Bound state influence on long-time power law decay in open quantum systems

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Outline:

Open quantum systems (OQS) – prototype model

Topic I – Exceptional Points in OQS (Markovian dynamics)

- Prototype model – discrete spectrum
- Generalized Puiseux expansion at the exceptional points (EPs)
- Spontaneous appearance of time irreversibility at real-valued EP

Number of EPs in a given open quantum system:

- Number of EPs in simple tight-binding models with impurities
- Question: Number of EPs in arbitrary open quantum systems?

Outline:
Topic II – Bound state influence on long-time dynamics in OQS (Non-Markovian)

Deviations from exponential decay in quantum mechanics:

- Short time scales – quantum Zeno and anti-Zeno effects
- Long time scales – connection with continuum threshold

Survival Probability Formalism and Physical Motivation:

- Relevant studies in the literature

Prototype model – linear case:

- Bound state transition to anti-bound state (virtual state)
- Long time dynamics: long-time near zone $P(t) \sim t^{-1}$
- Long-time far zone $P(t) \sim t^{-3}$
- Timescale set by Δ_Q – gap between bound state and threshold

Side-coupled impurity model:

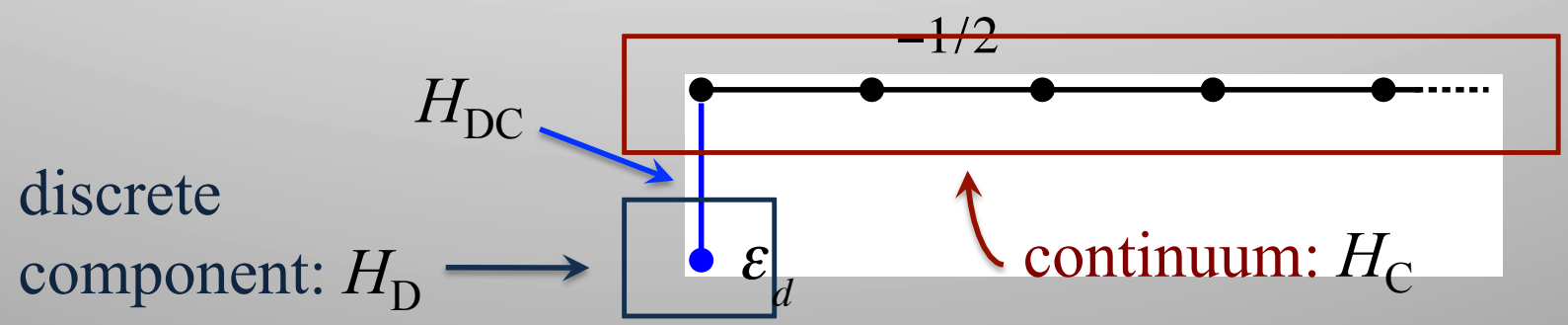
- Bound state trapping below threshold

Open Quantum Systems

Open quantum system consists of:

- Discrete system H_D
- Embedded in a larger system (continuum) H_C
- Coupled via H_{DC}

Prototype Model: semi-infinite chain with end-point impurity

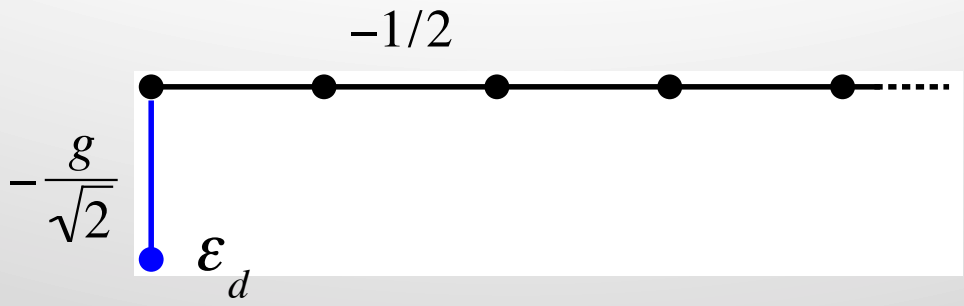


$$H_D = \varepsilon_d d^+ d$$

$$H_C = -\frac{1}{2}\sum_{i=1}^{\infty}(c_i^+ c_{i+1} + c_{i+1}^+ c_i)$$

Open Quantum Systems: Prototype model

Prototype:



$$H = H_D + H_C + H_{DC}$$

$$H = \varepsilon_d d^+ d - \frac{1}{2}\sum_{i=1}^{\infty}(c_i^+ c_{i+1} + c_{i+1}^+ c_i) - \frac{g}{\sqrt{2}}(c_1^+ d + d^+ c_1)$$

Topic I: Exceptional Points in OQS

Formalism for Exceptional Points in finite Hamiltonians:

Tosio Kato, *Perturbation Theory for Linear Operators*, Springer-Verlag, Berlin (1980), pp. 62-66.

Exceptional points (EPs) in open quantum systems:

- Associated with the **discrete sector** of the OQS spectrum
- Branch points of a **cut in parameter space** shared by two (or more) discrete eigenvalues
- Can be found as the roots of the **system discriminant**
- Real-valued EPs → associated with the appearance of the **resonant state**

(note that real-valued EPs cannot occur in Hermitian systems)

Prototype model: discrete spectrum

take continuum limit and introduce half-chain Fourier series:

$$H = \varepsilon_d d^\dagger d + \int_0^\pi \varepsilon_k c_k^\dagger c_k + g \int_0^\pi V_k (c_k^\dagger d + d^\dagger c_k)$$

$(N \to \infty)$

Continuum:

$k \in [0, \pi]$ on $\varepsilon_k = -\cos k$

Obtain the discrete spectrum from:

$$\left\langle d \left| \frac{1}{z - H} \right| d \right\rangle = \frac{1}{z - \varepsilon_d - \Sigma(z)}$$

yields quadratic polynomial

Prototype: Discrete eigenvalues and discriminant

Quadratic dispersion yields:

$$z_{\pm}(\varepsilon_d, g) = \varepsilon_d \frac{1-g^2}{1-2g^2} \pm g^2 \frac{\sqrt{\varepsilon_d^2 - (1-2g^2)}}{1-2g^2}$$

System discriminant:

$$\boxed{D(\varepsilon_d, g) = -4g^4\left(1-2g^2\right)\left(\varepsilon_d^2 - (1-2g^2)\right)}$$

$\boxed{\varepsilon_d^2 - (1-2g^2) = 0}$ gives two EPs: $\varepsilon_d = \bar{\varepsilon}_{\pm} \equiv \pm\sqrt{1-2g^2}$

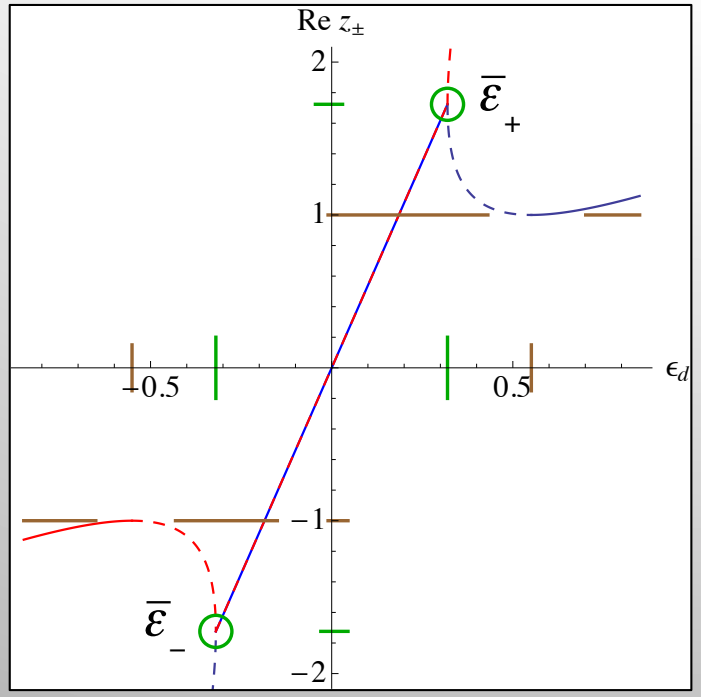
For $g < 1/\sqrt{2}$ $\left(g > 1/\sqrt{2}\right)$ these EPs are real-valued (pure imaginary).

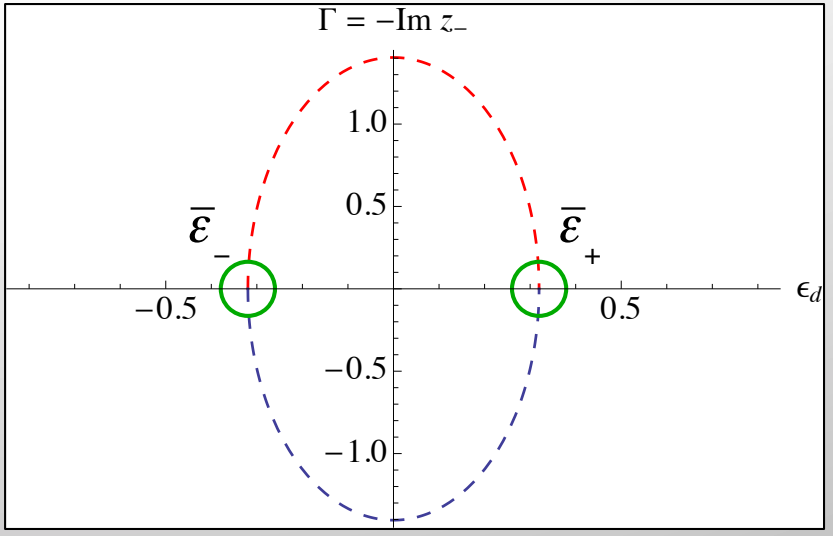
We will focus on real-valued case $g < 1/\sqrt{2}$ for now.

$g = 1/\sqrt{2}$ ➔ special linear case (return to this in Topic II).

Discrete spectrum: eigenvalue expansion at EP

$g < 1/\sqrt{2}$ case





$$f_2(\varepsilon_d, g) \equiv \varepsilon_d^2 - (1 - 2g^2) = (\varepsilon_d - \bar{\varepsilon}_+)(\varepsilon_d - \bar{\varepsilon}_-)$$

Generalized Puiseux expansion in the vicinity of $\varepsilon_d \approx \bar{\varepsilon}_\pm$

$$z_s = \frac{1 + \bar{\varepsilon}_\pm^2}{2\bar{\varepsilon}_\pm} + s\frac{1 - \bar{\varepsilon}_\pm^2}{2\bar{\varepsilon}_\pm^2}\left(f_2(\varepsilon_d, g)\right)^{1/2} + \frac{1}{2\bar{\varepsilon}_\pm}\sum_{n=2}^{\infty}\left(\frac{s\left(f_2(\varepsilon_d, g)\right)^{1/2}}{\bar{\varepsilon}_\pm}\right)^n \qquad (s = \pm)$$

QPT analogy for the real-valued EPs

decay rate
appears at the EPs: $\left|\varepsilon_d\right| < 1 - 2g^2$

$$z_s = \frac{1+\bar{\varepsilon}_\pm^2}{2\bar{\varepsilon}_\pm} + s\frac{1-\bar{\varepsilon}_\pm^2}{2\bar{\varepsilon}_\pm^2}\left(f_2(\varepsilon_d, g)\right)^{1/2} + \frac{1}{2\bar{\varepsilon}_\pm}\sum_{n=2}^{\infty}\left(\frac{s\left(f_2(\varepsilon_d, g)\right)^{1/2}}{\bar{\varepsilon}_\pm}\right)^n$$

QPT analogy: decay rate → order parameter

(*PT* spontaneous symmetry breaking)

Transition from *localized/anti-localized* states to *resonant state*: mimics the ordinary |*k*> states (definite chirality).

S. Garmon, I. Rotter, N. Hatano, and D. Segal, Int. J. Theor. Phys., DOI: 10.1007/s10773-012-1240-5; **arXiv: 1107.1759**

Number of Exceptional Points in a finite, closed system

Recall, for simple ***closed*** system:

$$H_{\text{closed}} = \begin{bmatrix} \varepsilon_1 & \Delta/2 \\ \Delta/2 & \varepsilon_2 \end{bmatrix}$$

Eigenvalue equation $H\,\boldsymbol{\psi} = \boldsymbol{\varepsilon}\,\boldsymbol{\psi}$ gives:

$$\bar{\varepsilon}_{\pm} = \frac{\varepsilon_1 + \varepsilon_2 \pm \sqrt{\left(\varepsilon_1 - \varepsilon_2\right)^2 - \Delta^2}}{2}$$

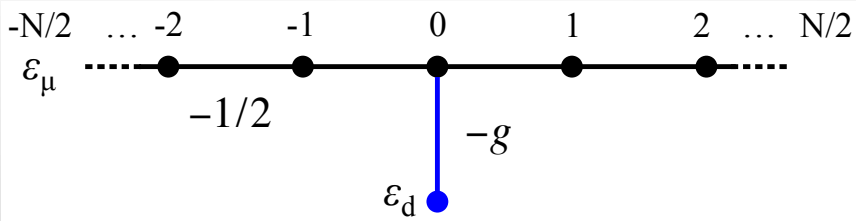
with **<u>two</u>** EPs: $\varepsilon_1 - \varepsilon_2 = \pm\Delta$

For generic closed system represented by *n*-dimensional Hamiltonian: $n\,(n-1)$ EPs

Kato, *Perturbation Theory for Linear Operators*, Springer-Verlag, Berlin (1980).

Effective finite-dimensional Hamiltonian for open quantum systems

For open quantum systems, such as:



We may obtain an (ε-dependent) effective Hamiltonian:

$$H_{\text{eff}}(\varepsilon) = \begin{bmatrix} \varepsilon_d & -g \\ -g & \varepsilon - \sqrt{\varepsilon^2 - 1} \end{bmatrix}$$

- **<u>isospectral</u>** with original Hamiltonian

- obtained by: Feshbach projection operator technique,
  point-contact technique

N. Hatano, Fortschr. Phys., DOI: 10.1002/prop.201200064 (2012).

Number of Exceptional Points in OQS - 1

Obtain the finite spectrum as solutions:

$$H_{\text{eff}}(\varepsilon)\,\Psi = \varepsilon\,\Psi$$

Results in a **4th order** equation for the present system:

Therefore – 4 x 3 = 12 EPs!

Number of Exceptional Points in OQS - 2

Easy to extrapolate for dispersion in the leads $\varepsilon_k = -\cos k$:

- 1 solution for each site N_D in discrete sector
- 1 solution for each distinct, *non-degenerate* chain N_C
- multiply by 2 for each non-degenerate chain

$$2^{Nc}(N_C + N_D) - \text{th order polynomial}$$

Therefore:

$$\boxed{2^{Nc}(N_C + N_D)\left[2^{Nc}(N_C + N_D) - 1\right] \quad \text{EPs}}$$

S. Garmon, I. Rotter, N. Hatano, and D. Segal, Int. J. Theor. Phys., DOI: 10.1007/s10773-012-1240-5; **arXiv: 1107.1759**

Proposed Question:

How many exceptional points are there in a *generic* open quantum system?

Topic II: Bound state influence on long-time power law decay

For decades it has been known that deviations from exponential decay exist in quantum systems *at least* on very short and very long time scales.

C. B. Chiu, B. Misra, and E. C. G. Sudarshan, Phys. Rev. D **16**, 520 (1977).

J. Martorell, J. G. Muga, and D. W. L. Spring, Lect. Notes. Phys. **789**, 239 (2009).

Short time scales typically give rise to parabolic decay: $P(t) \sim t^2$

- Quantum Zeno effect ➔ repeated measurements result in decelerated decay
- quantum anti-Zeno effect ➔ accelerated decay
- Experimental confirmation – ultra-cold sodium atoms initially trapped in accelerating optical potential:

S. R. Wilkinson, C. F. Bharucha, M. C. Fischer, K. W. Madison, P. R. Morrow, Q. Niu, B. Sunduram, and M. G. Raizen, Nature (London) **387**, 575 (1997).

M. C. Fischer, B. Gutiérrez-Medina, and M. G. Raizen, Phys. Rev. Lett. **87**, 040402 (2001).

Long-time deviations from exponential decay

Long time deviations intimately connected with the continuum threshold.

- Mathematically proven for quantum systems:

L. A. Khalfin, Soc. Phys. JETP **6**, 1053 (1958).

M. N. Hack, Phys. Lett. A **90**, 220 (1982).

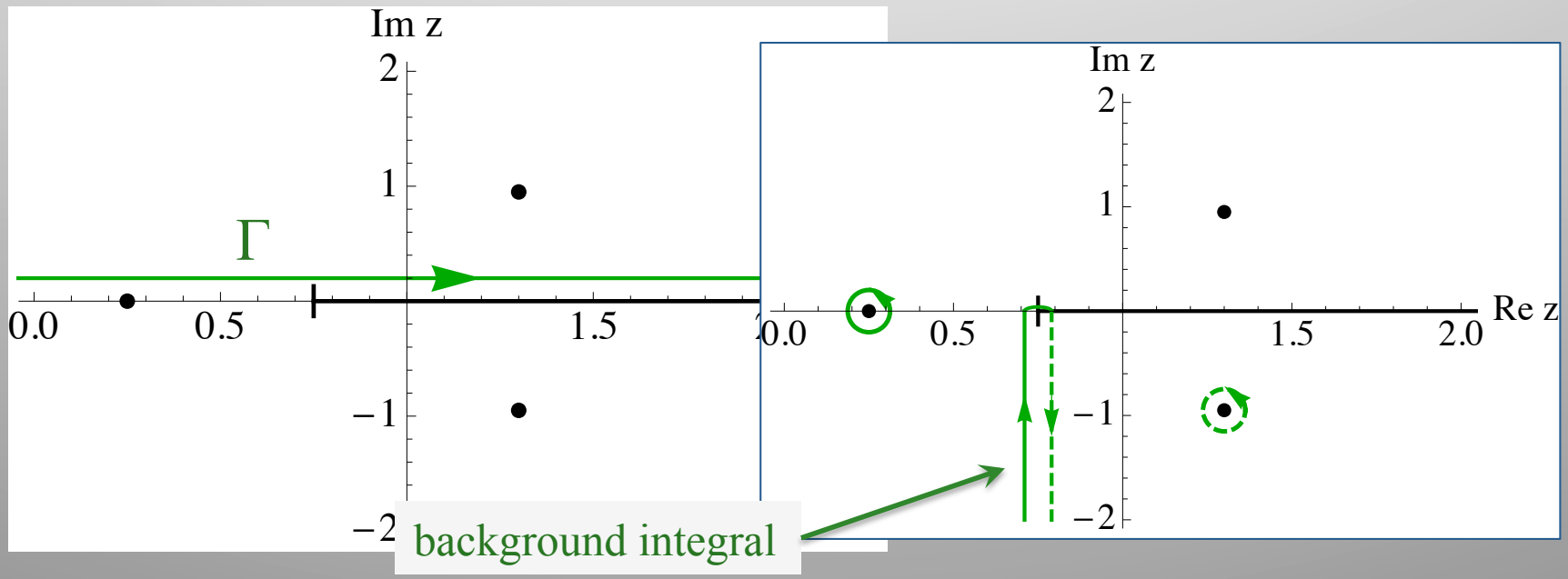
- Typically gives rise to inverse power law decay
- Typical asymptotic decay law: $P(t) \sim t^{-3}$
- Recent experimental verification: luminescence decay properties of dissolved organic materials following laser excitation:

C. Rothe, S. I. Hintschich and A. P. Monkman, Phys. Rev. Lett. **96**, 163601 (2006).

Formalism: survival probability for an initially prepared state

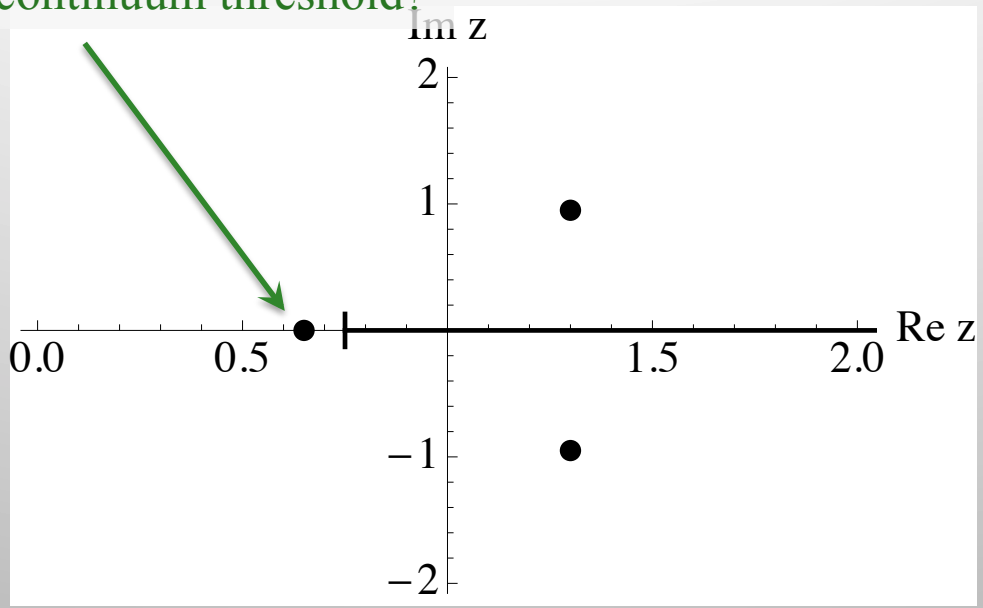
Survival probability: $P(t) = |A(t)|^2$

$$A(t) = \langle \psi_0 | e^{-iHt} | \psi_0 \rangle = \frac{1}{2\pi i} \int_\Gamma dz\, e^{-izt} \left\langle \psi_0 \left| \frac{1}{z - H} \right| \psi_0 \right\rangle$$



Physical motivations: bound state at threshold

question: what happens as bound state approaches continuum threshold?



Answer: the long-time non-exponential decay effects will be amplified as bound state approaches the threshold.

Note that bound state transitions to anti-bound state (2nd sheet) after reaching threshold

Relevant studies in the literature

T. Jittoh, S. Matsumoto, J. Sato, Y. Sako, and K. Takeda, Phys. Rev. A **71**, 012109 (2005).

Radial potential: for *s*-wave component, as energy of initially prepared state approaches threshold, **exponential decay suppressed completely**.

(However, they do not consider bound states).

Victor Dinu, Arne Jensen, and Gheorge Nenciu, J. Math. Phys. **50**, 013516 (2009).

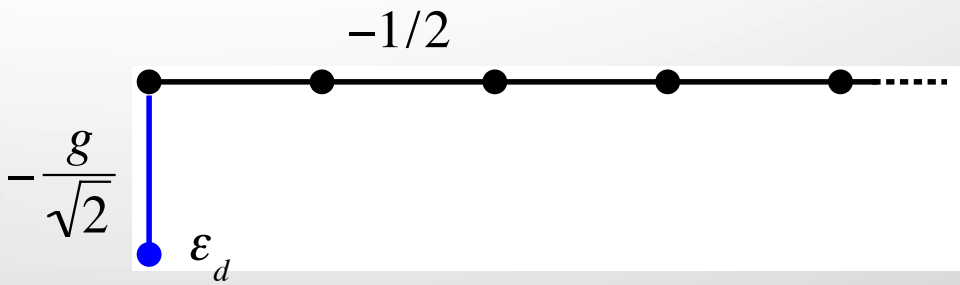
From mathematical physics perspective, authors study a bound state near threshold. Unfortunately, they make several unphysical assumptions.

(e.g. Discrete unperturbed energy appearing at threshold cannot form a bound state below threshold??)

Other relevant studies ➔ TBA

Special case of prototype model: linear dispersion

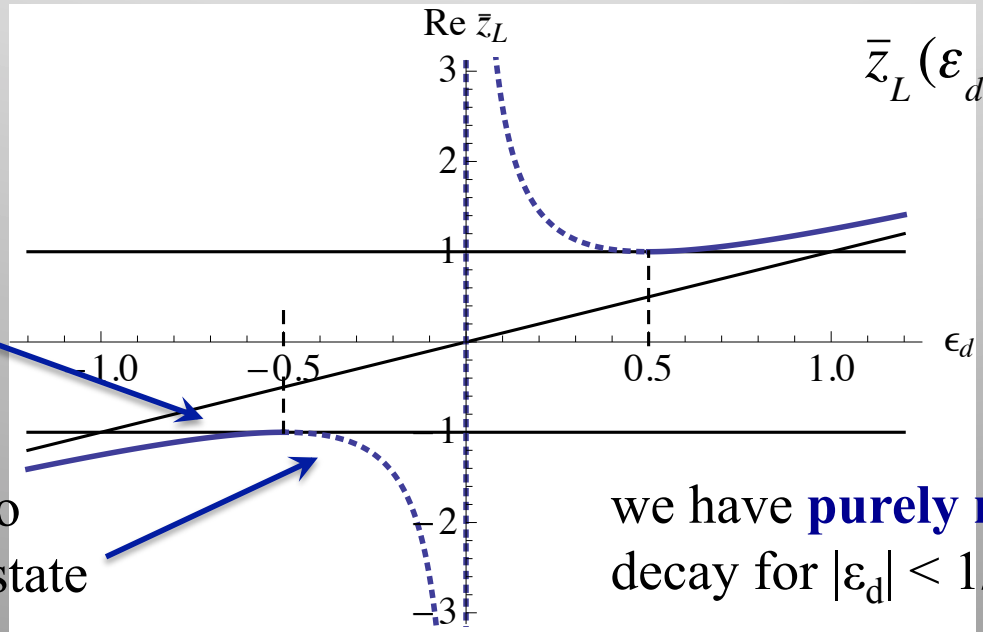
Return to prototype:



choose special case $g = 1/\sqrt{2}$

Yields a simplified linear dispersion with solution:

$$\bar{z}_L(\varepsilon_d) = \varepsilon_d + \frac{1}{4\varepsilon_d}$$



bound state

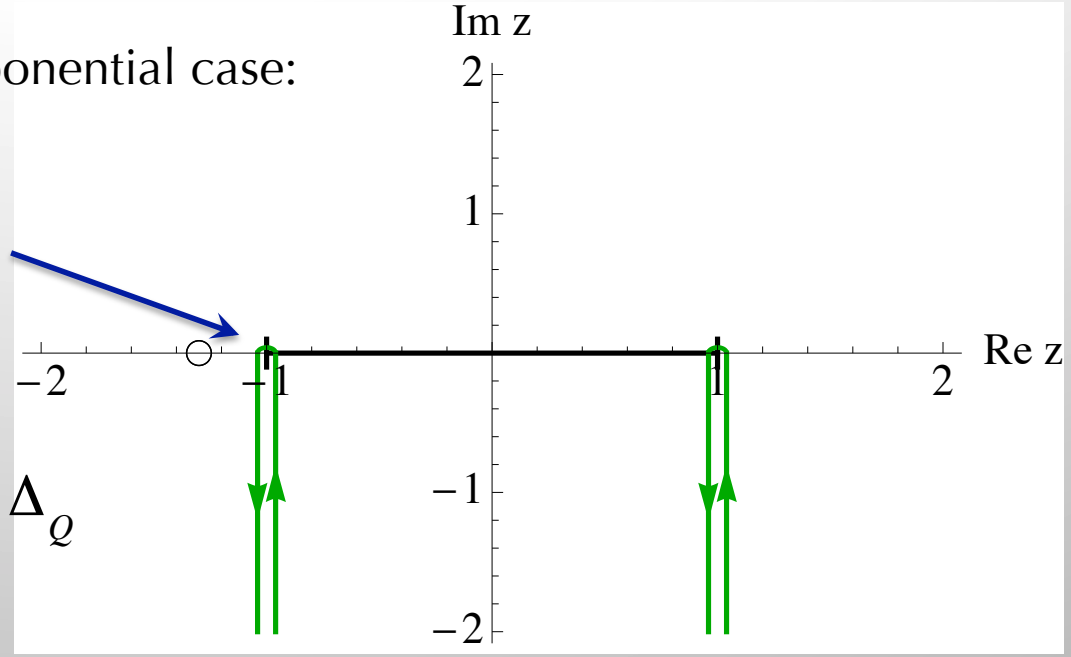
transitions to anti-bound state

we have **purely non-exponential** decay for $|\varepsilon_d| < 1/2$

Long-time dynamics for prototype model

Focus on the purely non-exponential case:

vicinity of lower threshold



define $\bar{z}_L \equiv -1 + \Delta_Q$

$$A_{th}^{-}(t) = \frac{1}{2\pi i}\left[\int_{-1}^{-1-i\infty} dz\, \frac{e^{-izt}}{\eta^{\mathrm{I}}(\mathrm{z})} - \int_{-1-i\infty}^{-1} dz\, \frac{e^{-izt}}{\eta^{\mathrm{II}}(\mathrm{z})}\right]$$

$$= \frac{1}{2\pi i \varepsilon_d}\int_{-1}^{-1-i\infty} dz\, e^{-izt}\, \frac{\sqrt{z^2-1}}{z-\bar{z}_L(\Delta_Q)}$$

Long-time dynamics: near zone and far zone

$$A_{th}^{-}(t) = \frac{e^{-it}}{2\pi i \varepsilon_d t^2} \int_0^\infty dz\, e^{-s} \frac{\sqrt{s^2 - 2its}}{\Delta_Q + i\frac{s}{t}}$$

Consider the timescale: $1 << t << (\Delta_Q)^{-1}$ (Long-time 'near zone')

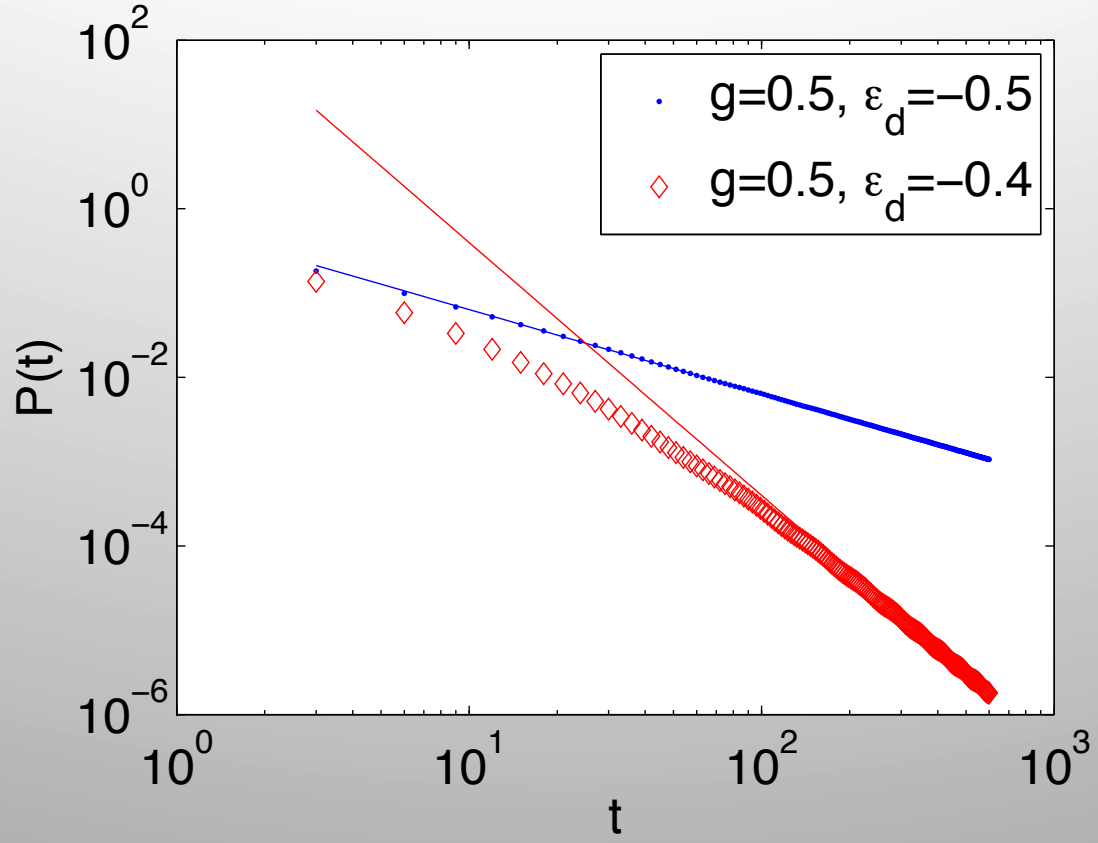
$$\left|A_{th}^{-}(t)\right|^2 \sim t^{-1}$$

Asymptotic limit: $(\Delta_Q)^{-1} << t$ (Long-time 'far zone')

$$\left|A_{th}^{-}(t)\right|^2 \sim t^{-3}$$

Note that for $\Delta_Q = 0$, the near zone becomes fully asymptotic

Long-time dynamics: numerical results for prototype model



S. Garmon, T. Petrosky, L. Simine, and D. Segal, Fort. Physik, DOI: 10.1002/prop.201200077; **arXiv:1204.6141**.

Long-time dynamics for general open quantum systems

Similar effect observed in the following works:

S. Longhi, Phys. Rev. Lett. **97**, 110402 (2006).

S. Garmon, Ph.D. thesis, University of Texas at Austin (2007).

Axel D. Dente, Raúl A. Bustos-Marún, and Horacio M. Pastawski, Phys. Rev. A **78**, 062116 (2008).

Straight-forward to demonstrate: time scale separating near and far zones should *always* be inversely related to Δ_Q in OQS

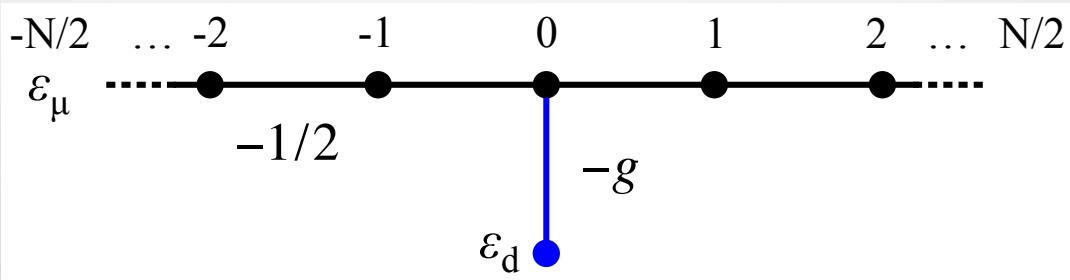
S. Garmon, T. Petrosky, L. Simine, and D. Segal, Fort. Physik, DOI: 10.1002/prop.201200077; **arXiv:1204.6141**.

The transition from bound to anti-bound states also leads to a maximum in the local density of states:

Raúl A. Bustos-Marún, Eduardo A. Coronado, and Horacio M. Pastawski, Phys. Rev. B **82**, 035434 (2010).

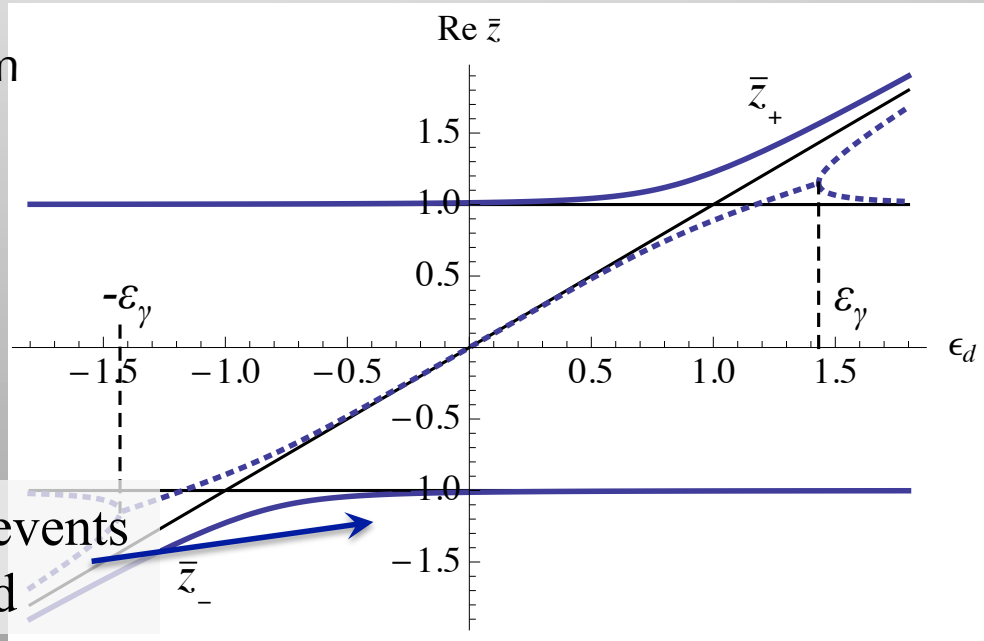
Further demonstration: bound state trapped below threshold

Side-coupled impurity model (or T-model):



We again find dispersion from resolvent method:

$$z - \varepsilon_d = \frac{g^2}{\sqrt{z^2 - 1}}$$



van Hove DOS singularity prevents bound state reaching threshold

Long-time dynamics for bound state trapped below threshold

Bound state eigenvalue expansion:

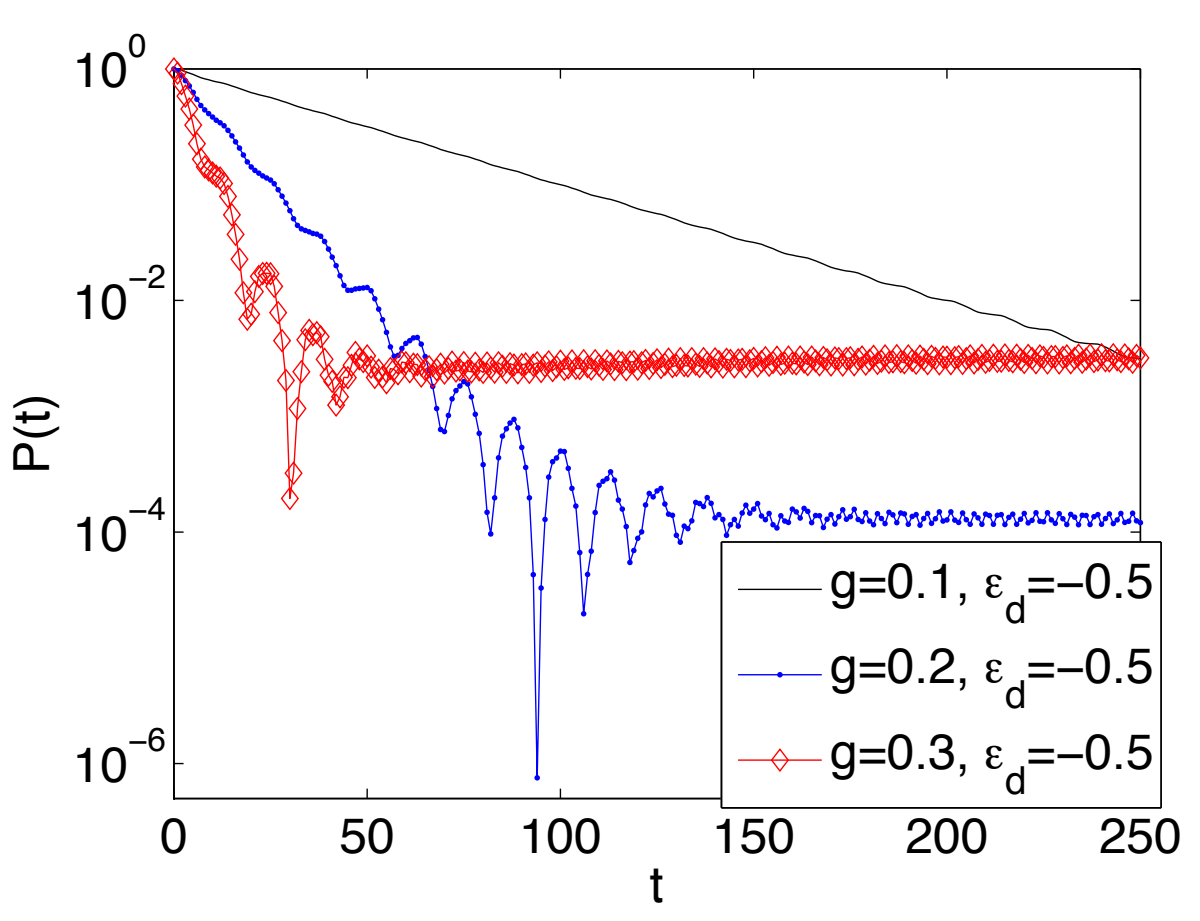
$$\bar{z}_{-} = -1 - \tilde{\Delta}_Q + O(g^8) \text{ with } \tilde{\Delta}_Q \equiv \frac{1}{2(1+\varepsilon_d)^2} g^4$$

In the near zone:

$$\left| A_{th}^{-}(t) \right|^2 = \frac{\tilde{\Delta}_Q^2}{2\pi g^2 t} = \frac{g^4}{2\pi(1+\varepsilon_d)^4 t}$$

Hence closing the gap requires ε_d goes to infinity, which kills the effect in any case.

Long-time dynamics: numerical results for side-coupled impurity model



Due to bound states, resonance, difficult to see much

Conclusions

Topic I – EPs in OQS

- Generalization of Kato's expression for eigenvalue expansion in the vicinity of EPs

- QPT analogy at real-valued EPs:
  - Decay rate as order parameter
  - Channel correlations and dynamical critical exponent

- Number of EPs in an OQS with quadratic dispersion: $2^{N_C}(N_C + N_D)\,(2^{N_C}(N_C + N_D) - 1)$

Conclusions

Topic II – Bound state influence on long time dynamics in OQS

- Bound state transition to anti-bound state at continuum threshold
- Purely non-exponential dynamics when only anti-bound states are present
- Long time dynamics for prototype model:
  - Long-time near zone: $P(t) \sim t^{-1}$
  - Long-time far zone: $P(t) \sim t^{-3}$
- Amplification of non-Markovian decay as bound state transitions to anti-bound state; near zone becomes asymptotic dynamics