

# Stationary and time-dependent spectral renormalization method

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#### Spectral renormalization method for the solution of the Kohn-Sham equation

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# Goal of Talk

# Modest:

- Solve Kohn-Sham equations using spectral renormalization method;
- Use time-dependent spectral renormalization to simulate time-dependent DFT.

Ambitious: Use the machinery developed above to study

- Many-body (strongly interacting) Anderson localization;
- PT symmetric DFT or DFT with complex potentials.
- Topological physics in the presence of strong interaction.

# Spectral renormalization method

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# Spectral renormalization method for computing self-localized solutions to nonlinear systems

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#### PHYSICAL REVIEW A 97, 032134 (2018)

# Computing eigenfunctions and eigenvalues of boundary-value problems with the orthogonal spectral renormalization method

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# A toy model: Gross-Pitaevskii equation

Models Bose-Einstein condensation at zero temperature

$$i\psi_t = -\psi_{xx} + x^2\psi + |\psi|^2\psi$$
$$\psi(x,t) = \phi(x)e^{-iEt}$$
$$-\phi_{xx} + x^2\phi + |\phi|^2\phi = E\phi$$
$$\int |\phi|^2 dx = N$$

Goal: compute the eigenfunctions  $\phi$  and eigen energy E



Iteration scheme Give  $\varphi_1$  equals random numbers Compute  $R_1$ Compute  $E_1$  $c\varphi - \varphi_{xx} + x^2\varphi + |R|^2|\varphi|^2\varphi = c\varphi + E\varphi$ Update  $|R_n|^2 = \frac{N}{\int |\varphi_n|^2}$  $E_{n} = \frac{\int |\varphi_{n,x}|^{2} + \int x^{2} |\varphi_{n}|^{2} + |R_{n}|^{2} \int |\varphi_{n}|^{4}}{\int |\varphi_{n}|^{2}}$  $\hat{\varphi}_{n+1} = \left(\frac{c+E_n}{c+k^2}\right)\hat{\varphi}_n - \frac{1}{c+k^2}F[x^2\varphi_n + |R_n|^2|\varphi_n|^2\varphi_n]$ 



# Time dependent spectral renormalization

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## Time-dependent spectral renormalization method

CrossMark

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- Bridge between theory and numerics
- The same method is used to solve linear/nonlinear eigenvalues problems as well as time dependent problems,
- Used to detect singularities for ODEs and PDEs,
- Allows inclusion of physics on demand in the form of conservation laws.

## Evolution equation:

$$\frac{\partial \psi}{\partial t} = \mathcal{L}\psi + \mathcal{N}[\psi]$$

Initial condition:

$$\psi(x,t=0) = f(x)$$

^

Conservative PDE:

$$\int_{\Omega} Q_j[\psi(x,t)]dx = C_j$$

Dissipative PDE:

$$\frac{d}{dt} \int_{\Omega} X_j[\psi(x,t)] dx = \int_{\Omega} J_j[\psi(x,t)] dx$$

Duhamel's principle:

$$\psi(x,t) = S(t)f(x) + \int_0^t d\tau S(t-\tau)\mathcal{N}\left[\psi(x,\tau)\right]$$

Picard iteration:

$$\psi_{n+1}(x,t) = S(t)f(x) + \int_0^t d\tau S(t-\tau)\mathcal{N}[\psi_n(x,\tau)]$$
$$S(t) \equiv e^{t\mathcal{L}}, \quad t \ge 0$$

Semigroup operator:

Time dependent renormalization:  $\psi(x,t) = R(t)\phi(x,t)$ 

$$\phi(x,t) = \frac{S(t)f(x)}{R(t)} + \frac{1}{R(t)} \int_0^t d\tau S(t-\tau) \mathcal{N}\left[R(\tau)\phi(x,\tau)\right]$$

Renormalized Picard iteration:

$$\phi_{n+1}(x,t) = \frac{S(t)f(x)}{R_n(t)} + \frac{1}{R_n(t)} \int_0^t d\tau S(t-\tau) \mathcal{N}\left[R_n(\tau)\phi_n(x,\tau)\right]$$

$$\int_{\Omega} Q_j[R(t)\phi(x,t)]dx = C_j$$

$$\frac{d}{dt} \int_{\Omega} X_j[R(t)\phi(x,t)] dx = \int_{\Omega} J_j[R(t)\phi(x,t)] dx$$

## Evaluate the time integral

$$G(x, \tau) \equiv \mathcal{N}[R(\tau)\phi(x, \tau)]$$

$$I(x,t) \equiv \int_0^t d\tau S(t-\tau)G(x,\tau) \qquad \hat{I}(k,t) = \int_0^t d\tau e^{(t-\tau)\hat{\mathcal{L}}(k)}\hat{G}(k,\tau)$$

$$\hat{I}(k, t_{m+1}) = e^{\Delta t \hat{\mathcal{L}}(k)} \left[ \hat{I}(k, t_m) + \int_{t_m}^{t_{m+1}} d\tau e^{(t_m - \tau)\hat{\mathcal{L}}(k)} \hat{G}(k, \tau) \right],$$

$$\hat{G}(k,\tau) = \hat{G}(k,t_m) + \frac{1}{\Delta t} \left[ \hat{G}(k,t_{m+1}) - \hat{G}(k,t_m) \right] (\tau - t_m) .$$

$$\hat{I}(k, t_{m+1}) = e^{\Delta t \hat{\mathcal{L}}(k)} \left[ \hat{I}(k, t_m) + A\hat{G}(k, t_m) + B\hat{G}(k, t_{m+1}) \right],$$

$$\psi_{t} = i\psi_{xx} + 2i|\psi|^{2}\psi$$
  

$$\psi_{ex}(x,t) = \operatorname{sech}(x+2\xi t)e^{-i[\xi x + (\xi^{2}-1)t]}$$
  

$$\psi(x,t) = R(t)\phi(x,t)$$
  
power: 
$$\int_{-\infty}^{+\infty} dx|\psi|^{2} = C_{1}, \qquad |R_{n}(t)|^{2} = \frac{C_{1}}{\int_{-\infty}^{+\infty} |\phi_{n}(x,t)|^{2}dx}$$
  
momentum: 
$$\operatorname{Im} \int_{-\infty}^{+\infty} dx\psi\psi_{x}^{*} = C_{2} \qquad |R_{n}(t)|^{2} = \frac{C_{2}}{\int_{-\infty}^{+\infty} \phi_{n}(x,t)\phi_{n}^{*}(x,t)dx}$$
  
Hamiltonian: 
$$\int_{-\infty}^{+\infty} dx \left[|\psi_{x}|^{2} - |\psi|^{4}\right] = C_{3} \quad |R_{n}(t)|^{4} \int_{-\infty}^{+\infty} |\phi_{nx}(x,t)|^{4}dx - |R_{n}(t)|^{2} \int_{-\infty}^{+\infty} |\phi_{n}(x,t)|^{2}dx + C_{3} = 0$$
  

$$\phi_{n+1}(x,t) = \frac{S(t)f(x)}{R_{n}(t)} + \frac{2i}{R_{n}(t)} \int_{0}^{t} d\tau |R_{n}(\tau)|^{2}R_{n}(\tau)|\phi_{n}(x,\tau)|^{2}\phi_{n}(x,\tau)$$



### **Snapshot of iteration**



**Fig. 5.** The error evolution in the solution E(t), power P(t), momentum M(t), and Hamiltonian H(t). The value of R(t) is found using conservation of power (row 1 of Table 1), momentum (row 2 of Table 1), and Hamiltonian (row 3 of Table 1 with negative sign) in panels (a), (b), and (c), respectively. The computational parameters are:  $\xi = 2, T = 7, M = 1000, L = 100, N = 1024$ .

## Dissipative PDE: Burgers' equation

$$\psi_t = -\psi\psi_x + \nu\psi_{xx}$$

$$\psi(x,t) = -2\nu \frac{u_x(x,t)}{u(x,t)} \qquad \qquad u_t(x,t) = \nu u_{xx}(x,t)$$

$$\psi(x,0) = f(x) = -\frac{\nu \cos(x)}{1 + \frac{1}{2}\sin(x)} \qquad \psi_{\text{ex}}(x,t) = -\frac{\nu \cos(x)e^{-\nu t}}{1 + \frac{1}{2}\sin(x)e^{-\nu t}}$$

$$\frac{d}{dt} \int_0^{2\pi} \psi^2(x,t) dx = -2\nu \int_0^{2\pi} \psi_x^2(x,t) dx$$

## Burgers' Renormalization

$$\begin{split} \psi(x,t) &= R(t)\phi(x,t) \qquad \frac{d(\theta_1 R^2)}{dt} = -2\nu\theta_2 R^2 \\ \theta_1(t) &= \int_0^{2\pi} \phi^2(x,t) dx \neq 0 \qquad \theta_2(t) = \int_0^{2\pi} \phi_x^2(x,t) dx \\ R^2(t) &= \frac{R^2(0)\theta_1(0)}{\theta_1(t)} \exp\left(-2\nu \int_0^t \frac{\theta_2(\tau)}{\theta_1(\tau)} d\tau\right) \\ \hat{\phi}_{n+1}(k,t) &= \frac{1}{R_n(t)} e^{-\nu t k^2} \hat{f}(k) + \frac{1}{R_n(t)} \hat{I}_n(k,t) \end{split}$$

$$\hat{I}(k,t_{m+1}) = e^{-\nu\Delta tk^2} \left\{ \hat{I}(k,t_m) - AR^2(t_m)F\left[\phi(x,t_m)\phi_x(x,t_m)\right] - BR^2(t_{m+1})F\left[\phi(x,t_{m+1})\phi_x(x,t_{m+1})\right] \right\} ,$$

## **Detecting singularities for ODEs**

$$\dot{x} = x^2, \quad x(0) = x_0 \qquad \qquad x(t) = \frac{1}{\frac{1}{x_0} - t}$$

Duhamel's formulation

$$x(t) = x_0 + \int_0^t x^2(\tau) d\tau$$

$$x(t) = Ry(t)$$
  $y(t) = \frac{1}{R} \left[ x_0 + R^2 \int_0^t y^2(\tau) \right] d\tau$ 

$$\int_{0}^{T} \varphi(t) y_{n}(t) dt = \frac{x_{0}}{R_{n}} \int_{0}^{T} \varphi(t) dt + R_{n} \int_{0}^{T} dt \varphi(t) \left[ \int_{0}^{t} y_{n}^{2}(\tau) d\tau \right]$$
$$y_{n+1}(t) = \frac{1}{R_{n}} \left[ x_{0} + R_{n}^{2} \int_{0}^{t} y_{n}^{2}(\tau) \right] d\tau$$



Anderson localization of strongly interacting systems?

## Anderson localization of non interacting systems

Consider the linear Schrödinger equation governing the motion of an electron in a periodic crystal

 $i\partial_t \psi = -\partial_x^2 \psi + V(x)\psi \qquad \psi : \mathbb{R}^+ \times \mathbb{R} \to \mathbb{C}$  $\psi(x,0) = \psi_0(x) \qquad -\infty < x < +\infty$  $V(x) = V(x+a) \qquad V : \mathbb{R} \to \mathbb{R} \quad (\text{smooth})$ 

 $\psi(t,x) = \phi(x,E)\exp(-iEt)$   $E \in \mathbb{R}$ 

$$-\partial_x^2 \phi + V(x)\phi = E\phi$$

Boundary conditions:  $\phi$  is bounded as  $x \rightarrow \pm \infty$ 

### **Floquet-Bloch theory and band-gap structure**

The spectrum of 
$$-\partial_x^2 + V(x)$$
 acting on  $L^2(\mathbb{R})$ 

is real, bounded from below, tends to positive infinity, is absolutely continuous, and consists of the union of closed intervals called spectral bands separated by spectral gaps.

$$-\partial_x^2 \phi + V(x)\phi = E\phi$$
  

$$\phi_n(x,k) = \varphi_n(x,k(E))e^{ik(E)x}$$
  

$$\varphi_n(x+a,k) = \varphi_n(x,k)$$
  

$$\left[-\left(\frac{d}{dx}+ik\right)^2 + V(x)\right]\varphi_n(x,k) = E_n(k)\varphi_n(x,k)$$

 $E_1(k) \le E_2(k) \le \dots \le E_m(k) \le \dots$ 

 $\varphi_n(x,k)$  is complex and bounded function of x

If k(E) is real then φ<sub>n</sub>(x,k(E)) is a bounded function of x k(E) is in a spectral band
If k(E) is imaginary, then φ<sub>n</sub>(x,k(E)) is unbounded in x

k(E) is in a spectral gap

A wave propagates freely through the medium Ballistic Transport/Diffraction

### Transport in random lattices

#### Classical behavior

Random impurities in the crystalline structure scatter the electron and give rise to a random walk motion of the electron as if they were classical billiard balls. This is the mechanism behind diffusion and Ohm's law.

#### Quantum behavior

$$-\partial_x^2 \phi + [V(x) + V_{\omega}(x)]\phi = E\phi$$
$$V(x) = V(x + a)$$

 $\{V_{\omega}\}_{\omega\in\Omega}$  is a collection of random potentials chosen from the set  $\Omega$  with probability measure  $P(\omega)$ 

The wave is coherently scattered by defects, Constructive interference of multiple scatterings

The transmission probability of a propagating wave through a disordered medium decays when the strength of the disorder potential reaches a critical value and leads to Anderson localization.



# Experimental difficulties?

Anderson localization in disordered atomic lattices is difficult to observed

**Reasons: Anderson localization requires** 

> a disordered potential which is time independent;

> No many body interactions

# LETTERS

# Transport and Anderson localization in disordered two-dimensional photonic lattices

Tal Schwartz<sup>1</sup>, Guy Bartal<sup>1</sup>, Shmuel Fishman<sup>1</sup> & Mordechai Segev<sup>1</sup>



**Figure 1** | **Transverse localization scheme. a**, A probe beam entering a disordered lattice, which is periodic in the two transverse dimensions (*x* and *y*) but invariant in the propagation direction (*z*). In the experiment described here, we use a triangular (hexagonal) photonic lattice with a periodicity of 11.2  $\mu$ m and a refractive-index contrast of ~5.3 × 10<sup>-4</sup>. The lattice is induced optically, by transforming the interference pattern among three plane wave

$$P \equiv \left[ \int I(x,y,L)^2 dx dy \right] / \left[ \int I(x,y,L) dx dy \right]^2,$$

units of P=inverse area



### Anderson Localization and Nonlinearity in One-Dimensional Disordered Photonic Lattices

Yoav Lahini,<sup>1,\*</sup> Assaf Avidan,<sup>1</sup> Francesca Pozzi,<sup>2</sup> Marc Sorel,<sup>2</sup> Roberto Morandotti,<sup>3</sup> Demetrios N. Christodoulides,<sup>4</sup> and Yaron Silberberg<sup>1</sup>





#### Anderson Localization and Nonlinearity in One-Dimensional Disordered Photonic Lattices

Yoav Lahini,<sup>1,\*</sup> Assaf Avidan,<sup>1</sup> Francesca Pozzi,<sup>2</sup> Marc Sorel,<sup>2</sup> Roberto Morandotti,<sup>3</sup> Demetrios N. Christodoulides,<sup>4</sup> and Yaron Silberberg<sup>1</sup>



#### nature

# LETTERS

# Direct observation of Anderson localization of matter waves in a controlled disorder

Juliette Billy<sup>1</sup>, Vincent Josse<sup>1</sup>, Zhanchun Zuo<sup>1</sup>, Alain Bernard<sup>1</sup>, Ben Hambrecht<sup>1</sup>, Pierre Lugan<sup>1</sup>, David Clément<sup>1</sup>, Laurent Sanchez-Palencia<sup>1</sup>, Philippe Bouyer<sup>1</sup> & Alain Aspect<sup>1</sup>



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## Numerical study of one-dimensional and interacting Bose–Einstein condensates in a random potential

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red slop=0.344, disorder strength=2 blue slop=0.306, disorder strength=4 full straight line slop=0.4  $\beta = 1$ 

# Anderson localization for NLS equation

Mathematical formulation:

$$iu_t = -u_{xx} + V_w(x)u + g|u|^2u, \quad g > 0$$
  
 $V_w(x)$  is a random potential

Assume that the initial condition u(x, 0) is well localized Prove (or dis prove) the following statement: For any  $0 < \epsilon \ll 1$  with probability  $1 - \epsilon$  on the space of the potentials  $sup_{x,t}|e^{a|x|}u(x,t)| < C(\epsilon) < \infty$  for some a > 0Random and dynamic optimal transport approach?

# **PT** symmetric DFT?



What about non Hermitian ``Hamiltonians", do they describe physical reality? VOLUME 80, NUMBER 24

#### Real Spectra in Non-Hermitian Hamiltonians Having $\mathcal{PT}$ Symmetry

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The condition of self-adjointness ensures that the eigenvalues of a Hamiltonian are real and bounded below. However, if one replaces this condition by the weaker condition of  $\mathcal{PT}$  symmetry, one obtains new infinite classes of Hamiltonians whose spectra are also real and positive. The classical and quantum properties of some of these Hamiltonians are discussed in this paper.

 $-\psi''(x) - (ix)^N \psi(x) = E\psi(x).$ 



FIG. 1. Energy levels of the Hamiltonian  $H = p^2 - (ix)^N$  as a function of the parameter N. There are three regions: When  $N \ge 2$  the spectrum is real and positive. The lower bound of this region, N = 2, corresponds to the harmonic oscillator, whose energy levels are  $E_n = 2n + 1$ . When 1 < N < 2, there are a finite number of real positive eigenvalues and an infinite number of complex conjugate pairs of eigenvalues. As N decreases from 2 to 1, the number of real eigenvalues decreases; when  $N \le 1.42207$ , the only real eigenvalue is the ground-state energy. As N approaches  $1^+$ , the ground-state energy diverges. For  $N \le 1$  there are no real eigenvalues.

## Introduction to PT symmetry

Parity operator: 
$$Pf(x) = f(-x)$$
  
Time reversel operator:  $Tf(x) = f^*(x)$ 

Time reversal operator:  $Tf(x) = f^*(x)$ 

PT operator: 
$$PTf(x) = f^*(-x)$$

Definition of *PT* symmetric operators: Let *A* be a linear operator. We say the *A* is *PT* symmetric if

$$[PT, A] = 0$$

$$A = -\frac{d^2}{dx^2} + V(x) \qquad V^*(-x) = V(x)$$

Definition of *unbroken PT* symmetry Let *A* be a linear operator. We say that *A* has *unbroken PT* symmetry if *A* and *PT* share the same eigenfunctions.

Theorem: If a *PT* symmetric linear operator *A* has an unbroken *PT* symmetry, then its spectrum is real.

Proof: 
$$PTu = \alpha u$$
  $Au = \lambda u$   
 $PT(Au) = PT(\lambda u) = \lambda^* PTu = \lambda^* \alpha u$   
 $PT(Au) = APTu = A\alpha u = \alpha \lambda u$   
 $\lambda^* = \lambda$ 

$$(f,g)_{CPT} = \int_{-\infty}^{+\infty} dx f^{CPT}(x)g(x)$$
  
It gives positive definite norm and  
Unitary evolution  
$$[C,H] = 0$$
  
$$[C,PT] = 0$$

Can *PT* symmetric Hamiltonians (with exact PT symmetry) be considered as a Extension of quantum mechanics?

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#### **Complex Extension of Quantum Mechanics**

Carl M. Bender,<sup>1</sup> Dorje C. Brody,<sup>2</sup> and Hugh F. Jones<sup>2</sup> <sup>1</sup>Department of Physics, Washington University, St. Louis, Missouri 63130 <sup>2</sup>Blackett Laboratory, Imperial College, London SW7 2BZ, United Kingdom (Received 12 August 2002; published 16 December 2002)

Requiring that a Hamiltonian be Hermitian is overly restrictive. A consistent physical theory of quantum mechanics can be built on a complex Hamiltonian that is not Hermitian but satisfies the less restrictive and more physical condition of space-time reflection symmetry ( $\mathcal{PT}$  symmetry). One might expect a non-Hermitian Hamiltonian to lead to a violation of unitarity. However, if  $\mathcal{PT}$  symmetry is not spontaneously broken, it is possible to construct a previously unnoticed symmetry C of the Hamiltonian. Using C, an inner product whose associated norm is positive definite can be constructed. The procedure is general and works for any  $\mathcal{PT}$ -symmetric Hamiltonian. Observables exhibit  $C\mathcal{PT}$  symmetry, and the dynamics is governed by unitary time evolution. This work is not in conflict with conventional quantum mechanics but is rather a complex generalization of it.

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PACS numbers: 11.30.Er, 03.65.-w, 03.65.Ge, 02.60.Lj

# *PT* symmetry in Optics Normalized $i\frac{\partial\Psi}{\partial z} + \frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi = 0 \qquad \left(V(x) = V^*(-x)\right)$ **Paraxial Wave Equation of Diffraction** $\begin{cases} \operatorname{Re}\left\{V\left(x\right)\right\} \propto n_{R}(x) & \text{Index profile} \\ \operatorname{Im}\left\{V\left(x\right)\right\} \propto n_{I}(x) & \text{Gain-loss profile} \end{cases}$ Symmetric mode $n_R(x)$ $n_{I}(x)$ G Transparent $\mathcal{PT}$ waveguide

### Beam Dynamics in $\mathcal{PT}$ Symmetric Optical Lattices

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#### Optical Solitons in $\mathcal{PT}$ Periodic Potentials

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We investigate the effect of nonlinearity on beam dynamics in parity-time ( $\mathcal{PT}$ ) symmetric potentials. We show that a novel class of one- and two-dimensional nonlinear self-trapped modes can exist in optical  $\mathcal{PT}$  synthetic lattices. These solitons are shown to be stable over a wide range of potential parameters. The transverse power flow within these complex solitons is also examined.

DOI: 10.1103/PhysRevLett.100.030402

PACS numbers: 03.65.Ge, 11.30.Er, 42.65.Sf, 42.65.Tg

$$V(x) = \cos^2(x), \qquad W(x) = W_0 \sin(2x). \qquad i \frac{\partial \psi}{\partial z} + \frac{\partial^2 \psi}{\partial x^2} + [V(x) + iW(x)]\psi + |\psi|^2\psi = 0,$$

## Bandstucture of a *PT* optical lattice\*

 $\begin{cases} If & V_0 \le 0.5 \ real \ eigenvalues \\ If & V_0 > 0.5 \ complex \ eigenvalues \end{cases}$ 



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physics

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#### Observation of $\mathcal{PT}$ -Symmetry Breaking in Complex Optical Potentials

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Observation of  $\mathcal{PT}$ -breaking in a passive coupler

Observation of  $\mathcal{PT}$ -breaking in an active coupler

## **Observation of parity-time symmetry in optics**

Christian E. Rüter<sup>1</sup>, Konstantinos G. Makris<sup>2</sup>, Ramy El-Ganainy<sup>2</sup>, Demetrios N. Christodoulides<sup>2</sup>, Mordechai Segev<sup>3</sup> and Detlef Kip<sup>1</sup>\*



# Experimental realization of $\mathcal{PT}$ -lattice

Parity–time synthetic photonic lattices, <u>A. Regensburger, C. Bersch,</u> <u>A. Miri, G. Onishchukov,</u> <u>D. N. Christodoulides</u>, and <u>U. Peschel</u> Nature, 488, 167–171 (09 August 2012)



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# **Non-Hermitian physics and PT symmetry**

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In recent years, notions drawn from non-Hermitian physics and parity-time (PT) symmetry have attracted considerable attention. In particular, the realization that the interplay between gain and loss can lead to entirely new and unexpected features has initiated an intense research effort to explore non-Hermitian systems both theoretically and experimentally. Here we review recent progress in this emerging field, and provide an outlook to future directions and developments.



## ARTICLE

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# Constant-intensity waves and their modulation instability in non-Hermitian potentials

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THE JOURNAL OF CHEMICAL PHYSICS 125, 124104 (2006)

## **Density functional theory of complex transition densities**

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Letter

pubs.acs.org/JPCL

## Calculating the Lifetimes of Metastable States with Complex Density Functional Theory

Yongxi Zhou and Matthias Ernzerhof\*

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## **Open-system Kohn-Sham density functional theory**

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# LETTER

# Photonic Floquet topological insulators

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Topological insulators are a new phase of matter<sup>1</sup>, with the striking property that conduction of electrons occurs only on their surfaces<sup>1-3</sup>. In two dimensions, electrons on the surface of a topological insulator are not scattered despite defects and disorder, providing robustness akin to that of superconductors. Topological insulators are predicted to have wide-ranging applications in fault-tolerant quantum computing and spintronics. Substantial effort has been directed towards realizing topological insulators for electromagnetic waves<sup>4-13</sup>. One-

# **Topological insulator laser: Experiments**

Miguel A. Bandres,\* Steffen Wittek,\* Gal Harari,\* Midya Parto, Jinhan Ren, Mordechai Segev,† Demetrios N. Christodoulides,† Mercedeh Khajavikhan†

# **Topological DFT?**

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## **Topological insulators**

Topological insulators are materials that are insulating in their interior but can support the flow of electrons on their surface. The underlying cause is time-reversal symmetry: their physics is independent of whether time is flowing backward or forward. These surface states are robust, maintained even in the presence of surface defects.

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