DYNAMICAL COMPOSITION LAW FOR BOUNDARY CONDITIONS OF A QUANTUM CAVITY

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Work with:

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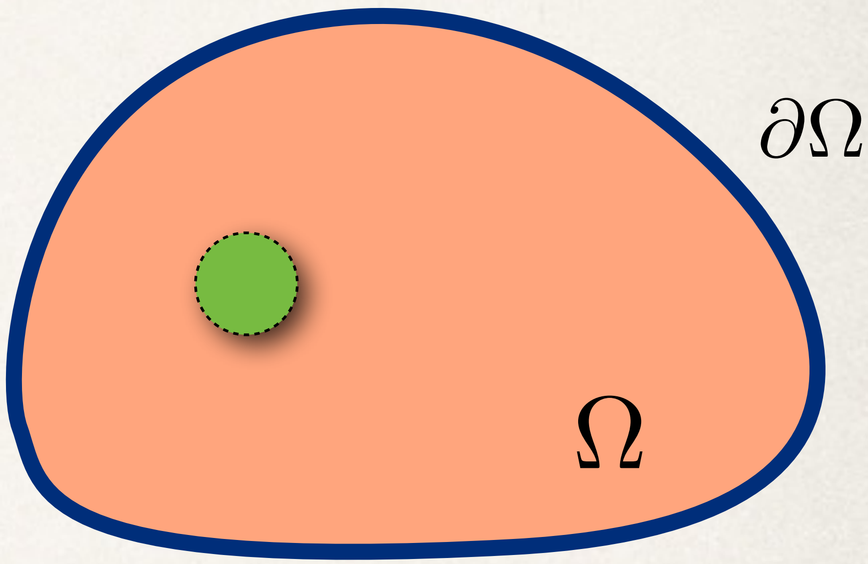
Bari, Napoli, Zaragoza

Policeta - San Rufo, 11 July 2016

Napoli 2002

Outline

- Alternating Boundary Conditions
- Operators vs Quadratic Forms
- Quantum b.c.: A particle on a segment
- Quantum b.c.: A particle in a cavity
- Limit dynamics
- Composition Law of Boundary Conditions



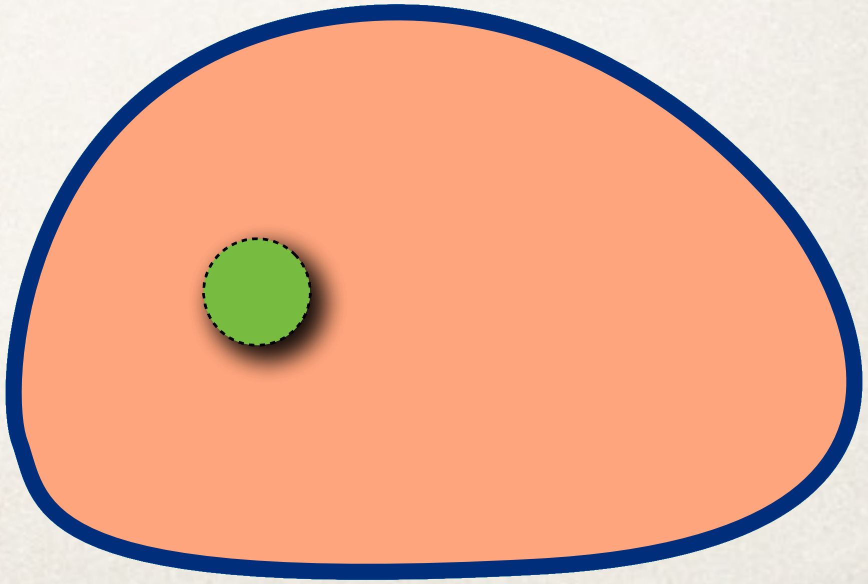
Alternating Boundary Conditions

$$T_1 := T_{U_1} = \frac{p^2}{2m} = -\frac{1}{2m}\Delta_{U_1} \qquad T_2 := T_{U_2} = \frac{p^2}{2m} = -\frac{1}{2m}\Delta_{U_2}$$

$$\underbrace{\left(\mathrm{e}^{-\mathrm{i}tT_1/N}\mathrm{e}^{-\mathrm{i}tT_2/N}\right)\left(\mathrm{e}^{-\mathrm{i}tT_1/N}\mathrm{e}^{-\mathrm{i}tT_2/N}\right)\dots\left(\mathrm{e}^{-\mathrm{i}tT_1/N}\mathrm{e}^{-\mathrm{i}tT_2/N}\right)}_{N\ \text{times}}$$

$$N \to \infty$$

$$\left(\mathrm{e}^{-\mathrm{i}tT_1/N}\mathrm{e}^{-\mathrm{i}tT_2/N}\right)^N \longrightarrow \ ?$$



Product Formulae

Trotter (1959)

Suppose that $C = A + B$ is (essentially) self-adjoint on

$$D(C) = D(A) \cap D(B)$$

then
$$\left(\mathrm{e}^{-\mathrm{i}tA/N}\mathrm{e}^{-\mathrm{i}tB/N}\right)^N \to \mathrm{e}^{-\mathrm{i}tC}$$

Unfortunately, on $D(T_U) \cap D(T_V)$

$T = (T_U + T_V)/2$ has infinite s.a. extensions T_W

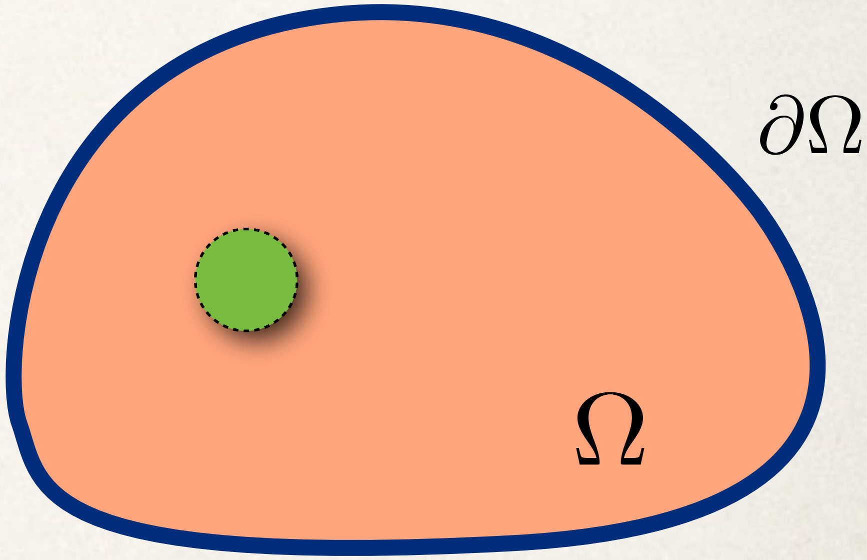
$$\left(\mathrm{e}^{-\mathrm{i}tT_U/N}\mathrm{e}^{-\mathrm{i}tT_V/N}\right)^N \to \mathrm{e}^{-\mathrm{i}2tT_W}$$???

Product Formulae

On $D(T_U) \cap D(T_V)$

$T = (T_U + T_V)/2$ has infinite s.a. extensions T_W

$$\left(\mathrm{e}^{-\mathrm{i}tT_U/N}\mathrm{e}^{-\mathrm{i}tT_V/N}\right)^N \to \mathrm{e}^{-\mathrm{i}2tT_W} \quad ???$$



$\psi|_{\partial\Omega} = 0$ Dirichlet

$\partial_\nu \psi|_{\partial\Omega} = 0$ Neumann

Dirichlet + Neumann $\psi|_{\partial\Omega} = \partial_\nu \psi|_{\partial\Omega} = 0$???

Product Formulae

Consider the expectation value of the kinetic energy

$$t_1(\psi) = \langle \psi \,|T_{U_1} \psi \rangle \qquad t_2(\psi) = \langle \psi \,|T_{U_2} \psi \rangle$$

Quadratic forms

$$D(t_1) \cap D(t_2)$$

dense

$$t_{U_3} := t_3 = \frac{t_1 + t_2}{2}$$

real quadratic form

$$t_3(\psi) = \langle \psi \,|T_{U_3} \psi \rangle \qquad T_{U_3} := T_3 = \frac{(T_1 \dot{+} T_2)}{2}$$

self-adjoint!

Product Formulae

$$T_3 = \frac{(T_1 \dot{+} T_2)}{2}$$

$$\left(\mathrm{e}^{-\mathrm{i}tT_1/N}\mathrm{e}^{-\mathrm{i}tT_2/N}\right)^N \to \mathrm{e}^{-\mathrm{i}2tT_3}$$

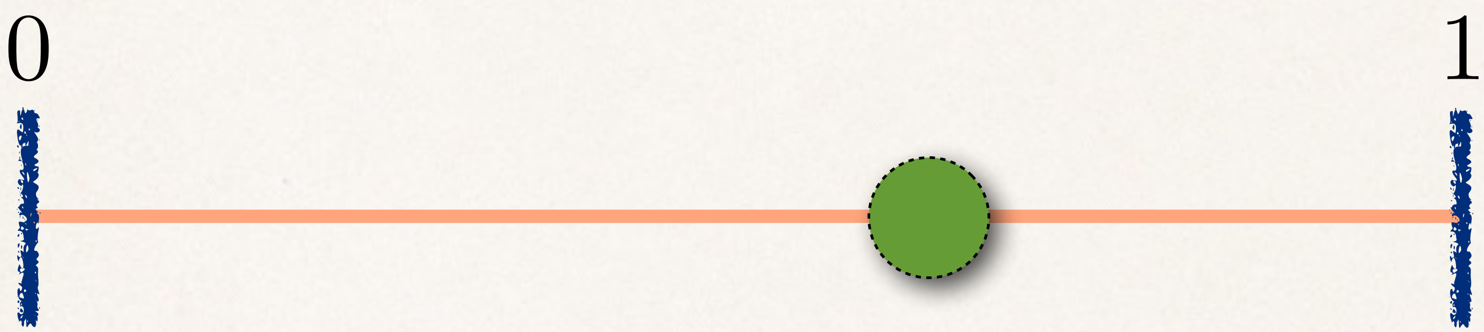
T. Kato (1978)
M.L. Lapidus (1982)

Composition law of boundary conditions

Objective: $$T_3 = \frac{(T_1 \dot{+} T_2)}{2}$$

Need to compute $$\frac{t_1 + t_2}{2}$$

A quantum particle on a segment



test functions
compact support

$$H = T = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

$$D(T) = \mathcal{D}(0,1)$$

What happens at the boundary?

$$D(T^*) = \{\psi \in L^2(0,1), \psi'' \in L^2(0,1)\} = H^2[0,1]$$

Kinetic energy quadratic form

$$t(\psi) = \langle \psi | T\psi \rangle = -\frac{\hbar^2}{2m} \int_0^1 \overline{\psi(x)} \psi''(x) \mathrm{d}x$$

$$= \frac{\hbar^2}{2m} \left(\int_0^1 |\psi'(x)|^2 \mathrm{d}x - \overline{\psi(1)}\psi'(1) + \overline{\psi(0)}\psi'(0) \right)$$

$$= \frac{\hbar^2}{2m} \left(\|\psi'\|^2 + \langle \varphi | \dot{\varphi} \rangle_{\mathbb{C}^2} \right)$$

$$\varphi = \begin{pmatrix} \psi(0) \\ \psi(1) \end{pmatrix} \qquad \dot{\varphi} = \begin{pmatrix} \psi'(0) \\ -\psi'(1) \end{pmatrix}$$

Kinetic energy quadratic form

$$t(\psi) = \frac{\hbar^2}{2m} \left(\|\psi'\|^2 + \langle \varphi | \dot{\varphi} \rangle_{\mathbb{C}^2} \right)$$

Boundary conditions $\quad \mathrm{Im}\, \langle \varphi | \dot{\varphi} \rangle = 0$

$$i\,(I + U)\,\varphi = (I - U)\,\dot{\varphi} \qquad U \in \mathrm{U}(2)$$

Quantum Boundary Conditions
and
Self-adjoint extensions

$$T_U\psi = -\frac{\hbar^2}{2m}\psi'' \qquad\qquad U \in \mathrm{U}(2)$$

$$i\,(I+U)\,\varphi = (I-U)\,\dot{\varphi}$$

$$\varphi = \begin{pmatrix}\psi(0)\\ \psi(1)\end{pmatrix} \qquad\qquad \dot{\varphi} = \begin{pmatrix}\psi'(0)\\ -\psi'(1)\end{pmatrix}$$

M. Asorey, A. Ibort, G. Marmo, Int. J. Mod. Phys. A **20**, 1001 (2005)

Quantum Boundary Conditions
and
Self-adjoint extensions

Self-adjoint extensions

$\updownarrow$

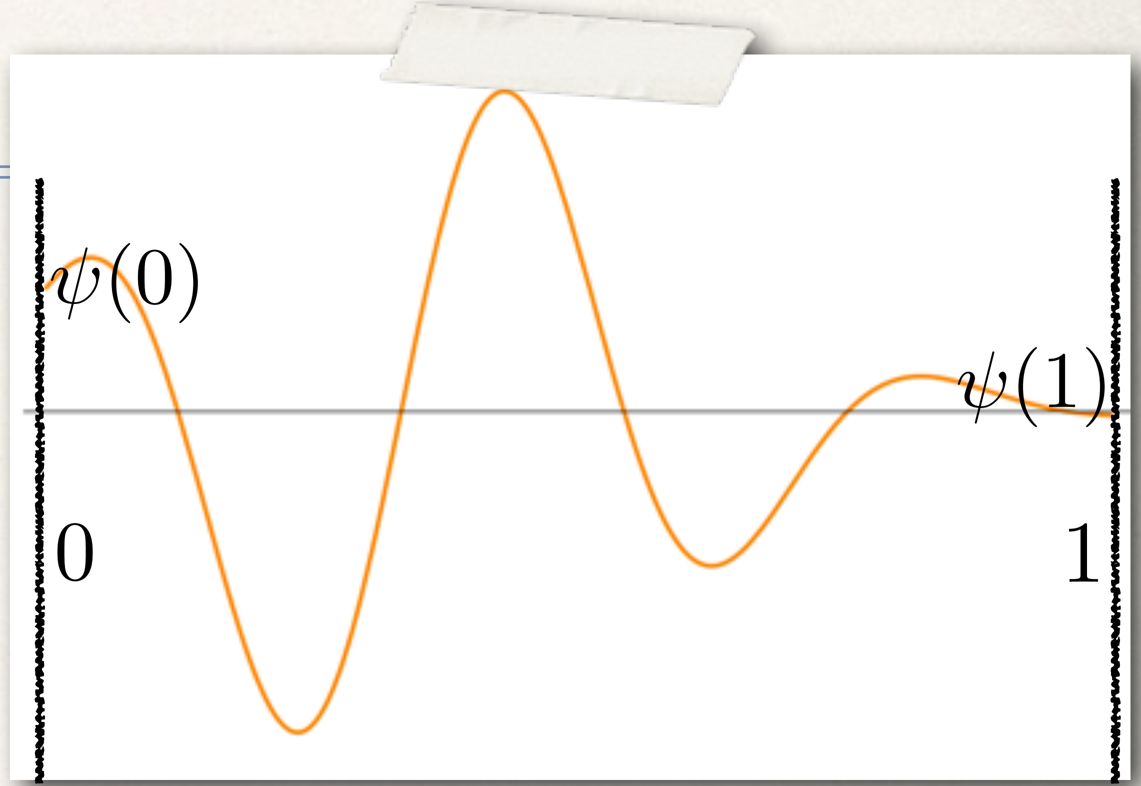
Unitary matrices at the boundary

$$i\,(I + U)\,\varphi = (I - U)\,\dot{\varphi} \qquad\qquad U \in \mathrm{U}(2)$$

M. Asorey, A. Ibort, G. Marmo, Int. J. Mod. Phys. A **20**, 1001 (2005)

Examples

$$i\,(I+U)\begin{pmatrix}\psi(0)\\ \psi(1)\end{pmatrix} = (I-U)\begin{pmatrix}\psi'(0)\\ -\psi'(1)\end{pmatrix}$$



Dirichlet

$$U = I \qquad \psi(0) = 0 = \psi(1)$$

Robin

$$U = -e^{-i\alpha} I$$

$$\alpha \in \mathbb{R} \qquad \begin{cases}\psi'(0) = -\tan\frac{\alpha}{2}\,\psi(0),\\ \psi'(1) = \tan\frac{\alpha}{2}\,\psi(1)\end{cases}$$

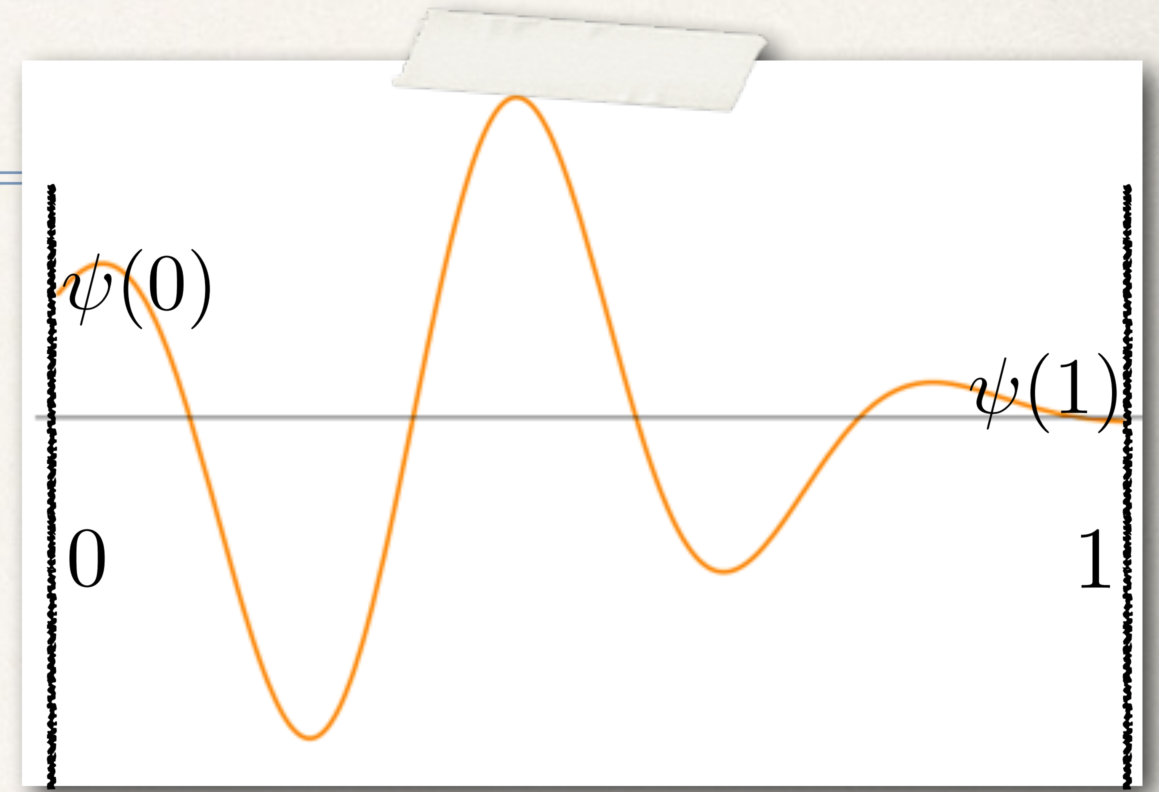
Neumann

$$U = -I$$

$$\psi'(0) = 0 = \psi'(1)$$

Examples

$$i\,(I+U)\begin{pmatrix}\psi(0)\\ \psi(1)\end{pmatrix} = (I-U)\begin{pmatrix}\psi'(0)\\ -\psi'(1)\end{pmatrix}$$



Dirichlet+Robin

$$U = \begin{pmatrix} 1 & 0 \\ 0 & -\mathrm{e}^{-\mathrm{i}\alpha} \end{pmatrix} \qquad \begin{cases} \psi(0) = 0 \\ \psi'(1) = \tan\frac{\alpha}{2}\,\psi(1) \end{cases}$$

$$\alpha \in \mathbb{R}$$

Antiperiodic

$$U = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \begin{cases} \psi(0) = -\psi(1) \\ \psi'(0) = -\psi'(1) \end{cases}$$

Periodic

$$U = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$$

$$\begin{cases} \psi(0) = \psi(1) \\ \psi'(0) = \psi'(1) \end{cases}$$

Role of the eigenvalue 1

$$i\,(\mathbb{I}+U)\,\varphi = (\mathbb{I}-U)\,\dot{\varphi} \qquad \varphi = \begin{pmatrix}\psi(0)\\ \psi(1)\end{pmatrix} \quad \dot{\varphi} = \begin{pmatrix}\psi'(0)\\ -\psi'(1)\end{pmatrix}$$

Suppose 1 is not an eigenvalue of U

$$\dot{\varphi} = K_U \varphi \qquad K_U = i(I+U)(I-U)^{-1} = \mathbf{C}^{-1}(U)$$

Cayley transform

$$\mathbf{C}(K) = (K-iI)(K+iI)^{-1} \qquad \mathbf{C}^{-1}(V) = i(I+V)(I-V)^{-1}$$

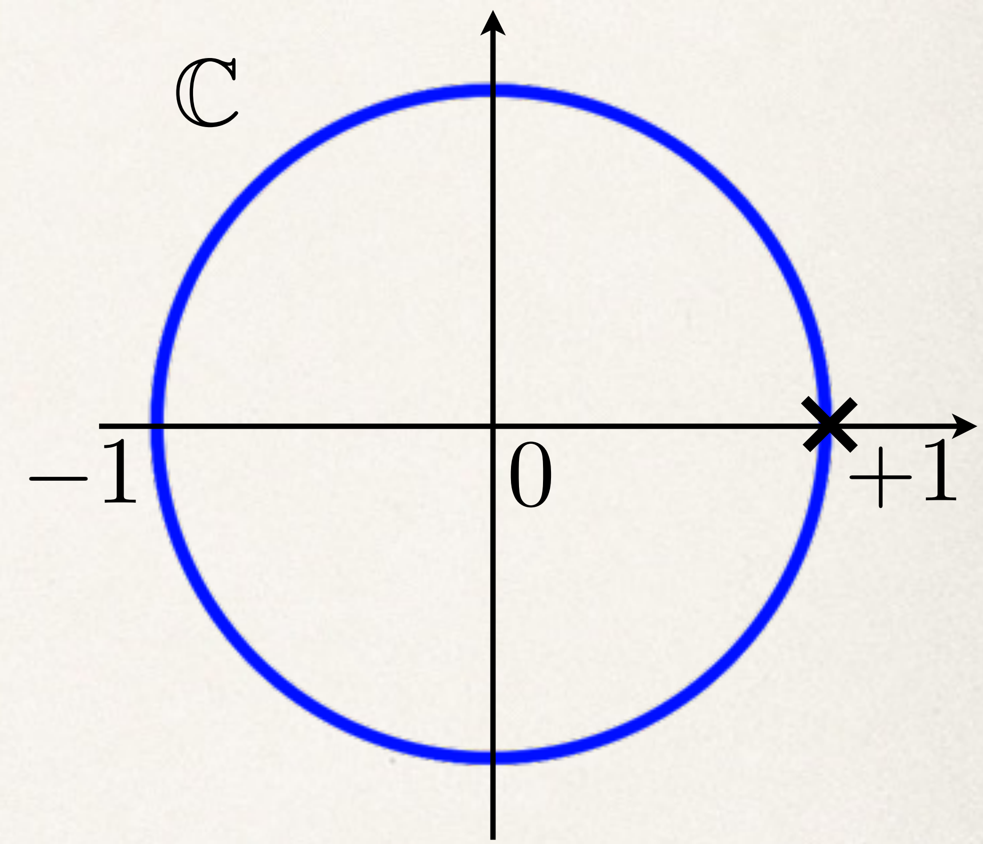
Role of the eigenvalue 1

P_U eigenprojection of eigenvalue 1

$$U = P_U + V_U$$

$$V_U = Q_U \, U \, Q_U$$

Warning: P_U or Q_U can be 0



$$i\,(\mathbb{I} + U)\,\varphi = (\mathbb{I} - U)\,\dot{\varphi} \qquad \Longleftrightarrow \qquad \begin{cases} P\varphi = 0, \\ i(I+V)Q\varphi = (I-V)Q\dot{\varphi} \end{cases}$$

Role of the eigenvalue 1

$$i\,(\mathbb{I}+U)\,\varphi = (\mathbb{I}-U)\,\dot{\varphi} \qquad \Longleftrightarrow \qquad \begin{cases} P_U\,\varphi = 0, \\ \dot{\varphi} = K_U \varphi, \end{cases}$$

$$K_U = \mathbf{C}^{-1}(V_U)Q_U = i(I+V_U)(I-V_U)^{-1}Q_U$$

$$\boxed{\textbf{Partial Cayley transform}}$$

$$\mathbf{C}(K) = (K-iI)(K+iI)^{-1} \qquad \mathbf{C}^{-1}(V) = i(I+V)(I-V)^{-1}$$

Kinetic energy

Boundary conditions:

$$t_U(\psi) = \frac{1}{2m}\left(\|\psi'\|^2 + \langle \varphi | \dot{\varphi} \rangle_{\mathbb{C}^2} \right)$$

$$\begin{cases} P_U\,\varphi = 0, \\ \dot{\varphi} = K_U \varphi, \end{cases}$$

$$\boxed{\begin{aligned} t_U(\psi) &= \frac{1}{2m}\left(\|\psi'\|^2 + \langle \varphi | K_U \varphi \rangle_{\mathbb{C}^2} \right) \\ D(t_U) &= \{\psi \in H^1(0,1) \,|\, P_U \varphi = 0\} \end{aligned}}$$

M. Asorey, P. F., G. Marmo, S. Pascazio J. Phys. A: Math. Theor. **46** (2013) 102001

Quadratic Forms vs Operators

$$t_U(\psi) = \frac{1}{2m}\left(\|\psi'\|^2 + \langle \varphi | K_U \varphi \rangle_{\mathbb{C}^2} \right)$$

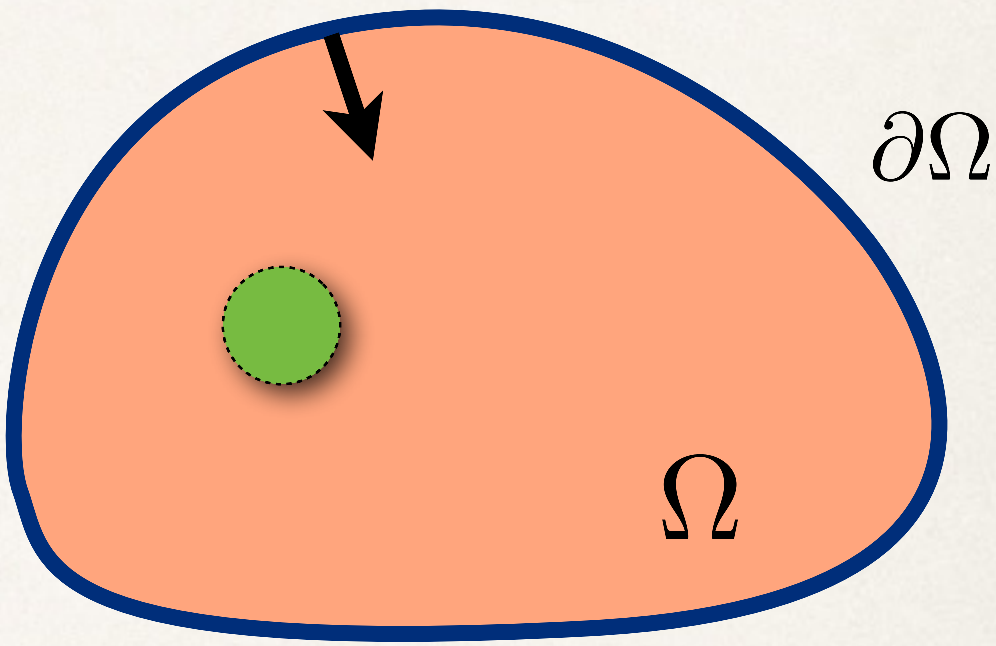
$$D(t_U) = \{\psi \in H^1(0,1) \,|\, P_U \varphi = 0\}$$

$$D(T_U) = \{\psi \in H^2(0,1) \,|\, i(I+U)\varphi = (I-U)\dot{\varphi}\}$$

$U = P_U + \mathbf{C}(K_U) Q_U$ $\quad P_U$ eigenprojection of U on 1

A particle in a cavity

$$H = T = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\Delta$$



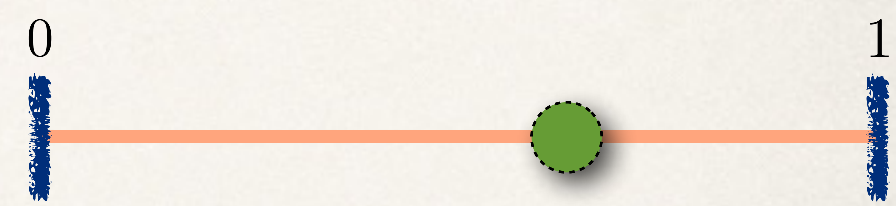
Dirichlet b.c.

$$D(H_D) = \{\psi \in H^2(\Omega) \,:\, \psi|_{\partial\Omega} = 0\}.$$

What are the other physical realizations?

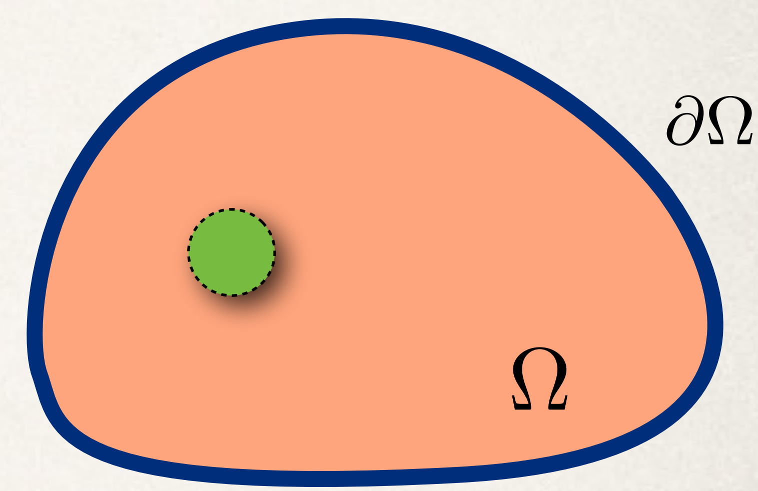
A particle in a cavity

Differences with the 1D case



- The boundary is infinite dimensional
- Much richer situation
- Mathematically: (unbounded) operators on the borders; Domains

VS



Example: Robin Boundary Conditions

$$\psi'(0) = \alpha_0 \psi(0)$$
$$\psi'(1) = \alpha_1 \psi(1)$$

$$\frac{\partial \psi}{\partial \nu}(x) = \alpha(x)\psi(x)$$
$$x \in \partial\Omega$$

More generally: $$\frac{\partial \psi}{\partial \nu}(x) = K\,\psi(x)$$ K operator on the boundary

A useful decomposition

$$D(T^*) = \{\psi \in L^2(\Omega), \Delta\psi \in L^2(\Omega)\}$$ quite irregular…

Every $\psi \in D(T^*)$ can be split into:

$$\boxed{\psi = \psi_D + \psi_0}$$

harmonic function

$\psi_0 \in N(T^*) = N(\Delta)$

such that:

$$\begin{cases} -\Delta\psi = -\Delta\psi_D \\ \psi|_{\partial\Omega} = \psi_0|_{\partial\Omega} \end{cases} \iff \begin{cases} -\Delta\psi_0 = 0 \\ \psi_D|_{\partial\Omega} = 0 \end{cases}$$

Dirichlet b.c.

A useful decomposition

$$\boxed{\psi = \psi_D + \psi_0}$$

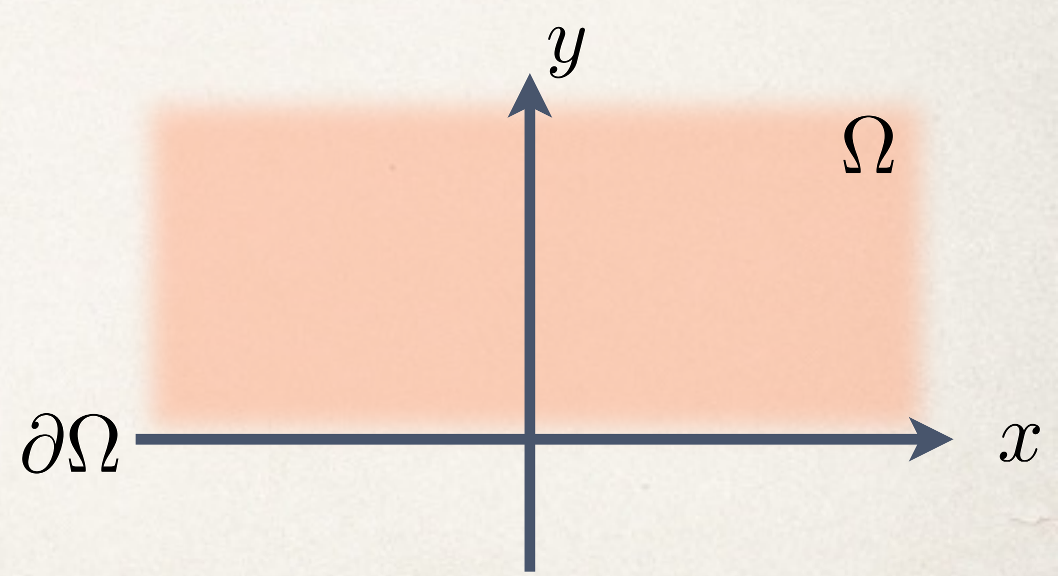
$$\begin{cases} -\Delta\psi_0 = 0 \\ \psi_D|_{\partial\Omega} = 0 \end{cases}$$

ψ_0 is harmonic

ψ_0 is extremely regular in Ω $\quad \not\Longrightarrow \quad$ ψ_0 is regular on $\partial\Omega$

$$\Omega = \mathbb{R}^2_+ \qquad f(x,y) = \frac{1}{(x+iy)}$$

$$-\Delta f = 0 \qquad \boxed{\lim_{y\downarrow 0} f(z) = P.V.\frac{1}{x} - i\pi\delta(x)}$$



Distributions on the boundary!

Quadratic Form

Expectation value of the kinetic energy

$$-\Delta\psi_0 = 0$$
$$\psi = \psi_D + \psi_0$$
$$\partial_\nu\psi = \nu \cdot (\nabla\psi)\,|_{\partial\Omega}$$

$$t(\psi) \propto -\langle\psi|\Delta\psi\rangle = -\langle\psi|\Delta\psi_D\rangle$$
$$= \int_\Omega \overline{\nabla\psi} \cdot \nabla\psi_D \mathrm{d}x + \int_{\partial\Omega} \overline{\psi}\,\partial_\nu\psi_D \mathrm{d}S$$
$$= \int_\Omega \overline{\nabla\psi}_D \cdot \nabla\psi_D \mathrm{d}x + \int_{\partial\Omega} \overline{\psi}\,\partial_\nu\psi_D \mathrm{d}S$$
$$= \|\nabla\psi_D\|^2 + \langle\psi|\partial_\nu\psi_D\rangle_{L^2(\partial\Omega)}$$

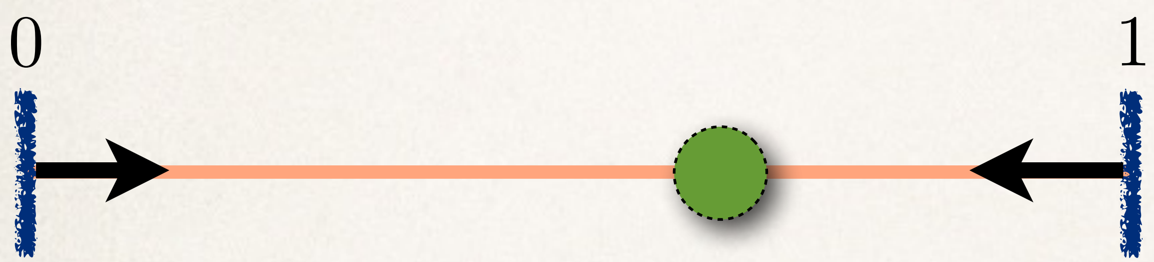
Gauss - Green's formula

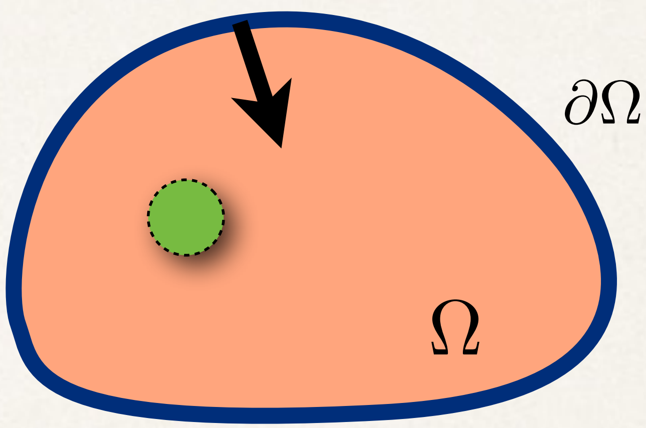
bulk

boundary

1D vs multiD

Expectation value of the kinetic energy





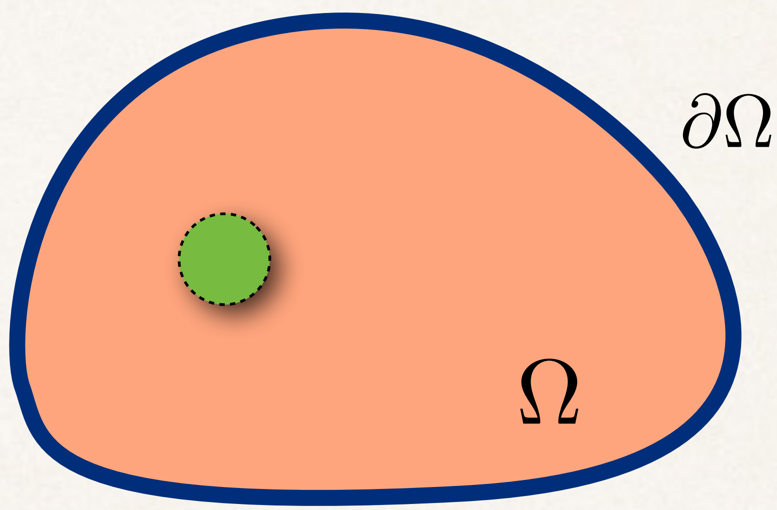
$$t(\psi) = \frac{\hbar^2}{2m}\left(\|\psi'\|^2 + \langle\varphi|\dot\varphi\rangle_{\mathbb{C}^2}\right)$$

$$\varphi = \begin{pmatrix}\psi(0)\\ \psi(1)\end{pmatrix} \qquad \dot\varphi = \begin{pmatrix}\psi'(0)\\ -\psi'(1)\end{pmatrix}$$

$$t(\psi) = \frac{\hbar^2}{2m}\left(\|\nabla\psi_D\|^2 + \langle\psi\,|\partial_\nu\psi_D\rangle\right)$$

$$\begin{cases}\varphi = \psi|_{\partial\Omega}\\ \dot\varphi = \partial_\nu\psi_D\end{cases}$$

A quantum particle in a cavity



$$T_U = -\frac{\hbar^2}{2m}\Delta \qquad\qquad U \in \mathcal{U}\left(\mathcal{H}_{\partial\Omega}\right)$$

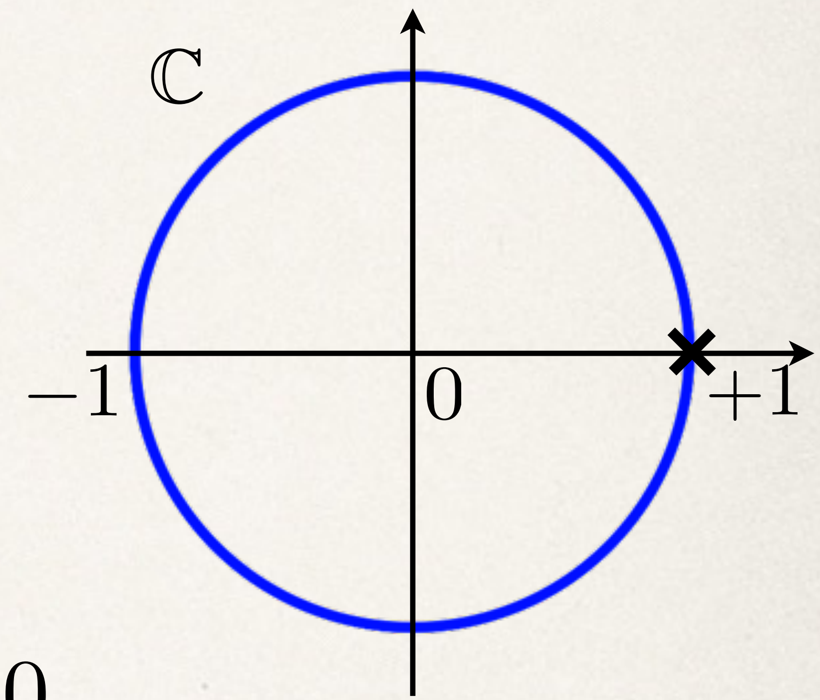
$$D(T_U) = \{\psi \in D(T^*) \,|\, i(U+I)\varphi = (I-U)\,\dot{\varphi}\,\}$$

A quantum particle in a cavity

P_U eigenprojection of eigenvalue 1

P_U could be infinite dimensional

$$\boxed{\begin{aligned} U &= P_U + V_U \\ V_U &= Q_U\, U\, Q_U \end{aligned}}$$

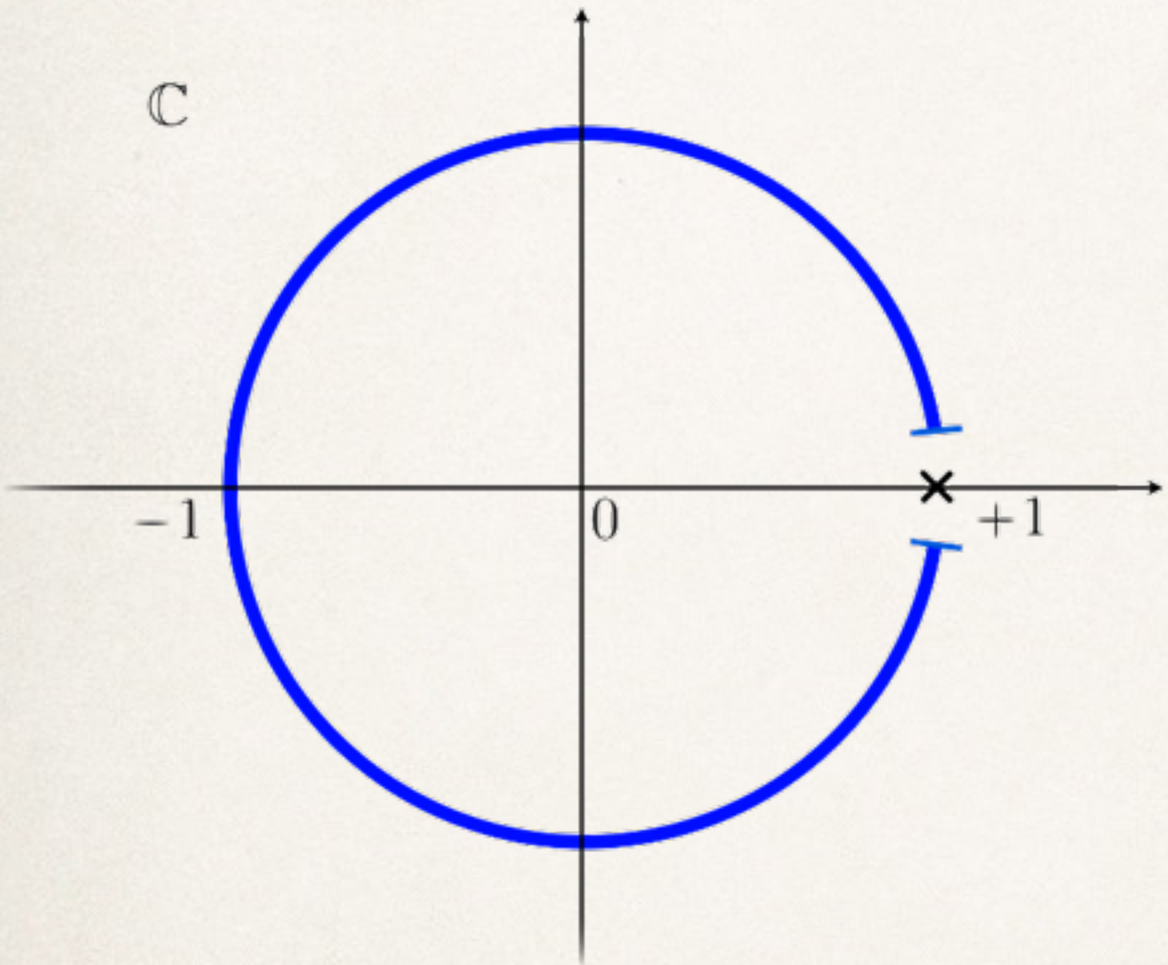


$$i\,(\mathbb{I} + U)\,\varphi = (\mathbb{I} - U)\,\dot{\varphi} \quad \Longleftrightarrow \quad \begin{cases} P_U\,\varphi = 0, \\ \dot{\varphi} = K_U \varphi, \end{cases}$$

$$K_U = \mathbf{C}^{-1}(V_U)Q_U = i(I + V_U)(I - V_U)^{-1}Q_U$$

...may be unbounded

A quantum particle in a cavity



Working assumption

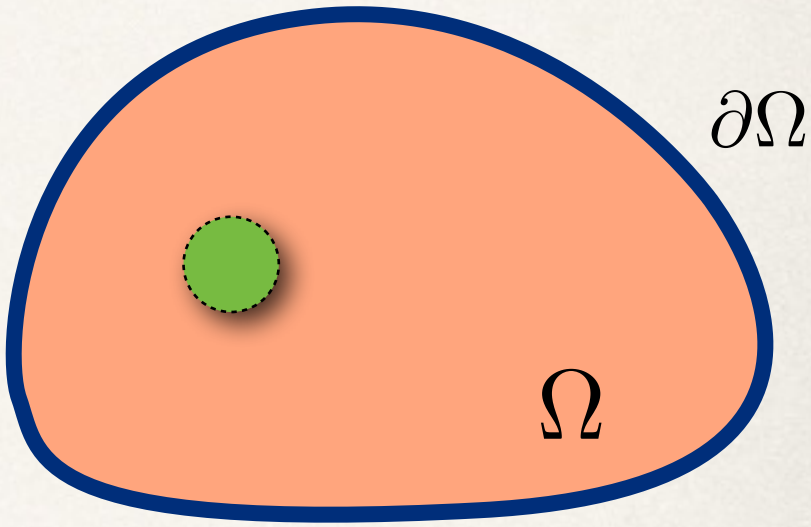
Gapped spectrum around 1

$$K_U = \mathbf{C}^{-1}(V_U)Q_U = i(I + V_U)(I - V_U)^{-1}Q_U$$

bounded

Kinetic Energy

Fix a physical realization T_U



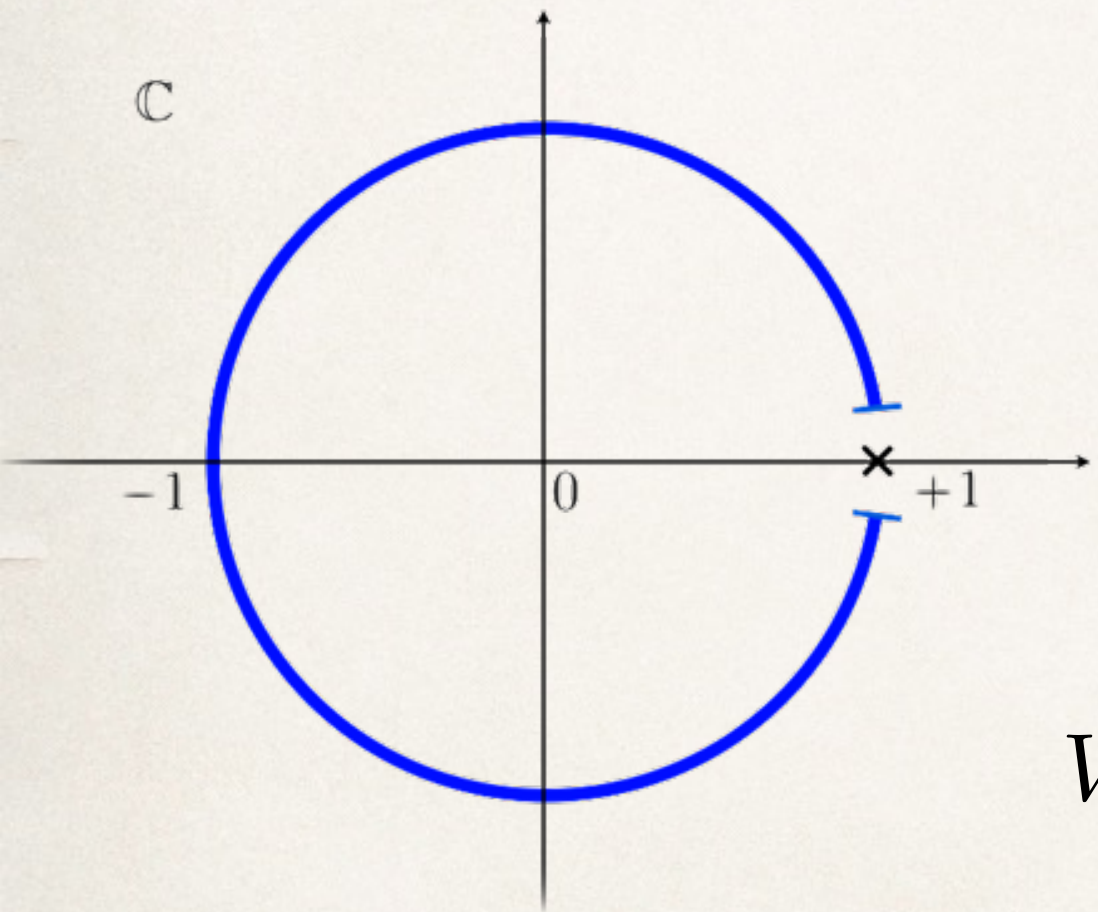
$$\begin{cases} P_U\,\varphi = 0, \\ \dot\varphi = K_U\varphi \end{cases}$$

$$t_U(\psi) = \frac{\hbar^2}{2m}\left(\|\nabla\psi_D\|^2 + \langle\varphi\,|\dot\varphi\rangle\right) = \frac{\hbar^2}{2m}\left(\|\nabla\psi_D\|^2 + \langle\varphi\,|K_U\varphi\rangle\right)$$

real closed quadratic form

$$D(t_U) = \{\psi \in H_0^1(\Omega) + \ker(T^*)\,|\,P_U\varphi = 0\}$$

Ingredients



$$U_i = P_i + V_i \qquad i = 1, 2$$

$$t_i(\psi) = \frac{\hbar^2}{2m}\left(\|\nabla\psi_D\|^2 + \langle\varphi\,|K_i\,\varphi\rangle \right)$$

$$D(t_i) = \{\psi\,|\,P_i\varphi = 0\}$$

$$V_i = Q_i\,U_i\,Q_i \qquad K_i = \mathbf{C}^{-1}(V_i)Q_i$$

bounded, since gapped spectrum

Form sum

Objective: $$T_3 = \frac{(T_1 \dot{+} T_2)}{2}$$

Need to compute $$\frac{t_1 + t_2}{2}$$

$$\frac{t_1(\psi) + t_2(\psi)}{2} = \|\nabla \psi_D\|^2 + \langle \varphi | K_3 \varphi \rangle,$$

$$K_3 = \frac{1}{2}\left(K_1 + K_2\right)$$

Limit dynamics

$$\frac{t_1(\psi)+t_2(\psi)}{2} = \|\nabla\psi_D\|^2 + \langle\varphi|K_3\varphi\rangle$$

lower bounded quadratic form

$$D(t_1)\cap D(t_2) = \{\psi \,|\, P_1\varphi = P_2\varphi = 0\} = \{\psi \,|\, P_3\varphi = 0\}$$

$$U_3 = P_3 + \mathbf{C}(K_3)Q_3 \qquad\qquad U_3 \in \mathcal{U}(\mathcal{H}_{\partial\Omega})$$

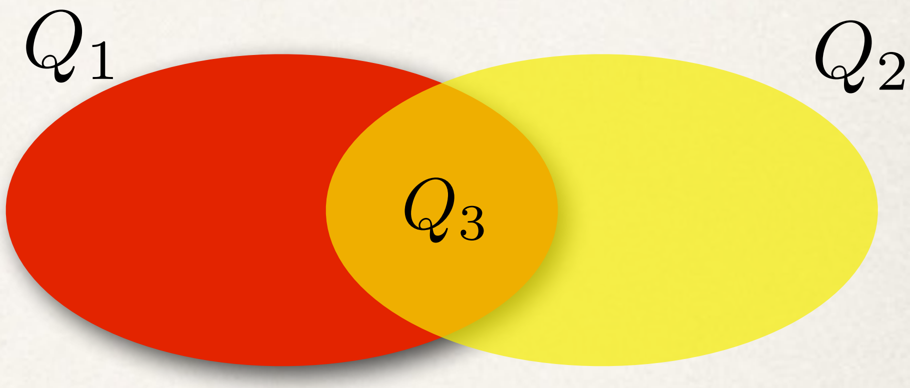
$$\frac{t_1+t_2}{2} = \langle\psi, T_{U_3}\psi\rangle$$

$$D(T_{U_3}) = \{\psi \in D(T^*) \,|\, i(I+U_3)\varphi = (I-U_3)\dot\varphi\}$$

Limit dynamics

$$U_3 = P_3 + \mathbf{C}(K_3)Q_3$$

$$Q_3\varphi = \varphi \iff \begin{cases} Q_1\varphi = \varphi \\ Q_2\varphi = \varphi \end{cases}$$



Q_3 is the projection on $\mathrm{Ran}(Q_3) = \mathrm{Ran}(Q_1) \cap \mathrm{Ran}(Q_2)$

$$Q_3 = Q_1 \wedge Q_2 \qquad\qquad P_3 = I - Q_3 = P_1 \vee P_2$$

P_3 is the eigenprojection of U_3 with eigenvalue 1

Limit dynamics

$$\left(\mathrm{e}^{-\mathrm{i}tT_1/N}\mathrm{e}^{-\mathrm{i}tT_2/N}\right)^N \to \mathrm{e}^{-\mathrm{i}2tT_3}$$

$$T_3 = \frac{(T_1 \dot{+} T_2)}{2} \qquad U_3 \in \mathcal{U}(\mathcal{H}_{\partial\Omega})$$

$$D(T_{U_3}) = \{\psi \in D(T^*) \,|\, i(I + U_3)\varphi = (I - U_3)\dot{\varphi}\}$$

$$\boxed{U_3 = P_3 + \mathbf{C}\left(\frac{\mathbf{C}^{-1}(V_1)Q_1 + \mathbf{C}^{-1}(V_2)Q_2}{2}\right)Q_3}$$

Composition law

$$\left(\mathrm{e}^{-\mathrm{i}tT_1/N}\mathrm{e}^{-\mathrm{i}tT_2/N}\right)^N \to \mathrm{e}^{-\mathrm{i}2tT_3} \qquad U_3 = U_1 \star U_2$$

$$\boxed{\begin{gathered} U_1 \star U_2 = P_{12} + \mathbf{C}\left(\frac{\mathbf{C}^{-1}(V_1)Q_1 + \mathbf{C}^{-1}(V_2)Q_2}{2}\right)Q_{12} \\ P_{12} = P_1 \vee P_2 \qquad Q_{12} = Q_1 \wedge Q_2 \end{gathered}}$$

$$U_i = P_i + V_i \qquad V_i = Q_i\, U_i\, Q_i \qquad i = 1, 2$$

Cayley transform

$$\mathbf{C}(K) = (K - iI)(K + iI)^{-1} \qquad \mathbf{C}^{-1}(V) = i(I + V)(I - V)^{-1}$$

Some properties

$$\boxed{\begin{gathered} U_1 \star U_2 = P_{12} + \mathbf{C}\left(\frac{\mathbf{C}^{-1}(V_1)Q_1 + \mathbf{C}^{-1}(V_2)Q_2}{2}\right)Q_{12} \\ P_{12} = P_1 \vee P_2 \qquad\qquad Q_{12} = Q_1 \wedge Q_2 \end{gathered}}$$

$P_1 = I, \quad Q_1 = 0$ Dirichlet

$$\boxed{I \star U_2 = I}$$

$P_{12} = I \vee P_2 = I, \quad Q_{12} = 0 \wedge Q_2 = 0$ Dirichlet absorbing

Some properties

$$U_1 \star U_2 = P_{12} + \mathbf{C}\left(\frac{\mathbf{C}^{-1}(V_1)Q_1 + \mathbf{C}^{-1}(V_2)Q_2}{2}\right)Q_{12}$$

$$P_{12} = P_1 \vee P_2 \qquad\qquad Q_{12} = Q_1 \wedge Q_2$$

In general P_{12} is increasing and Q_{12} is decreasing

If $P_1 \neq P_2$ is then P_{12} strictly increasing

Outlook

- Free particle in a cavity
- S.a. extensions in terms of unitaries on the boundary
- Limit dynamics of alternating b.c.
- Applications
- Extension to the Dirac Operator