A globalized Newton method for the optimal control of multiple interacting fermions

Greg von Winckel

Institut für Mathematik und Wissenschaftliches Rechnen
Karl-Franzens Universität Graz

October 12, 2011

Outline

- Single particle dynamics and control problem

Outline

- Single particle dynamics and control problem
- Two or more fermions

Outline

- Single particle dynamics and control problem
- Two or more fermions
- Discretization methods

Outline

- Single particle dynamics and control problem
- Two or more fermions
- Discretization methods
- Lagrangian and optimality conditions

Outline

- Single particle dynamics and control problem
- Two or more fermions
- Discretization methods
- Lagrangian and optimality conditions
- Reduced model method

Outline

- Single particle dynamics and control problem
- Two or more fermions
- Discretization methods
- Lagrangian and optimality conditions
- Reduced model method
- Numerical results for test cases

Single particle

Dynamics described by time-dependent Schrödinger equation

$$i\partial_t \psi(x,t) = -\partial_x^2 \psi + V(x,t)\psi(x,t)$$

Single particle

Dynamics described by time-dependent Schr̈odinger equation

$$i\partial_t\psi(x,t) = -\partial_x^2\psi + V(x,t)\psi(x,t)$$

Any influence on the wavefunction is via potential $V(x,t)$

Single particle

Dynamics described by time-dependent Schr̈odinger equation

$$i\partial_t \psi(x,t) = -\partial_x^2 \psi + V(x,t)\psi(x,t)$$

Any influence on the wavefunction is via potential $V(x,t)$

Typical goal:

Single particle

Dynamics described by time-dependent Schr̈odinger equation

$$i\partial_t \psi(x,t) = -\partial_x^2 \psi + V(x,t)\psi(x,t)$$

Any influence on the wavefunction is via potential $V(x,t)$

Typical goal:

Given $\psi(x,0)$, find $V(x,t)$ such that $\psi(x,T) \approx \tilde{\psi}(x)$

Single particle

Dynamics described by time-dependent Schr̈odinger equation

$$i\partial_t \psi(x,t) = -\partial_x^2 \psi + V(x,t)\psi(x,t)$$

Any influence on the wavefunction is via potential $V(x,t)$

Typical goal:

Given $\psi(x,0)$, find $V(x,t)$ such that $\psi(x,T) \approx \tilde{\psi}(x)$

$$\mathcal{P}\psi(x,T) = \left(\psi(\cdot,T), \tilde{\psi}\right)\tilde{\psi}(x)$$

Single particle

Dynamics described by time-dependent Schrödinger equation

$$i\partial_t\psi(x,t) = -\partial_x^2\psi + V(x,t)\psi(x,t)$$

Any influence on the wavefunction is via potential $V(x,t)$

Typical goal:

Given $\psi(x,0)$, find $V(x,t)$ such that $\psi(x,T) \approx \tilde{\psi}(x)$

$$\mathcal{P}\psi(x,T) = \left(\psi(\cdot,T),\tilde{\psi}\right)\tilde{\psi}(x)$$

Want to make $\|\mathcal{P}\psi(\cdot,T)\|^2 \to 1$

Single particle

Dynamics described by time-dependent Schr̈odinger equation

$$i\partial_t\psi(x,t) = -\partial_x^2\psi + V(x,t)\psi(x,t)$$

Any influence on the wavefunction is via potential $V(x,t)$

Typical goal:

Given $\psi(x,0)$, find $V(x,t)$ such that $\psi(x,T) \approx \tilde{\psi}(x)$

$$\mathcal{P}\psi(x,T) = \left(\psi(\cdot,T),\tilde{\psi}\right)\tilde{\psi}(x)$$

Want to make $\|\mathcal{P}\psi(\cdot,T)\|^2 \to 1$

State transition: $\tilde{\psi}$ and $\psi(x,0)$ are eigenfunctions

Two identical particles

TDSE for two identical particles

$$i\partial_t \psi(x_1, x_2, t) = \left\{ -(\partial_{x_1}^2 + \partial_{x_2}^2) + V(x_1, x_2, t) \right\} \psi(x_1, x_2, t)$$

Two identical particles

TDSE for two identical particles

$$i\partial_t\psi(x_1, x_2, t) = \left\{-(\partial^2_{x_1} + \partial^2_{x_2}) + V(x_1, x_2, t)\right\}\psi(x_1, x_2, t)$$

Invariance of $|\psi|$ under permutation

$$|\psi(x_1, x_2)|^2 = |\psi(x_2, x_1)|^2 \;\Rightarrow\; \psi(x_2, x_1) = \psi(x_1, x_2)e^{i\theta}$$

Two identical particles

TDSE for two identical particles

$$i\partial_t\psi(x_1, x_2, t) = \left\{-(\partial^2_{x_1} + \partial^2_{x_2}) + V(x_1, x_2, t)\right\}\psi(x_1, x_2, t)$$

Invariance of $|\psi|$ under permutation

$$|\psi(x_1, x_2)|^2 = |\psi(x_2, x_1)|^2 \;\Rightarrow\; \psi(x_2, x_1) = \psi(x_1, x_2)e^{i\theta}$$

Let P be the permutation operator

$$P\psi(x_1, x_2) = \psi(x_2, x_1) = e^{i\theta}\psi(x_1, x_2)$$

Two identical particles

TDSE for two identical particles

$$i\partial_t\psi(x_1, x_2, t) = \left\{-(\partial_{x_1}^2 + \partial_{x_2}^2) + V(x_1, x_2, t)\right\}\psi(x_1, x_2, t)$$

Invariance of $|\psi|$ under permutation

$$|\psi(x_1, x_2)|^2 = |\psi(x_2, x_1)|^2 \;\Rightarrow\; \psi(x_2, x_1) = \psi(x_1, x_2)e^{i\theta}$$

Let P be the permutation operator

$$P\psi(x_1, x_2) = \psi(x_2, x_1) = e^{i\theta}\psi(x_1, x_2)$$

Two permutations

$$P^2\psi(x_1, x_2) = P\psi(x_2, x_1) = e^{i2\theta}\psi(x_1, x_2) = \psi(x_1, x_2)$$

Two identical particles

TDSE for two identical particles

$$i\partial_t\psi(x_1, x_2, t) = \left\{-(\partial_{x_1}^2 + \partial_{x_2}^2) + V(x_1, x_2, t)\right\}\psi(x_1, x_2, t)$$

Invariance of $|\psi|$ under permutation

$$|\psi(x_1, x_2)|^2 = |\psi(x_2, x_1)|^2 \;\Rightarrow\; \psi(x_2, x_1) = \psi(x_1, x_2)e^{i\theta}$$

Let P be the permutation operator

$$P\psi(x_1, x_2) = \psi(x_2, x_1) = e^{i\theta}\psi(x_1, x_2)$$

Two permutations

$$P^2\psi(x_1, x_2) = P\psi(x_2, x_1) = e^{i2\theta}\psi(x_1, x_2) = \psi(x_1, x_2)$$

Parity relations

$$\psi(x_1, x_2) = \pm\psi(x_2, x_1)$$

Two fermions

Without interaction $V(x_1, x_2, t) = V(x_1, t) + V(x_2, t)$

$$i\partial_t \psi_1(x_1, t) = [-\partial_{x_1}^2 + V(x_1, t)]\psi_1(x_1, t)$$
$$i\partial_t \psi_2(x_2, t) = [-\partial_{x_2}^2 + V(x_2, t)]\psi_2(x_2, t)$$

Two fermions

Without interaction $V(x_1, x_2, t) = V(x_1, t) + V(x_2, t)$

$$i\partial_t \psi_1(x_1, t) = [-\partial_{x_1}^2 + V(x_1, t)]\psi_1(x_1, t)$$
$$i\partial_t \psi_2(x_2, t) = [-\partial_{x_2}^2 + V(x_2, t)]\psi_2(x_2, t)$$

Two particle wavefunction

$$\psi(x_1, x_2, t) = \psi_1(x_1, t)\psi_2(x_2, t) - \psi_1(x_2, t)\psi_1(x_2, t)$$

Two fermions

Without interaction $V(x_1, x_2, t) = V(x_1, t) + V(x_2, t)$

$$i\partial_t\psi_1(x_1, t) = [-\partial_{x_1}^2 + V(x_1, t)]\psi_1(x_1, t)$$
$$i\partial_t\psi_2(x_2, t) = [-\partial_{x_2}^2 + V(x_2, t)]\psi_2(x_2, t)$$

Two particle wavefunction

$$\psi(x_1, x_2, t) = \psi_1(x_1, t)\psi_2(x_2, t) - \psi_1(x_2, t)\psi_1(x_2, t)$$

More generally: n fermions

$$\psi(x_1, \ldots, x_n, t) = \det \begin{pmatrix} \psi_1(x_1, t) & \cdots & \psi_n(x_1, t) \\ \vdots & \ddots & \vdots \\ \psi_1(x_n, t) & \cdots & \psi_n(x_n, t) \end{pmatrix}$$

Two fermions

Without interaction $V(x_1, x_2, t) = V(x_1, t) + V(x_2, t)$

$$i\partial_t\psi_1(x_1, t) = [-\partial_{x_1}^2 + V(x_1, t)]\psi_1(x_1, t)$$
$$i\partial_t\psi_2(x_2, t) = [-\partial_{x_2}^2 + V(x_2, t)]\psi_2(x_2, t)$$

Two particle wavefunction

$$\psi(x_1, x_2, t) = \psi_1(x_1, t)\psi_2(x_2, t) - \psi_1(x_2, t)\psi_1(x_2, t)$$

More generally: n fermions

$$\psi(x_1, \ldots, x_n, t) = \det \begin{pmatrix} \psi_1(x_1, t) & \cdots & \psi_n(x_1, t) \\ \vdots & \ddots & \vdots \\ \psi_1(x_n, t) & \cdots & \psi_n(x_n, t) \end{pmatrix}$$

$$\psi(x_1, \ldots, x_n, t) = 0, \quad \text{if } x_j = x_k \text{ for some } 1 \leqslant j, k \leqslant n$$

TDSE for n fermions

$$\left\{ -\Delta + \sum_{j=1}^{n} \left(V^c(x_j, t) + \sum_{k>j}^{n} V^i(x_j, x_k) \right) \right\} \psi_i(\mathbf{x}) = \lambda_i \psi_i(\mathbf{x})$$

TDSE for n fermions

$$\left\{ -\Delta + \sum_{j=1}^{n} \left(V^c(x_j, t) + \sum_{k>j}^{n} V^i(x_j, x_k) \right) \right\} \psi_i(\mathbf{x}) = \lambda_i \psi_i(\mathbf{x})$$

where

$$\Delta = \partial_{x_1}^2 + \cdots \partial_{x_n}^2$$

TDSE for n fermions

$$\left\{-\Delta + \sum_{j=1}^{n} \left(V^c(x_j, t) + \sum_{k>j}^{n} V^i(x_j, x_k) \right) \right\} \psi_i(\mathbf{x}) = \lambda_i \psi_i(\mathbf{x})$$

where

$$\Delta = \partial_{x_1}^2 + \cdots \partial_{x_n}^2$$

The confining/control potential $V^c(x, t)$ affects all particles

TDSE for n fermions

$$\left\{-\Delta + \sum_{j=1}^{n}\left(V^c(x_j,t) + \sum_{k>j}^{n} V^i(x_j,x_k)\right)\right\}\psi_i(\mathbf{x}) = \lambda_i \psi_i(\mathbf{x})$$

where

$$\Delta = \partial_{x_1}^2 + \cdots \partial_{x_n}^2$$

The confining/control potential $V^c(x,t)$ affects all particles

Coulombic interaction

$$V^i(x_j,x_k) = \frac{q}{|x_j - x_k|} \approx \frac{q}{\sqrt{(x_j-x_k)^2+\epsilon^2}}$$

q is electronic charge

Eigenfunctions - square well without interaction

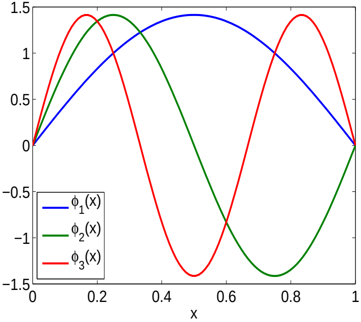


Figure: Single particle: states $|1\rangle$, $|2\rangle$, and $|3\rangle$

Eigenfunctions - square well without interaction

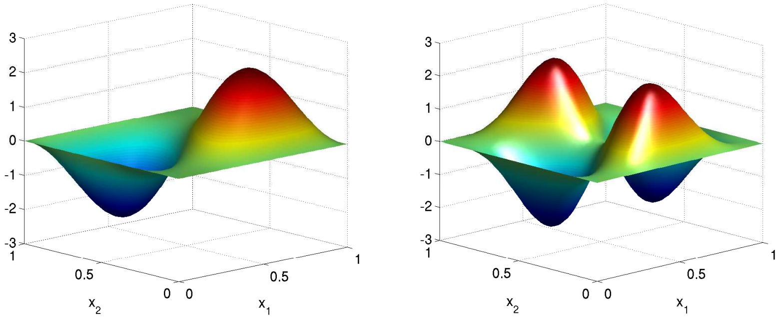


Figure: Two particles: state $|1,2\rangle$ and $|1,3\rangle$

Eigenfunctions - square well without interaction

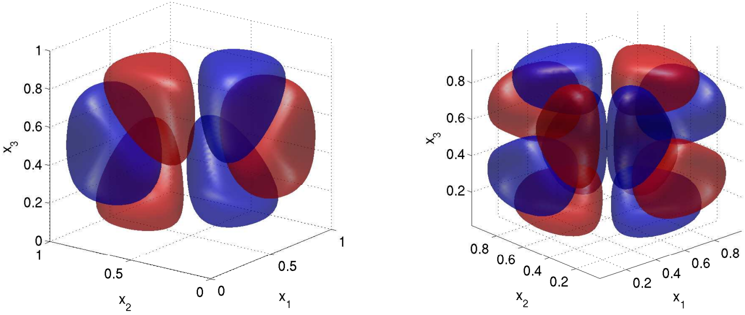


Figure: Three particles: state $|1, 2, 3\rangle$ and $|1, 2, 4\rangle$

Spatial discretization - one dimension

Legendre G-NI discretization

$$\psi(x) \approx \psi_p(x) = \sum_{k=1}^{p} \hat{\psi}_k \ell_k(x)$$

Legendre G-NI discretization

$$\psi(x) \approx \psi_p(x) = \sum_{k=1}^{p} \hat{\psi}_k \ell_k(x)$$

The Lagrange polynomials are

$$\ell_j(x) = \prod_{\substack{k=0 \\ k \neq j}}^{p+1} \frac{x - x_k}{x_j - x_k}, \quad j = 0, \ldots, p+1$$

End points excluded for homogeneous Dirichlet conditions

Spatial discretization - one dimension

Legendre G-NI discretization

$$\psi(x) \approx \psi_p(x) = \sum_{k=1}^{p} \hat{\psi}_k \ell_k(x)$$

The Lagrange polynomials are

$$\ell_j(x) = \prod_{\substack{k=0 \\ k \neq j}}^{p+1} \frac{x - x_k}{x_j - x_k}, \quad j = 0, \ldots, p+1$$

End points excluded for homogeneous Dirichlet conditions
The Legendre-Gauss-Lobatto nodes are

$$\{x_0, \ldots, x_{p+1}\} = \{x | P'_{p+1}(x) = 0\} \cup \{\pm 1\}$$

where $P_k(x)$ is the kth Legendre polynomial

Spatial discretization - one dimension

Legendre G-NI discretization

$$\psi(x) \approx \psi_p(x) = \sum_{k=1}^{p} \hat{\psi}_k \ell_k(x)$$

The Lagrange polynomials are

$$\ell_j(x) = \prod_{\substack{k=0 \\ k \neq j}}^{p+1} \frac{x - x_k}{x_j - x_k}, \quad j = 0, \dots, p+1$$

End points excluded for homogeneous Dirichlet conditions
The Legendre-Gauss-Lobatto nodes are

$$\{x_0, \dots, x_{p+1}\} = \{x | P'_{p+1}(x) = 0\} \cup \{\pm 1\}$$

where $P_k(x)$ is the kth Legendre polynomial
The weights are

$$w_k = \frac{1}{(p+1)(p+2)} \frac{2}{[P_{p+1}(x_k)]^2}$$

Spatial discretization - one particle

Weak form of generalized eigenvalue problem

$$\sum_{k=1}^{p} [(\ell_j', \ell_k') + (\ell_j, V^c \ell_k)] \hat{\psi}_k = \lambda \sum_{k=1}^{p} [(\ell_j, \ell_k) \hat{\psi}_k$$

Spatial discretization - one particle

Weak form of generalized eigenvalue problem

$$\sum_{k=1}^{p}[(\ell_j', \ell_k') + (\ell_j, V^c \ell_k)]\hat{\psi}_k = \lambda \sum_{k=1}^{p}[(\ell_j, \ell_k)\hat{\psi}_k$$

Stiffness matrix $\tilde{\mathbf{K}}_{jk} = (\ell_j', \ell_k')$

Spatial discretization - one particle

Weak form of generalized eigenvalue problem

$$\sum_{k=1}^{p}[(\ell_j', \ell_k') + (\ell_j, V^c \ell_k)]\hat{\psi}_k = \lambda \sum_{k=1}^{p}[(\ell_j, \ell_k)\hat{\psi}_k$$

Stiffness matrix $\tilde{\mathbf{K}}_{jk} = (\ell_j', \ell_k')$

Confining potential $\tilde{\mathbf{V}}^{\mathbf{c}}_{jk} = (\ell_j, V^c \ell_k)$

Spatial discretization - one particle

Weak form of generalized eigenvalue problem

$$\sum_{k=1}^{p} [(\ell_j', \ell_k') + (\ell_j, V^c \ell_k)]\hat{\psi}_k = \lambda \sum_{k=1}^{p} [(\ell_j, \ell_k)\hat{\psi}_k$$

Stiffness matrix $\tilde{\mathbf{K}}_{jk} = (\ell_j', \ell_k')$

Confining potential $\tilde{\mathbf{V}}^{\mathbf{c}}_{jk} = (\ell_j, V^c \ell_k)$

Mass matrix $\tilde{\mathbf{M}}_{jk} = (\ell_j, \ell_k)$

Spatial discretization - one particle

Weak form of generalized eigenvalue problem

$$\sum_{k=1}^{p} [(\ell_j', \ell_k') + (\ell_j, V^c \ell_k)]\hat{\psi}_k = \lambda \sum_{k=1}^{p} [(\ell_j, \ell_k)\hat{\psi}_k$$

Stiffness matrix $\tilde{\mathbf{K}}_{jk} = (\ell_j', \ell_k')$

Confining potential $\tilde{\mathbf{V}}^{\mathbf{c}}_{jk} = (\ell_j, V^c \ell_k)$

Mass matrix $\tilde{\mathbf{M}}_{jk} = (\ell_j, \ell_k)$

Compute inner products with quadrature

$$\tilde{\mathbf{M}}_{jk} = \sum_{i=1}^{p} \ell_j(x_i)\ell_k(x_i)w_i, \quad \tilde{\mathbf{K}}_{jk} = \sum_{i=1}^{p} \ell_j'(x_i)\ell_k'(x_i)w_i$$

Spatial discretization - one particle

Weak form of generalized eigenvalue problem

$$\sum_{k=1}^{p}[(\ell_j', \ell_k') + (\ell_j, V^c \ell_k)]\hat{\psi}_k = \lambda \sum_{k=1}^{p}[(\ell_j, \ell_k)\hat{\psi}_k$$

Stiffness matrix $\tilde{\mathbf{K}}_{jk} = (\ell_j', \ell_k')$

Confining potential $\tilde{\mathbf{V}}^{\mathbf{c}}_{jk} = (\ell_j, V^c \ell_k)$

Mass matrix $\tilde{\mathbf{M}}_{jk} = (\ell_j, \ell_k)$

Compute inner products with quadrature

$$\tilde{\mathbf{M}}_{jk} = \sum_{i=1}^{p} \ell_j(x_i)\ell_k(x_i)w_i, \quad \tilde{\mathbf{K}}_{jk} = \sum_{i=1}^{p} \ell_j'(x_i)\ell_k'(x_i)w_i$$

All variable coefficient matrices are *diagonal*.

Spatial discretization - one particle

The mass matrix just contains the weights

$$\tilde{\mathbf{M}}_{jk} = w_j \delta_{jk}$$

Spatial discretization - one particle

The mass matrix just contains the weights

$$\tilde{\mathbf{M}}_{jk} = w_j \delta_{jk}$$

Trivial Cholesky factorization

$$\tilde{\mathbf{M}} = \mathbf{R}^\top \mathbf{R}, \quad \mathbf{R}_{jk} = \sqrt{w_j}\delta_{jk}$$

Spatial discretization - one particle

The mass matrix just contains the weights

$$\tilde{\mathbf{M}}_{jk} = w_j \delta_{jk}$$

Trivial Cholesky factorization

$$\tilde{\mathbf{M}} = \mathbf{R}^\top \mathbf{R}, \quad \mathbf{R}_{jk} = \sqrt{w_j}\delta_{jk}$$

The mass matrix is now the identity

$$[\mathbf{K} + \mathbf{V^c}]\hat{\varphi} = \lambda\hat{\varphi}, \quad \mathbf{K} = \mathbf{R}^{-\top}\tilde{\mathbf{K}}\mathbf{R}^{-1}, \quad \mathbf{V^v} = \mathbf{R}^{-\top}\tilde{\mathbf{V}}^{\mathbf{c}}\mathbf{R}^{-1}$$

This is algebraically equivalent to collocation

Spatial discretization - n particles

In principle need p^n grid points...

Spatial discretization - n particles

In principle need p^n grid points...

however, (anti)symmetry relations reduce the number of basis functions to N_p

$$N_p = \begin{pmatrix} p \\ n \end{pmatrix} = \frac{p!}{n!(p-n)!}$$

Spatial discretization - n particles

In principle need p^n grid points...

however, (anti)symmetry relations reduce the number of basis functions to N_p

$$N_p = \binom{p}{n} = \frac{p!}{n!(p-n)!}$$

Build a set of indices containing all unique n-tuples

Spatial discretization - n particles

In principle need p^n grid points...

however, (anti)symmetry relations reduce the number of basis functions to N_p

$$N_p = \left(\begin{array}{c} p \\ n \end{array} \right) = \frac{p!}{n!(p-n)!}$$

Build a set of indices containing all unique n-tuples

Can do this with one MATLAB command

```
map=nchoosek(1:p,n);
```

Spatial discretization - n particles

In principle need p^n grid points...

however, (anti)symmetry relations reduce the number of basis functions to N_p

$$N_p = \begin{pmatrix} p \\ n \end{pmatrix} = \frac{p!}{n!(p-n)!}$$

Build a set of indices containing all unique n-tuples

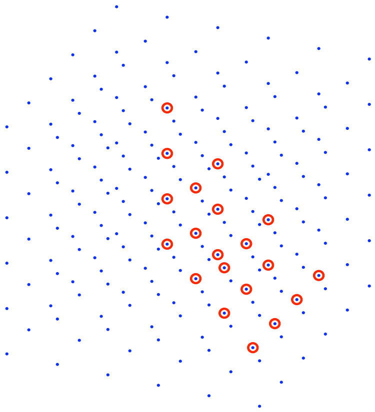
Can do this with one MATLAB command

```
map=nchoosek(1:p,n);
```

This returns an $N_p \times n$ matrix of all n-tuples, which happen to be the n-dimensional indices of grid points in the simplex.

3-tuples for $p = 6$

j	j_1	j_2	j_3
1	1	2	3
2	1	2	4
3	1	2	5
4	1	2	6
5	1	3	4
6	1	3	5
7	1	3	6
8	1	4	5
9	1	4	6
10	1	5	6
11	2	3	4
12	2	3	5
13	2	3	6
14	2	4	5
15	2	4	6
16	2	5	6
17	3	4	5
18	3	4	6
19	3	5	6
20	4	5	6



n particle stiffness matrix elements

n particle trial function φ is a Slater determinant of L^2-normalized Lagrange polynomials.

n particle stiffness matrix elements

n particle trial function φ is a Slater determinant of L^2-normalized Lagrange polynomials.

$$(\partial_{x_\gamma}\varphi_j, \partial_{x_\gamma}\varphi_k) = K^\gamma_{jk}$$

n particle stiffness matrix elements

n particle trial function φ is a Slater determinant of L^2-normalized Lagrange polynomials.

$$(\partial_{x_\nu}\varphi_j, \partial_{x_\nu}\varphi_k) = K^\nu_{jk}$$

Löwden rule for Slater inner products

$$K^\nu_{jk} = \det\begin{pmatrix} \delta_{j_1,k_1} & \cdots & \delta_{j_1,k_{\nu-1}} & K_{j_1,k_\nu} & \delta_{j_1,k_{\nu+1}} & \cdots & \delta_{j_1,k_n} \\ \vdots & & \vdots & \vdots & \vdots & & \vdots \\ \delta_{j_n,k_1} & \cdots & \delta_{j_n,k_{\nu-1}} & K_{j_n,k_\nu} & \delta_{j_n,k_{\nu+1}} & \cdots & \delta_{j_n,k_n} \end{pmatrix}$$

n particle stiffness matrix elements

n particle trial function φ is a Slater determinant of L^2-normalized Lagrange polynomials.

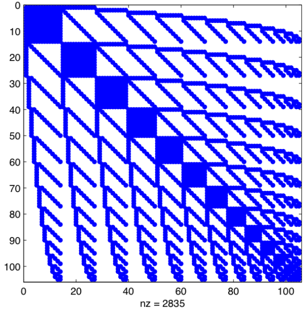
$$(\partial_{x_\nu}\varphi_j, \partial_{x_\nu}\varphi_k) = K^\nu_{jk}$$

Löwden rule for Slater inner products

$$K^\nu_{jk} = \det \begin{pmatrix} \delta_{j_1,k_1} & \cdots & \delta_{j_1,k_{\nu-1}} & K_{j_1,k_\nu} & \delta_{j_1,k_{\nu+1}} & \cdots & \delta_{j_1,k_n} \\ \vdots & & \vdots & \vdots & \vdots & & \vdots \\ \delta_{j_n,k_1} & \cdots & \delta_{j_n,k_{\nu-1}} & K_{j_n,k_\nu} & \delta_{j_n,k_{\nu+1}} & \cdots & \delta_{j_n,k_n} \end{pmatrix}$$

n particle stiffness matrix elements are taken directly from the single particle matrix with possible sign change

Stiffness matrix sparsity pattern



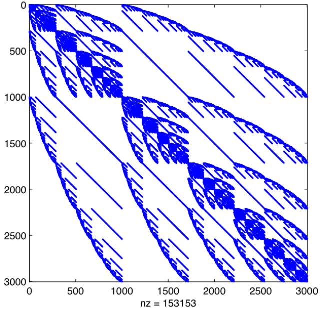


Figure: Left: $p = 15$ and $n = 2$, Right: $p = 15$ and $n = 5$

Stiffness matrix sparsity pattern

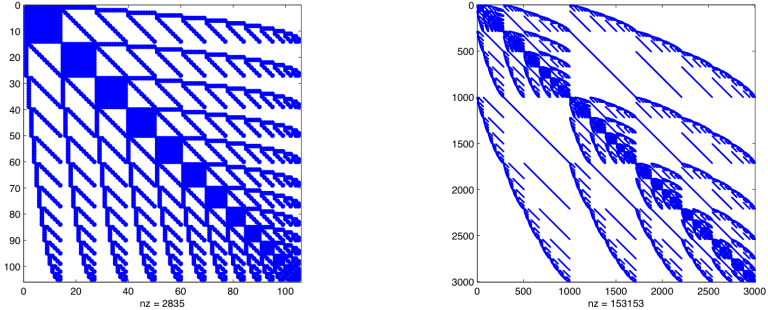


Figure: Left: $p = 15$ and $n = 2$, Right: $p = 15$ and $n = 5$

The off-diagonal sparsity pattern is that of the Johnson Graph's adjacency matrix

Discretization

Semi-discrete state equation

$$i\psi_t = \{\mathbf{H}_0 + u(t)\mathbf{V^c}\}\psi, \quad \psi \in \mathbb{C}^{N_p}$$

Discretization

Semi-discrete state equation

$$i\psi_t = \{\mathbf{H}_0 + u(t)\mathbf{V^c}\}\psi, \quad \psi \in \mathbb{C}^{N_p}$$

Compute $N_s << N_p$ eigenpairs (Λ, Φ) of stationary Hamiltonian

$$\mathbf{H}_0\Phi = \Phi\Lambda, \quad \Phi \in \mathbb{R}^{N_p \times N_s}, \quad \Lambda \in \mathbb{R}^{N_s \times N_s}$$

Discretization

Semi-discrete state equation

$$i\psi_t = \{\mathbf{H}_0 + u(t)\mathbf{V^c}\}\psi, \quad \psi \in \mathbb{C}^{N_p}$$

Compute $N_s << N_p$ eigenpairs (Λ, Φ) of stationary Hamiltonian

$$\mathbf{H}_0\Phi = \Phi\Lambda, \quad \Phi \in \mathbb{R}^{N_p \times N_s}, \quad \Lambda \in \mathbb{R}^{N_s \times N_s}$$

Reduced order model

$$iy_t = \{\Lambda + u(t)\mathbf{X}\}y, \quad y \in \mathbb{C}^{N_s}, \quad \mathbf{X} = \Phi^\top \mathbf{V^c}\Phi$$

Discretization

Semi-discrete state equation

$$i\psi_t = \{\mathbf{H}_0 + u(t)\mathbf{V^c}\}\psi, \quad \psi \in \mathbb{C}^{N_p}$$

Compute $N_s << N_p$ eigenpairs (Λ, Φ) of stationary Hamiltonian

$$\mathbf{H}_0\Phi = \Phi\Lambda, \quad \Phi \in \mathbb{R}^{N_p \times N_s}, \quad \Lambda \in \mathbb{R}^{N_s \times N_s}$$

Reduced order model

$$iy_t = \{\Lambda + u(t)\mathbf{X}\}y, \quad y \in \mathbb{C}^{N_s}, \quad \mathbf{X} = \Phi^\top \mathbf{V^c}\Phi$$

More compactly

$$y_t = \mathbf{A}(t)y, \quad \mathbf{A}(t) = -i\{\Lambda + u(t)\mathbf{X}\}$$

Discretization and the Lagrangian

Modified Crank-Nicolson time stepping

$$\left(I - \frac{\delta t}{4}[A_k + A_{k+1}]\right) y_k = \left(I + \frac{\delta t}{4}[A_k + A_{k-1}]\right) y_{k-1}$$

Discretization and the Lagrangian

Modified Crank-Nicolson time stepping

$$\left(I - \frac{\delta t}{4}[A_k + A_{k+1}]\right) y_k = \left(I + \frac{\delta t}{4}[A_k + A_{k-1}]\right) y_{k-1}$$

This becomes the kth equality constraint

$$e_k(y_k, y_{k-1}, u_k, u_{k-1}) = 0$$

Discretization and the Lagrangian

Modified Crank-Nicolson time stepping

$$\left(I - \frac{\delta t}{4}[A_k + A_{k+1}]\right) y_k = \left(I + \frac{\delta t}{4}[A_k + A_{k-1}]\right) y_{k-1}$$

This becomes the kth equality constraint

$$e_k(y_k, y_{k-1}, u_k, u_{k-1}) = 0$$

$$L(y, \bar{y}, u, \lambda, \bar{\lambda}) = 1 - \bar{y}_n^\top P y_n + \frac{1}{2} u^\top W u + \sum_{k=1}^{N} \lambda_k^\top e_k + \bar{\lambda}_k^\top \bar{e}_k$$

First-order optimality conditions

State equation

$$\left(I - \frac{\delta t}{4}[A_k + A_{k-1}]\right) y_k = \left(I + \frac{\delta t}{4}[A_k + A_{k-1}]\right) y_{k-1}$$

First-order optimality conditions

State equation

$$\left(I - \frac{\delta t}{4}[A_k + A_{k-1}]\right) y_k = \left(I + \frac{\delta t}{4}[A_k + A_{k-1}]\right) y_{k-1}$$

Adjoint equation

$$\left(I - \frac{\delta t}{4}[A_k + A_{k-1}]\right) \lambda_k = \left(I + \frac{\delta t}{4}[A_k + A_{k+1}]\right) \lambda_{k+1}$$

First-order optimality conditions

State equation

$$\left(I - \frac{\delta t}{4}[A_k + A_{k-1}]\right) y_k = \left(I + \frac{\delta t}{4}[A_k + A_{k-1}]\right) y_{k-1}$$

Adjoint equation

$$\left(I - \frac{\delta t}{4}[A_k + A_{k-1}]\right) \lambda_k = \left(I + \frac{\delta t}{4}[A_k + A_{k+1}]\right) \lambda_{k+1}$$

Final condition $\lambda_N = P\bar{y}_N$

First-order optimality conditions

State equation

$$\left(I - \frac{\delta t}{4}[A_k + A_{k-1}]\right) y_k = \left(I + \frac{\delta t}{4}[A_k + A_{k-1}]\right) y_{k-1}$$

Adjoint equation

$$\left(I - \frac{\delta t}{4}[A_k + A_{k-1}]\right) \lambda_k = \left(I + \frac{\delta t}{4}[A_k + A_{k+1}]\right) \lambda_{k+1}$$

Final condition $\lambda_N = P\bar{y}_N$

Control equation and reduced gradient

$$\nabla \tilde{J}(u) = Wu - \frac{\delta t}{2}\mathrm{Im}[\xi] = 0$$

$$\xi_k = \lambda_k^\top \mathbf{X}(y_k + y_{k-1}) + \lambda_{k+1}^\top \mathbf{X}(y_{k+1} + y_k)$$

Second-order optimality conditions

KKT system

$$\begin{pmatrix} L_{yy} & 0 & L_{yu} & 0 & L_{y\bar{\lambda}} \\ 0 & L_{\bar{y}\bar{y}} & L_{\bar{y}u} & L_{\bar{y}\lambda} & 0 \\ L_{uy} & L_{u\bar{y}} & L_{uu} & L_{u\lambda} & L_{u\bar{\lambda}} \\ 0 & L_{\lambda\bar{y}} & L_{\lambda u} & 0 & 0 \\ L_{\bar{\lambda}y} & 0 & L_{\bar{\lambda}u} & 0 & 0 \end{pmatrix} \begin{pmatrix} \delta y \\ \delta\bar{y} \\ \delta u \\ \delta\lambda \\ \delta\bar{\lambda} \end{pmatrix} = - \begin{pmatrix} 0 \\ 0 \\ L_u \\ 0 \\ 0 \end{pmatrix}$$

Second-order optimality conditions

KKT system

$$\begin{pmatrix} L_{yy} & 0 & L_{yu} & 0 & L_{y\bar{\lambda}} \\ 0 & L_{\bar{y}\bar{y}} & L_{\bar{y}u} & L_{\bar{y}\lambda} & 0 \\ L_{uy} & L_{u\bar{y}} & L_{uu} & L_{u\lambda} & L_{u\bar{\lambda}} \\ 0 & L_{\lambda\bar{y}} & L_{\lambda u} & 0 & 0 \\ L_{\bar{\lambda}y} & 0 & L_{\bar{\lambda}u} & 0 & 0 \end{pmatrix} \begin{pmatrix} \delta y \\ \delta\bar{y} \\ \delta u \\ \delta\lambda \\ \delta\bar{\lambda} \end{pmatrix} = - \begin{pmatrix} 0 \\ 0 \\ L_u \\ 0 \\ 0 \end{pmatrix}$$

Differential change in state and adjoint

$$\begin{aligned} \delta y &= -L_{\bar{\lambda}y}^{-1} L_{\bar{\lambda}u} \delta u \\ \delta\lambda &= -L_{\bar{y}\lambda}\delta\lambda^{-1}[L_{\bar{y}u}\delta u + L_{\bar{y}\bar{y}}\delta\bar{y}] \end{aligned}$$

Second-order optimality conditions

KKT system

$$\begin{pmatrix} L_{yy} & 0 & L_{yu} & 0 & L_{y\bar{\lambda}} \\ 0 & L_{\bar{y}\bar{y}} & L_{\bar{y}u} & L_{\bar{y}\lambda} & 0 \\ L_{uy} & L_{u\bar{y}} & L_{uu} & L_{u\lambda} & L_{u\bar{\lambda}} \\ 0 & L_{\lambda\bar{y}} & L_{\lambda u} & 0 & 0 \\ L_{\bar{\lambda}y} & 0 & L_{\bar{\lambda}u} & 0 & 0 \end{pmatrix} \begin{pmatrix} \delta y \\ \delta\bar{y} \\ \delta u \\ \delta\lambda \\ \delta\bar{\lambda} \end{pmatrix} = - \begin{pmatrix} 0 \\ 0 \\ L_u \\ 0 \\ 0 \end{pmatrix}$$

Differential change in state and adjoint

$$\delta y = -L_{\bar{\lambda}y}^{-1} L_{\bar{\lambda}u} \delta u$$
$$\delta\lambda = -L_{\bar{y}\lambda} \delta\lambda^{-1} [L_{\bar{y}u} \delta u + L_{\bar{y}\bar{y}} \delta\bar{y}]$$

Action of reduced Hessian

$$[\nabla^2 \tilde{J}(u)]\delta u = L_{uu} \delta u + 2\mathrm{Re}[L_{uy} \delta y + L_{u\lambda} \delta\lambda]$$

Second-order optimality conditions

KKT system

$$\begin{pmatrix} L_{yy} & 0 & L_{yu} & 0 & L_{y\bar{\lambda}} \\ 0 & L_{\bar{y}\bar{y}} & L_{\bar{y}u} & L_{\bar{y}\lambda} & 0 \\ L_{uy} & L_{u\bar{y}} & L_{uu} & L_{u\lambda} & L_{u\bar{\lambda}} \\ 0 & L_{\lambda\bar{y}} & L_{\lambda u} & 0 & 0 \\ L_{\bar{\lambda}y} & 0 & L_{\bar{\lambda}u} & 0 & 0 \end{pmatrix} \begin{pmatrix} \delta y \\ \delta\bar{y} \\ \delta u \\ \delta\lambda \\ \delta\bar{\lambda} \end{pmatrix} = - \begin{pmatrix} 0 \\ 0 \\ L_u \\ 0 \\ 0 \end{pmatrix}$$

Differential change in state and adjoint

$$\delta y = -L_{\bar{\lambda}y}^{-1} L_{\bar{\lambda}u} \delta u$$
$$\delta\lambda = -L_{\bar{y}\lambda}\delta\lambda^{-1}[L_{\bar{y}u}\delta u + L_{\bar{y}\bar{y}}\delta\bar{y}]$$

Action of reduced Hessian

$$[\nabla^2 \tilde{J}(u)]\delta u = L_{uu}\delta u + 2\mathrm{Re}[L_{uy}\delta y + L_{u\lambda}\delta\lambda]$$

Iteratively compute Newton direction with symmetric LQ method

$$[\nabla^2 \tilde{J}(u)]\delta u = -\nabla\tilde{J}(u)$$

Initial step length

Conventional wisdom: start with $a_0 = 1$ for Newton and quasi-Newton methods.

Initial step length

Conventional wisdom: start with $a_0 = 1$ for Newton and quasi-Newton methods.

The tracking part of the cost functional is bounded between 0 and 1 for all controls by virtue of the unitarity of the state equation

Initial step length

Conventional wisdom: start with $a_0 = 1$ for Newton and quasi-Newton methods.

The tracking part of the cost functional is bounded between 0 and 1 for all controls by virtue of the unitarity of the state equation

The cost functional is bounded from below by the regularization term.

Initial step length

Conventional wisdom: start with $a_0 = 1$ for Newton and quasi-Newton methods.

The tracking part of the cost functional is bounded between 0 and 1 for all controls by virtue of the unitarity of the state equation

The cost functional is bounded from below by the regularization term.

This amounts to a quadratic polynomial and we can write

$$J(\mathbf{u} + a\mathbf{d}) \geqslant m_2 a^2 + m_1 a + m_0$$

Initial step length

Conventional wisdom: start with $a_0 = 1$ for Newton and quasi-Newton methods.

The tracking part of the cost functional is bounded between 0 and 1 for all controls by virtue of the unitarity of the state equation

The cost functional is bounded from below by the regularization term.

This amounts to a quadratic polynomial and we can write

$$J(\mathbf{u} + a\mathbf{d}) \geqslant m_2 a^2 + m_1 a + m_0$$

Where the coefficients are given by $m_0 = \frac{\gamma}{2}\mathbf{u}^\top \mathbf{K}\mathbf{u} - J(\mathbf{u}) \leqslant 0$, $m_1 = \gamma \mathbf{u}^\top \mathbf{K}\mathbf{d}$, and $m_2 = \frac{\gamma}{2}\mathbf{d}^\top \mathbf{K}\mathbf{d}$.

Initial step length

Conventional wisdom: start with $a_0 = 1$ for Newton and quasi-Newton methods.

The tracking part of the cost functional is bounded between 0 and 1 for all controls by virtue of the unitarity of the state equation

The cost functional is bounded from below by the regularization term.

This amounts to a quadratic polynomial and we can write

$$J(\mathbf{u} + a\mathbf{d}) \geqslant m_2 a^2 + m_1 a + m_0$$

Where the coefficients are given by $m_0 = \frac{\gamma}{2}\mathbf{u}^\top \mathbf{K}\mathbf{u} - J(\mathbf{u}) \leqslant 0$, $m_1 = \gamma \mathbf{u}^\top \mathbf{K}\mathbf{d}$, and $m_2 = \frac{\gamma}{2}\mathbf{d}^\top \mathbf{K}\mathbf{d}$.

We can establish an upper bound on the maximum feasible step length

$$a_{\max} = \frac{\sqrt{m_1^2 - 4m_0 m_2} - m_1}{2m_2}$$

A priori estimate

Before evaluating $J(\mathbf{u} + a\mathbf{d})$, for some a, we know what the maximum feasible a can be to satisfy the SWC. This gives an a priori estimate on whether the cost functional is locally quadratic.

A priori estimate

Before evaluating $J(\mathbf{u} + a\mathbf{d})$, for some a, we know what the maximum feasible a can be to satisfy the SWC. This gives an a priori estimate on whether the cost functional is locally quadratic.

In particular, if $a_{\text{max}} < 1$, $J(\mathbf{u})$ is not locally quadratic.

A priori estimate

Before evaluating $J(\mathbf{u} + a\mathbf{d})$, for some a, we know what the maximum feasible a can be to satisfy the SWC. This gives an a priori estimate on whether the cost functional is locally quadratic.

In particular, if $a_{\text{max}} < 1$, $J(\mathbf{u})$ is not locally quadratic.

Make an initial step length of $\min(1, a_{\text{max}})$.

Model Reduction: Connectivity of states

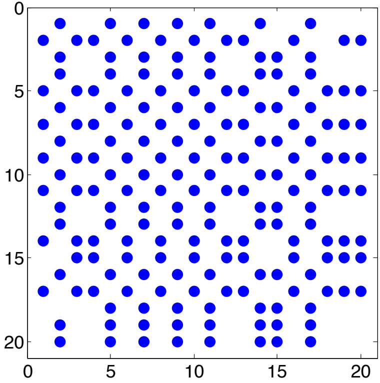


Figure: *Left:* Sparsity of interaction matrix $\mathbf{X}$.

Model Reduction: Connectivity of states

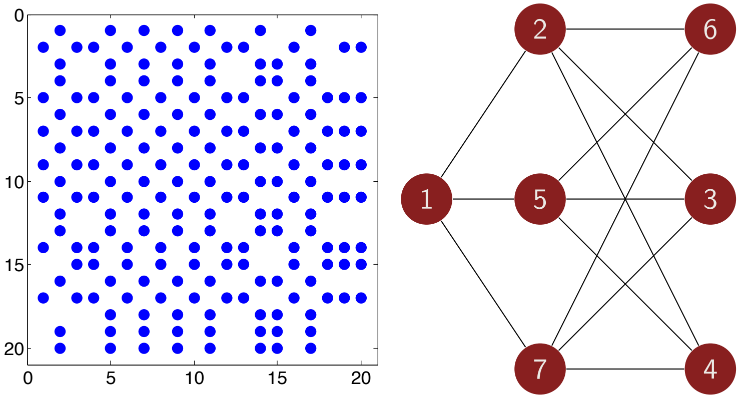


Figure: *Left:* Sparsity of interaction matrix $\mathbf{X}$. *Right:* Model reduction: Connectivity graph

Model reduction: Interaction picture

Time-dependent change of basis

$$y(t) = \exp(-i\Lambda t)z(t)$$

Model reduction: Interaction picture

Time-dependent change of basis

$$y(t) = \exp(-i\Lambda t)z(t)$$

Obtain new equation for $z(t)$

$$\dot{z}(t) = -iu(t)\exp(i\Lambda t)\mathbf{X}\exp(-i\Lambda t)z(t)$$

Model reduction: Interaction picture

Time-dependent change of basis

$$y(t) = \exp(-i\Lambda t) z(t)$$

Obtain new equation for $z(t)$

$$\dot{z}(t) = -iu(t) \exp(i\Lambda t) \mathbf{X} \exp(-i\Lambda t) z(t)$$

Write time-dependent interaction matrix

$$\tilde{\mathbf{X}}(t) = \exp(i\Lambda t) \mathbf{X} \exp(-i\Lambda t), \quad \tilde{\mathbf{X}}_{jk}(t) = \mathbf{X}_{jk} \exp i\omega_{jk} t$$

Where $\omega_{jk} = \lambda_j - \lambda_k$.

Model reduction: Interaction picture

Time-dependent change of basis

$$y(t) = \exp(-i\Lambda t)z(t)$$

Obtain new equation for $z(t)$

$$\dot{z}(t) = -iu(t)\exp(i\Lambda t)\mathbf{X}\exp(-i\Lambda t)z(t)$$

Write time-dependent interaction matrix

$$\tilde{\mathbf{X}}(t) = \exp(i\Lambda t)\mathbf{X}\exp(-i\Lambda t), \quad \tilde{\mathbf{X}}_{jk}(t) = \mathbf{X}_{jk}\exp i\omega_{jk}t$$

Where $\omega_{jk} = \lambda_j - \lambda_k$.
Write in integral form

$$z(T) = z(0) - i\int_0^t u(t)\tilde{\mathbf{X}}(t)z(t)dt$$

Model reduction: Interaction picture

We don't know $u(t)$ and $z(t)$ in advance.

We don't know $u(t)$ and $z(t)$ in advance.

However, $\tilde{\mathbf{X}}(t)$ is known and

$$\hat{\mathbf{X}} = \int_0^T \tilde{\mathbf{X}}_{jk}(t)dt, \quad \hat{\mathbf{X}}_{jk} = \mathbf{X}_{jk} \frac{\exp(i\omega_{jk}T) - 1}{i\omega_{jk}}$$

Model reduction: Interaction picture

We don't know $u(t)$ and $z(t)$ in advance.

However, $\tilde{\mathbf{X}}(t)$ is known and

$$\hat{\mathbf{X}} = \int_0^T \tilde{\mathbf{X}}_{jk}(t)dt, \quad \hat{\mathbf{X}}_{jk} = \mathbf{X}_{jk}\frac{\exp(i\omega_{jk}T) - 1}{i\omega_{jk}}$$

The $\hat{\mathbf{X}}_{jk}$ are like an inverse *cost* associated with the transition $|j\rangle \to |k\rangle$ or indicates how strongly the interaction couples the two states.

Model reduction: Interaction picture

We don't know $u(t)$ and $z(t)$ in advance.

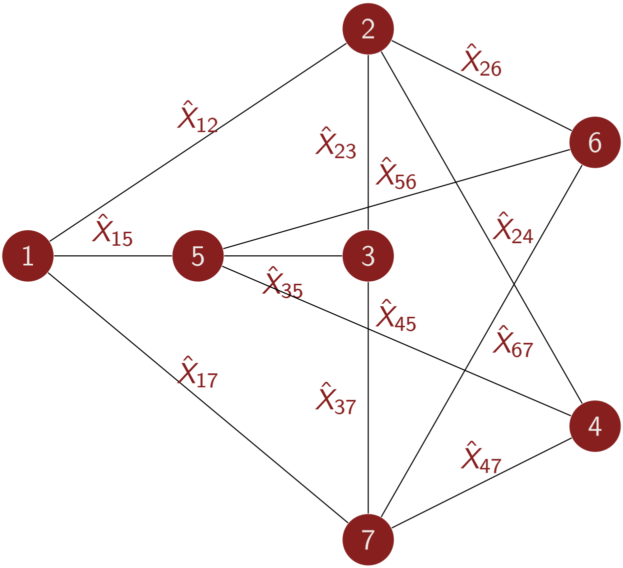
However, $\tilde{\mathbf{X}}(t)$ is known and

$$\hat{\mathbf{X}} = \int_0^T \tilde{\mathbf{X}}_{jk}(t)dt, \quad \hat{\mathbf{X}}_{jk} = \mathbf{X}_{jk} \frac{\exp(i\omega_{jk}T) - 1}{i\omega_{jk}}$$

The $\hat{\mathbf{X}}_{jk}$ are like an inverse *cost* associated with the transition $|j\rangle \rightarrow |k\rangle$ or indicates how strongly the interaction couples the two states.

Rank the connections of other states based on strength of coupling.

Model reduction: State coupling



Model reduction: Coupling strength

Heuristic idea: normalize coupling strength of state to self as 1.

Model reduction: Coupling strength

Heuristic idea: normalize coupling strength of state to self as 1.

The states most strongly coupled to e_i will have largest magnitude

$$r_1 = |e_i + \hat{\mathbf{X}} e_i|$$

This if for a single step from e_i to each other state.

Model reduction: Coupling strength

Heuristic idea: normalize coupling strength of state to self as 1.

The states most strongly coupled to e_i will have largest magnitude

$$r_1 = |e_i + \hat{\mathbf{X}} e_i|$$

This if for a single step from e_i to each other state.

Can have transition from e_i to e_j via intermediate state

$$r_2 = |e_i + \hat{\mathbf{X}} e_i + \hat{\mathbf{X}}^2 e_i|$$

Model reduction: Coupling strength

Heuristic idea: normalize coupling strength of state to self as 1.

The states most strongly coupled to e_i will have largest magnitude

$$r_1 = |e_i + \hat{\mathbf{X}} e_i|$$

This if for a single step from e_i to each other state.

Can have transition from e_i to e_j via intermediate state

$$r_2 = |e_i + \hat{\mathbf{X}} e_i + \hat{\mathbf{X}}^2 e_i|$$

Assuming any number of steps between intermediate states

$$r_\infty = \left| \sum_{j=0}^{\infty} \hat{\mathbf{X}}^j e_i \right|$$

Model reduction: Coupling strength

Heuristic idea: normalize coupling strength of state to self as 1.

The states most strongly coupled to e_i will have largest magnitude

$$r_1 = |e_i + \hat{\mathbf{X}} e_i|$$

This if for a single step from e_i to each other state.

Can have transition from e_i to e_j via intermediate state

$$r_2 = |e_i + \hat{\mathbf{X}} e_i + \hat{\mathbf{X}}^2 e_i|$$

Assuming any number of steps between intermediate states

$$r_\infty = \left| \sum_{j=0}^{\infty} \hat{\mathbf{X}}^j e_i \right| = |(\mathbf{I} - \hat{\mathbf{X}})^{-1} e_i|$$

Sort elements of r_∞ in descending order.

Model reduction: Coupling strength

Example: order of states coupled to e_1 from strongest to weakest

$$\{1, 2, 7, 5, 3, 14, 11, 8, 4, 10, 9, 16, 12, 20, 15, 13, 6, 17, 18, 19\}$$

Model reduction: Coupling strength

Example: order of states coupled to e_1 from strongest to weakest

$$\{1, 2, 7, 5, 3, 14, 11, 8, 4, 10, 9, 16, 12, 20, 15, 13, 6, 17, 18, 19\}$$

Solve control problem with n_1 most coupled states to initial state. Obtain u_1^*.

Model reduction: Coupling strength

Example: order of states coupled to e_1 from strongest to weakest

$$\{1, 2, 7, 5, 3, 14, 11, 8, 4, 10, 9, 16, 12, 20, 15, 13, 6, 17, 18, 19\}$$

Solve control problem with n_1 most coupled states to initial state. Obtain u_1^*.

Augment state space to n_2, use u_1^* as initial guess. Obtain u_2^*.

Model reduction: Coupling strength

Example: order of states coupled to e_1 from strongest to weakest

$$\{1, 2, 7, 5, 3, 14, 11, 8, 4, 10, 9, 16, 12, 20, 15, 13, 6, 17, 18, 19\}$$

Solve control problem with n_1 most coupled states to initial state. Obtain u_1^*.

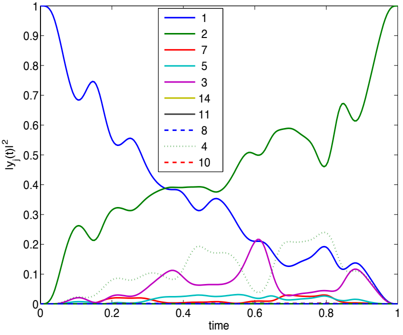
Augment state space to n_2, use u_1^* as initial guess. Obtain u_2^*.

Repeat until affect of augmenting state space on cost is less than tolerance.

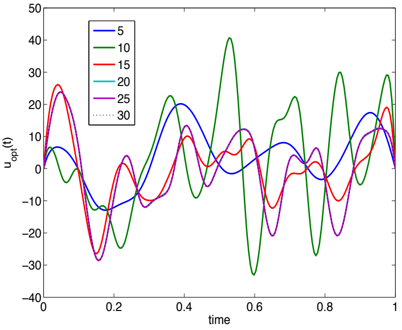
Numerical results - including $\exp(i\omega T)$

Here we have the state transition of the two particle system

$$|1,2\rangle \longrightarrow |1,3\rangle$$



(a) State occupancy vs. time

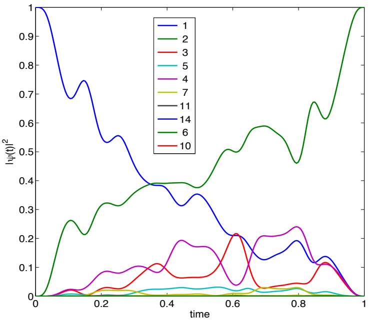


(b) Optimal control with refinement

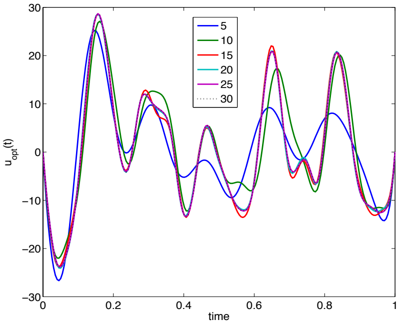
Numerical results - excluding $\exp(i\omega T)$

Here we have the state transition of the two particle system

$$|1,2\rangle \rightarrow |1,3\rangle$$



(c) State occupancy vs. time

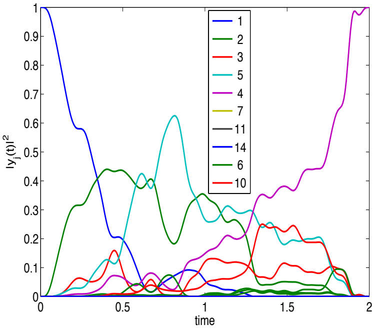


(d) Optimal control with refinement

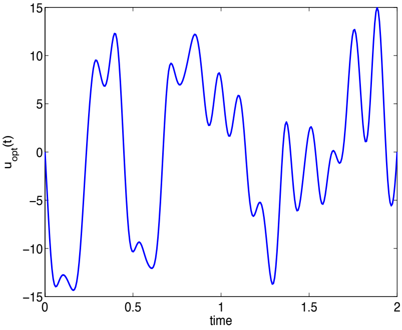
Numerical results - two particles

Here we have the state transition of the two particle system

$$|1,2\rangle \longrightarrow |1,4\rangle$$



(e) State occupancy vs. time

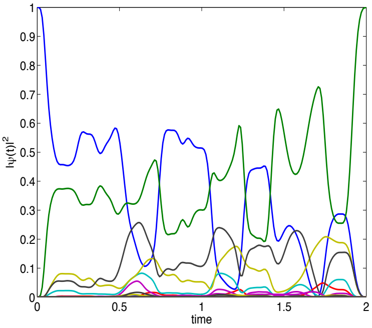


(f) Optimal control (50 modes)

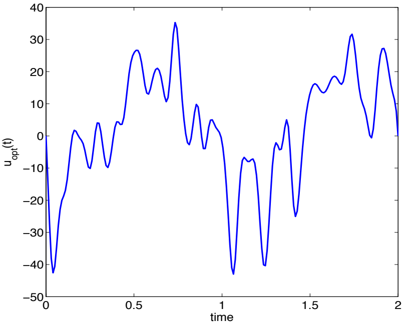
Numerical results - four particles

Here we have the state transition of the four particle system

$$|1,2,3,4\rangle \rightarrow |1,2,3,5\rangle \text{ state 1 to state 2}$$



(g) State occupancy vs. time

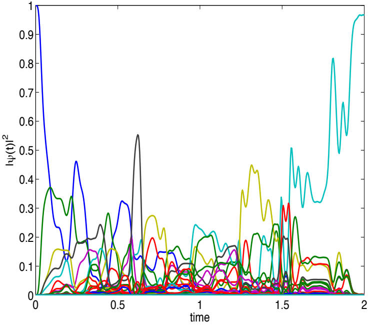


(h) Optimal control (50 modes)

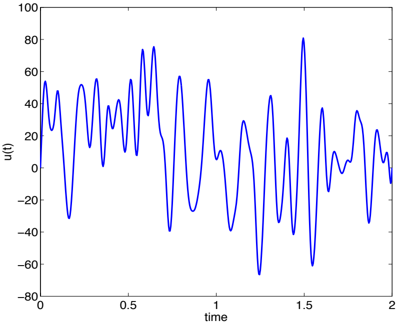
Numerical results - four particles

Here we have the state transition of the four particle system

$$|1,2,3,4\rangle \rightarrow |1,2,3,6\rangle \text{ state 1 to state 4}$$



(i) State occupancy vs. time



(j) Optimal control (50 modes)

Continuing work

- Extension to Gauß-Runge-Kutta time stepping

Continuing work

- Extension to Gauß-Runge-Kutta time stepping
- Automated update to state basis

Continuing work

- Extension to Gauß-Runge-Kutta time stepping
- Automated update to state basis
- Incorporation of spin

Continuing work

- Extension to Gauß-Runge-Kutta time stepping
- Automated update to state basis
- Incorporation of spin
- SR1-Trust region method may require less CPU time

Thank you for your attention