Complex eigenvalue problem of the Liouvillian of an open quantum dot system

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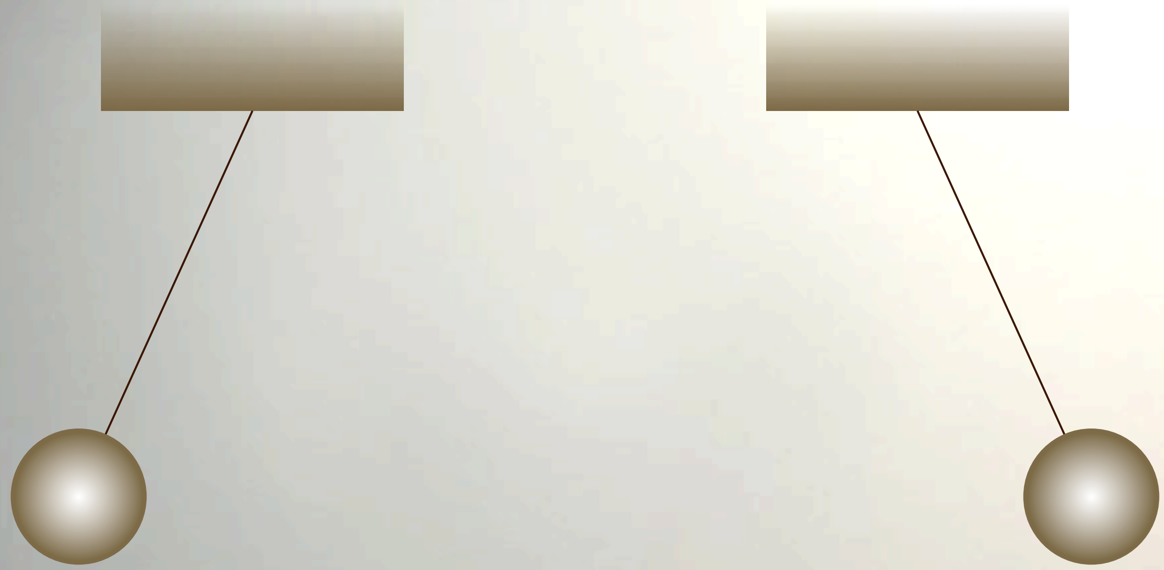
Arrow of Time



Before? After?

Time-reversal symmetry

Arrow of Time

Second law of thermodynamics

Arrow of Time

Equation of motion:
Time reversal symmetry

↓ ?

State of the universe:
Breaking of time reversal symmetry

Open quantum systems

Equation of motion: Time reversal symmetry

Its solutions: Can break the symmetry

Standard Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\psi(x)=E\psi(x)$$

Resonance: $E = E_{\mathrm{r}} - i\Gamma/2$

Anti-resonance: $E = E_{\mathrm{r}} + i\Gamma/2$

Complex eigenvalue problem

For a very simple open quantum dot system, we (numerically) exactly solve the complex eigenvalue problems of

1. the Hamiltonian and
2. the Liouvillian.

To find the arrow of time

•Finite System + Infinite Heat Bath

Traces out the heat bath

+ Markov approx., Perturbation expansion

Time-reversal symmetry is broken somewhere.

•Finite System (quantum dot)

+ Infinite System (lead)

Complex eigenvalue problem:

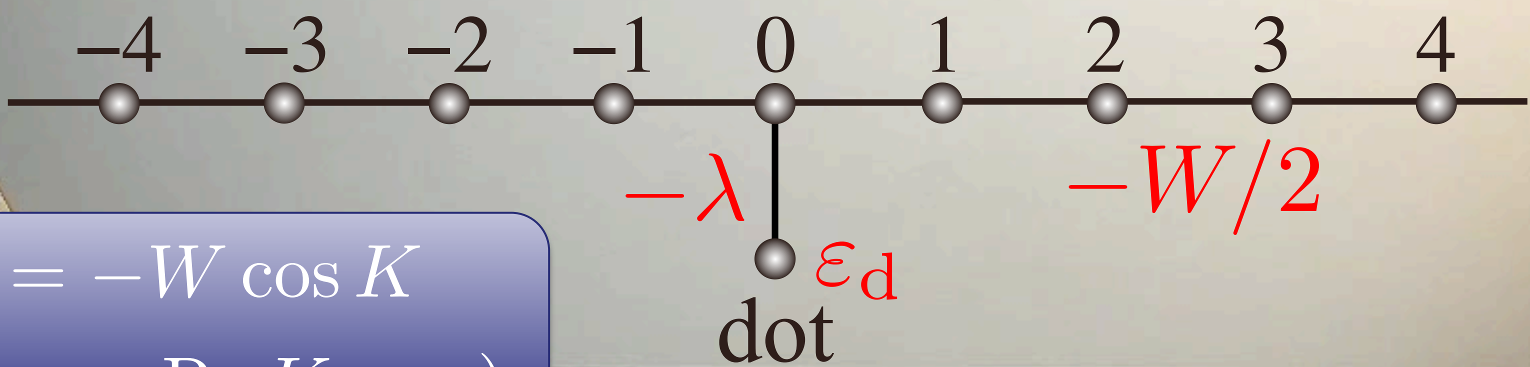
everything microscopically.

Spontaneous breaking of time-reversal symmetry.

Open quantum dot system

Tight-binding model

$$H = -\frac{W}{2}\sum_{-\infty}^{\infty}\left(|x+1\rangle\langle x| + |x\rangle\langle x+1|\right) - \lambda\left(|\mathrm{d}\rangle\langle 0| + |0\rangle\langle \mathrm{d}|\right) + \varepsilon_{\mathrm{d}}|\mathrm{d}\rangle\langle \mathrm{d}|$$



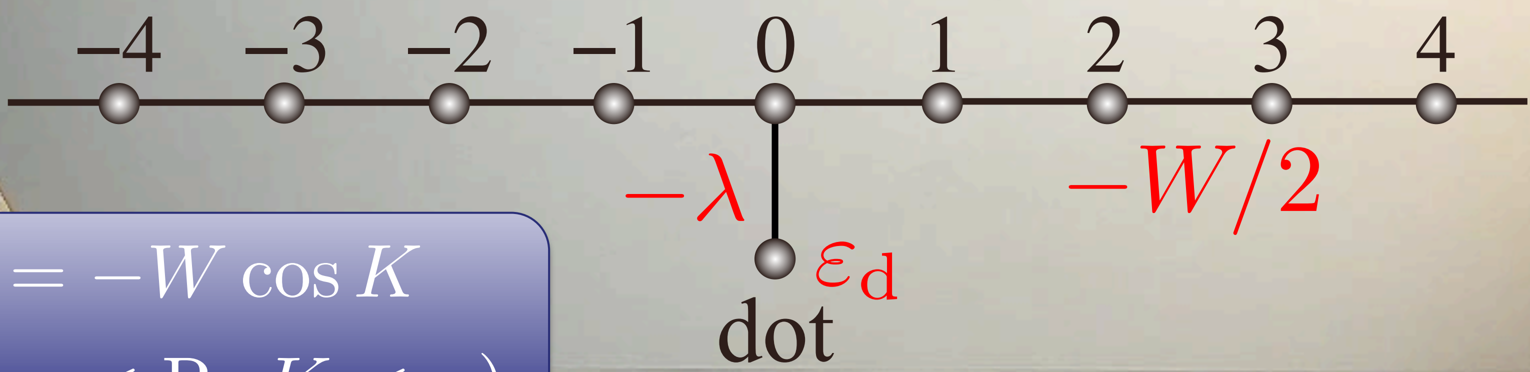
$E = -W\cos K$

$(-\pi < \mathrm{Re}\, K < \pi)$

Complex eigenvalues of the Hamiltonian

$$H\psi_n = E_n\psi_n, \quad E_n \in \mathbb{C}$$

Two methods
1. Siegert boundary condition
2. Feshbach formalism

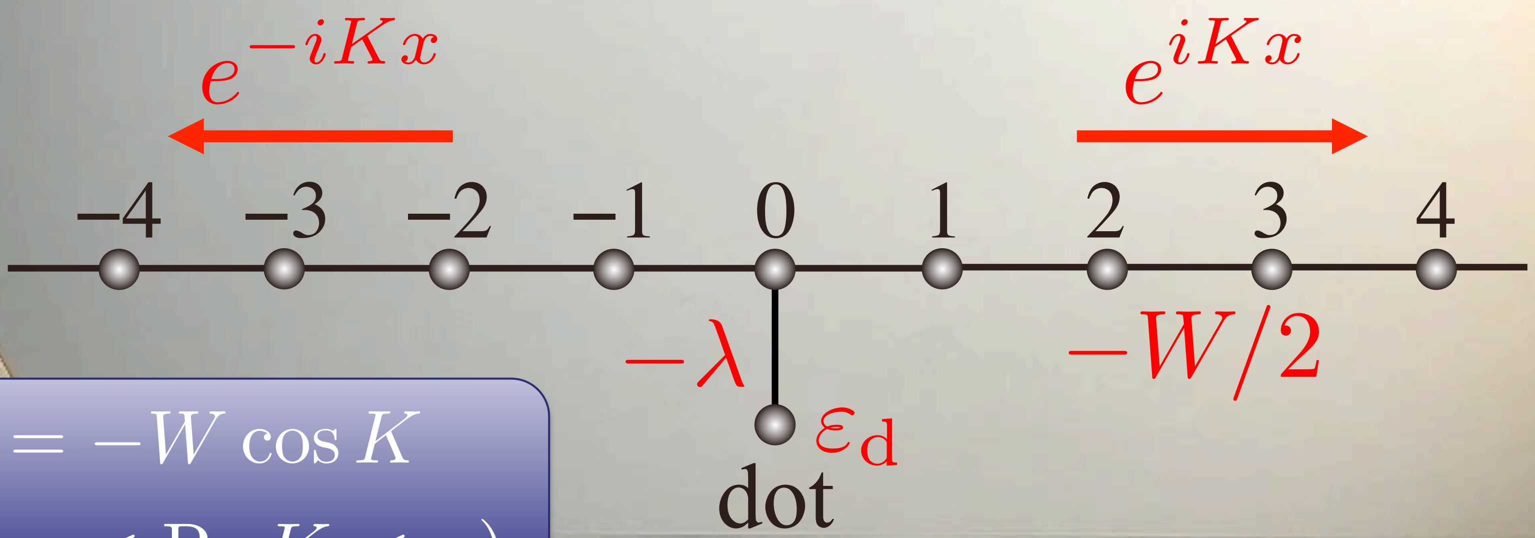


$$E = -W\cos K$$
$$(-\pi < \mathrm{Re}\,K < \pi)$$

Siegert boundary condition

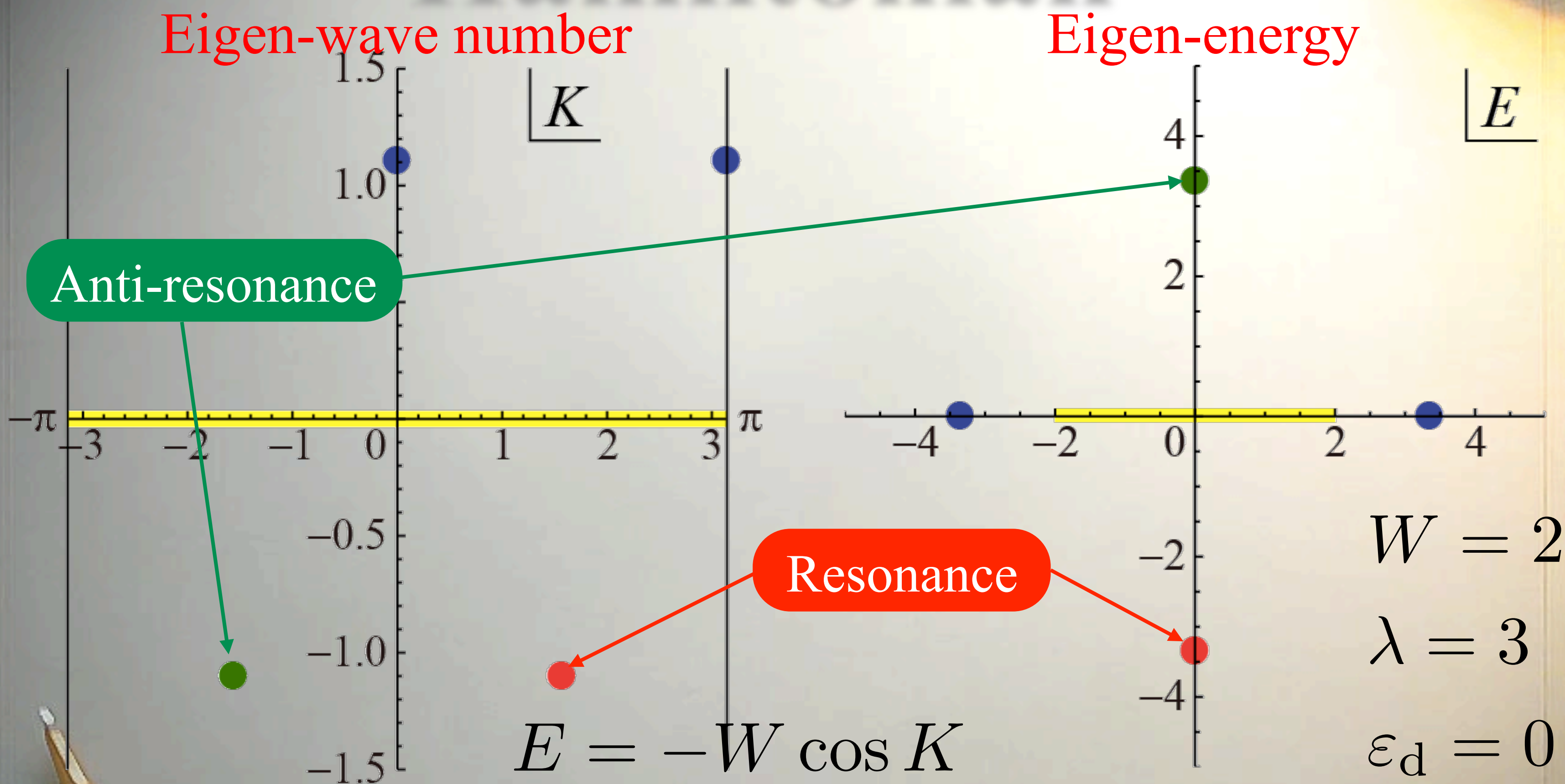
Resonance:
Eigenstate with outgoing waves only.

$$\psi(x) \simeq e^{iK|x|}$$



$$E = -W\cos K$$
$$(-\pi < \mathrm{Re}\,K < \pi)$$

Complex eigenvalues of the Hamiltonian



$E = -W \cos K$

$W = 2$

$\lambda = 3$

$\varepsilon_{\mathrm{d}} = 0$

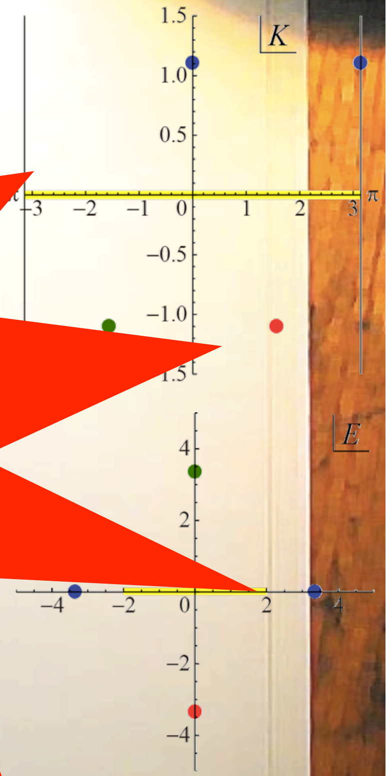
$\psi(x) \simeq e^{iK|x|}$

$\mathrm{Re}\, K_n \gtrless 0 \Leftrightarrow \mathrm{Im}\, E_n \lessgtr 0$

Resonant state as a stationary eigenstate

N. Hatano, K. Sasada, H. Nakamura and T. Petrosky, Prog. Theor. Phys. **119** (2008) 187

$$\langle x|\Psi_n(t)\rangle \sim e^{iK_n|x|}e^{-iE_n t}$$



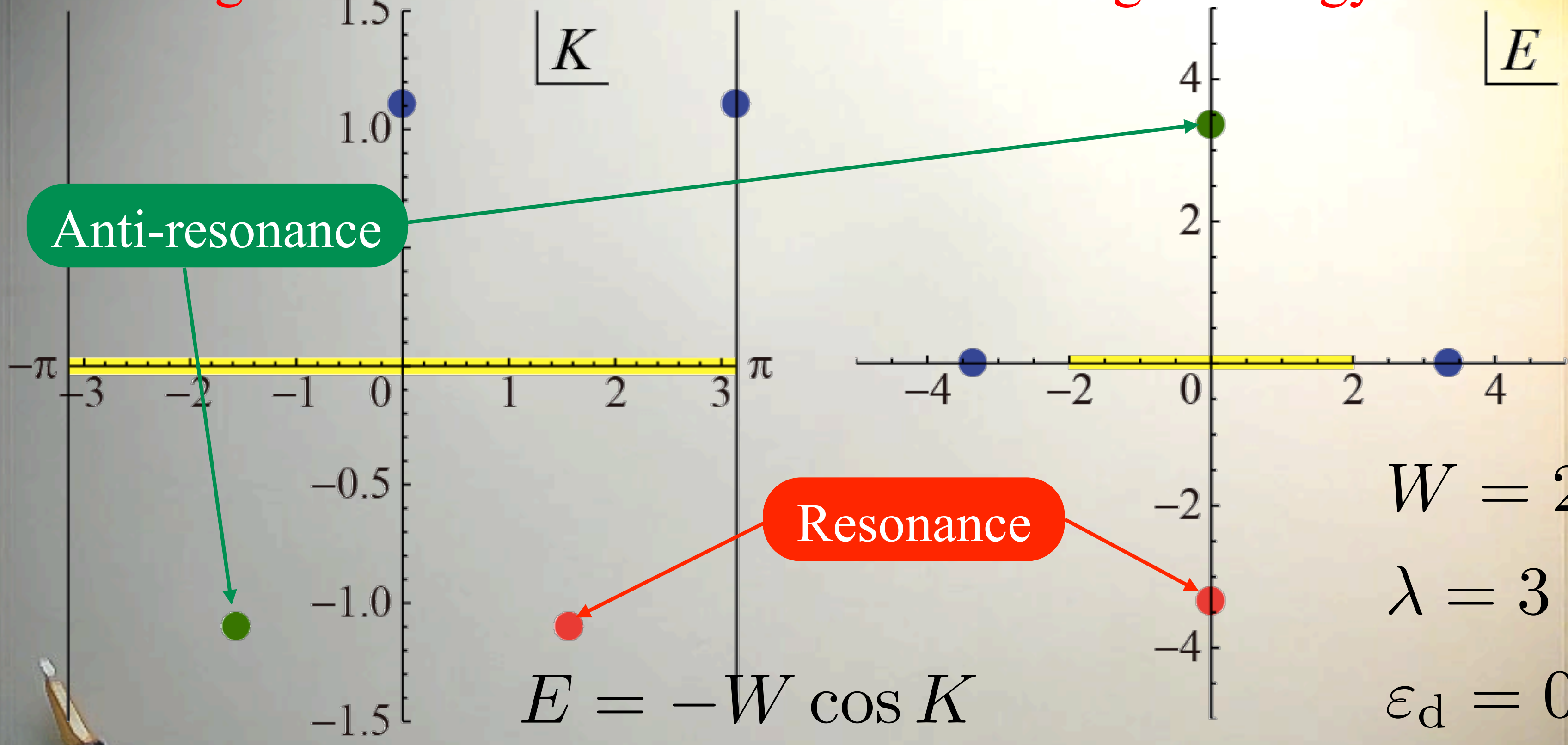
Breaking of time-reversal symmetry

Re $K_n \gtrless 0$ ... $E_n \gtrless$

"Anti-resonant state" as an eigenstate

Complex eigenvalues of the Hamiltonian

Eigen-wave number Eigen-energy



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Origin of the non-Hermiticity

N. Hatano, K. Sasada, H. Nakamura and T. Petrosky, Prog. Theor. Phys. **119** (2008) 187

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

Functional space of normalizable fns. → The operator H is Hermitian.

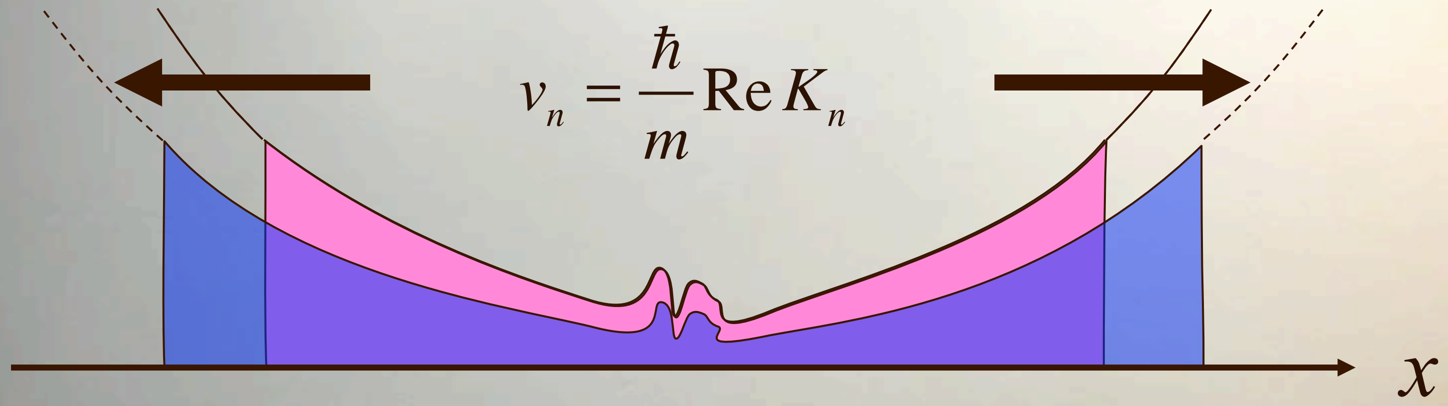
Functional space of unnormalizable fns. ← The operator H is non-Hermitian.

Probability Conservation

N. Hatano, K. Sasada, H. Nakamura and T. Petrosky, Prog. Theor. Phys. **119** (2008) 187

$$\psi(x) \simeq e^{iK|x|} \text{ with } \operatorname{Im} K < 0$$

$$|\langle x|\Psi_n(t)\rangle|^2 \simeq e^{2|\operatorname{Im} K_n||x|-2|\operatorname{Im} E_n|t}$$



Probabilistic Interpretation

Feshbach Formalism

Rotter; Ploszajczak; Petrosky & Prigogine

$$H|\psi\rangle = E|\psi\rangle \;\Rightarrow\; H_{\mathrm{eff}}(E)\,(P|\psi\rangle) = E\,(P|\psi\rangle)$$

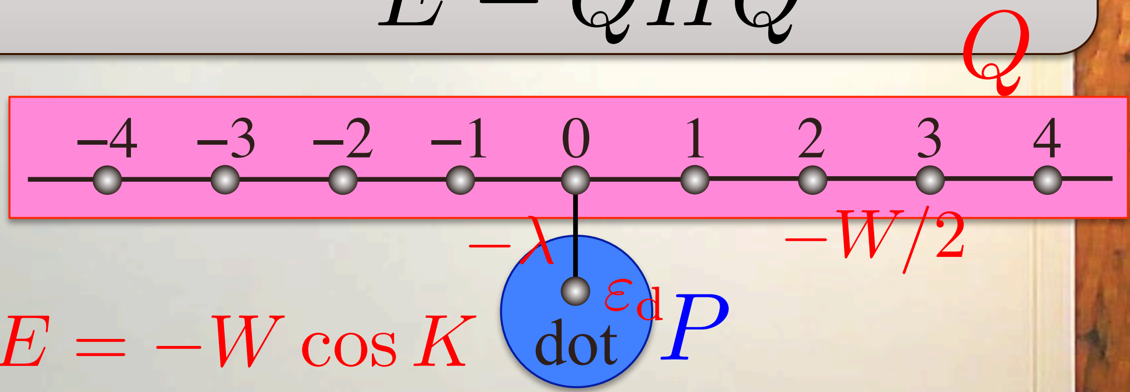
$$H_{\mathrm{eff}}(E) = PHP + PHQ\frac{1}{E - QHQ}QHP$$

$$PHP = \varepsilon_{\mathrm{d}}$$

$$QHP = -\lambda|0\rangle\langle \mathrm{d}|$$

$$PHQ = -\lambda|\mathrm{d}\rangle\langle 0|$$

$$QHQ = -\frac{W}{2}\sum_{x=-\infty}^{\infty}\left(|x+1\rangle\langle x| + |x\rangle\langle x+1|\right)$$

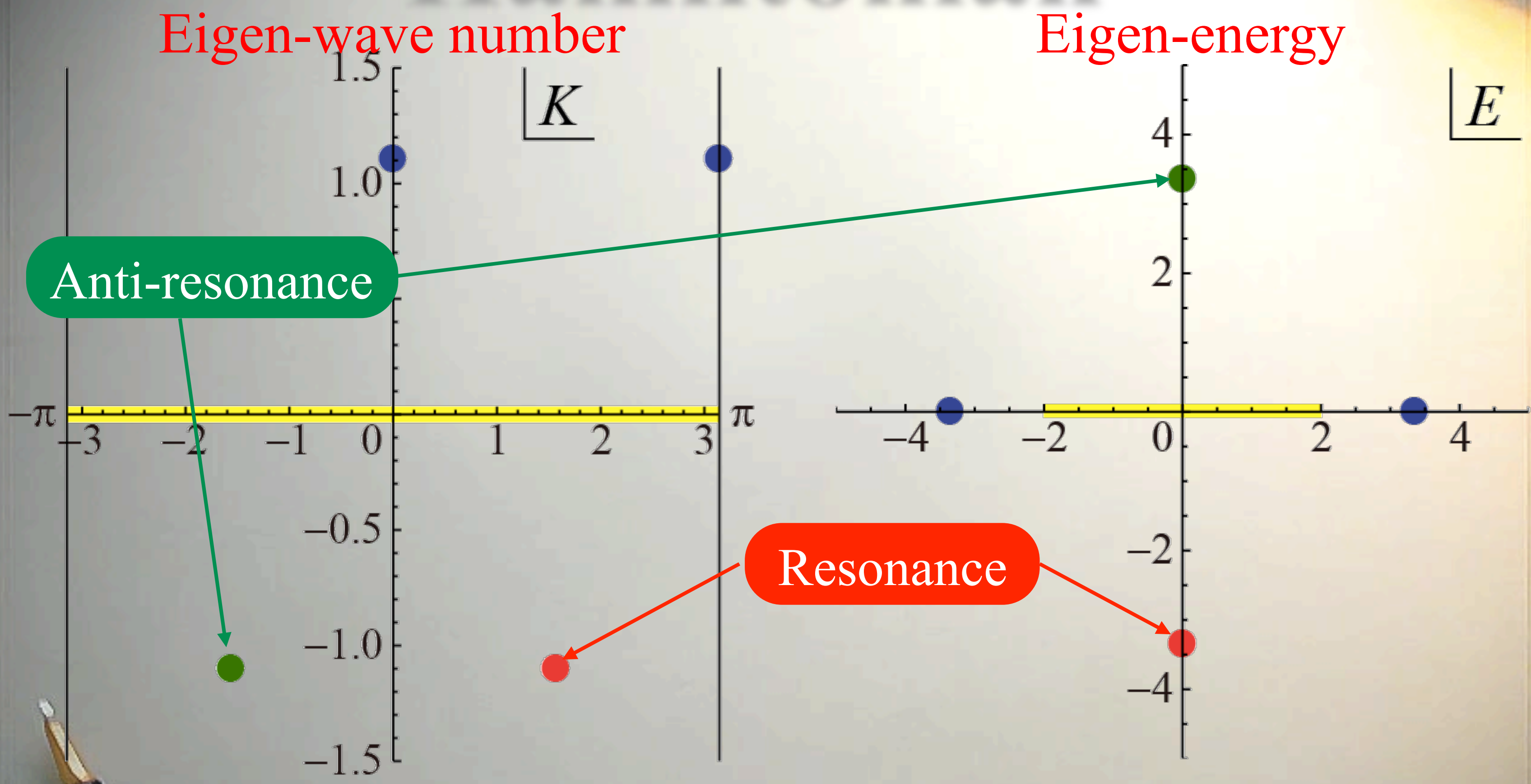


$$E = -W\cos K$$

$$PHQ\frac{1}{E - QHQ}QHP = \frac{\lambda^2|\mathrm{d}\rangle\langle \mathrm{d}|}{E + We^{iK}}$$

Hidden non-Hermiticity

Complex eigenvalues of the Hamiltonian



$$\psi(x) \simeq e^{iK|x|}$$

$$\mathrm{Re}\, K_n \gtrless 0 \Leftrightarrow \mathrm{Im}\, E_n \lessgtr 0$$

Approach to equilibrium

$$\rho(t) \to \rho_{\mathrm{eq}} \equiv \frac{1}{Z}\sum_n e^{-\beta E_n}|n\rangle\langle n|$$

Mixed state

Liouville-von Neumann equation

$$i\hbar\frac{d\rho}{dt} = [H,\rho] =: L\rho$$

$$L\rho_n = z_n\rho_n, \quad z_n \in \mathbb{C}$$

$$\rho(t) \simeq \rho_{\mathrm{eq}} + e^{-(\mathrm{Im}\, z_1)t}\rho_1$$

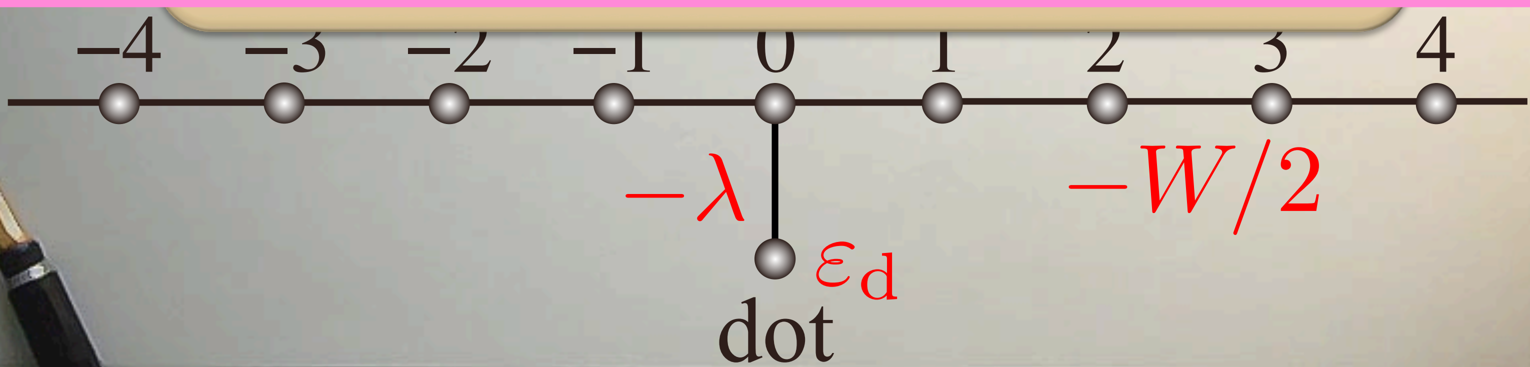
Complex eigevalues of the Liouvillian

$$L\rho_n = z_n \rho_n, \quad z_n \in \mathbb{C}$$

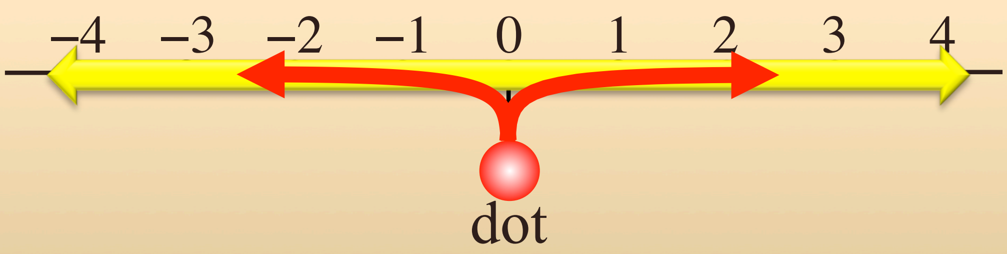
"Trivial" eigenvalues $z_{mn} = E_m - E_n$ exist.

Do "Non-trivial" eigenvalues exist?

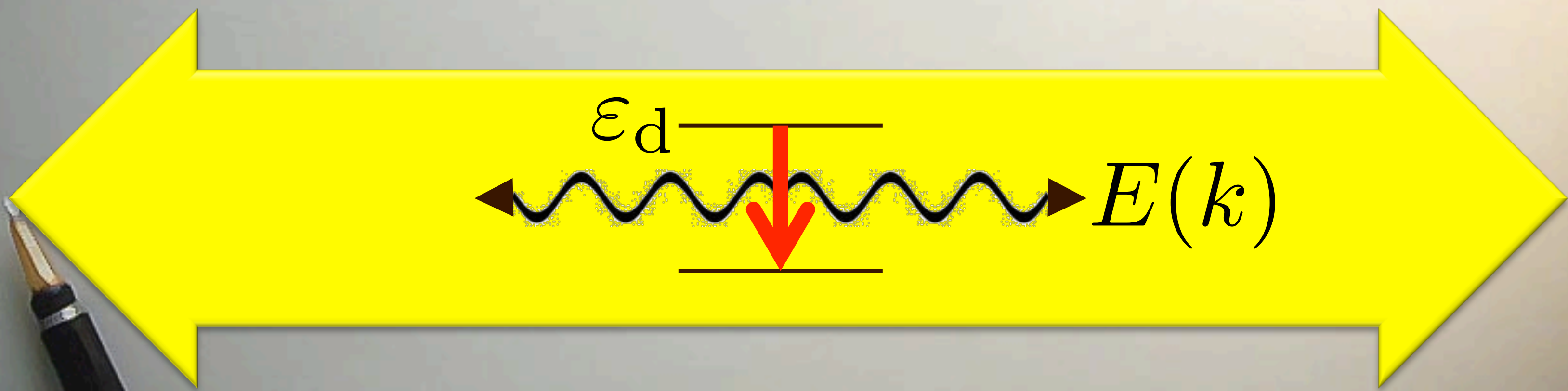
(whose eigenstates must be mixed states)



Relaxation to laser field?



"Non-trivial" relaxation constant possible



Bra-ket states for the Liovillian

T. Petrosky, I. Prigogine

$$i\hbar\frac{d\rho}{dt} = [H,\rho] =: L\rho$$

$$H|n\rangle = E_n|n\rangle$$
$$\langle m|n\rangle = \delta_{mn}$$
$$\sum_n |n\rangle\langle n| = 1$$

$$L|m,n\rangle\rangle = z_{mn}|m,n\rangle\rangle$$
$$\langle\langle m,n|k,l\rangle\rangle = \delta_{mk}\delta_{ln}$$
$$\sum_{m,n} |m,n\rangle\rangle\langle\langle m,n| = 1$$

$$|m,n\rangle\rangle := |m\rangle\langle n|$$
$$z_{mn} = E_m - E_n$$
$$\langle\langle A|B\rangle\rangle := \mathrm{Tr}\, A^\dagger B$$

Feshbach fm. for the Liouvillian

R. Nakano, T. Mori, N. Hatano, T. Petrosky

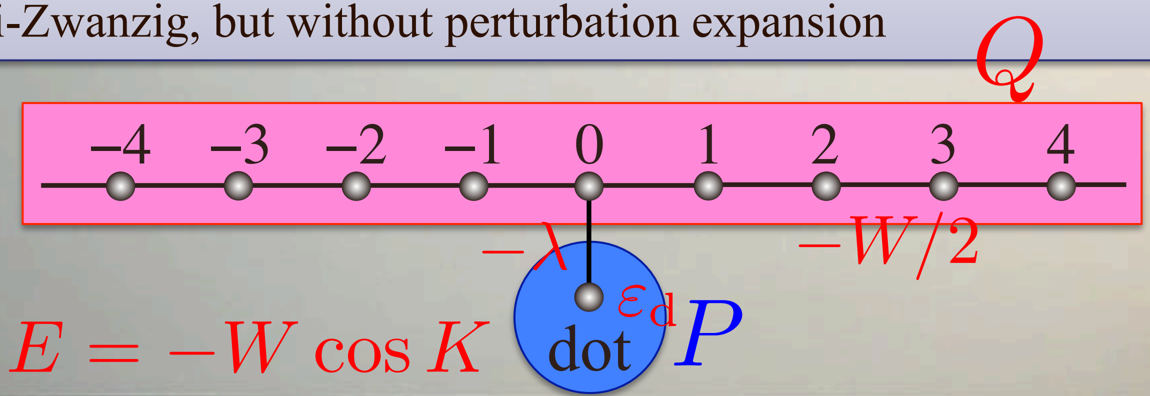
$$L|\rho\rangle\!\rangle = z|\rho\rangle\!\rangle$$

$$\Downarrow$$

$$L_{\text{eff}}(z)\left(P_L|\rho\rangle\!\rangle\right) = z\left(P_L|\rho\rangle\!\rangle\right)$$

$$L_{\text{eff}}(z) = P_L L P_L + P_L L Q_L \frac{1}{z - Q_L L Q_L} Q_L L P_L$$

Same as Mori-Zwanzig, but without perturbation expansion



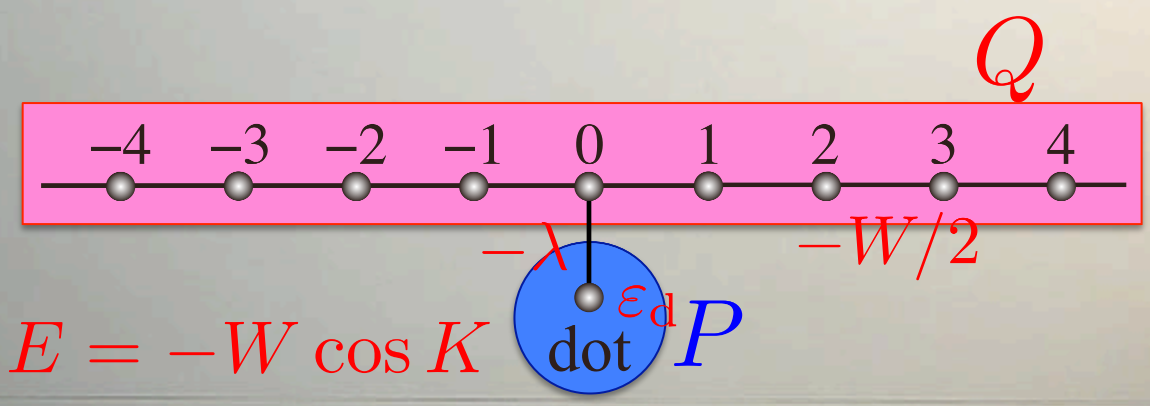
Intertwining of bras and kets

R. Nakano, T. Mori, N. Hatano, T. Petrosky

$$P_L + Q_L = 1 \quad \text{where} \quad P_L = P \times P$$

$$Q_L = Q \times Q + Q \times P + P \times Q$$

Kets and bras intertwine with each other



Retarded and advanced Green's fn.

R. Nakano, T. Mori, N. Hatano, T. Petrosky

$$\frac{1}{z-L} = \frac{1}{2\pi i}\int_{-\infty}^{\infty} d\zeta \frac{1}{\zeta + \frac{z}{2} - H} \times \frac{1}{\zeta - \frac{z}{2} - H}$$

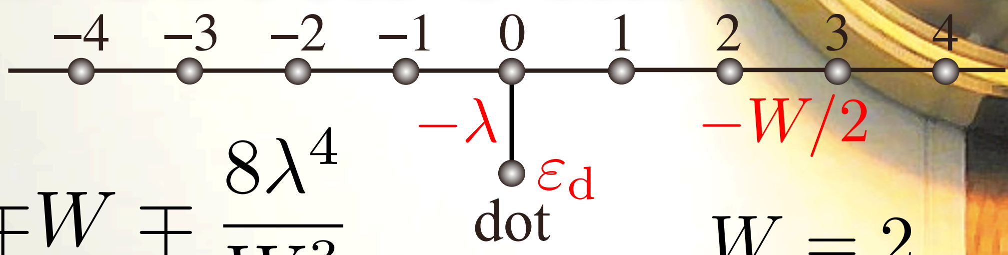
Green's fn.
4 types

= Retarded / Advanced × Retarded / Advanced

$$G^{\mathrm{RR}}(z) = \left(G^{\mathrm{AA}}(z^*)\right)^*$$

$$G^{\mathrm{RA}}(z) = \left(G^{\mathrm{AR}}(z^*)\right)^*$$

RR and RA Green's fns.



$$E_{\text{bound}} \simeq \mp 2.0001 = \mp W \mp \frac{8\lambda^4}{W^3}$$

$$W = 2$$

$$\lambda = 0.1$$

$$E_{\text{res}}, E_{\text{anti-res}} \simeq \mp i0.005 = \mp i\frac{\lambda^2}{W}$$

$$\varepsilon_{\mathrm{d}} = 0$$

(by T. Mori)

equation	numerical	perturbational
$L_{\text{eff}}^{\text{RA}}(z) = z$	$\pm 0.0005\cdots$	$E_{\text{res}}, E_{\text{anti-res}}$
$L_{\text{eff}}^{\text{RR}}(z) = z$	$-i0.01\cdots$	$E_{\text{res}} - E_{\text{anti-res}}$
	$-i0.00382\cdots$	$-i(3-\sqrt{5})\lambda^2/W$

Non-trivial eigenvalue!

Summary

- Definition and physics of resonance
- Breaking of the time-reversal symmetry
- Feshbach formalism for the Liouvillian
- Non-trivial eigenvalue

  for an atom in a laser field?

- Siegert b. c. for the Liouvillian?