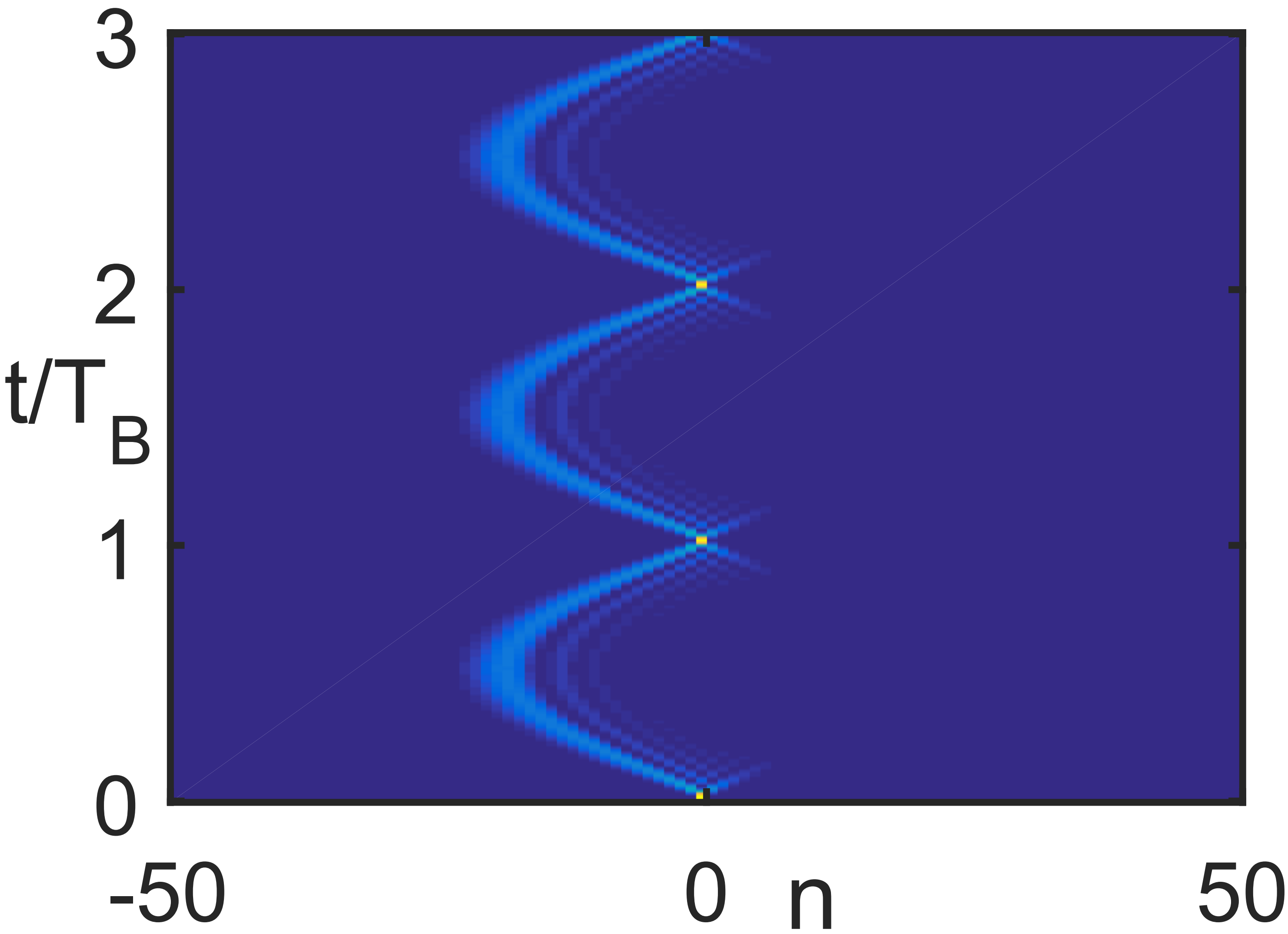
Propagation of single site initial state in Hermitian case



Quasiclassical dynamics not valid, but can be explained as classical ensemble

T. Hartmann, F. Keck, S. Mossmann, and H.J. Korsch, New J. Phys. 6 (2004) 2

Breathing modes in a Hatano-Nelson lattice

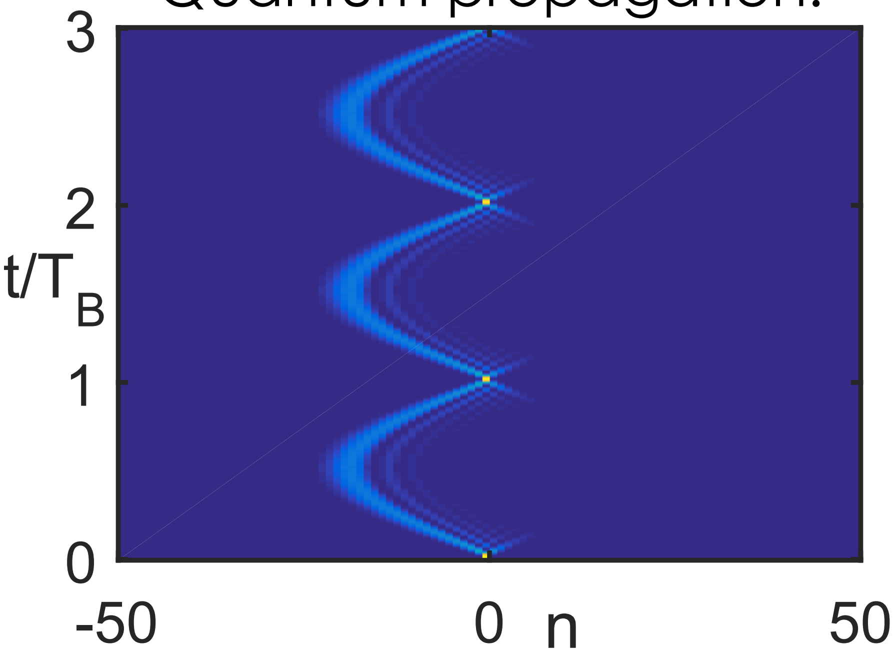


Quasiclassical breathing mode

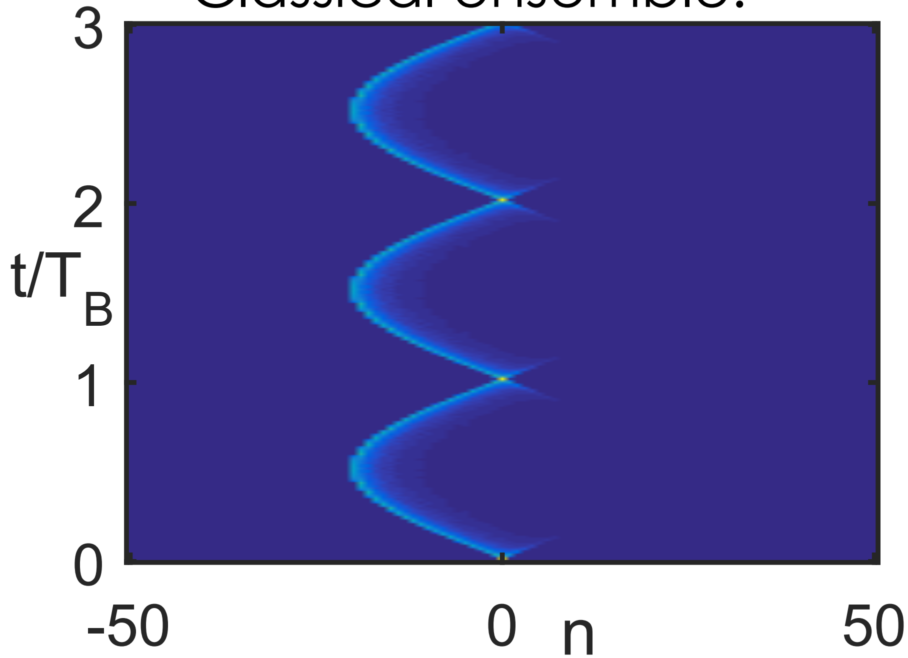
★Interpret Fourier transform of initially localised state as (incoherent) ensemble of infinitely narrow momentum wavepackets!

$$\delta_n = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{e}^{\mathrm{i}pn}\mathrm{d}p$$

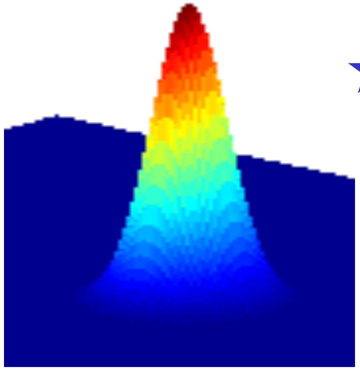
Quantum propagation:



Classical ensemble:



Summary

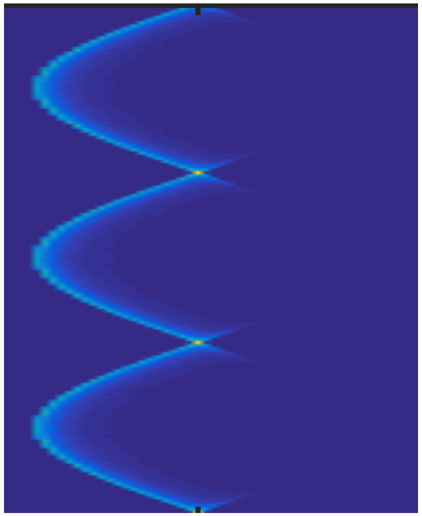


★Non-Hermitian QM: decay, PT-symmetry

★Semiclassical limit of Gaussian states: Phase space equipped with metric

★Quadratic Taylor expansion of Hamiltonian around central trajectory: Classical dynamics

★Non-Hermitian semiclassical limit - Dissipative dynamics coupled to evolution of metric (i.e. beam width)



★Explains non-Hermitian Bloch oscillations

Summary

★Non-Hermitian QM: decay, PT-symmetry

★Semiclassical limit of Gaussian states:

Thank you for your attention
and
Stay safe and sane!

Dissipative dynamics coupled to evolution of metric (i.e. beam width)

★Explains non-Hermitian Bloch oscillations