Self-adjoint extension in quantum mechanics & non-Rydberg spectra of 1D hydrogen atom

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Plan of the talk

- Short introduction to self-adjoint operators
- Singular interaction on a line
- Quantum graph vertices
- Self-adjoint extension of 1D 1/|x| potential
- non-Rydberg spectra of 1D hydrogen

Self-adjointness

- **Quiz:** Quantum mechanics on $x \in [0,L]$
  Let's have $\psi(0) = \psi(L) = 0$
  Eigenstates of $H = -\dfrac{d^2}{dx^2}$,i.e. $\psi_n(x) = \sin\dfrac{n\pi x}{L}$ are
  not eigenstates of $p = \dfrac{1}{i}\dfrac{d}{dx}$ though $H = p^2$
  In fact, spectra of p is *nil*

  Why?

- **Ans:** Operator to be observable, *Hermiticity is not enough*. Has to be <u>*self-adjoint*</u>

  Condition for Hilbert operator & <u>vector</u>

Self-adjointness for *p*

Condition for Hilbert operator & vector

- $$\int_0^L dx \phi^*(x) \frac{1}{i} \frac{d}{dx} \psi(x)$$ $\psi, \phi \in \mathrm{L}^2(0,L)$

$$= -i\left[\phi^*(L)\psi(L) - \phi^*(0)\psi(0)\right] + \int_0^L dx \left(\frac{1}{i}\frac{d}{dx}\phi(x)\right)^* \psi(x)$$

- To make p Hermite $\langle \phi | p\psi \rangle = \langle p\phi | \psi \rangle$
  we can have $\psi(L) = \psi(0) = 0$ & arbitrary $\phi(0), \phi(L)$

  self-adjoint extension ↓ $D(p) \subset D(p^*)$: *not symmetric*

  or we can have $\psi(L) = e^{i\chi}\psi(0)$ & $\phi(L) = e^{i\chi}\phi(0)$

  Self-adjoint: $D(p) = D(p^*)$: *symmetric*

Self-adjointness for H

- $$\int_0^L dx\phi^*(x)\left(-\frac{d^2}{dx^2}\right)\psi(x) - \int_0^L dx\left(-\frac{d^2}{dx^2}\phi(x)\right)^*\psi(x)$$
$$= -\left[\phi^*(L)\psi'(L) - \phi'^*(L)\psi(L) - \phi^*(0)\psi'(0) + \phi'^*(0)\psi(0)\right]$$

$$H = -\frac{d^2}{dx^2}$$

- To make H <u>self-adjoint</u>, namely, H Hermitian, $H = H^*$ and $D(H) = D(H^*)$, we need to impose

$$W[\phi^*(L), \psi(L)] - W[\phi^*(0), \psi(0)] = 0$$

Wronskian $W[\phi(x), \psi(x)] = \phi(x)\psi'(x) - \phi'(x)\psi(x)$

Self-adjointness for H

- $$\int_0^L dx\phi^*(x)\left(-\frac{d^2}{dx^2}\right)\psi(x) - \int_0^L dx\left(-\frac{d^2}{dx^2}\phi(x)\right)^*\psi(x)$$
$$= -\left[\phi^*(L)\psi'(L) - \phi'^*(L)\psi(L) - \phi^*(0)\psi'(0) + \phi'^*(0)\psi(0)\right]$$

$$H = -\frac{d^2}{dx^2}$$

- To make H <u>self-adjoint</u>, namely, H Hermitian, $H = H^*$ and $D(H) = D(H^*)$, we need to impose

$$J(L) - J(0) = 0$$

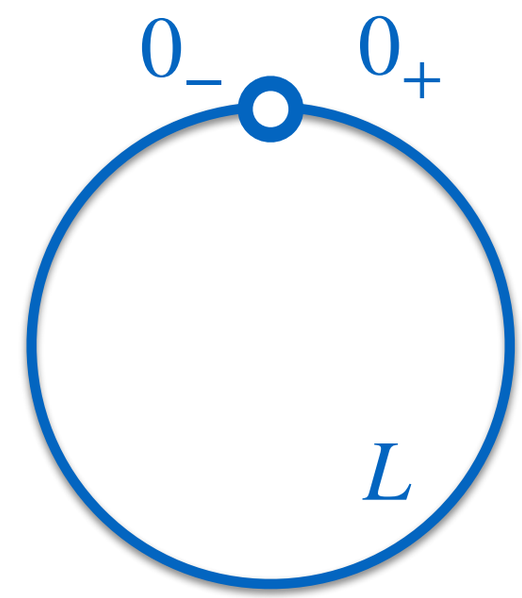
$\psi(x)$: solutions of Schödinger eq.

probability flux $J(x) = i\left(\psi^*(x)\psi'(x) - \psi'^*(x)\psi(x)\right)$

Self-adjointness for H

- Consider free particle on a *ring with a defect*

$$H = -\frac{d^2}{dx^2}$$



- To make H self-adjoint

$$\psi^*(0_-)\psi'(0_-) - \psi'^*(0_-)\psi(0_-) = \psi^*(0_+)\psi'(0_+) - \psi'^*(0_+)\psi(0_+)$$

or

$$J(0_+) - J(0_-) = 0$$

probability flux $J(x) = i\left(\psi^*(x)\psi'(x) - \psi'^*(x)\psi(x)\right)$

$\psi(x)$: solutions of Schödinger eq.

Point interaction on a line

- Consider free particle on a R\{0}

$$H = -\frac{d^2}{dx^2}$$

- To make H self-adjoint

$$\psi^*(0_-)\psi'(0_-) - \psi'^*(0_-)\psi(0_-) = \psi^*(0_+)\psi'(0_+) - \psi'^*(0_+)\psi(0_+)$$

- This includes

$$\psi'(0_+) - \psi'(0_-) = \upsilon\psi(0_+) = \upsilon\psi(0_-)$$

Dirac's δ function potential

υ real parameter

$\upsilon = 0$: free connection

Point interaction on a line

- Consider free particle on a R\{0}

$$H = -\frac{d^2}{dx^2}$$

- To make H self-adjoint

$$\psi^*(0_-)\psi'(0_-) - \psi'^*(0_-)\psi(0_-) = \psi^*(0_+)\psi'(0_+) - \psi'^*(0_+)\psi(0_+)$$

- Connection condition for **general point interaction** includes exotic $\psi(0_+) - \psi(0_-) = u\psi'(0_+) = u\psi'(0_-)$

Seba's δ' potential

u real parameter

Point interaction on a line

- Consider free particle on a R\{0}

$$H = -\frac{d^2}{dx^2}$$

- To make H self-adjoint

$$\psi^*(0_-)\psi'(0_-) - \psi'^*(0_-)\psi(0_-) = \psi^*(0_+)\psi'(0_+) - \psi'^*(0_+)\psi(0_+)$$

- Connection condition for **general point interaction** includes exotic $\psi(0_+) = t\psi(0_-), \quad \psi'(0_+) = (1/t)\psi'(0_-)$

u real parameter

Scale invariant point potential

Point interaction on a line

- Free particle on a R\{0}

$$\psi^*(0_-)\psi'(0_-) - \psi'^*(0_-)\psi(0_-) = \psi^*(0_+)\psi'(0_+) - \psi'^*(0_+)\psi(0_+)$$

- Define $\Psi_1 = \begin{pmatrix} \psi(0_+) \\ \psi(0_-) \end{pmatrix}$, $\Psi_2 = \begin{pmatrix} \psi'(0_+) \\ -\psi'(0_-) \end{pmatrix}$; flux cons.

  equiv. to $\Psi_1^\dagger \Psi_2 = \Psi_2^\dagger \Psi_1 \rightarrow \left|\Psi_1 + i\Psi_2\right| = \left|\Psi_1 - i\Psi_2\right|$

  Von Neumann's construction

- $U\left(\Psi_1 + i\Psi_2\right) = \Psi_1 - i\Psi_2$, $U \in U(2)$ 4-param. family

  or $(U - I)\Psi_2 - (U + I)\Psi_1 = 0$ connection cond.

Generized point interaction: detailed analysis in wider context

Summary (1)

- Self-adjointness is the condition for an operator to be an observable
- In 1D, self-adjointness of Laplacian operator is equivalent to flux conservation
- Applied to R\{0}, self-adjoint extension of Laplacian yields generalized point interaction on a line

Quantum graph

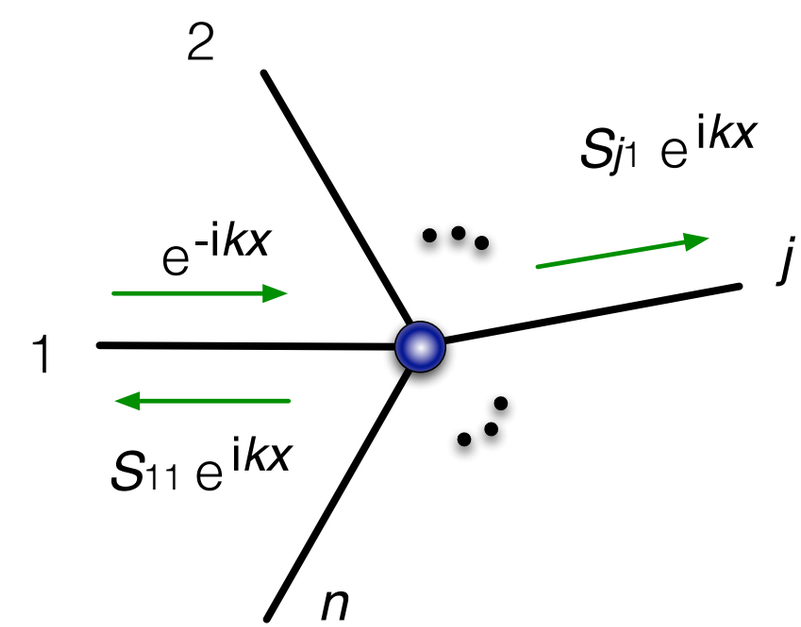
- Quantum particle on graph (lines & nodes)

  "mathematical physics" aspect

  - Minimal extension of 1-dim quantum mechanics

    "applicational" aspect

  - Model of single electron device



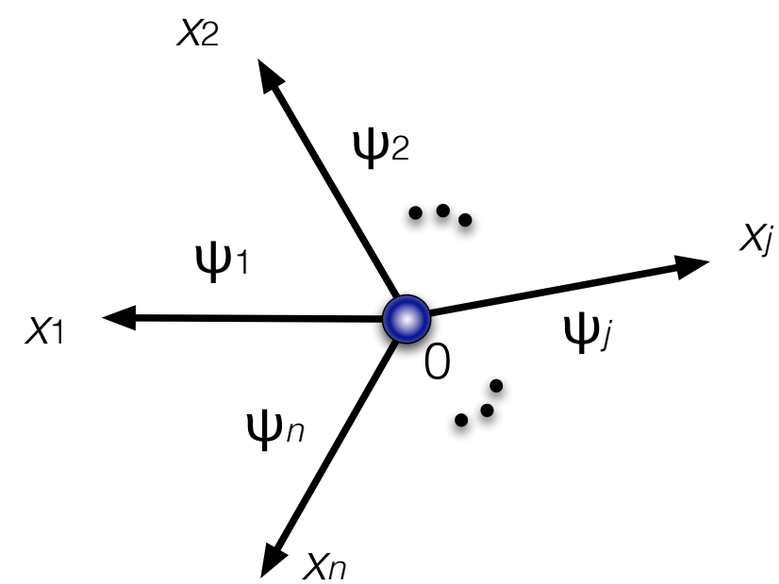
- free motion on line
  —» physics is in vertices

- Nontrivial phenomena
  «— scale invariance

Connection condition

- At the node, define

$$\Psi = \begin{pmatrix} \psi_1(0_+) \\ \vdots \\ \psi_n(0_+) \end{pmatrix} \qquad \Psi' = \begin{pmatrix} \psi_1'(0_+) \\ \vdots \\ \psi_n'(0_+) \end{pmatrix}$$



- flux conservation ψ* ψ'= ψ'* ψ (Self-adjoint extension)

$A\,\psi + B\,\psi' = 0$
$\mathrm{rank}(A, B) = n, \quad AB^* = BA^*$

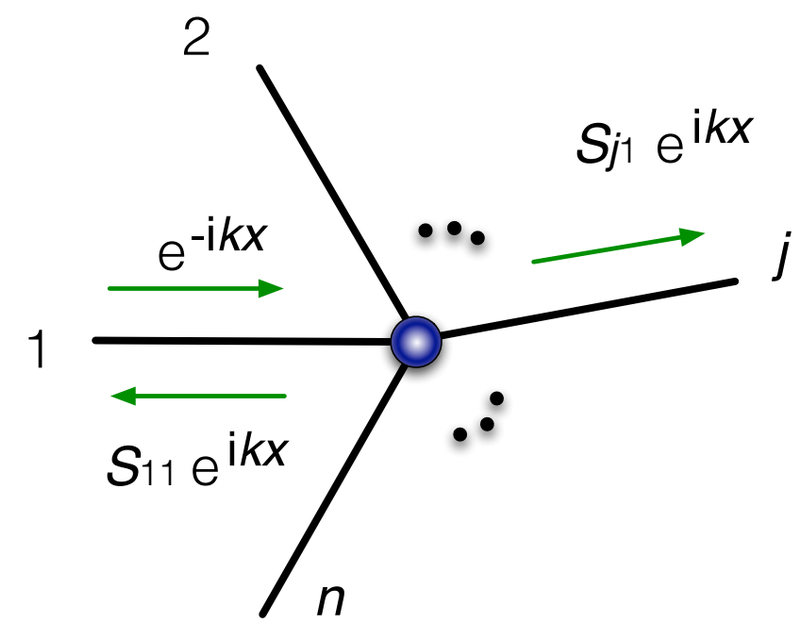
(Kostrykin & Schader, 99)
: n^2 parameters

- ψ, ψ' different dimension : scale anomaly

Scattering matrix

- Scattering from *j*-th to *i*-th lines

$$\psi_i^{(j)}(x_i) = e^{-\mathrm{i}kx_i} + \mathcal{S}_{ii} e^{\mathrm{i}kx_i} \qquad (i = j)$$
$$= \mathcal{S}_{ij}\, e^{\mathrm{i}kx_i} \qquad (i \neq j)$$



- Scattering matrix S(k) from

  $A\,\psi + B\,\psi' = 0$

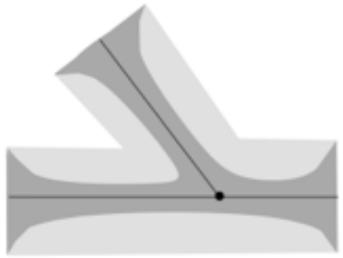
  —> $A(S(k) + I) + ik\,B(S(k) - I) = 0$

$$(\Psi^{(1)} \dots \Psi^{(n)}) = \mathcal{S}(k) + I$$
$$(\Psi'^{(1)} \dots \Psi'^{(n)}) = ik\mathcal{S}(k) - ikI$$

- $$\mathcal{S}(k) = -\frac{1}{A + \mathrm{i}kB}(A - \mathrm{i}kB)$$

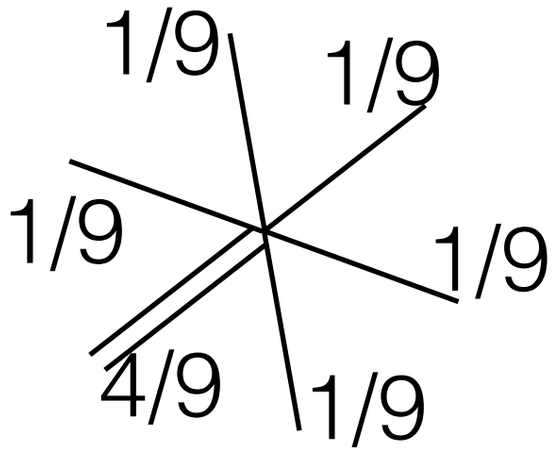
Free connection

- "normal" or "free" connection : thin tube limit
  $\psi_1(0) = \psi_2(0) = \ldots = \psi_n(0)$
  $\psi_1'(0) + \psi_2'(0) + \ldots + \psi_n'(0) = 0$



  transm. $S_{ij}(k) = -2/n$, refl. $S_{jj}(k) = 1-2/n$

- dual "free·" exists
  $\psi_1(0) + \psi_2(0) + \ldots + \psi_n(0) = 0$
  $\psi_1'(0) = \psi_2'(0) = \ldots = \psi_n'(0)$



  transm. $S_{ij}(k) = 2/n$, refl. $S_{jj}(k) = -1+2/n$

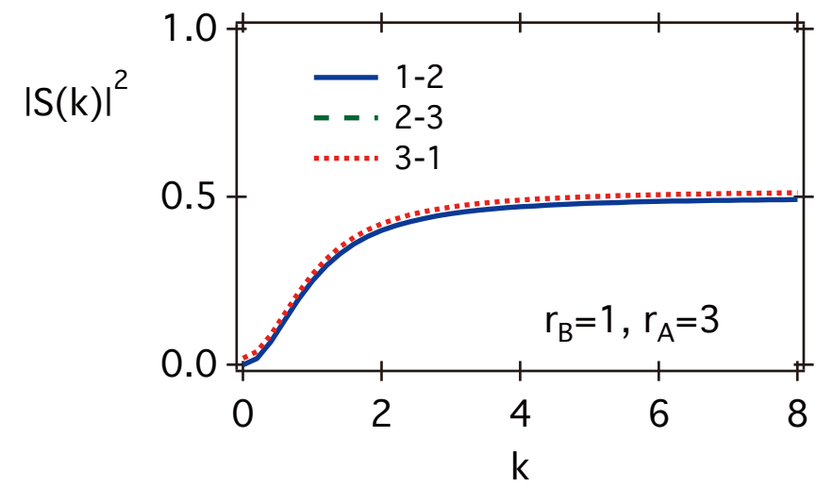
total reflection at $n \longrightarrow \infty$

Delta & delta-prime vertices

- delta connection free + obstacle v : [1/*L*] length scale

$$\psi_1(0) = \psi_2(0) = \ldots = \psi_n(0)$$
$$\psi_1'(0) + \psi_2'(0) + \ldots + \psi_n'(0) = v\,\psi(0)$$

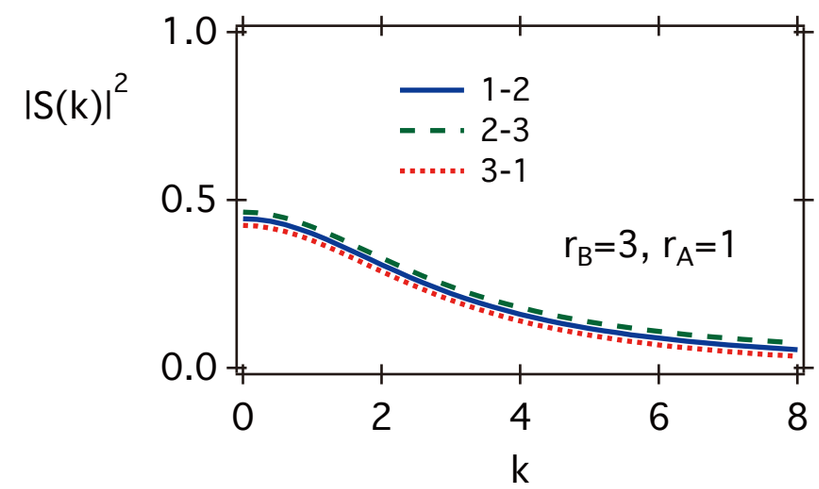
discontinuous ψ' high-pass filter



- delta-prime connection u : [*L*]

$$\psi_1(0) + \psi_2(0) \ldots + \psi_n(0) = u\,\psi'(0)$$
$$\psi_1'(0) = \psi_2'(0) = \ldots = \psi_n'(0)$$

discontinuous ψ low-pass filter



Scale invariant vertices

- Extension of free node with scale invariant parameters
  $\psi_1(0) = 1/t_2\, \psi_2(0) = \ldots = 1/t_n\, \psi_n(0)$
  $\psi_1'(0) + t_2\, \psi_2'(0) + \ldots + t_n\, \psi_n'(0) = 0$

  Branching ratio controlled by $|t_n|^2$

  —> k-independent scattering (Fulop & Tsutsui '00)

- Their "dual" partners
  $\psi_1(0) + t_2\, \psi_2(0) + \ldots + t_n\, \psi_n(0) = 0$
  $\psi_1'(0) = 1/t_2\, \psi_2'(0) = \ldots = 1/t_n\, \psi_n'(0)$

- Mixed types ($\{1,..,m\}$ $\{m+1,..,n\}$) also exist (m=1,...,n)

General vertex

- General KS connection condition rewritten with two numbers {*m*, *m*'} as

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} S & 0 \\ -T^\dagger & I^{(n-m)} \end{pmatrix} \Psi$$

or

$$\begin{pmatrix} \underline{S} & 0 \\ -\underline{T}^\dagger & I^{(n-m')} \end{pmatrix} \Psi' = \begin{pmatrix} I^{(m')} & \underline{T} \\ 0 & 0 \end{pmatrix} \Psi$$

S : delta [1/*L*]

$\underline{S}$: delta-prime [*L*]

T , $\underline{T}$: FT param [1]

- *T* : *m* x (*n*-*m*) complex, *S* : *m* x *m* Hermitian
  $\underline{T}$: *m*' x (*n*-*m*') complex, $\underline{S}$: *m*' x *m*' Hermitian

- *m* + *m*' = *n* + *s* ; *s* = rank(*S*) = rank($\underline{S}$)

Known vertices in ST form

- delta : $\{m=1, m'=n\}$

$$\begin{pmatrix} 1 & 1 & \cdots & 1 \\ 0 & 0 & \cdots & 0 \\ \vdots & & \ddots & \\ 0 & 0 & \cdots & 0 \end{pmatrix} \Psi' = \begin{pmatrix} s & 0 & \cdots & 0 \\ -1 & 1 & & 0 \\ \vdots & & \ddots & \vdots \\ -1 & 0 & \cdots & 1 \end{pmatrix} \Psi$$

- delta-prime : $\{m=1, m'=n\}$

$$\begin{pmatrix} \underline{s} & 0 & \cdots & 0 \\ -1 & 1 & & 0 \\ \vdots & & \ddots & \vdots \\ -1 & 0 & \cdots & 1 \end{pmatrix} \Psi' = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 0 & 0 & \cdots & 0 \\ \vdots & & \ddots & \\ 0 & 0 & \cdots & 0 \end{pmatrix} \Psi$$

S, $\underline{S}$: coupling strength

T, $\underline{T}$: FT parameter

- FT $\{m=1, m'=n\text{-}1\}$

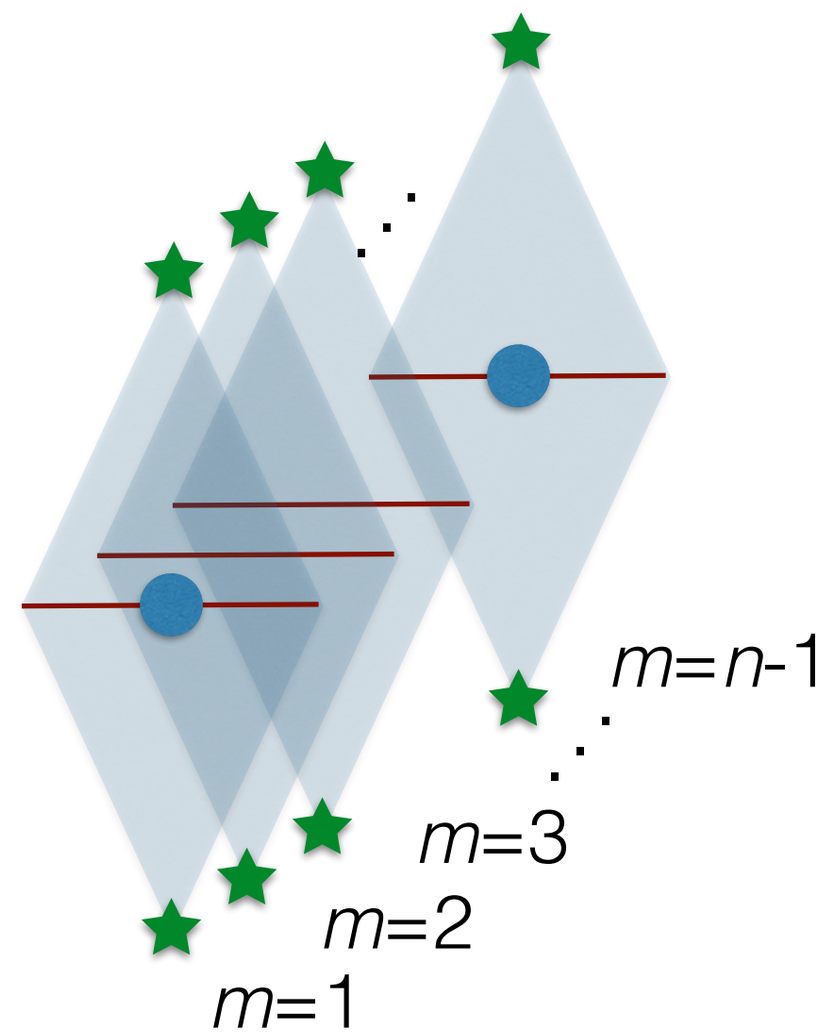
$$\begin{pmatrix} 1 & t_2 & \cdots & t_n \\ 0 & 0 & \cdots & 0 \\ \vdots & & \ddots & \\ 0 & 0 & \cdots & 0 \end{pmatrix} \Psi' = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ -t_1^* & 1 & & 0 \\ \vdots & & \ddots & \vdots \\ -t_n^* & 0 & \cdots & 1 \end{pmatrix} \Psi$$

FT $\{m=2, m'=n\text{-}2\}$

$$\begin{pmatrix} 1 & 0 & t_{13} & \cdots & t_{1n} \\ 0 & 1 & t_{23} & \cdots & t_{2n} \\ 0 & & 0 & & 0 \\ \vdots & & & \ddots & \\ 0 & & \cdots & & 0 \end{pmatrix} \Psi' = \begin{pmatrix} 0 & 0 & \cdots & & 0 \\ 0 & 0 & & & \\ -t_{13}^* & -t_{23}^* & 1 & & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ -t_{1n}^* & -t_{2n}^* & 0 & \cdots & 1 \end{pmatrix} \Psi$$

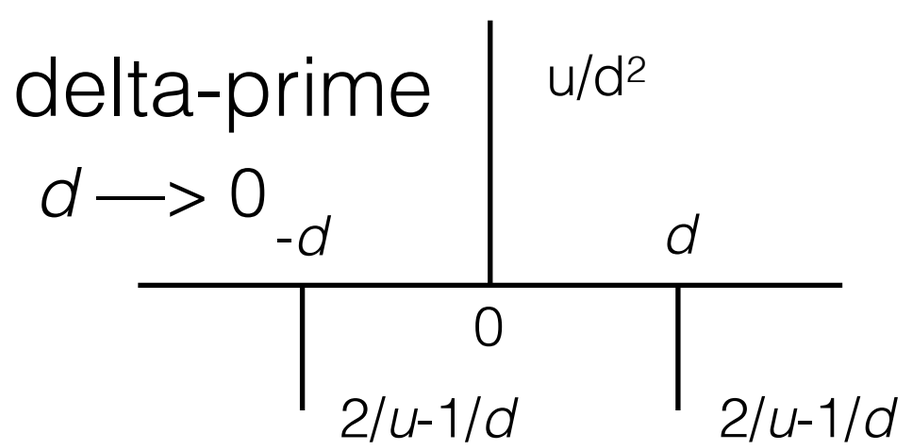
Charting parameter space

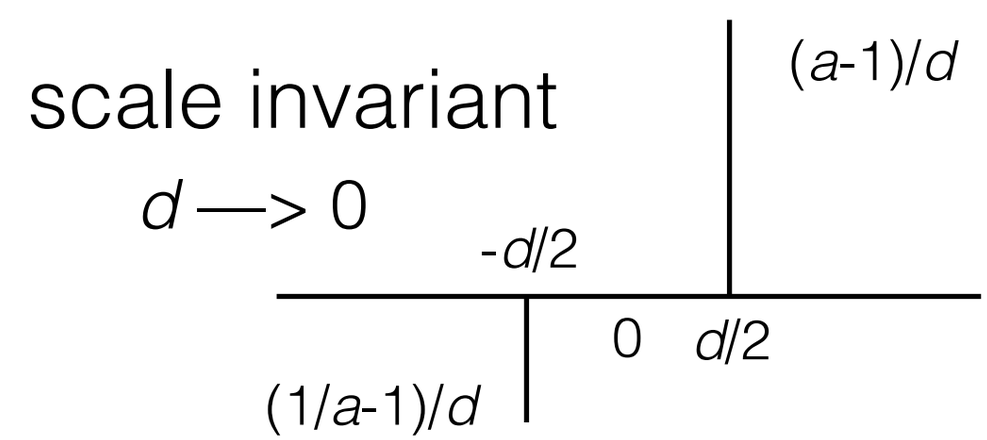
- n^2-dim parameter space divides into $m = 0, \ldots, n$ shells
- Classical scale invariance kept in only special subfamilies
  - scale invariant family
  - disconnected conditions
  - free connection



Dimensional transmutation

- $n = 2$ delta $\psi_+' - \psi_-' = v\,\psi_+ = v\,\psi_-$ $v : [1/L]$
- $n = 2$ delta-prime $\psi_+ - \psi_- = u\,\psi'_+ = u\,\psi'_-$ $u : [L]$
- $n = 2$ scale invariant $\psi_+' = a\,\psi_-'$, $\psi_+ = (1/a)\,\psi_-$ $a : [1]$

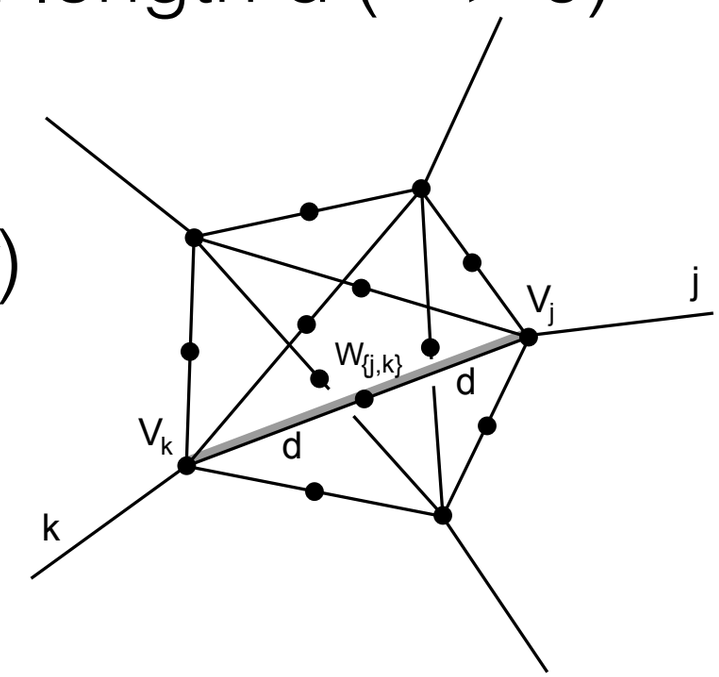




Emergence of scale with strength renormalization

Exotic vertex from deltas

- Finite approximation scheme for general vertex
  - -- cut node, connect all pairs by lines of length d (—> 0)
  - -- n δs [v_j] at new nodes,
  - -- $n(n\text{-}1)/2$ δs[w_{jk}] at the center of (j, k)
  - -- $n(n\text{-}1)/2$ vector potentials [A_{jk}] on (j, k)
  - -- $v_j = \gamma_j + \beta_j/d$, $A_{ij} = \eta/d$, $w_{jk} = \beta_{jk}/d + \eta_{jk}/d^2$



- Norm-resolvent convergence proved
  - $R^{Ap}(k^2)$: resolvent on $L^2(G_d)$;
  - $R(k^2)$: resolvent on $L^2(\ (R_+)^n\ )$
  - $R^E(k^2) = R(k^2) + 0$
  - $\| R^E(k^2) - R^{Ap}(k^2) \| \rightarrow 0+$

$$G_d = (\mathbb{R}^+)^n \oplus (0,d)^{\frac{n(n-1)}{2}}$$

$n + 2\, n(n\text{-}1)/2 = n^2$

Inverse scattering

- Scale invariant vertex $\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} 0 & 0 \\ -T^\dagger & I^{(n-m)} \end{pmatrix} \Psi$ yields

  Hermite & unitary $\mathcal{S} = -I^{(n)} + 2 \begin{pmatrix} I^{(m)} \\ T^\dagger \end{pmatrix} \left(I^{(m)} + TT^\dagger \right)^{-1} \begin{pmatrix} I^{(m)} & T \end{pmatrix}$

- Any Hermite & unitary matrix S with rank(S+I(n))=m

$$\mathcal{S} + I^{(n)} = \begin{pmatrix} I^{(m)} \\ T^\dagger \end{pmatrix} M \begin{pmatrix} I^{(m)} & T \end{pmatrix}$$

$$(\mathcal{S} + I^{(n)})^2 = 2(\mathcal{S} + I^{(n)})$$

$$M = 2(I^{(m)} + TT^\dagger)^{-1}$$

- Inverse problem through diagonalization

$$\mathcal{S} = X_m^{-1} Z_m X_m \qquad X_m = \begin{pmatrix} I^{(m)} & T \\ T^\dagger & -I^{(n-m)} \end{pmatrix} \; Z_m = \begin{pmatrix} I^{(m)} & 0 \\ 0 & -I^{(n-m)} \end{pmatrix}$$

Equitransmitting S-matrix

- Design quantum graph with given (Hermit & unitary) *S*
- Consider Hermitian unitary matrix of the form

$$\mathcal{S} = \frac{1}{N}\begin{pmatrix} \pm d & e^{\mathrm{i}\phi_{12}} & \cdots & e^{\mathrm{i}\phi_{1n}} \\ e^{\mathrm{i}\phi_{21}} & \pm d & \cdots & e^{\mathrm{i}\phi_{1n}} \\ \vdots & & \ddots & \vdots \\ e^{\mathrm{i}\phi_{n1}} & \cdots & & \pm d \end{pmatrix}$$

- Also consider *S* with real elements
- What is the maximum & minimum value of *d*?
  -- largest (darkest) : *d*=n/2-1
  -- known brightest : *d*=1 (*n*=4,8,12...) , *d*=0 (*n*=2,6,10...)

Most reflective case

- largest value *d*=*n*/2-1 free connection *m*=1

$$\mathcal{S}(k) = \begin{pmatrix} \frac{2}{n} - 1 & \cdots & \frac{2}{n} \\ \vdots & \ddots & \vdots \\ \frac{2}{n} & \cdots & \frac{2}{n} - 1 \end{pmatrix} \longrightarrow T = \begin{pmatrix} 1 & \cdots & 1 \end{pmatrix}$$

- free' connection *m*=*n*-1

$$\mathcal{S}(k) = \begin{pmatrix} 1 - \frac{2}{n} & \cdots & -\frac{2}{n} \\ \vdots & \ddots & \vdots \\ -\frac{2}{n} & \cdots & 1 - \frac{2}{n} \end{pmatrix} \longrightarrow T = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}$$

- third case *m*=*n*/2

$$\mathcal{S}(k) = \begin{pmatrix} 1 - \frac{2}{n} & \cdots & -\frac{2}{n} & \frac{2}{n} & \cdots & \frac{2}{n} \\ \vdots & \ddots & & \vdots & & \vdots \\ -\frac{2}{n} & & 1 - \frac{2}{n} & \frac{2}{n} & \cdots & \frac{2}{n} \\ \frac{n}{2} & & \frac{n}{2} & -1 + \frac{n}{2} & \cdots & \frac{2}{n} \\ \vdots & & \vdots & & \ddots & \vdots \\ \frac{2}{n} & \cdots & \frac{2}{n} & & \cdots & -1 + \frac{2}{n} \end{pmatrix} \longrightarrow T = \frac{2}{n} \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & & \vdots \\ 1 & \cdots & 1 \end{pmatrix}$$

Hadamard & Conference

- Reflectionless & equiscattering quantum graphs with real S matrix elements

$$\mathcal{S} = \frac{1}{\sqrt{5}} \begin{pmatrix} 0 & -1 & -1 & -1 & 1 & 1 \\ -1 & 0 & -1 & 1 & -1 & 1 \\ -1 & -1 & 0 & 1 & 1 & -1 \\ -1 & 1 & 1 & 0 & 1 & 1 \\ 1 & -1 & 1 & 1 & 0 & 1 \\ 1 & 1 & -1 & 1 & 1 & 0 \end{pmatrix}$$

Hadamard matrix: n=4, 8, 12, 16,...

$$T = \frac{1}{\sigma + 1} \begin{pmatrix} \sigma & 1 & 1 & 1 \\ 1 & \sigma & 1 & 1 \\ 1 & 1 & \sigma & 1 \\ 1 & 1 & 1 & \sigma \end{pmatrix}$$

$\sigma = \sqrt{2} - 1$ Silver mean

$\gamma = (\sqrt{5} - 1)/2$ Golden mean

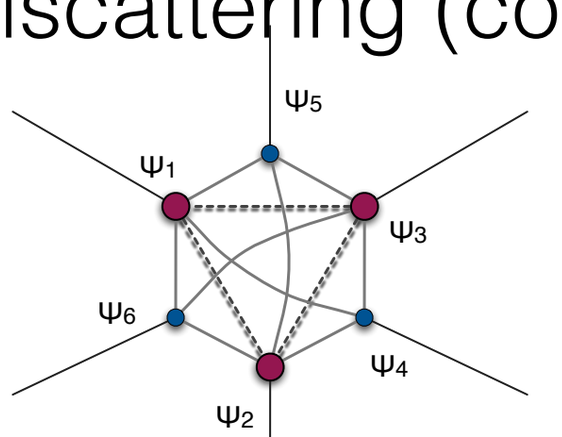
$$T = \begin{pmatrix} 1 & 1+\gamma & 1+\gamma \\ 1+\gamma & 1 & 1+\gamma \\ 1+\gamma & 1+\gamma & 1 \end{pmatrix}$$

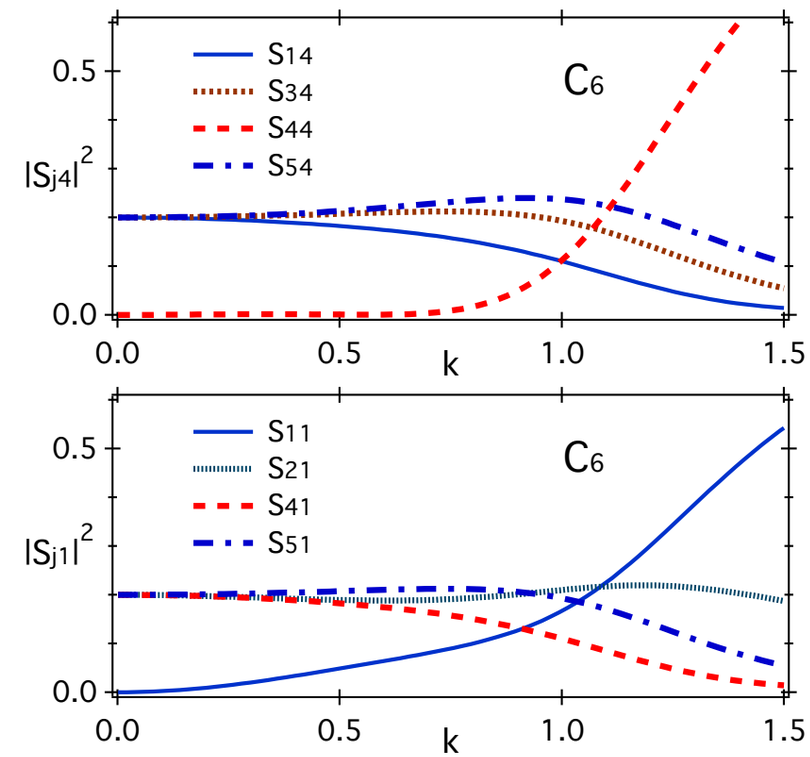
Conference matrix: n=6, 10, 14, 18,...

$$\mathcal{S} = \frac{1}{\sqrt{8}} \begin{pmatrix} 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 \end{pmatrix}$$

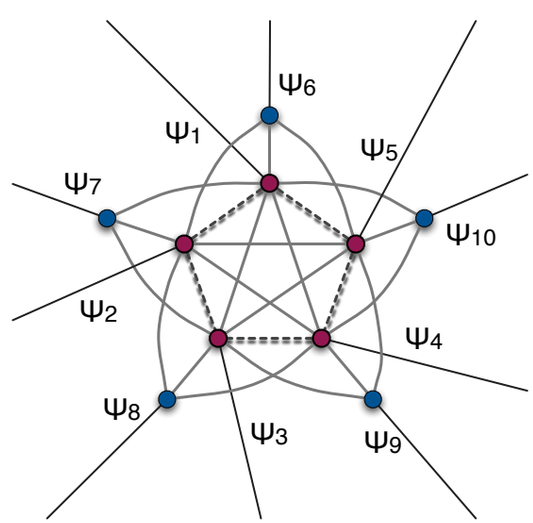
Finite construction

- *n*=6 reflectionless and equiscattering (conference)

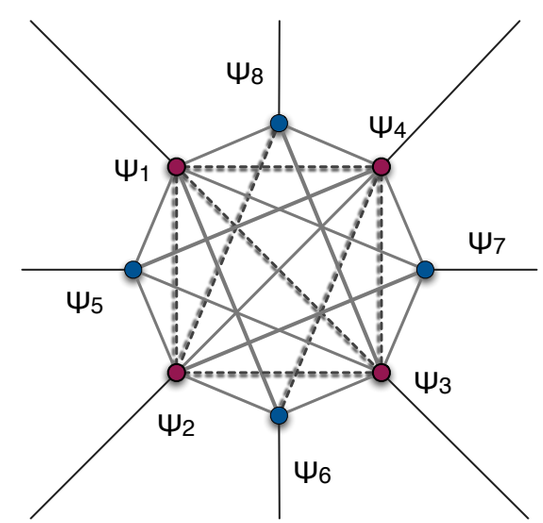




- *n*=10 conference



n=8 equiscattering (Hadamard)



Some examples

- n=6

$$F_6 = \begin{pmatrix} 2 & -1 & -1 & 1 & 1 & 1 \\ -1 & 2 & -1 & 1 & 1 & 1 \\ -1 & -1 & 2 & 1 & 1 & 1 \\ 1 & 1 & 1 & -2 & 1 & 1 \\ 1 & 1 & 1 & 1 & -2 & 1 \\ 1 & 1 & 1 & 1 & 1 & -2 \end{pmatrix} \qquad H_6 = \begin{pmatrix} 1 & -1 & -1 & i & 1 & 1 \\ -1 & 1 & -1 & 1 & i & 1 \\ -1 & -1 & 1 & 1 & 1 & i \\ -i & 1 & 1 & -1 & 1 & 1 \\ 1 & -i & 1 & 1 & -1 & 1 \\ 1 & 1 & -i & 1 & 1 & -1 \end{pmatrix} \qquad C_6 = \begin{pmatrix} 0 & -1 & -1 & -1 & 1 & 1 \\ -1 & 0 & -1 & 1 & -1 & 1 \\ -1 & -1 & 0 & 1 & 1 & -1 \\ -1 & 1 & 1 & 0 & 1 & 1 \\ 1 & -1 & 1 & 1 & 0 & 1 \\ 1 & 1 & -1 & 1 & 1 & 0 \end{pmatrix}$$

- n=8

$$\begin{pmatrix} A & B \\ B^\dagger & -A \end{pmatrix}$$

$$\begin{pmatrix} 3 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & 3 & -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & -1 & 3 & -1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 3 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -3 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & -3 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & -3 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & -3 \end{pmatrix} \begin{pmatrix} 1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ -1 & -1 & 1 & -1 & 1 & 1 & -1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 & 1 & 1 & 1 & -1 \end{pmatrix} \begin{pmatrix} 0 & -i & i & -i & i & -i & i & -i \\ i & 0 & i & i & i & i & i & i \\ -i & -i & 0 & i & -i & -i & i & i \\ i & -i & -i & 0 & i & -i & -i & i \\ -i & -i & i & -i & 0 & i & -i & i \\ i & -i & i & i & -i & 0 & -i & -i \\ -i & -i & -i & i & i & i & 0 & -i \\ i & -i & -i & -i & -i & i & i & 0 \end{pmatrix}$$

Further example

- n=10

$$\begin{pmatrix} 4 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ -1 & 4 & -1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & 4 & -1 & -1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 4 & -1 & 1 & 1 & 1 & 1 & 1 \\ -1 & -1 & -1 & -1 & 4 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & -4 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & -4 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & -4 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -4 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & -4 \end{pmatrix} \qquad \begin{pmatrix} 2 & -1 & -1 & -1 & -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & 2 & -1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 \\ -1 & -1 & 2 & -1 & -1 & 1 & 1 & -1 & 1 & 1 \\ -1 & -1 & -1 & 2 & -1 & 1 & 1 & 1 & -1 & 1 \\ -1 & -1 & -1 & -1 & 2 & 1 & 1 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 & 1 & -2 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & 1 & 1 & -2 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & 1 & 1 & 1 & -2 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & -2 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & -2 \end{pmatrix}$$

$$\begin{pmatrix} 1 & -1 & -1 & -1 & -1 & -1 & i & -i & -i & i \\ -1 & 1 & -1 & -1 & -1 & i & -1 & -i & i & -i \\ -1 & -1 & 1 & -1 & -1 & -i & -i & -1 & i & i \\ -1 & -1 & -1 & 1 & -1 & -i & i & i & -1 & -i \\ -1 & -1 & -1 & -1 & 1 & i & -i & i & -i & -1 \\ -1 & -i & i & i & -i & -1 & 1 & 1 & 1 & 1 \\ -i & -1 & i & -i & i & 1 & -1 & 1 & 1 & 1 \\ i & i & -1 & -i & -i & 1 & 1 & -1 & 1 & 1 \\ i & -i & -i & -1 & i & 1 & 1 & 1 & -1 & 1 \\ -i & i & -i & i & -1 & 1 & 1 & 1 & 1 & -1 \end{pmatrix} \qquad \begin{pmatrix} 0 & -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 & 1 \\ -1 & 0 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & 0 & -1 & -1 & 1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 0 & 1 & 1 & 1 & 1 & -1 & 1 \\ -1 & 1 & -1 & 1 & 0 & 1 & 1 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 & 1 & 0 & 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & 1 & 1 & 1 & 0 & -1 & 1 & -1 \\ 1 & 1 & -1 & 1 & 1 & -1 & -1 & 0 & 1 & 1 \\ 1 & 1 & 1 & -1 & 1 & -1 & 1 & 1 & 0 & -1 \\ 1 & 1 & 1 & 1 & -1 & 1 & -1 & 1 & -1 & 0 \end{pmatrix}$$

Hadamard conjecture+

- What type of equiscatt. & reflectionless graphs exist?

$$\mathcal{S} = \frac{1}{n}\begin{pmatrix} d & e^{\mathrm{i}\phi_{12}} & \cdots & e^{\mathrm{i}\phi_{1n}} \\ e^{\mathrm{i}\phi_{21}} & d & \cdots & e^{\mathrm{i}\phi_{1n}} \\ \vdots & & \ddots & \vdots \\ e^{\mathrm{i}\phi_{n-11}} & \cdots & -d & e^{\mathrm{i}\phi_{n-1n}} \\ e^{\mathrm{i}\phi_{n1}} & \cdots & e^{\mathrm{i}\phi_{nn-1}} & -d \end{pmatrix}$$

what *n* for INTEGER *d* with real *S* ?

possible *d* ?—> [0, *n*/2-1]

—> *d* = n/2-1 free connection

—> *d* = 1 equiscattering : Hadamard matrix

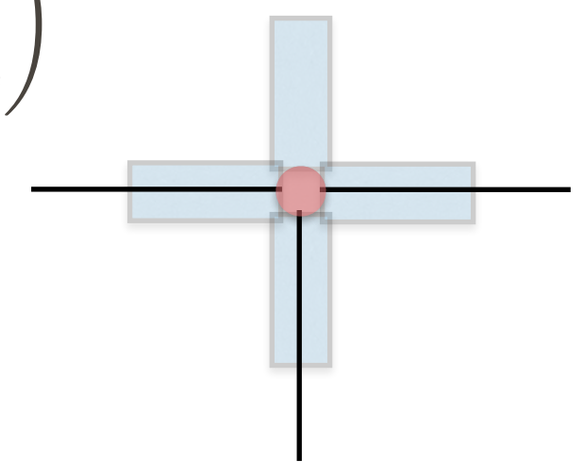
—> *d* = 0 no reflection : conference matrix

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} 0 & 0 \\ -T^\dagger & I^{(n-m)} \end{pmatrix} \Psi$$

Counter intuitive coupling

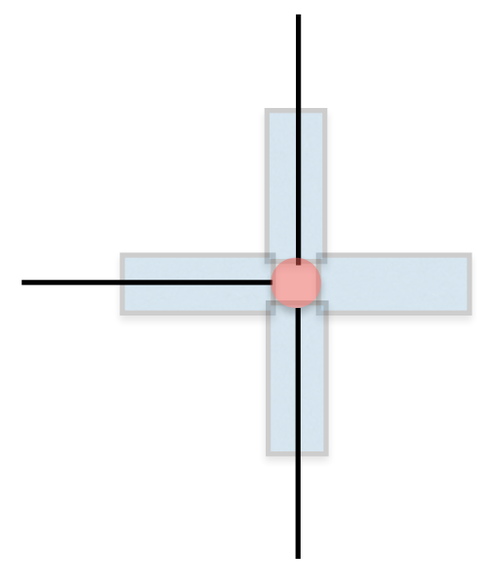
- Scale invariant n=4 graph with $T = \begin{pmatrix} a & a \\ a & -a \end{pmatrix}$

$$\mathcal{S} = \begin{pmatrix} \frac{1-2a^2}{1+2a^2} & 0 & \frac{2a}{1+2a^2} & \frac{2a}{1+2a^2} \\ 0 & \frac{1-2a^2}{1+2a^2} & \frac{2a}{1+2a^2} & -\frac{2a}{1+2a^2} \\ \frac{2a}{1+2a^2} & \frac{2a}{1+2a^2} & -\frac{1-2a^2}{1+2a^2} & 0 \\ \frac{2a}{1+2a^2} & -\frac{2a}{1+2a^2} & 0 & -\frac{1-2a^2}{1+2a^2} \end{pmatrix}$$



- In particular, with $a = \frac{1}{\sqrt{2}}$

$$\mathcal{S} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & -1 \\ 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{pmatrix}$$



pair-wise equiscattering
with no reflection

$\psi_1(0) + \psi_2(0) = 1/a\ \psi_3(0)$
$\psi_1(0) - \psi_2(0) = 1/a\ \psi_4(0)$
$\psi_1'(0) + a\,\psi_3'(0) + a\,\psi_4'(0) = 0$
$\psi_1'(0) + a\,\psi_3'(0) - a\,\psi_4'(0) = 0$

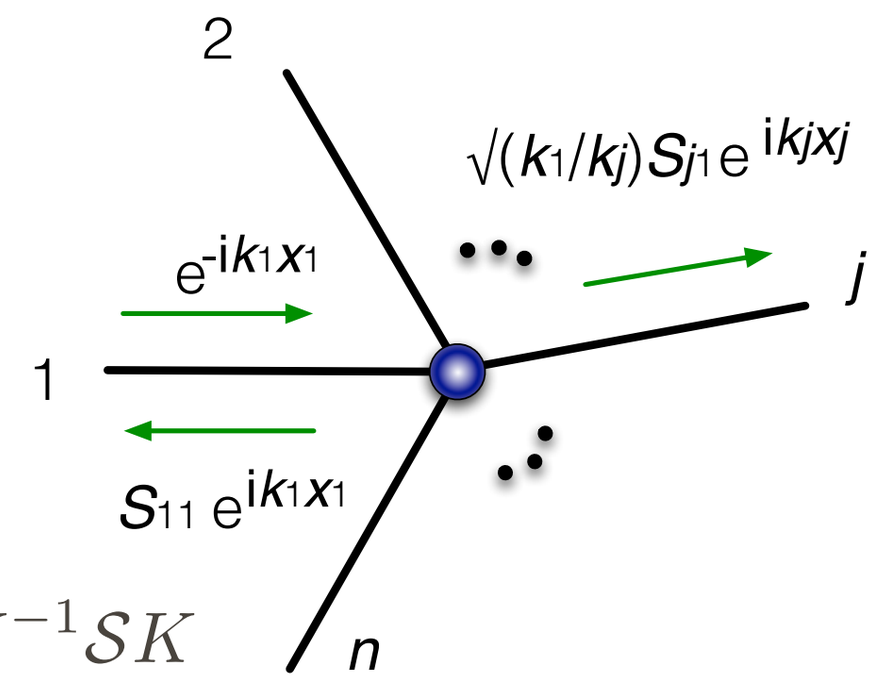
Potentials on lines

- Potential U_j on line j

$$k_j = \sqrt{k^2 - U_j}$$

$$\psi_i^{(j)}(x) = e^{-\mathrm{i}k_j x} + \mathcal{S}_{jj} e^{\mathrm{i}k_j x} \qquad \text{for } i = j$$

$$= \qquad \mathcal{S}_{ij}\sqrt{\frac{k_j}{k_i}} e^{\mathrm{i}k_i x} \qquad \text{for } i \neq j$$



- Define $K = \{\sqrt{k_i}\delta_{ij}\}$

  $A\,\psi + B\,\psi' = 0$

$$(\Psi^{(1)} \dots \Psi^{(n)}) = I^{(n)} + K^{-1}\mathcal{S}K$$

$$(\Psi'^{(1)} \dots \Psi'^{(n)}) = \mathrm{i}K^2 + \mathrm{i}K\mathcal{S}K$$

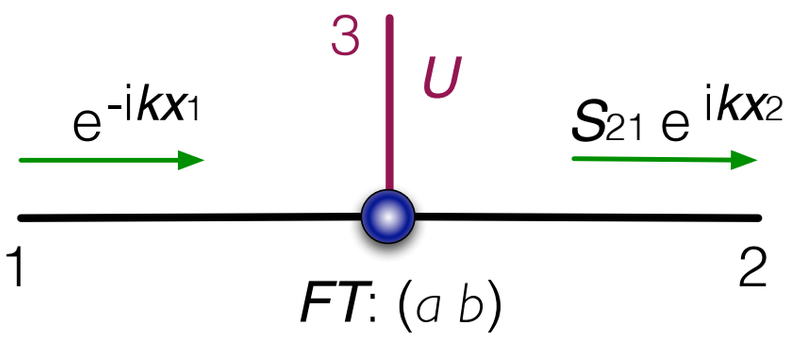
- Scattering matrix

$$\mathcal{S} = -(AK^{-1} + \mathrm{i}BK)^{-1}(AK^{-1} - \mathrm{i}BK)$$

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} 0 & 0 \\ -T^\dagger & I^{(n-m)} \end{pmatrix} \Psi$$

Threshold resonance

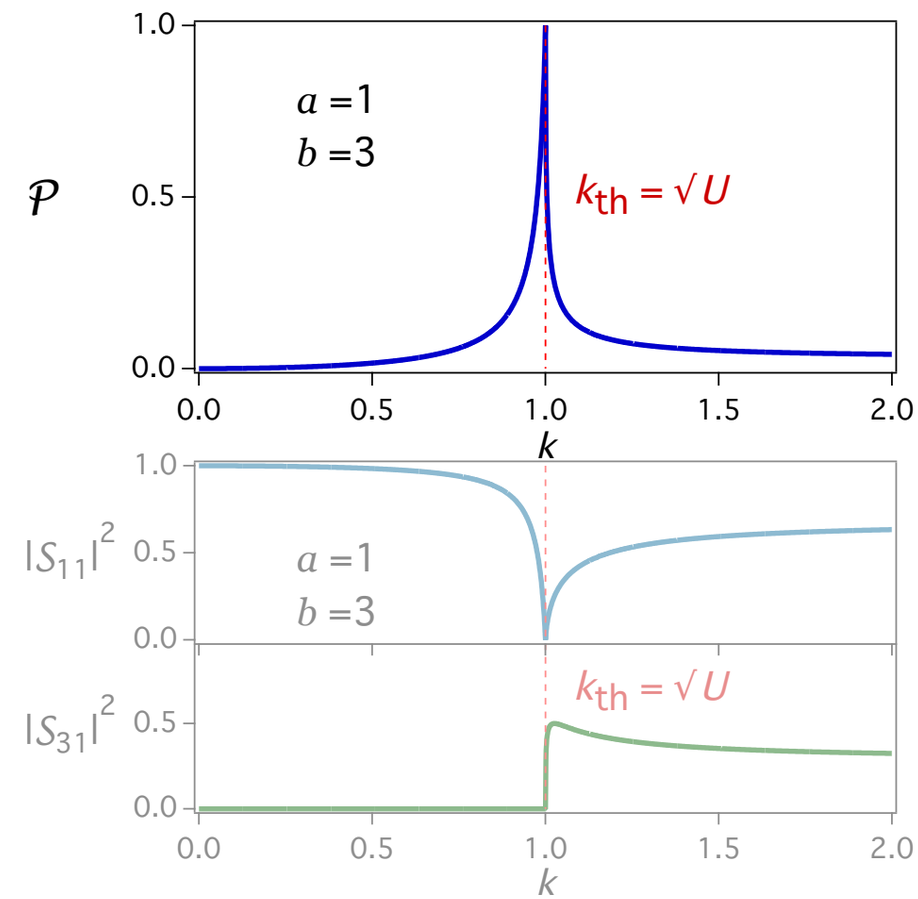
- N=3 Graph node $T = \begin{pmatrix} a & b \end{pmatrix}$ with external field U



- 1–> 2 transmission $P = |S_{21}|^2$

$$\mathcal{S}_{21}(k;U) = \frac{2a}{1 + a^2 + b^2\sqrt{1 - \frac{U}{k^2}}}$$

- $b >> a \geq 1$:
threshold resonance at $k_{th}=\sqrt{U}$



U-controlled monochromatic filtering

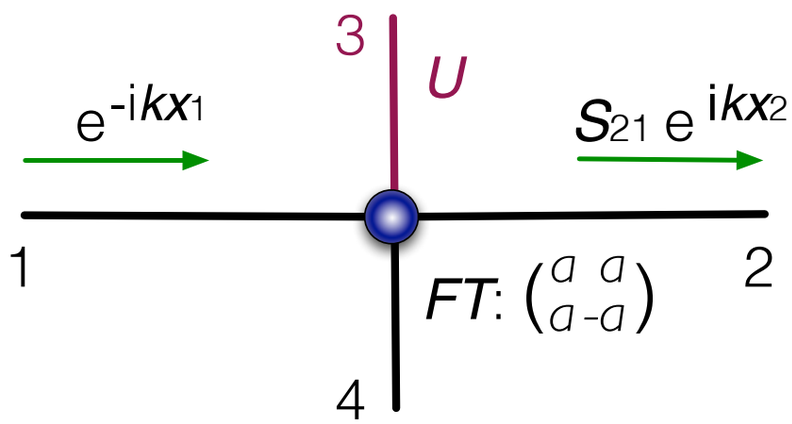
$$k_{\rm pol} = \frac{b^2}{\sqrt{b^4 - (1+a^2)^2}}\sqrt{U}$$

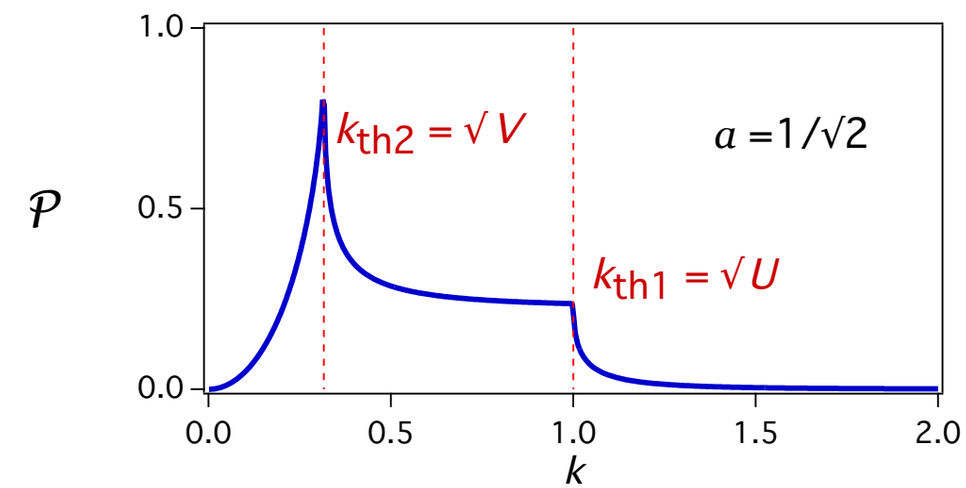
pole on unphysical surface

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} 0 & 0 \\ -T^\dagger & I^{(n-m)} \end{pmatrix} \Psi$$

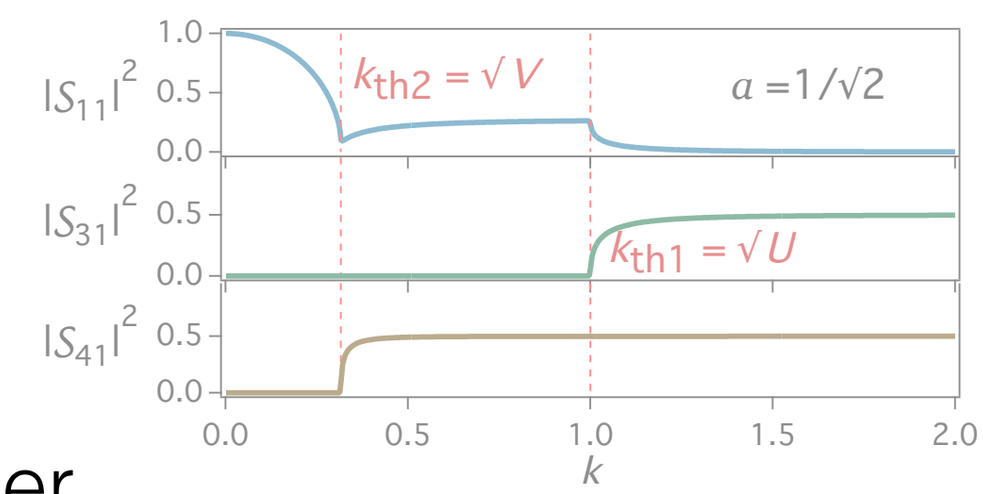
Controllable band filter

- N=4 Graph node $T = \begin{pmatrix} a & a \\ a & -a \end{pmatrix}$ with external field U, V





- 1–>2 transmission $P = |S_{21}|^2$
  Interference of 2 resonances

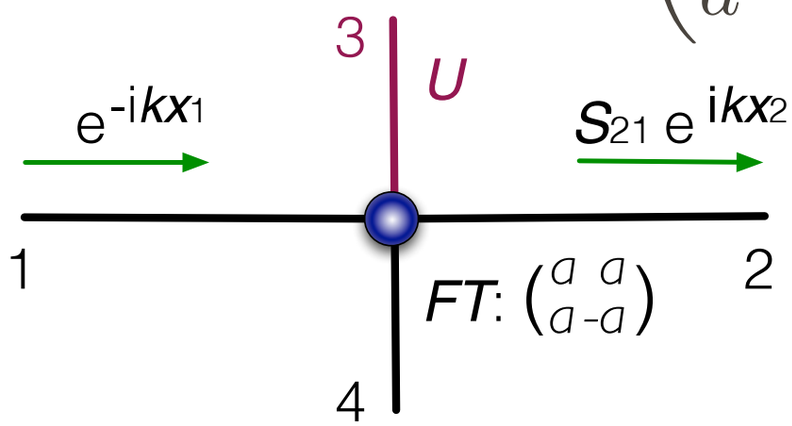


- No transm. when $V = U$
  $k^{(1)}_{th}=\sqrt{U}$, $k^{(2)}_{th}=\sqrt{V}$
  –» $[\sqrt{U}, \sqrt{V}]$ Band Filter

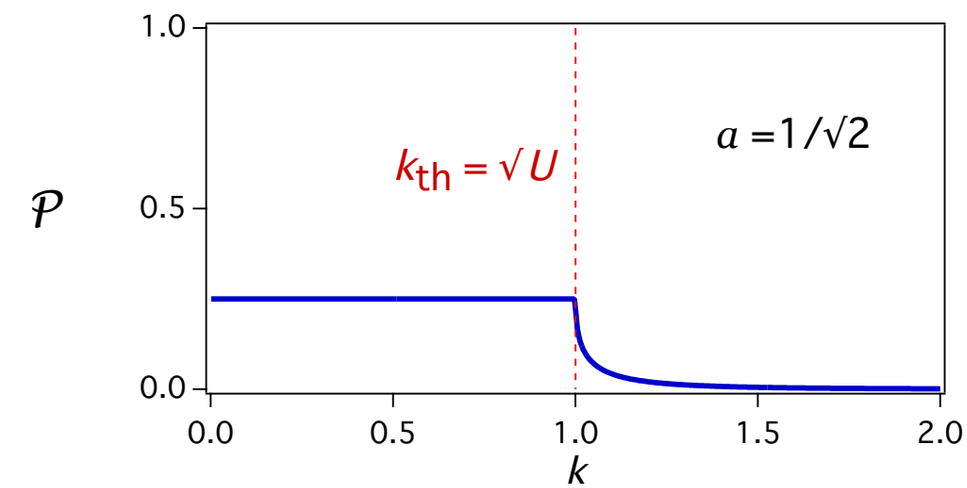
$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} 0 & 0 \\ -T^\dagger & I^{(n-m)} \end{pmatrix} \Psi$$

Controllable flat filter

- Graph node $T = \begin{pmatrix} a & a \\ a & -a \end{pmatrix}$ with external field U

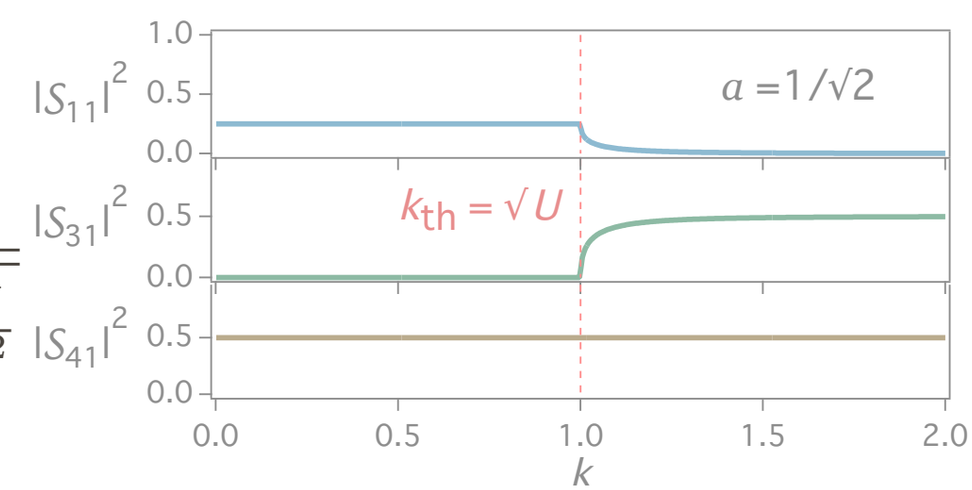


$$a = \frac{1}{\sqrt{2}}$$



- 1–>2 transmission $P = |S_{21}|^2$

$$\mathcal{S}_{21}(k;U) = \frac{2a^2\left(1-\sqrt{1-\frac{U}{k^2}}\right)}{(1+2a^2)+2a^2(1+2a^2)\sqrt{1-\frac{U}{k^2}}}$$

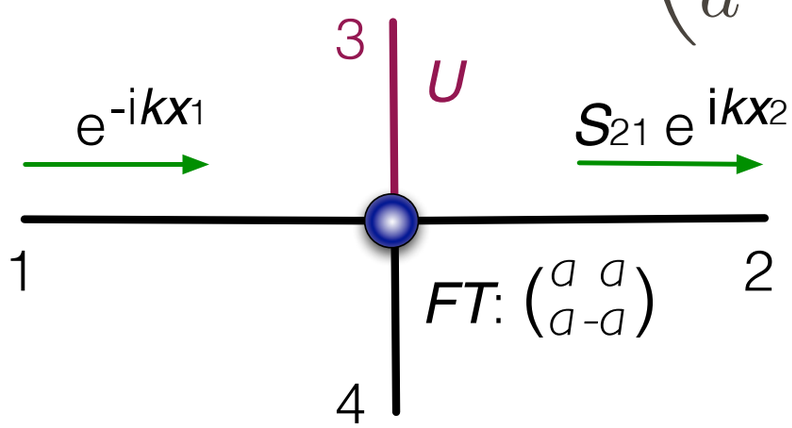


- [0,√U] flat band-filter

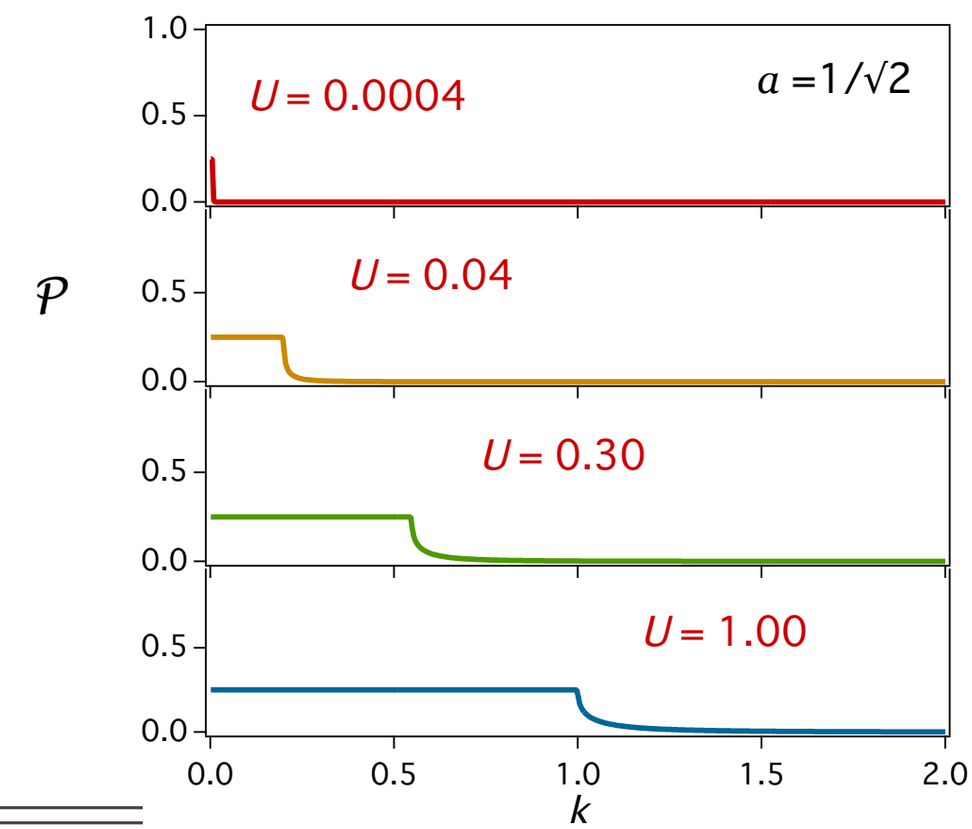
$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} 0 & 0 \\ -T^\dagger & I^{(n-m)} \end{pmatrix} \Psi$$

Controllable flat filter

- Graph node $T = \begin{pmatrix} a & a \\ a & -a \end{pmatrix}$ with external field U



$$a = \frac{1}{\sqrt{2}}$$

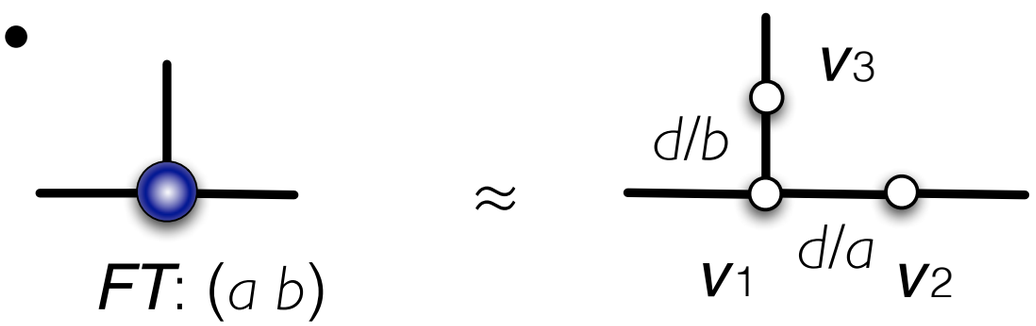


- 1–>2 transmission $P = |S_{21}|^2$

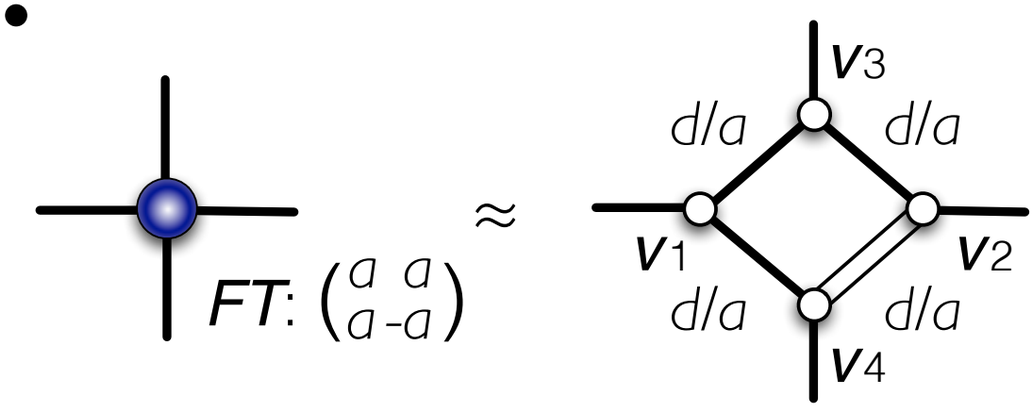
$$\mathcal{S}_{21}(k;U) = \frac{2a^2\left(1-\sqrt{1-\frac{U}{k^2}}\right)}{(1+2a^2)+2a^2(1+2a^2)\sqrt{1-\frac{U}{k^2}}}$$

- $[0,\sqrt{U}]$ flat band-filter

Finite graph realization

- Exotic vertex from delta vertices (+magnetic field)
- 

$$v_1 = [a(a-1) + b(b-1)]/d$$
$$v_2 = (1-a)/d$$
$$v_3 = (1-b)/d$$

- 

$$v_1 = v_2 = 2a(a-1)/d$$
$$v_3 = v_4 = (1-2a)/d$$

∗ No 1-»2 (interference) U=0

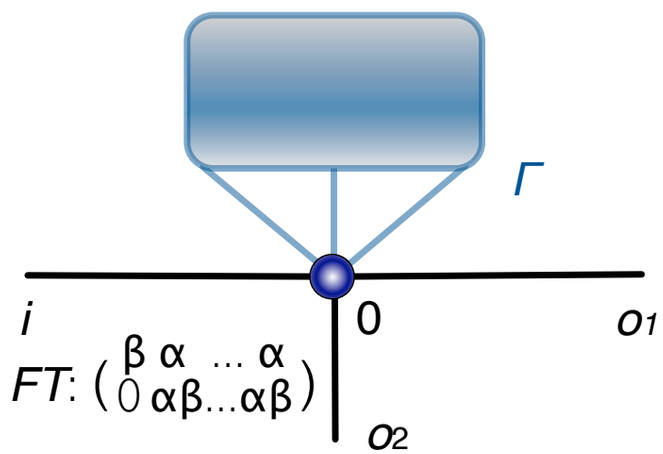
∗ No 1-»3 with added U > E

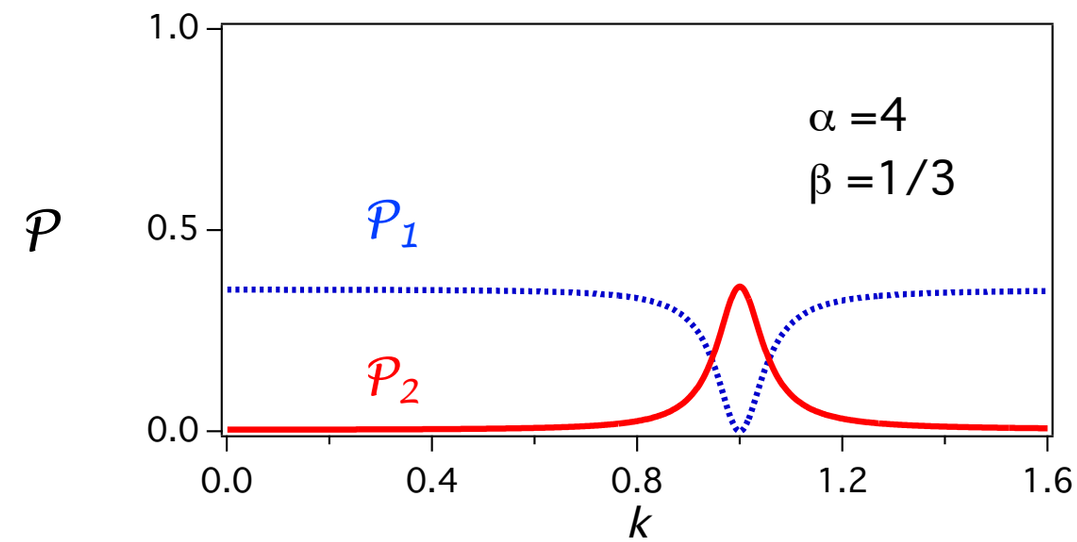
⟶ flux pushed to 1–>2

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} 0 & 0 \\ -T^\dagger & I^{(n-m)} \end{pmatrix} \Psi$$

Generalizations

- Generalized monochromatic spectral filter



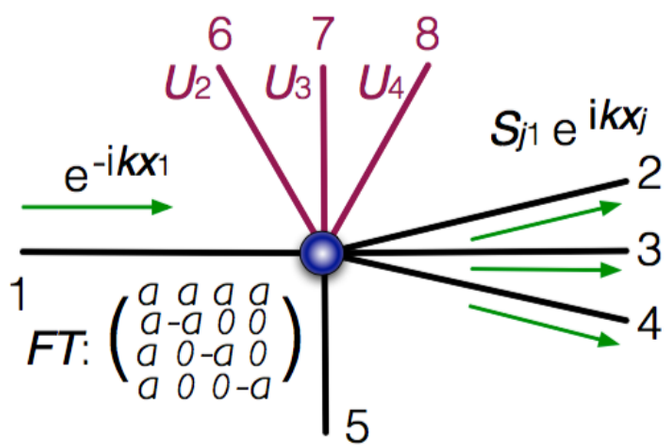


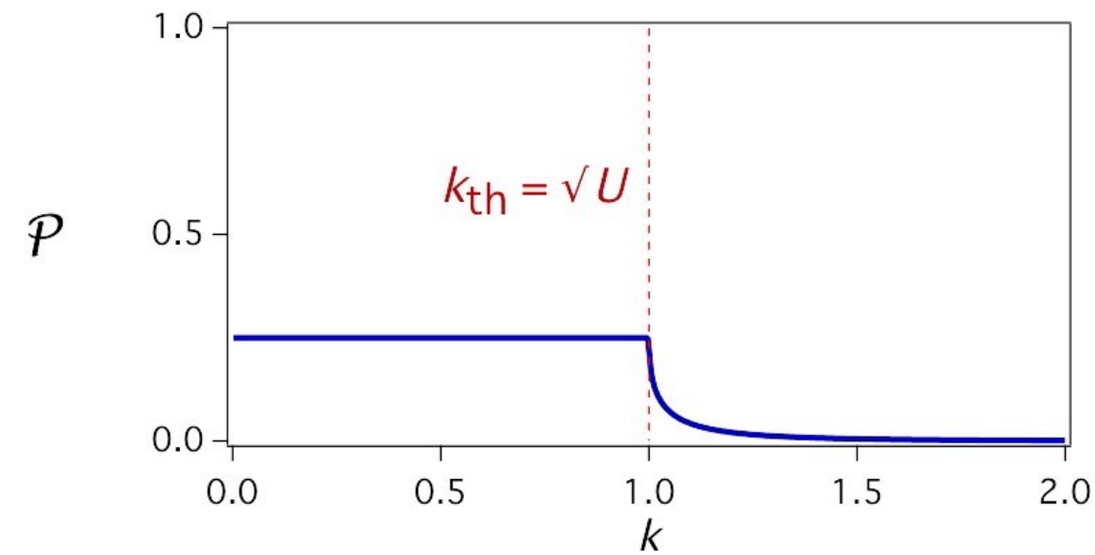
$$\begin{pmatrix} 1 & 0 & \beta & \alpha & \cdots & \alpha \\ 0 & 1 & 0 & \alpha\beta & \cdots & \alpha\beta \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ \vdots & & & & & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix} \begin{pmatrix} -\psi'_-(0) \\ \psi'_1(0) \\ \psi'_2(0) \\ \phi'_1(0) \\ \vdots \\ \phi'_n(0) \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ -\beta & 0 & 1 & 0 & \cdots & 0 \\ -\alpha & -\alpha\beta & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \ddots & \\ -\alpha & -\alpha\beta & 0 & 0 & \cdots & 1 \end{pmatrix} \begin{pmatrix} \psi_-(0) \\ \psi_1(0) \\ \psi_2(0) \\ \phi_1(0) \\ \vdots \\ \phi_n(0) \end{pmatrix}$$

$$\begin{pmatrix} I^{(m)} & T \\ 0 & 0 \end{pmatrix} \Psi' = \begin{pmatrix} 0 & 0 \\ -T^\dagger & I^{(n-m)} \end{pmatrix} \Psi$$

Generalizations

- Generalized flat-band spectral filter





only obtainable when "free *S*" has maximal # of zeros:

[Theorem] Maximal # of 0 for Hermitian & unitary matrix

$= (n\text{-}2)^2$ for odd n

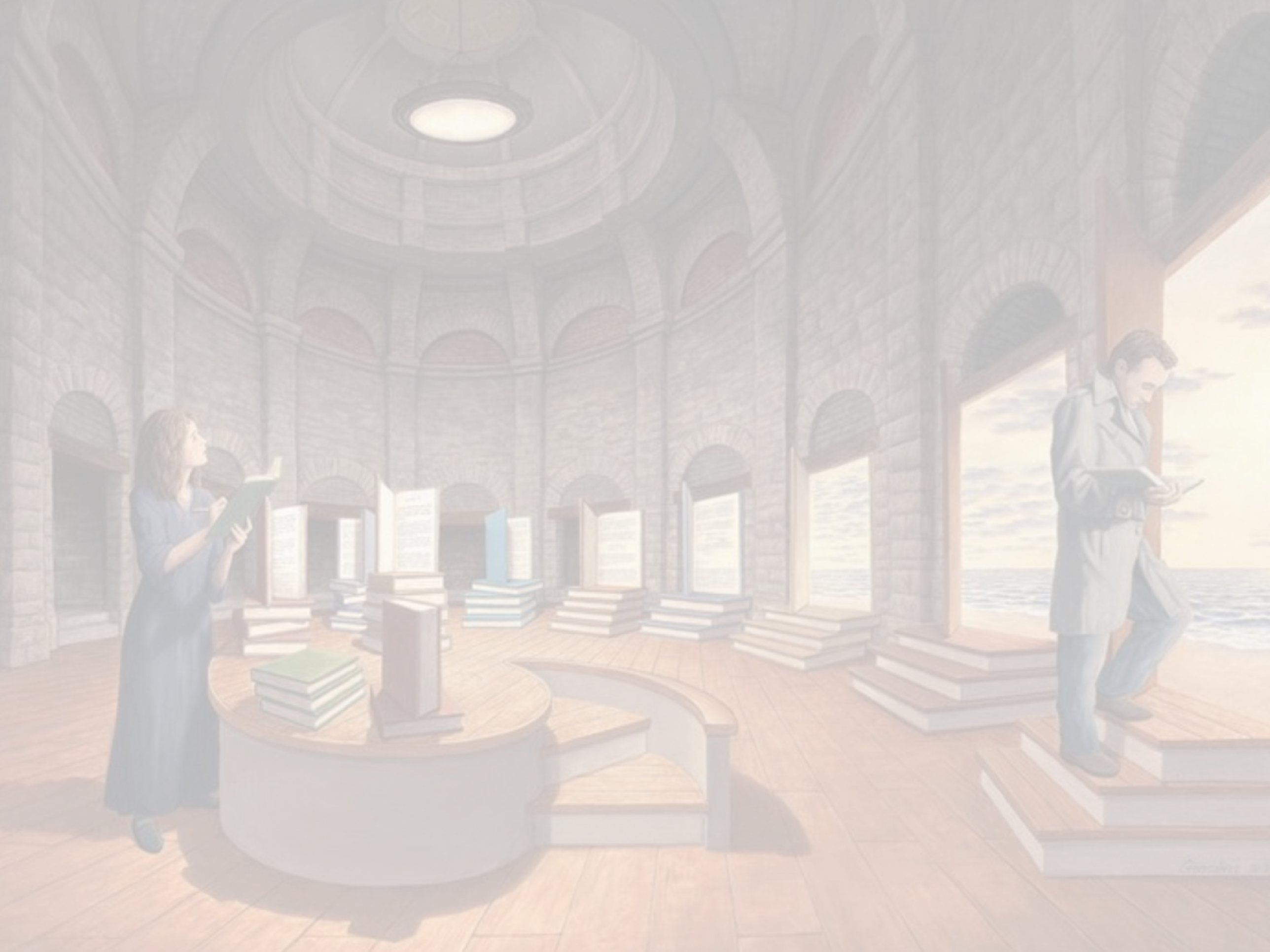
$= (n\text{-}2)^2+4$ for even n

Summary (2)

- Quantum graph vertices studied in detail
  --- exploration of n^2-parameter space
  --- physical realization of exotic quantum vertex

- Graph vertex with filtering properties discovered
  — controllable monochromatic spectral filter
  — controllable flat-band spectral filter

- Some useful classification of Hermitian & unitary matrices obtained



1D Coulomb problem

- With $\hbar = 1$, $e = k = m = 1$, 1D coulomb problem is

$$\psi''(x) + \left(\frac{1}{4} - \frac{\alpha}{|x|}\right)\psi(x) = 0$$

where $\alpha = \dfrac{1}{\sqrt{-2E}}$, $z = \dfrac{2}{\alpha}x$

convergent at $z \to \infty$

divergent at $z \to \infty$

- Solutions are given by Whittaker $W_{\alpha,\frac{1}{2}}(z)$, $M_{\alpha,\frac{1}{2}}(z)$:

$$\psi(z) = [\sin\Omega\Theta(-x) + \cos\Omega\Theta(x)]W_{\alpha,\frac{1}{2}}(z)$$

$\psi'(z)$ divegent at $z = 0$

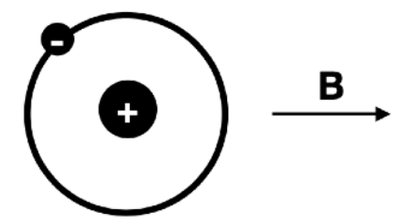
- Loudon (1982): Make $W_{\alpha,\frac{1}{2}}(0) = 0 \;\rightarrow \alpha = 1,2,3,...$

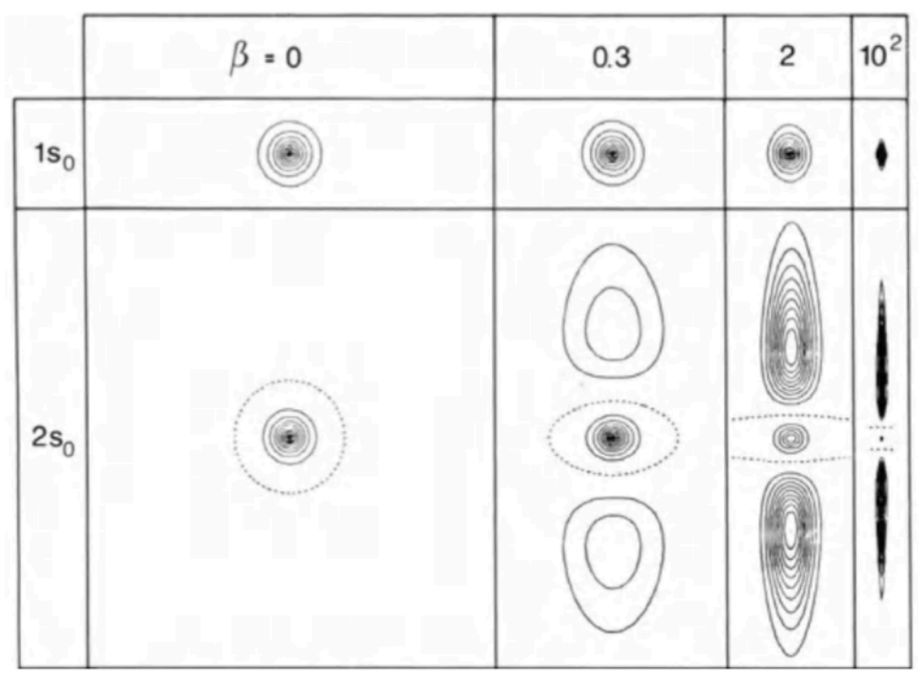
Rydberg spectra

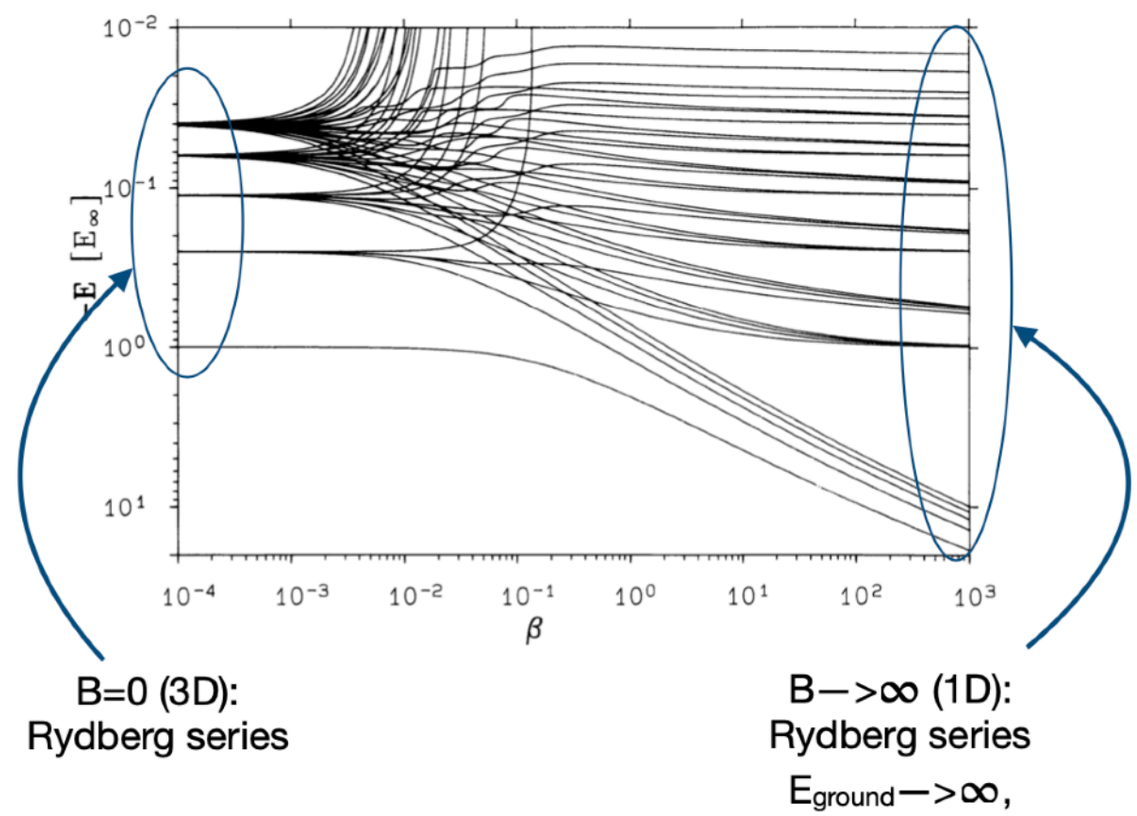
But different conditions kept being proposed since then..

1D Coulomb problem

- Hydrogen atom under magnetic field







- other occurence: nanowire, impurity CNT, superfluid surface e

1D Coulomb problem

- More general condition should exist other than arbitrary prescription $\psi(0) = 0$

- Self-adjoint extension of $H = -\frac{1}{2}\frac{d^2}{dx^2} - \frac{1}{|x|}$

  $\psi^*(0_-)\psi'(0_-) - \psi'^*(0_-)\psi(0_-) = \psi^*(0_+)\psi'(0_+) - \psi'^*(0_+)\psi(0_+)$

  cannot be used because of divergence

- Go back to Wronskian!

  $W[\psi^*(0_-), \psi(0_-)] - W[\psi^*(0_+), \psi(0_+)] = 0$

  $W[\phi(x), \psi(x)] = \phi(x)\psi'(x) - \phi'(x)\psi(x)$

1D Coulomb problem

- Auxiliary functions $H\varphi_j = E\varphi_j(x)$, $W[\varphi_1, \varphi_2] = 1$

$$W[\phi^*, \psi] = \begin{vmatrix} \phi^* & \phi'^* \\ \psi & \psi' \end{vmatrix} = \begin{vmatrix} \phi^* & \phi'^* \\ \psi & \psi' \end{vmatrix} \begin{vmatrix} \varphi_1' & \varphi_2' \\ -\varphi_1 & -\varphi_2' \end{vmatrix}$$

$$= W[\phi^*, \varphi_1]W[\psi, \varphi_2] - W[\phi^*, \varphi_2]W[\psi, \varphi_1]$$

- $\Psi_1 = \begin{pmatrix} W[\psi, \varphi_1]_{0+} \\ W[\psi, \varphi_1]_{0-} \end{pmatrix}$, $\Psi_2 = \begin{pmatrix} W[\psi, \varphi_2]_{0+} \\ W[\psi, \varphi_2]_{0-} \end{pmatrix}$

- Choose $\phi_1(x) = \dfrac{\beta}{2} M_{\beta,\frac{1}{2}}\left(\frac{2}{\beta}x\right)(\theta(x) - \theta(-x))$,

  $\phi_2(x) = -\Gamma(1-\beta) W_{\beta,\frac{1}{2}}\left(\frac{2}{\beta}x\right)$ with arbitrary β

1D Coulomb problem

- We find $\Psi_2 - \xi\Psi_1 = 0$
  $$\xi = -\frac{1}{\alpha} + 2\log\alpha - 2F(1-\alpha) + \frac{1}{\beta} + 2\log\beta + 2F(1-\beta)$$

- $W[\psi^*(0_-), \psi(0_-)] - W[\psi^*(0_+), \psi(0_+)] = 0$ is identical to
  $$(U - I)\Psi_2 - (U + I)\Psi_1 = 0, \quad U \in U(2) \quad \text{(4-parameter)}$$

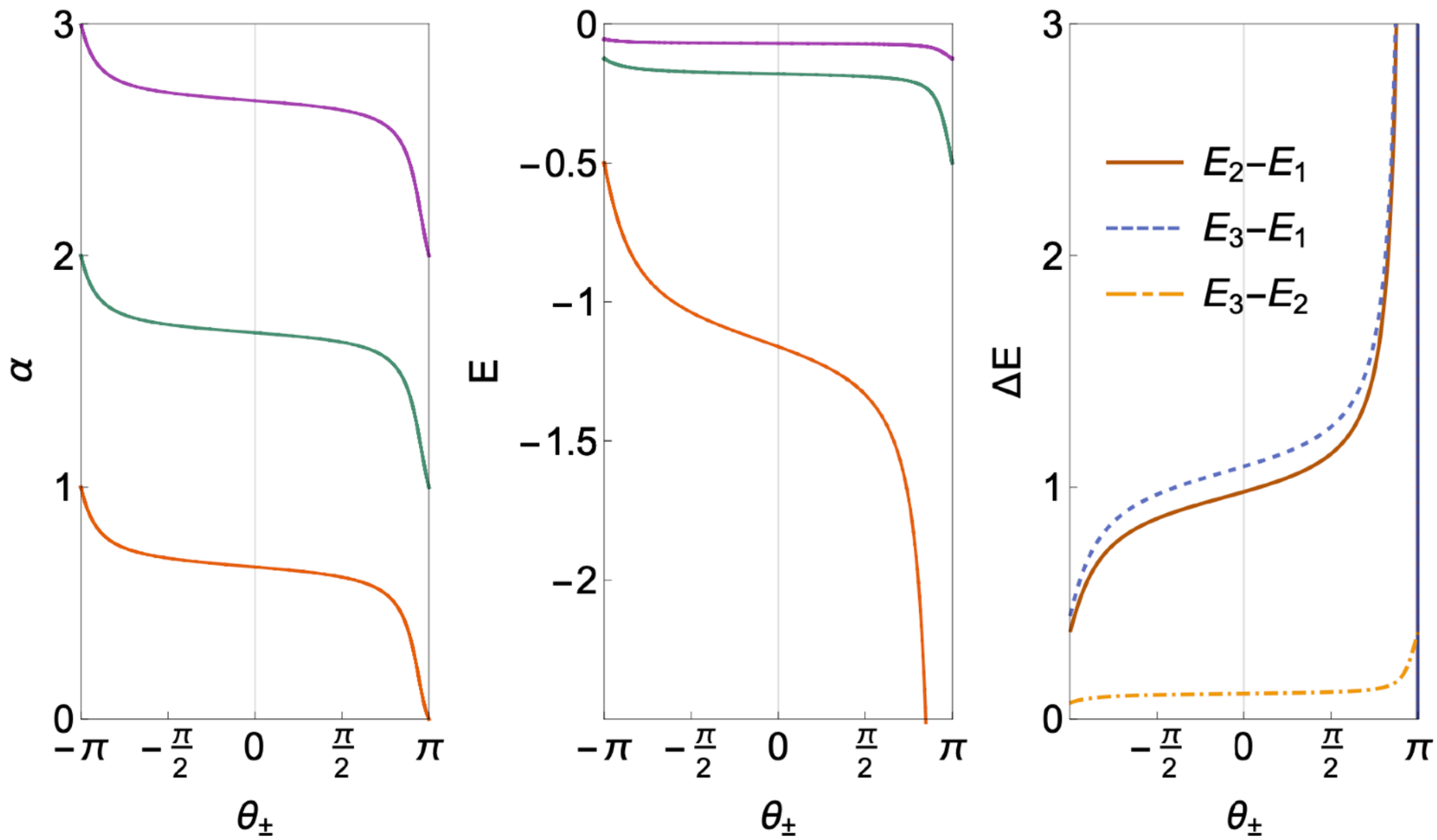
- Diagonalize $U = V^{-1}DV$ with parametrization
  $$D = \begin{pmatrix} e^{-i\theta_+} & 0 \\ 0 & e^{-i\theta_-} \end{pmatrix}, \; V = \begin{pmatrix} e^{i\lambda}\cos(\omega) & \sin(\omega) \\ -\sin(\omega) & e^{-i\lambda}\cos(\omega) \end{pmatrix}$$

1D Coulomb problem

- $\lambda = 0$
  $\omega = \Omega + (1 \mp 1)\frac{\pi}{4}$
  $\tan\left(\frac{\theta_\pm}{2}\right) = -\frac{1}{\alpha} - 2\log\left(\frac{2}{\alpha}\right) - 2F(1-\alpha) - 4\gamma$

- Reversing above, spectra & eigenfunctions obtained
  $(\alpha(\theta_+), \Omega = \omega), \ (\alpha(\theta_2), \Omega = \omega - \frac{\pi}{2})$
  [$\omega = \frac{\pi}{4}$ gives equal L/R weight]
  choice $\frac{1}{\beta} - 2\log(\beta) + 2F(1-\beta) = -4\gamma - 2\log(2)$ made

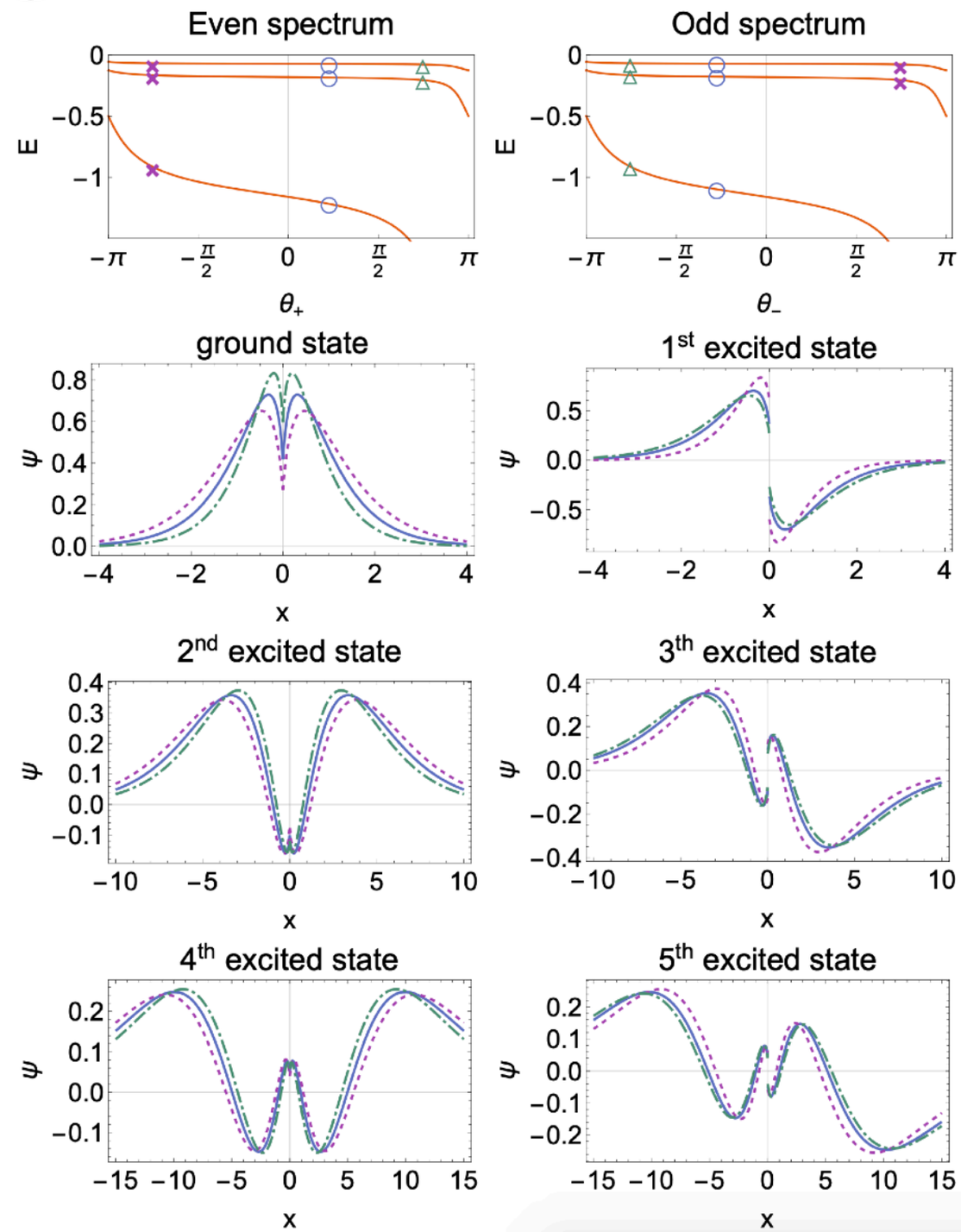
Non-Rydberg spectra



- parameters θ_+ & θ_- determins the spectra

Exotic eigenstates

- Even & odd states awy from Rydberg



○ —— $\tilde{\Omega} = \frac{\pi}{4}, \ \theta_- = -\frac{\pi}{4}, \ \theta_+ = \frac{\pi}{4}$

× ---- $\tilde{\Omega} = \frac{\pi}{4}, \ \theta_- = \frac{3\pi}{4}, \ \theta_+ = -\frac{3\pi}{4}$

▲ —·— $\tilde{\Omega} = \frac{\pi}{4}, \ \theta_- = -\frac{3\pi}{4}, \ \theta_+ = \frac{3\pi}{4}$

Exotic eigenstates

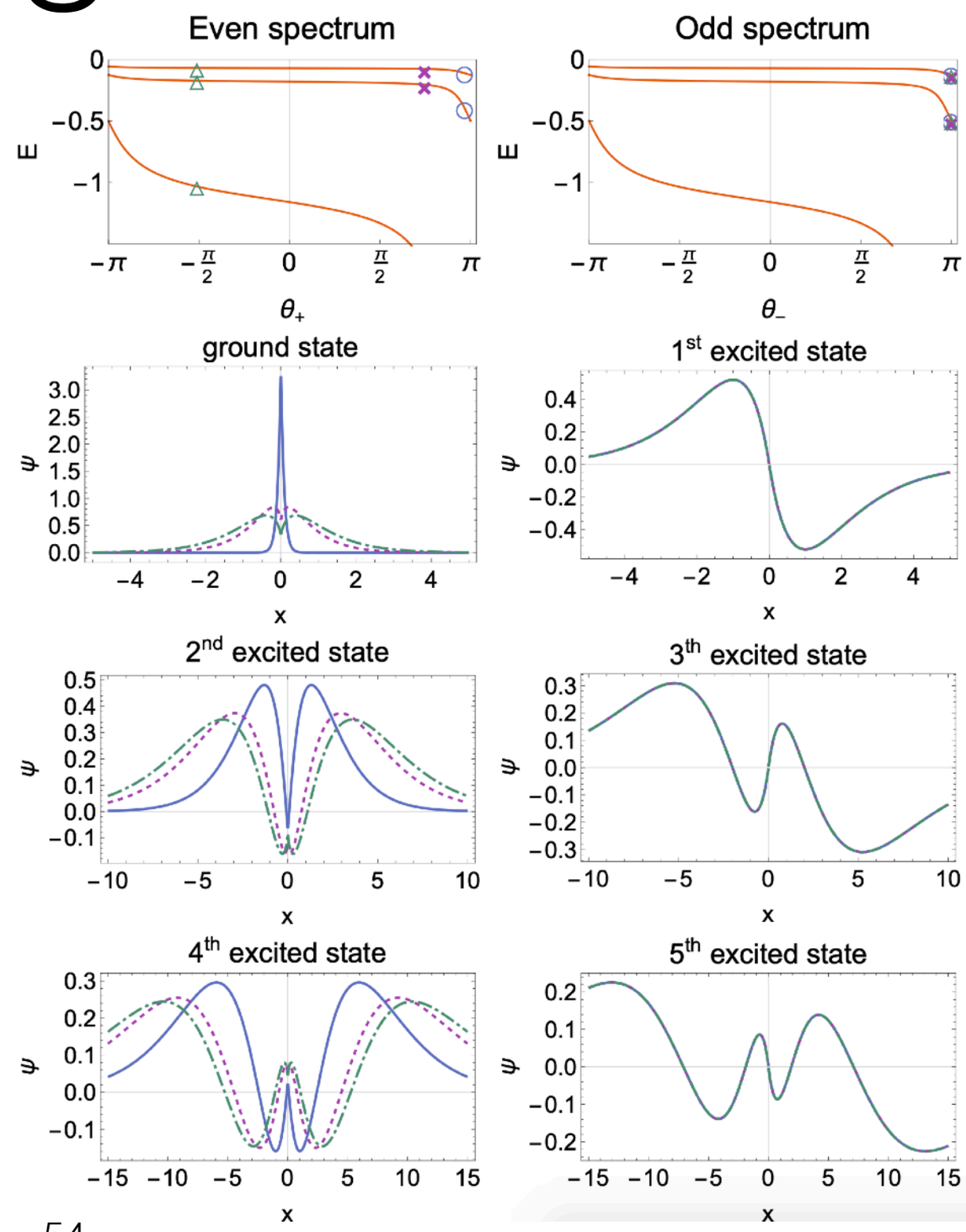
- Even states:
  far away from Rydberg

- Odd states:
  Rydberg

○ —— $\tilde{\Omega} = \frac{\pi}{4},\ \theta_- = \pi,\ \theta_+ = \pi$

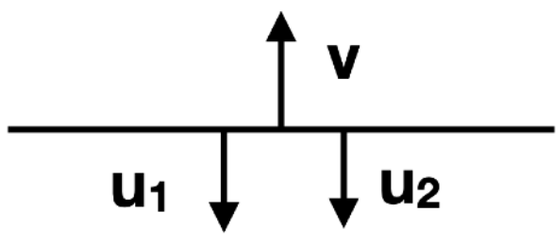
× ---- $\tilde{\Omega} = \frac{\pi}{4},\ \theta_- = \pi,\ \theta_+ = \frac{3\pi}{4}$

△ —·— $\tilde{\Omega} = \frac{\pi}{4},\ \theta_- = \pi,\ \theta_+ = -\frac{\pi}{2}$



Finite construction

- Cut-off coulomb at $-d < x < d$ and place three δs



$$R(\Omega) \equiv \frac{\psi(-d)}{\psi(d)} = \tan(\Omega),$$

$$Q(d,\alpha) \equiv \frac{\psi'(d)}{\psi(d)} = \frac{1}{\alpha} - \frac{\alpha}{d} - \frac{1}{d}\frac{W_{1+\alpha,\frac{1}{2}}(\frac{2d}{\alpha})}{W_{1+\alpha,\frac{1}{2}}(\frac{2d}{\alpha})}$$

$$= -\frac{1}{\alpha} - 2\log\left(\frac{2d}{\alpha}\right) - 2F(1-\alpha) - 4\gamma + \mathcal{O}\left(d\,(\log(d))^2\right).$$

Compare

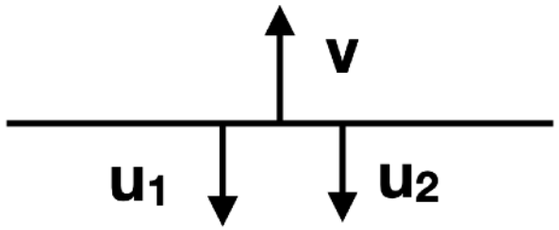
$$R_\pm(\Omega) = \tan\left(\omega + (1 \mp 1)\frac{\pi}{4}\right),$$

$$Q_\pm(d,\alpha) = \tan\left(\frac{\theta_\pm}{2}\right) - 2\log(d).$$

Finite construction

- Cut-off coulomb at $-d < x < d$ and place three δs

$$
\begin{aligned}
u_1 = &-\frac{1}{2\,d} - \log(d) \\
&+ \frac{1}{4}\left(1 + \sin(2\,\omega) + \cos(2\,\omega)\right)\tan\left(\frac{\theta_-}{2}\right) \\
&+ \frac{1}{4}\left(1 - \sin(2\,\omega) - \cos(2\,\omega)\right)\tan\left(\frac{\theta_+}{2}\right), \\
v = &-\frac{1}{d} + \frac{1}{d^2}\,\frac{\csc(2\,\omega)}{\tan\left(\frac{\theta_-}{2}\right) - \tan\left(\frac{\theta_+}{2}\right)}, \\
u_2 = &-\frac{1}{2\,d} - \log(d) \\
&+ \frac{1}{4}\left(1 + \sin(2\,\omega) - \cos(2\,\omega)\right)\tan\left(\frac{\theta_-}{2}\right) \\
&+ \frac{1}{4}\left(1 - \sin(2\,\omega) + \cos(2\,\omega)\right)\tan\left(\frac{\theta_+}{2}\right).
\end{aligned}
$$



Summary (3)

- Full solution of 1D Coulomb problem found
  — three-parameter family of self-adjoint extension
  — determine x=0 behavior & connection cond.
  — non-Rydberg spectra revealed

- One concrete procedure to construct exotic connection condition (in terms of 3 delta) found

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