# A fast numerical method for the operator solution of the generalized Rosen-Zener model

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Exploiting Algebraic and Geometric Structure in Time-Integration Methods
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# Shrödinger equation

In Nuclear Magnetic Resonance (NMR) applications, the quantum dynamic of particles is described by the Schrödinger equation

$$\hbar \frac{\partial |\Psi\rangle}{\partial t} = -iH|\Psi\rangle,$$

with $H$ the (time-dependent) Hamiltonian and $\Psi$ the wave function.

- Simulations are of great importance. They provide benchmarks for studies of new materials, and the development of new magnetic fields.
- $H$ size increases exponentially with the number of particles.
- $H$ is sparse and structured (Kronecker).

# Extended Rosen-Zener model

- The Rosen-Zener (RZ) model [Rosen, Zener, 1932] is of the highest importance as representative of two-level quantum systems.
- Important in Nuclear Magnetic Resonance (NMR) [Silver, Joseph, Hoult, 1984; Hioe, 1984] and Magnetic Resonance Imaging (MRI) [Zhang, Garwood et al., 2017].
- In [Koyseva et al., 2007; Vitanov, 2010] the RZ model was extended to multiple degenerate sets of states in the framework of quantum-state engineering $\rightarrow$ Large-size ODE.
- The extended RZ model has been used as a test model for numerical solvers of non-autonomous evolutions equations [Blanes, Casas, Thalhammer, 2017; Blanes, Casas, Murua, 2017; Auzinger et al., 2019; Bader et al., 2022]

# Extended Rosen-Zener model

Goal: compute $U(t) \in \mathbb{C}^{N\times N}$, $N = 2k$, the operator solution of:

$$\partial_t U(t) = -iH(t)U(t), \quad U(s) = I_N.$$

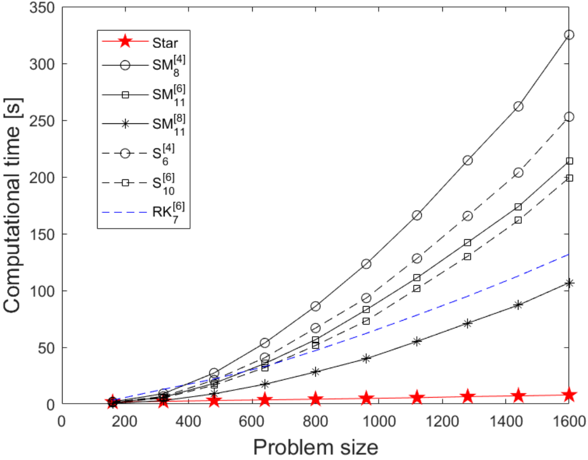
$$H(t) := \omega(t)\sigma_3 \otimes I_k + v(t)\sigma_1 \otimes M_k,$$

with the Pauli matrices $\sigma_j$ and $M_k \in \mathbb{R}^{k\times k}$:

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad M_k = \begin{bmatrix} 0 & 1 & & \\ 1 & 0 & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & 0 \end{bmatrix},$$

$$\sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \omega(t) := w_0 + \varepsilon \cos(\delta t), \; v(t) := \frac{v_0}{\cosh(t/T_0)}.$$

# A new (linear scaling?) algorithm: Preview



# Approach outline

| Problem | Linear ODE |
|---|---|
| ↓ | |
| New solution expression | $\star$-product |
| ↓ | |
| Discretization | Legendre polynomials |
| ↓ | |
| Matrix problem | Kronecker, low rank |
| ↓ | |
| Numerical solution | Iterative methods |

# The problem: two systems of linear ODEs

We will solve two related problems.
First, the quantum state vector case. Compute the $N$-size vector $\psi(t)$ solving:

$$\frac{\partial}{\partial t}\psi(t) = -H(t)\psi(t), \quad \psi(t_0) = \psi_0 \in \mathbb{C}^N, \quad t \in I = [t_0, t_f].$$

Second, the operator case. Compute the $N \times N$ matrix-valued function $U(t)$ solving

$$\frac{\partial}{\partial t}U(t) = -H(t)U(t), \quad U(t_0) = I_N, \quad t \in I = [t_0, t_f].$$

Note that $\psi(t) = U(t)\psi_0$.

We define the $\star$-product as [Giscard, P., Ryckebusch]

$$(f_2 \star f_1)(t,s) := \int_I f_2(t,\tau) f_1(\tau,s)\,\mathrm{d}\tau, \quad \Theta(t-s) = \begin{cases} 1, & t \geq s, \\ 0, & t < s \end{cases}$$

where $f_1(t,s), f_2(t,s)$ comes from a specific class of distributions: $f_j(t,s) = \tilde{f}_j(t,s)\Theta(t-s)$, $f_j$ analytic in $t,s \in I$.
Then the solution to the problems are:

$$U(t) = \hat{U}(t,t_0), \quad \psi(t) = \hat{U}(t,t_0)\psi_0,$$

with

$$\hat{U}(t,s) = \Theta(t-s) \star \left( I_N \delta(t-s) + iH(t)\Theta(t-s) \right)^{-\star}.$$

# Volterra Composition

§ 4. — **Risoluzione generale di equazioni integrali.**

9. Abbiasi una funzione analitica del tipo (1)

(1′) $$\mathbf{F}(z_1, z_2, \ldots, z_n).$$

Scriviamo l'equazione

(4) $$\mathbf{F}(z_1, z_2, \ldots, z_n) = 0.$$

$$S(x, y) = R(x, y) - \frac{1}{2} R^2(x, y) + \frac{1}{3} R^3(x, y) - \cdots + \frac{(-1)^n}{n} R^n(x, y) + \cdots$$

ove

$$R^n(x, y) = \int_x^y R^{n-1}(x, \xi)\, R(\xi, y)\, d\xi\,.$$

e non dovremo porre alcuna limitazione per i valori assoluti di $S(x, y)$, $R(x, y)$, purchè siano finiti.

10. Supponiamo in particolare che la (4′) sia un polinomio razionale e

[Volterra, Rend Lincei, 1910]

# Discretization: Legendre polynomial expansion

If $I = [-1, 1]$, $f(t, s)$ can be expanded in a 2D series:

$$f(t,s) = \tilde{f}(t)\Theta(t-s) \approx \sum_{k=0}^{m-1} \sum_{\ell=0}^{m-1} \alpha_{k,\ell} p_k(t) p_\ell(s),$$

with $p_k$ the orthonormal Legendre polynomials:

$$\int_{-1}^{1} p_k(\tau) p_\ell(\tau) d\tau = \delta_{k\ell},$$

and

$$\alpha_{k,l} = \int_{-1}^{1} p_k(\rho) \left( \int_{-1}^{1} f(\tau,\rho) p_\ell(\tau) d\tau \right) d\rho.$$

# Discretization: Legendre polynomial coefficients

The function is then represented by the matrix:

$$f(t,s) \to \begin{bmatrix} \alpha_{0,0} & \alpha_{0,1} & \cdots & \alpha_{0,m-1} \\ \alpha_{1,0} & \alpha_{1,1} & \cdots & \alpha_{1,m-1} \\ \vdots & \vdots & & \vdots \\ \alpha_{m-1,0} & \alpha_{m-1,1} & \cdots & \alpha_{m-1,m-1} \end{bmatrix} =: F$$

Note that

$$\begin{aligned} f(t,s) &\approx \sum_{k=0}^{m-1} \sum_{\ell=0}^{m-1} \alpha_{k,\ell} p_k(t) p_\ell(s) = \varphi_m(t)^T F \varphi_m(s) \\ &\approx \begin{bmatrix} p_0(t) & \dots & p_{m-1}(t) \end{bmatrix} F \begin{bmatrix} p_0(s) \\ \vdots \\ p_{m-1}(s) \end{bmatrix}. \end{aligned}$$

# Matrix problem: the resolvent

The discretized $\star$-product translates into the usual matrix algebra.

| | |
|---|---|
| $f(t,s)$ | $F_m$ |
| $1_\star = \delta(t-s)$ | $I_m$ |
| $f^{\star-1}$ | $F_m^{-1}$ |
| $g(t,s)$ | $G_m$ |
| $f \star g$ | $F_m G_m$ |
| $f + g$ | $F_m + G_m$ |
| $\Theta(t-s)$ | $T_m$ |
| $R_\star(f)$ | $(I_m - F_m)^{-1}$ |
| $\hat{U}(t,s)$ | $T_m(I_m - F_m)^{-1}$ |

# Kronecker structure and low-rank

In many applications, $H(t)$ is given as a sum of products:

$$H(t) = \sum_{j=0}^{s} H_j \times \tilde{f}_j(t),$$

with $H_j$ sparse matrices, and $\tilde{f}_j(t)$ analytic scalar functions. Our approach reformulates the problem as the linear system

$$\left( I_{Nm} + i \sum_{j=0}^{s} H_j \otimes F_j \right) \text{vec}(X) = \psi_0 \otimes \varphi_m(-1),$$

with vec the vectorization transformation and $F_j$ the Legendre discretization matrices. Equivelently, we have the matrix equation with a low-rank rhs (state vector case)

$$X + i \sum_{j=0}^{s} F_j X H_j^T = \varphi_m(-1) \psi_0^T.$$

# Matrix equation and the Rosen-Zener model

In the Rosen-Zener model for the state vector case we get the approximant:

$$\psi(t) \approx vec\left(\phi_M(t)^T T_M X\right), \quad t \in [-1, 1],$$

where $X \in \mathbb{C}^{M \times N}$ is the solution of the matrix equation

$$X + i\,\Omega_M X(\sigma_3 \otimes I_k) + i\,V_M X(\sigma_1 \otimes M_k) = \phi_M(-1)\psi_0^T,$$

with $\Omega_M$ and $V_M$ the $M \times M$ coefficient matrices of, respectively, $\omega(t)$ and $v(t)$.

# Numerical solution: Iterations for the state vector ODE

At this scope, we can derive from (18) the (implicit) iterates:

$$X_{n+1} + i\,\Omega_M X_{n+1}(\sigma_3 \otimes I_k) = -i\,V_M X_n(\sigma_1 \otimes M_k) + \phi_M(-1)\psi_0^T.$$

Thanks to the simple diagonal structure of the matrix $\sigma_3 \otimes I_k$, we get the *stationary iterative method*:

$$X_{n+1/2} = -i\,V_M X_n(\sigma_1 \otimes M_k) + \phi_M(-1)\psi_0^T;$$
$$X_{n+1} = G_1 X_{n+1/2} D_1 + G_2 X_{n+1/2} D_2,$$

with $X_0 = \phi_M(-1)\psi_0^T$ and

$$G_1 = (I_M + i\,\Omega_M)^{-1}, \quad D_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \otimes I_k,$$

$$G_2 = (I_M - i\,\Omega_M)^{-1}, \quad D_2 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \otimes I_k.$$

# Algorithm for the state vector

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**Require:** Error tolerance $tol > 0$ and svd truncation tolerance $trunc > 0$.

$L = \phi_M(-1)$; $R = \psi_0$;

$g = [G_1 L, G_2 L]$; $d = [D_1 R, D_2 R]$;

**while** $err \geq tol$ **do**

- $L = -i V_M L$; $R = (\sigma_1 \otimes M_k) R$; ▷ Iteration (6)
- $L = [G_1 L, G_2 L, g]$; $R = [D_1 R, D_2 R, d]$; ▷ Iteration (7)
- $L = Q_L R_L$; ▷ Economy-size QR decomposition
- $R_L = U S V^H$; ▷ Economy-size SVD decomposition
- $r = \min\{j : \sigma_j < trunc\}$, with $\text{diag}(\sigma_j) = S$;
- $L = Q_L U(:, 1:r) S(1:r, 1:r)$; ▷ Truncation
- $R = R$ conjugate$(V(:, 1:r))$; ▷ Truncation
- $b = L(R^T$ conjugate$(\psi_0))$; ▷ $b = (\psi_0^H \otimes I_M) vec(LR^T)$
- $err = \|b - b_{old}\|_2$ ▷ Cheap error estimate
- $b_{old} = b$;

**end while**

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$$X \approx LR^T$$

# Matrix equation and the Rosen-Zener model

In the Rosen-Zener model for the operator case we get the approximant:

$$U_{:,j}(t) \approx vec\left(\phi_M(t)^T T_M X^{(j)}\right),$$

where $U_{:,j}(t)$ is the $j$th column of $U(t)$. Here, $H^{(j)}$ is the solution of the equation

$$X + i\,\Omega_M X(\sigma_3 \otimes I_k) + i\,V_M X(\sigma_1 \otimes M_k) = \phi_M(-1)e_j,$$

i.e, the state vector equation with initial state $\psi_0 = e_j$.

# Algorithm for the operator solution

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**Require:** Error tolerance $tol > 0$ and svd truncation tolerance $trunc > 0$.

```
L = φ_M(−1);   R = I_n;
g = [G_1 L, G_2 L];   d = [D_1, D_2];
while err ≥ tol do
    L = −i V_M L;          R = (σ_1 ⊗ M_k) R;          ▷ Iteration (6)
    L = [G_1 L, G_2 L, g]; R = [D_1 R, D_2 R, d];      ▷ Iteration (7)
    L = Q_L R_L;                                       ▷ Economy-size QR decomposition
    R_L = U S V^H;                                     ▷ Economy-size SVD decomposition
    r = min{j : σ_j < trunc}, with diag(σ_j) = S;
    L = Q_L U(:, 1 : r) S(1 : r, 1 : r);               ▷ Truncation
    K = conjugate(V(:, 1 : r)) ⊗ I_N;
    R = RK;                                            ▷ Truncation
    b = L(R(1, 1 : N : 1 + (r − 1)N))^T;               ▷ b = X(:, 1)
    err = ||b − b_old||_2                              ▷ Cheap error estimate
    b_old = b;
end while
```

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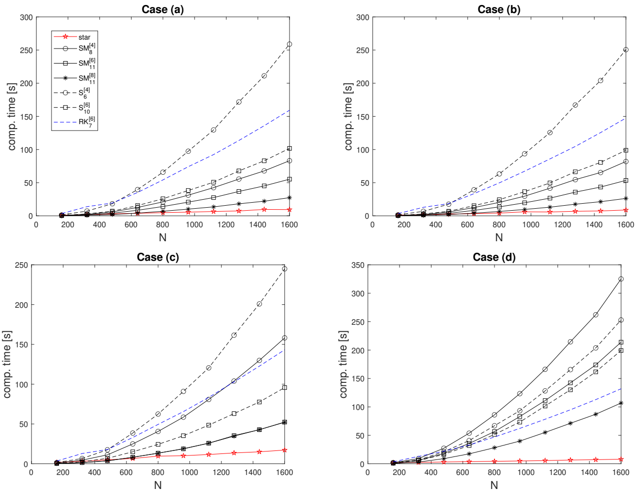
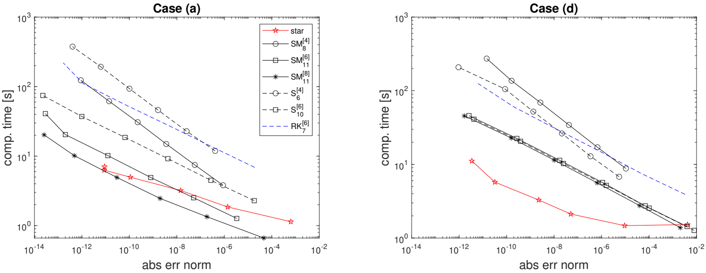
$$X^{(j)} \approx L\left(R(:, j : N : j + (r-1)N)\right)^T, \quad j = 1, \ldots, N.$$

# Comparison: size



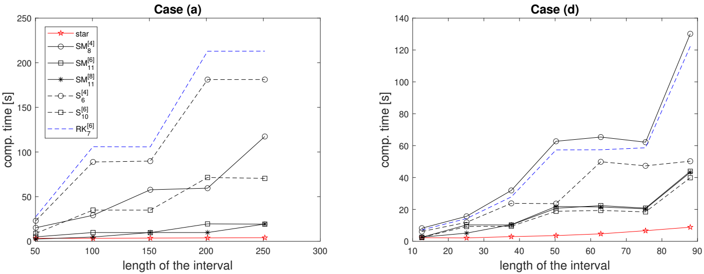

Error order $1e-7$. Examples and methods for the comparison from: [Blanes, Casas, Murua, The Journal of Chemical Physics, 2017]

# Comparison: accuracy




$N = 400$

# Comparison: interval length




$N = 400$, Error order $1e - 7$.

# Remarks

1. We introduce a new method for the operator solution of the Rosen-Zener model whose computational cost appears to scale linearly with the size of the problem.
2. The method seems to scale linearly also with the length of the domain if we do not include the discretization cost.
3. Probably because of the system condition number, the method cannot reach too high accuracy.
4. A method for the state vector case has also been introduced.
5. This proves that the new $\star$-approach to ODEs can play a crucial role in the resolution of increasingly large problems from quantum chemistry.

# References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- S. Pozza, arXiv:2302.11375 [math.NA] (2023).
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Projects

- Charles University PRIMUS research poject: *A Lanczos-like Method for the Time-Ordered Exponential, www.starlanczos.cz*.
- French ANR research project: *MAGICA (MAGnetic resonance techniques and Innovative Combinatorial Algebra)*.