Discretizing Schrodinger Type Operators with Spectral Accuracy on Quantum Graphs

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March 2, 2020

Quantum Mechanics 101

The Schrödinger equation

$$iu_t = -u_{xx} + f(x)$$

where $f(x)$ could be:

- Potential energy term: $V(x)u$
- Interaction between particles: $|u|^2 u$

Quantum Mechanics 101

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It is useful for modeling waves in thin branching structures

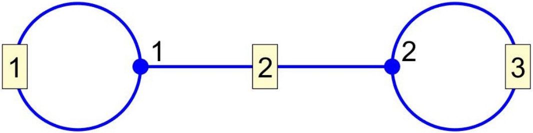
- Qubits in a quantum circuit
- Free electrons orbiting organic molecules
- Electromagnetic waves propagating through dielectric tubes

My Problem

Find time-periodic solutions to

$$iu_t = -u_{xx} - |u|^2 u$$

on



While I'm at it:

Solve $iu_t = -u_{xx} - |u|^2 u$ on *any* graphs with machine precision

Graphs

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  - $V =$ set of vertices v_j
  - $E =$ set of edges e_j

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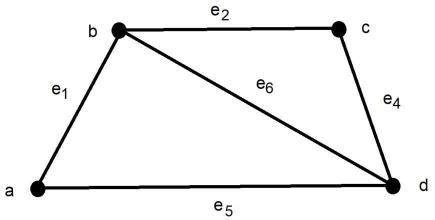
- Example
  - $V = \{a, b, c, d\}$
  - $E = \{(a, b), (b, c), (c, d), (b, d)\}$



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  - each edge has a length $l_j \in (0, \infty)$
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  - a metric graph
  - has a Schrödinger type operator on each edge

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↑ Schrödinger type operator

Example: Solutions on Graphs

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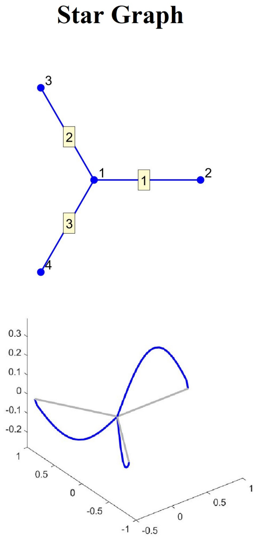

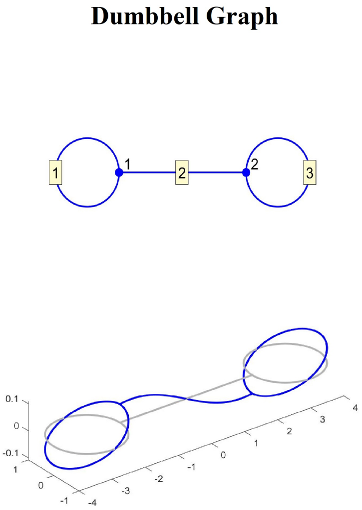

Vertex Conditions

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Possible conditions at a vertex v:

1) Leaf Nodes (Incident to **exactly one** edge)

- Boundary Condition
  - Dirichlet: $u_j(v) = 0$
  - Neumann: $u_j'(v) = 0$
  - Robin: $\alpha_j u_j(v) + u_j'(v) = 0$

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2) Internal Nodes (Incident to **more than one** edge)

- Matching Conditions
  - Continuity Condition: $u_j(v) = u_k(v)$
  - Current Conservation: $u_j'(v) = u_k'(v)$
    - Kirchoff: $\sum_{j=1}^{d_v} u_j'(v) = \sigma u_1(v)$

Numerically Defining Operators: Line

Problem: Solve for u when $x \in [0, \ell]$ in:

$$u_{xx} = f(x), \quad u(0) = a, \ u(\ell) = b$$

Discretized Problem: $D^2\vec{u} = \vec{f}$ where D is the discretized version of $\frac{d}{dx}$

We know D^2 and $\vec{f}$ so we can solve for $\vec{u}$.

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But how does do we enforce the boundary conditions?

Numerically Defining Operators: BCs

Popular method

- Row replacement
- Linear convergence

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Our Method

- Project information from n points to $n-2$ points
  - Method name: Rectangular Collocation
- Spectral convergence
  - $e_n \sim (\frac{\ell}{n})^n$

Rectangular Collocation

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1. Start with:
   - n discretization points that we are currently evaluating at $\{x_k\}_{k=1}^{n}$
   - $n-2$ discretization points we'd like to be working on instead $\{y_k\}_{k=1}^{n-2}$

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   Given discretization points $\{x_k\}_{k=1}^{n}$ the barycentric weights are:

$$w_k = \prod_{\substack{l=1 \\ l \neq k}}^{n} (x_k - x_l)^{-1} \qquad k = 1, ..., n$$

   The unique polynomial interpolating $\{(x_j, f_j)\}_{j=1}^{n}$ is:

$$p_{n-1}(y) = \frac{\sum_{k=1}^{n} (w_k/(y - x_k)) f_k}{\sum_{l=1}^{n} (w_k/(y - x_l))}$$

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$$\boldsymbol{w}_{n-2,1} = P_{n-2,n}\ \boldsymbol{v}_{n,1}$$

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$$(P_{n-2,n})_{j,k} = \begin{cases} \frac{w_k}{y_j - x_k}\left(\sum_{l=1}^{N} \frac{w_l}{y_j - x_l}\right)^{-1} & y_j \neq x_k \\ 1 & y_j = x_k \end{cases}$$

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$$P_{n-2,n}D^2_{n,n} = \text{Projected Second Derivative Matrix}$$

Numerically Defining Operators: Line

Problem: Solve for u when $x \in [0, \ell]$ in:

$$u_{xx} = f(x), \quad u(0) = a, \ \ u(\ell) = b$$

Discretized: $D^2\vec{u} = \vec{f}$ where D is the discretized version of $\frac{d}{dx}$

(*Still need to enforce the boundary conditions*)

Numerically Defining Operators: Line

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$$\underbrace{\begin{bmatrix} 1 & \dots & 0 \\ & \begin{bmatrix} & & \\ & PD^2 & \\ & & \end{bmatrix} & \\ 0 & \dots & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_{n-1} \\ u_n \end{bmatrix}}_{\vec{u}} = \underbrace{\begin{bmatrix} a \\ f_2 \\ \vdots \\ f_{n-1} \\ b \end{bmatrix}}_{\vec{f}}$$

Use some built in commands and solve $L\vec{u} = \vec{f}$ for $\vec{u}$

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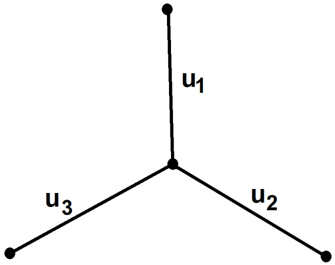
Use some built in commands and solve $L\vec{u} = \vec{f}$ for $\vec{u}$

Now glue some lines together and you have a quantum graph!

Numerically Defining Operators: Graph

Problem: Solve $u_{xx} = f(x)$ when x is in:



$$\begin{cases} u_1(l_1) = u_2(l_2) = u_3(l_3) = 0 & \text{Boundary Condition} \\ u_1(0) = u_2(0) = u_3(0) & \text{Continuity Condition} \\ u_1'(0) + u_2'(0) + u_3'(0) = 0 & \text{Current Conservation (Kirchoff Condition)} \end{cases}$$

Numerically Defining Operators: Graphs

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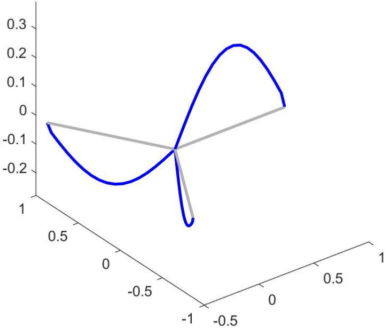
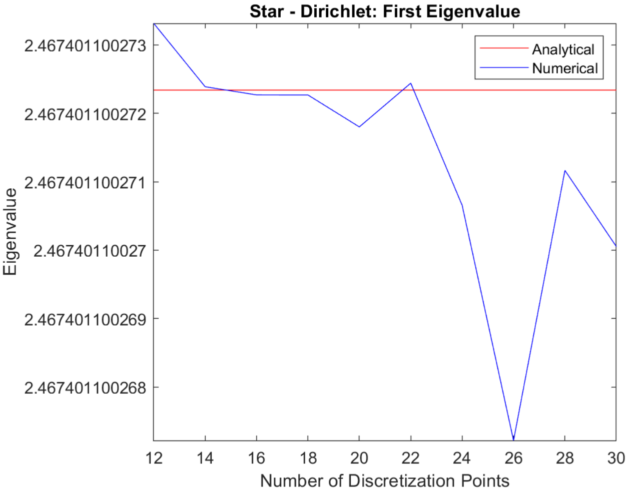
$$L = \begin{bmatrix} \begin{bmatrix} PD^2 & \dots & 0 \\ \vdots & PD^2 & \vdots \\ 0 & \dots & PD^2 \end{bmatrix} \\ \begin{bmatrix} & BC & \end{bmatrix} \\ \begin{bmatrix} & Continuity & \end{bmatrix} \\ \begin{bmatrix} & KC & \end{bmatrix} \end{bmatrix}$$

Numerically Defining Operators: Graphs

Use built in commands to solve $L\vec{u} = \vec{f}$:



Convergence of Spatial Operator



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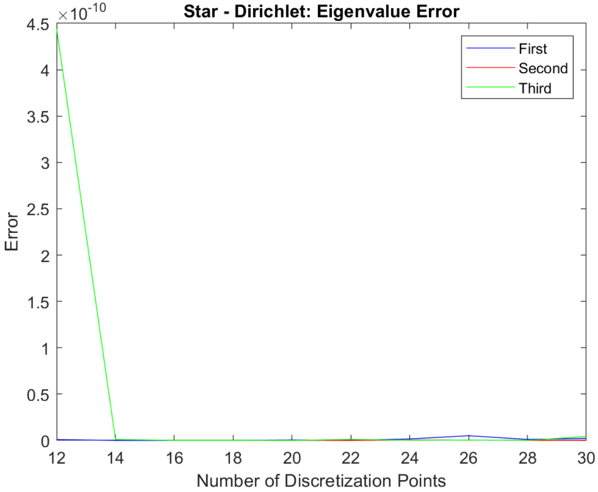

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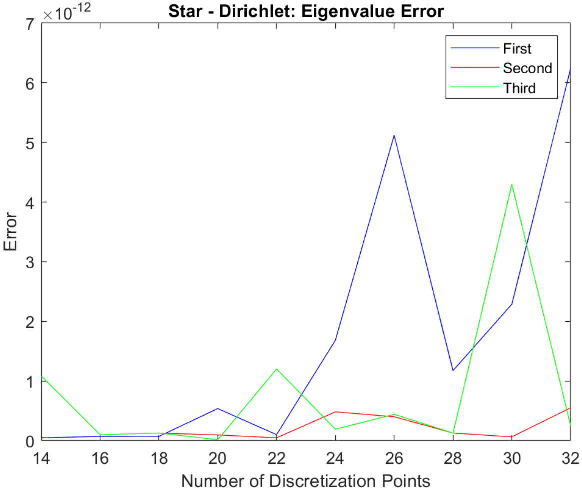

Time Evolution

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So you want you want to see what happens when time doesn't stand still? How interesting...

Challenges:

- Finding a time-stepper that matches the accuracy of our spatial solver
- Accounting for our spatial solver being on a new domain
- Coping with the non-linearity

Time Evolution: Linear

Step One: Ignore the non-linearity

We know how to solve $iu_t = -u_{xx}$ analytically
(Spoiler: Its solution is an exponential)

Time Evolution: Linear

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The Problem:

$$\begin{cases} iu_t = -u_{xx} \\ \text{vertex conditions} \\ u(x,0) = f(x) \end{cases}$$

The Discretized Problem:

$$\begin{cases} \dfrac{d\boldsymbol{u}}{dt} = -iD^2\boldsymbol{u} \\ B\boldsymbol{u} = 0 \\ u(\boldsymbol{x},0) = f(\boldsymbol{x}) \end{cases}$$

this means $\dfrac{d\boldsymbol{u}}{dt} \neq -i \underbrace{\begin{bmatrix} [& PD^2 &] \\ [& B &] \end{bmatrix}}_{L} \boldsymbol{u}$

Time Evolution: Linear

We need to project our solution

$$\widetilde{\boldsymbol{u}} = P_{M,N}\boldsymbol{u}$$

(Note: $P_{M,N} =$ zero matrix with $P_{n-2,n}$'s on its diagonal)

Can recover original solution using this:

$$\begin{bmatrix} P_{M,N} \\ L \end{bmatrix} \boldsymbol{u} = \begin{bmatrix} I_M \\ 0 \end{bmatrix} \widetilde{\boldsymbol{u}}$$

$$\Rightarrow \quad \boldsymbol{u} = \underbrace{\begin{bmatrix} P_{M,N} \\ L \end{bmatrix} \begin{bmatrix} I_M \\ 0 \end{bmatrix}}_{E} \widetilde{\boldsymbol{u}}$$

Time Evolution: Linear

Apply $P_{M,N}$ to both sides of: $\dfrac{d\boldsymbol{u}}{dt} = -iD^2\boldsymbol{u}$

$$\frac{d\widetilde{\boldsymbol{u}}}{dt} = -iP_{M,N}D^2E\widetilde{\boldsymbol{u}}$$

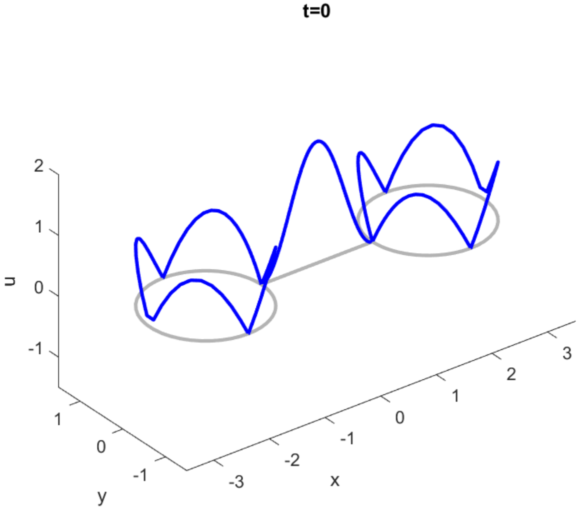
Use analytic knowledge and matrix exponentials to get solution:

$$\widetilde{\boldsymbol{u}} = \exp\left(-itP_{N-mj,N}D^2E\right)\widetilde{\boldsymbol{u}}(x,0)$$

Recover the actual solution:

$$\boldsymbol{u} = E\exp\left(-itP_{M,N}D^2E\right)P_{M,N}\boldsymbol{u}(x,0)$$

Time Evolution: $iu_t = -u_{xx}$



Time Evolution: Nonlinear

Step Two: Admit you have a problem

$$iu_t = -u_{xx} - |u|^2 u$$

Challenges:

- Most well-developed non-linear schemes are only fourth order
- The better schemes haven't been adjusted for DAEs

Time Evolution: Strang Splitting

Rewrite: $u_t = \mathcal{L}u + N(u,t)$

Solve separate problems

$$d_t \boldsymbol{v} = \mathcal{L}\boldsymbol{v} \qquad d_t \boldsymbol{w} = N\boldsymbol{w}$$

$$\boldsymbol{v}_n = e^{\mathcal{L}t}\boldsymbol{u}_{n-1} \qquad \boldsymbol{w}_n = F(Nt)\boldsymbol{u}_{n-1}$$

Second Order Scheme:

$$\boldsymbol{u}_n = e^{\mathcal{L}\frac{\Delta t}{2}} F(N\Delta t) e^{\mathcal{L}\frac{\Delta t}{2}} \boldsymbol{u}_{n-1}$$

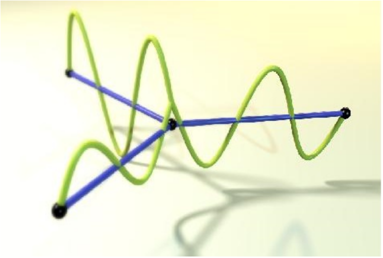
General Scheme:

$$\boldsymbol{u}_n = e^{c_1 \Delta t \mathcal{L}} F(d_1 t N) e^{c_2 \Delta t \mathcal{L}} F(d_2 \Delta t N) \ldots e^{c_k \Delta t L} F(d_k \Delta t N) \boldsymbol{u}_{n-1}$$

where c_i's and d_i's represent fractional time steps

Conclusion

- Developing tools to model Quantum Graphs is essential
- Rectangular Collocation is a superior method for solving PDE's with Schrödinger type operators
- Computationally efficient time stepping scheme come in two pieces
  - Use matrix exponentials for linear term
  - Account for non-linear term with a splitting scheme (I'll get on it)
- Will be ready to look for time periodic orbit solutions soon!



Thanks!

Special thanks to

- My advisor, Jeremy Marzuola
- My collaborator at NJIT, Roy Goodman
- And you guys for coming