Tensor train algorithms for quantum dynamics simulations of excited state nonadiabatic processes and quantum control

Victor S. Batista

Yale University, Department of Chemistry &
Energy Sciences Institute

NSF
DOE
NIH
AFOSR

The TT-SOFT Method

Multidimensional Nonadiabatic Quantum Dynamics

Samuel Greene and Victor S. Batista

Department of Chemistry, Yale University

Samuel Greene

The TT-SOFT Method

SOFT Propagation

$$\Psi(\mathbf{x}, t_0 + \tau) = \int \mathrm{d}\mathbf{x}' \, \langle \mathbf{x} | e^{-i\hat{H}\tau/\hbar} | \mathbf{x}' \rangle \, \Psi(\mathbf{x}', t_0),$$

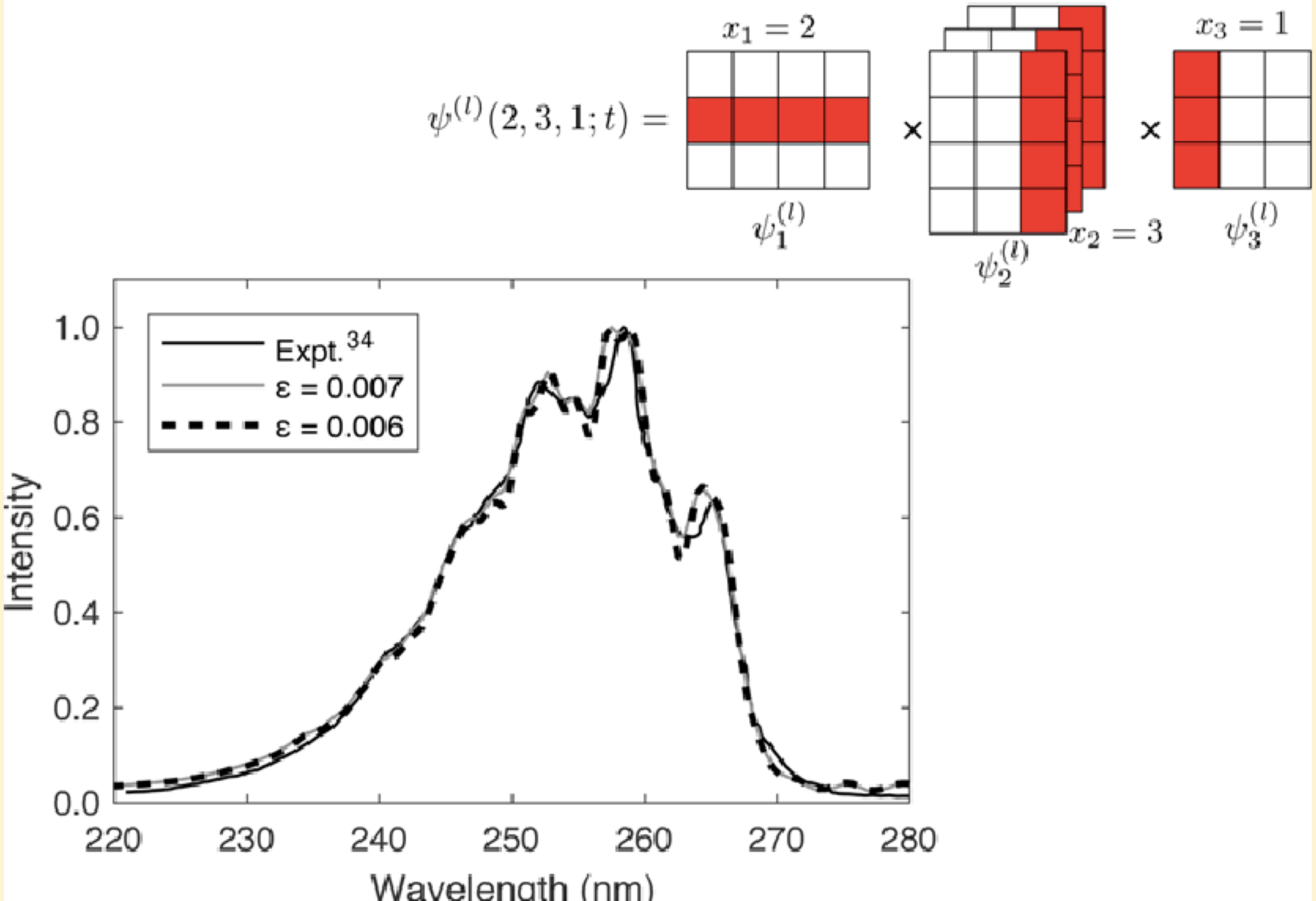
$$e^{-i\hat{H}\tau/\hbar} = e^{-i\hat{T}\tau/2\hbar} e^{-i\hat{V}\tau/\hbar} e^{-i\hat{T}\tau/2\hbar} + \mathcal{O}(\tau^3).$$

$$\hat{H} = \hat{T} + \hat{V},$$

$$\Psi(\mathbf{x}, t_0 + \tau) = \mathrm{IFT}\left[e^{-i\mathbf{p}\cdot\mathbf{m}^{-1}\cdot\mathbf{p}\tau/4\hbar} \, \mathrm{FT}\left[e^{-i\hat{V}(\mathbf{x}'')\tau/\hbar} \, \mathrm{IFT}\left[e^{-i\mathbf{p}\cdot\mathbf{m}^{-1}\cdot\mathbf{p}\tau/4\hbar} \, \mathrm{FT}\left[\Psi(\mathbf{x}', t_0)\right]\right]\right]\right]$$

TT Format

$$\psi^{(l)}(x_1, x_2, \ldots, x_d; t) = \sum_{\alpha_1, \alpha_2, \ldots, \alpha_{d-1}} \psi_1^{(l)}(x_1, \alpha_1; t)\psi_2^{(l)}(\alpha_1, x_2, \alpha_2; t) \cdots \psi_d^{(l)}(\alpha_{d-1}, x_d; t)$$



TT Format

Generic Tensor

$$A(i_1, i_2, \ldots, i_d) = \sum_{\alpha_1=1}^{r_1} \sum_{\alpha_2=1}^{r_2} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} A_1(i_1, \alpha_1) A_2(\alpha_1, i_2, \alpha_2) \cdots A_d(\alpha_{d-1}, i_d),$$

Wavepacket

$$\psi^{(l)}(x_1, x_2, \ldots, x_d; t) = \sum_{\alpha_1, \alpha_2, \ldots, \alpha_{d-1}} \psi_1^{(l)}(x_1, \alpha_1; t) \psi_2^{(l)}(\alpha_1, x_2, \alpha_2; t) \cdots \psi_d^{(l)}(\alpha_{d-1}, x_d; t)$$

Kinetic Propagator

$$U(\mathbf{p}) = e^{-i\mathbf{p}\cdot\mathbf{m}^{-1}\cdot\mathbf{p}\tau/2\hbar}, \qquad \mathbf{p} = (p_1, p_2, \ldots, p_d)$$

$$U(p_1, p_2, \ldots, p_d) = \sum_{\alpha_1, \alpha_2, \ldots, \alpha_{d-1}} U_1(p_1, \alpha_1) U_2(\alpha_1, p_2, \alpha_2) \cdots U_d(\alpha_{d-1}, p_d).$$

Multidimensional Vibronic Model

$$\hat{V} = \hat{V}_d + \hat{V}_c,$$

$$\hat{V}_c = \left(\sum_{i=1}^{d} c_i x_i + \sum_{i=1}^{d} \sum_{j=1}^{d} c_{ij} x_i x_j \right) (|1\rangle\langle 2| + |2\rangle\langle 1|)$$

$$\hat{V}_k = \left(E_k + \sum_{j=1}^{d} \frac{1}{2} m_j \omega_j x_j^2 + \sum_{i=1}^{d} a_i^k x_i + \sum_{i=1}^{d} \sum_{j=1}^{d} a_{ij}^k x_i x_j \right) |k\rangle\langle k|$$

25-Dimensional S_1/S_2 Wavepacket Components

$$\Psi(\mathbf{x},t) = \begin{pmatrix} \psi^{(1)}(\mathbf{x},t) \\ \psi^{(2)}(\mathbf{x},t) \end{pmatrix}$$

$$\begin{pmatrix} \psi''^{(1)}(\boldsymbol{x},t) \\ \psi''^{(2)}(\boldsymbol{x},t) \end{pmatrix} = e^{-iV\tau/\hbar} \begin{pmatrix} \psi'^{(1)}(\boldsymbol{x},t) \\ \psi'^{(2)}(\boldsymbol{x},t) \end{pmatrix}$$

$$e^{-iV\tau/\hbar} = \sum_{n=0}^{N} \frac{(-iV\tau/\hbar)^n}{n!}$$

Tensor-Train Split-Operator Fourier Transform (TT-SOFT) Method: Multidimensional Nonadiabatic Quantum Dynamics

Samuel M. Greene and Victor S. Batista

J. Chem. Theory Comput. 2017, **13**, 4034–4042

Survival Amplitude

$$C(t - t_0) = \langle \Psi(t_0) | \Psi(t) \rangle$$

dot product of tensor trains A and B

$$\sum_{i_1=1}^{n_1} \sum_{i_2=1}^{n_2} \cdots \sum_{i_d=1}^{n_d} A^*(i_1, i_2, \ldots, i_d) B(i_1, i_2, \ldots, i_d)$$

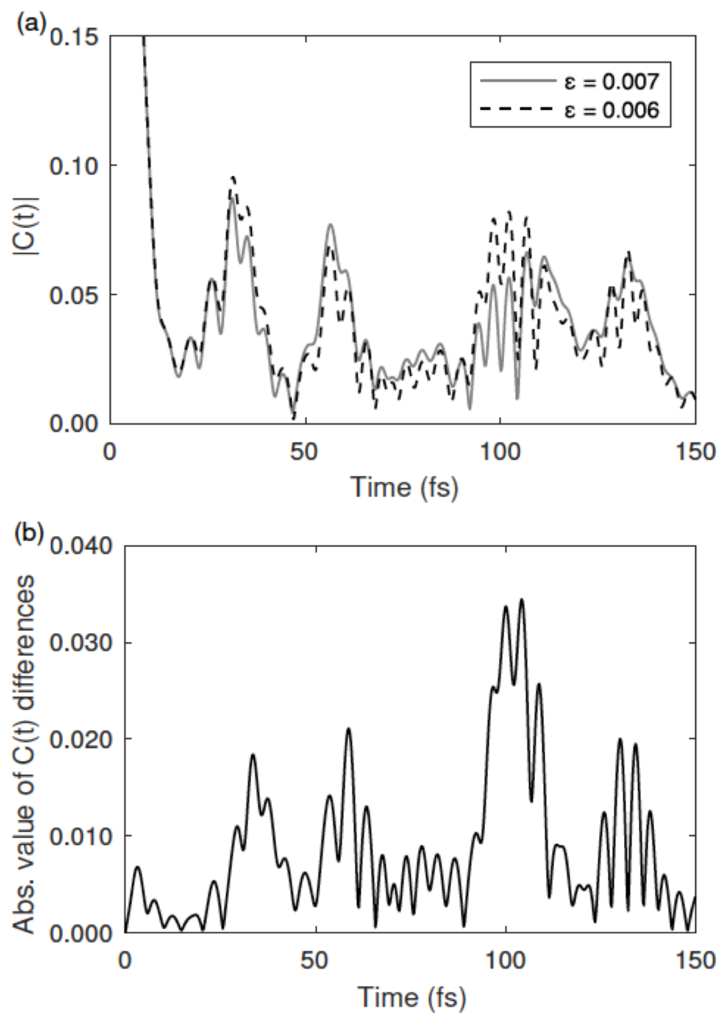
Photoabsorption Spectrum

$$I(\omega) \propto \omega \int_{-\infty}^{\infty} \mathrm{d}t \, C(t) e^{i\omega t}$$

Tensor-Train Split-Operator Fourier Transform (TT-SOFT) Method: Multidimensional Nonadiabatic Quantum Dynamics

Samuel M. Greene and Victor S. Batista

J. Chem. Theory Comput. 2017, **13**, 4034−4042



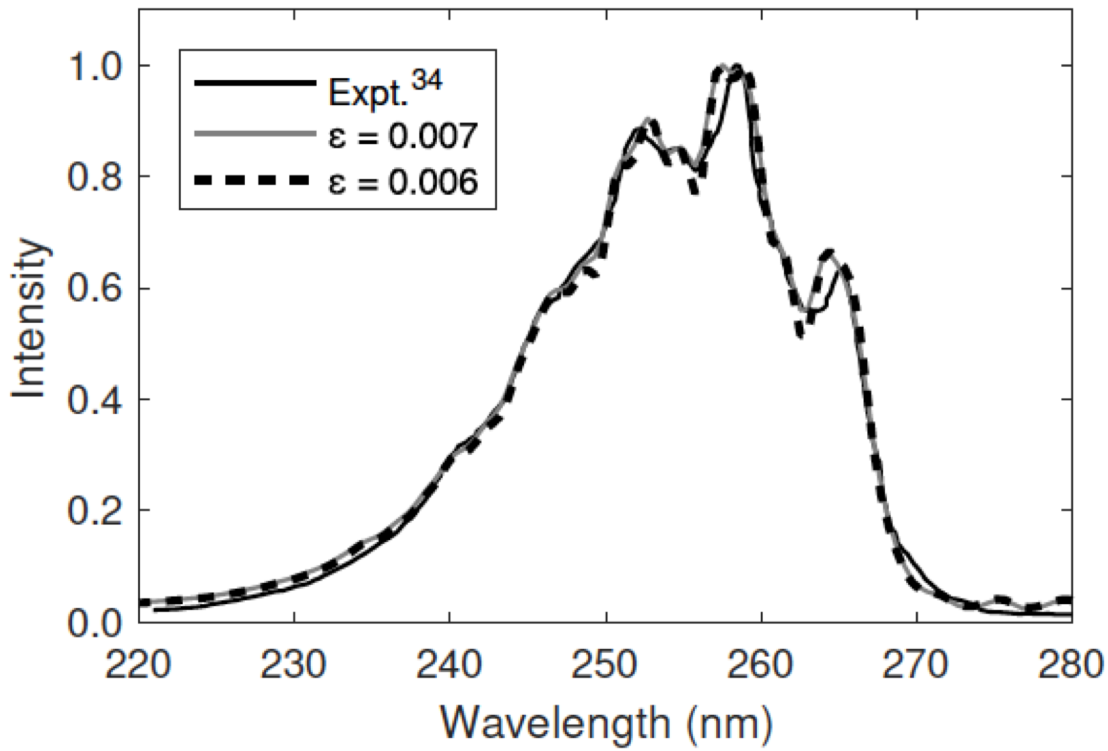
Tensor-Train Split-Operator Fourier Transform (TT-SOFT) Method: Multidimensional Nonadiabatic Quantum Dynamics

Samuel M. Greene and Victor S. Batista

J. Chem. Theory Comput. 2017, **13**, 4034−4042

Photoabsorption Spectrum

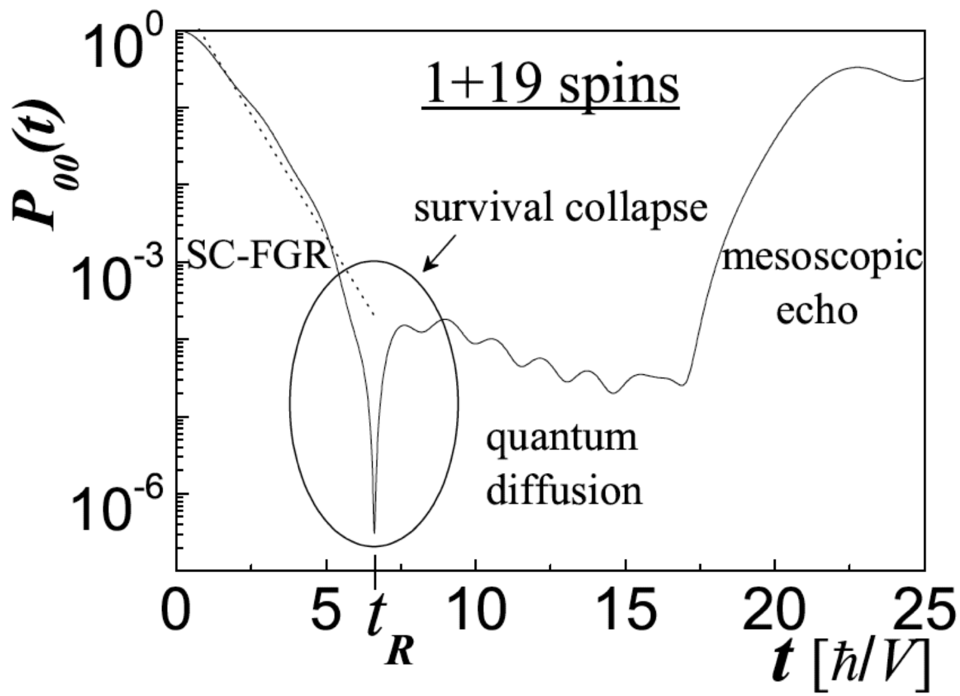
Comparison TT-SOFT versus Experimental Spectra of Pyrazine



Tensor-Train Split-Operator Fourier Transform (TT-SOFT) Method

DYNAMICS IN A NUCLEAR SPINS CHAIN

$$\hat{H} = \sum_{n=0}^{M-1} \hbar\Omega_n \hat{S}_n^z - \sum_{n=0}^{M-2} \frac{1}{2} J_{n+1,n} \left[\hat{S}_{n+1}^x \hat{S}_n^x + \hat{S}_{n+1}^y \hat{S}_n^y \right]$$



E. Rufeil Fiori, H.M. Pastawski *Chem. Phys. Lett.* 420: 35-41

Chebyshev Propagation

$$e^{-i\hat{H}t_m}\Psi_t = \sum_{k=0}^{N}(2-\delta_{k,0})J_k(t_m)(-i)^k T_k(\hat{H})\Psi_t$$

$$T_0\Psi_t = \Psi_t,$$

$$T_1\Psi_t = \hat{H}\Psi_t,$$

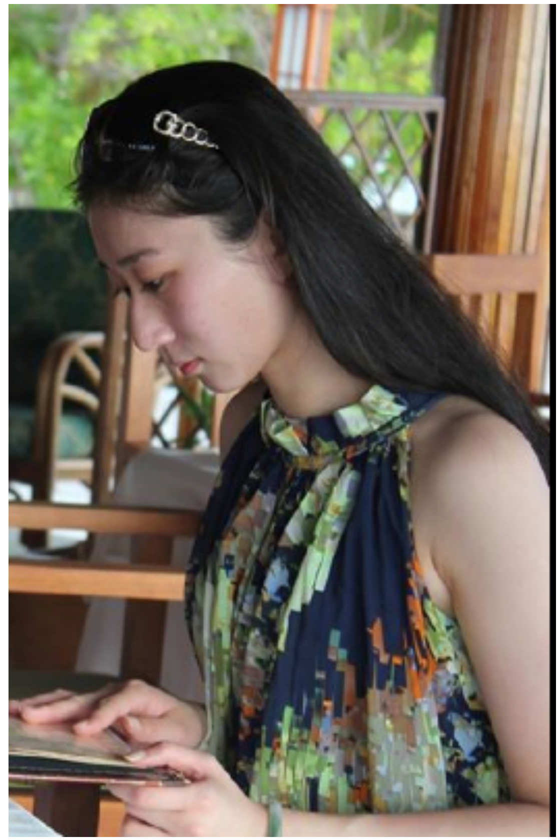
$$T_n\Psi_t = 2\hat{H}T_{n-1}\Psi_t - T_{n-2}\Psi_t,\ \text{for n} > 1$$

Chebyshev Propagation

```
function [cpol_tt] = cheb2(PE_tt,KE_tt,G_tt,Dp,Dm,dx,nx,dp,np,Npoly,eps)
% Chebyshev polynomials applied to state G_tt
cpol_tt{1}=G_tt;
cpol_tt{2}=round(times(PE_tt,G_tt),eps);
FT_G_tt=round(times(KE_tt,tt_FT(G_tt,dx,nx,1)),eps);
cpol_tt{2} = round((cpol_tt{2}+tt_FT(FT_G_tt,dp,np,-1))*2/Dm-G_tt*Dp/Dm,eps);
for j=3:Npoly
    cpol_tt{j}=round(2*times(PE_tt,cpol_tt{j-1}),eps);
    FT_G_tt=round(2*times(KE_tt,tt_FT(cpol_tt{j-1},dx,nx,1)),eps);
    cpol_tt{j} = round((cpol_tt{j}+tt_FT(FT_G_tt,dp,np,-1))*2/Dm
    ... -cpol_tt{j-1}*2*Dp/Dm,eps);
    cpol_tt{j} = round(cpol_tt{j}-cpol_tt{j-2},eps);
end
end
```

```
function [Gc_tt] = exp_cheb2(cpol_tt,t,Npoly,eps)
%  Chebyshev expansion of exp(-I*H*dt) applied to psi(xj)
Gc_tt=besselj(0,t)*cpol_tt{1};
for k=2:Npoly
    Gc_tt= round(Gc_tt+2*besselj(k-1,t)*cpol_tt{k}*(-1i)^(k-1),eps);
end
```

A Time-Sliced Thawed Gaussian Propagation Method for Simulations of Quantum Dynamics



Xiangmeng Kong and Victor S. Batista

Department of Chemistry, Yale University, New Haven, CT 06520-8107

Fast Gaussian Wavepacket Transform

$$\hat{\Psi}(p) = \sum_i g_i(p) \frac{g_i(p)}{\sum_j g_j^2(p)} \hat{\Psi}(p),$$

=1

$$= \sum_i g_i(p) \int dp' \delta(p'-p) \frac{g_i(p')}{\sum_j g_j^2(p')} \hat{\Psi}(p'),$$

$$= \sum_i g_i(p) \int dp' \left(\sum_k \frac{\Delta x}{2\pi} e^{-\imath(p-p')x_k} \right) \frac{g_i(p')}{\sum_j g_j^2(p')} \hat{\Psi}(p'),$$

$$= \sum_{i,k} \frac{\sqrt{\Delta x}}{\sqrt{2\pi}} g_i(p) e^{-\imath p x_k} \left(\int \frac{\sqrt{\Delta x}}{\sqrt{2\pi}} \frac{g_i(p') e^{\imath p' x_k}}{\sum_j g_j^2(p')} \hat{\Psi}(p') dp' \right)$$

$$= \sum_{i,k} \hat{\phi}_{i,k}(p) c_{i,k}.$$

$$c_{i,k} = \int \frac{\sqrt{\Delta x}}{\sqrt{2\pi}} \frac{g_i(p') e^{\imath p' x_k}}{\sum_i g_i^2(p')} \hat{\Psi}(p') dp'$$

FGWT

$$\hat{\phi}_{j,k}(p) = \frac{\sqrt{\Delta x}}{\sqrt{2\pi}} g_j(p) e^{-\imath p x_k} \qquad g_j(p) = e^{-(p-p_j)^2/\sigma^2}$$

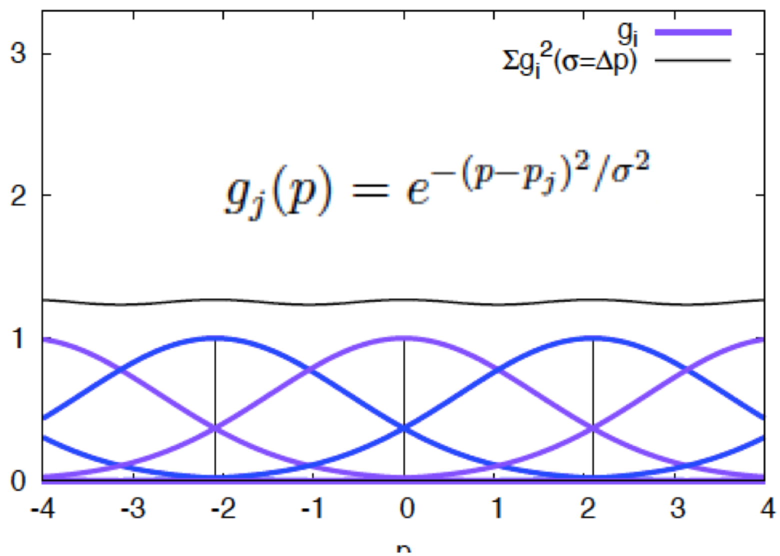
Qian, J.; Ying, L. Fast Gaussian Wavepacket Transforms and Gaussian Beams for the Schrödinger Equation. *J. Comp. Phys.* (2010) ***229***: 7848–7873.

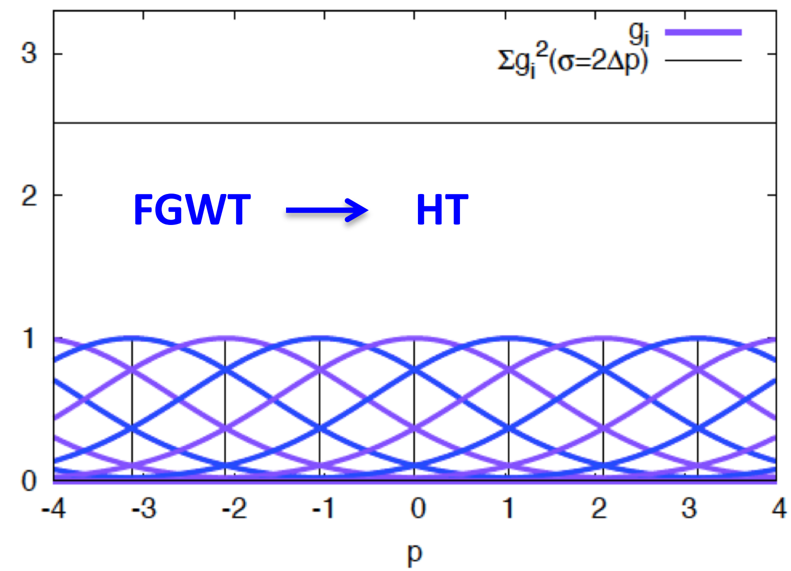
Kong, X.; Markmann, A.; Batista, V.S., A Time-Sliced Thawed Gaussian Propagation Method for Simulations of Quantum Dynamics. *J. Phys. Chem.* A 120: 3260-3269(2016).

Time Sliced Thawed Gaussian Propagation Method

Kong, X.; Markmann, A.; Batista, V.S., A Time-Sliced Thawed Gaussian Propagation Method for Simulations of Quantum Dynamics. *J. Phys. Chem.* A 120: 3260-3269(2016).

$$c_{i,k} = \int \frac{\sqrt{\Delta x}}{\sqrt{2\pi}} \frac{g_i(p') e^{ip' x_k}}{\sum_i g_i^2(p')} \hat{\Psi}(p') dp'$$





$$\Psi(x) = \pi^{-\frac{1}{4}} \alpha^{\frac{1}{4}} e^{-\frac{\alpha}{2}(x-x_0)^2 + ip_0(x-x_0)}$$

$$c_{j,k} = \frac{\sqrt{\Delta x}}{(\alpha\pi)^{1/4}} \frac{1}{S} \sqrt{\frac{\sigma^2 \alpha}{2\alpha + \sigma^2}} e^{-\frac{(p_j - p_0)^2}{(2\alpha+\sigma^2)}} e^{-\frac{\alpha\sigma^2 (x_0 - x_k)^2}{2(2\alpha+\sigma^2)}} e^{-i(x_0 - x_k)\frac{(2\alpha p_j + \sigma^2 p_0)}{(2\alpha+\sigma^2)}}$$

Time Sliced Thawed Gaussian Propagation Method

Kong, X.; Markmann, A.; Batista, V.S., A Time-Sliced Thawed Gaussian Propagation Method for Simulations of Quantum Dynamics. *J. Phys. Chem.* A 120: 3260-3269(2016).

$$\Psi(x) = \pi^{-\frac{1}{4}} \alpha^{\frac{1}{4}} e^{-\frac{\alpha}{2}(x-x_0)^2 + \imath p_0 (x-x_0)}$$

$$\Psi(x) = \sum_{j,k} c_{j,k} \phi_{j,k}(x)$$

↑

$$\begin{aligned} \phi_{j,k}(x) &= \frac{1}{\sqrt{2\pi}} \int \hat{\phi}_{j,k}(p) e^{\imath p x} dp, \\ &= \frac{\sqrt{\Delta x}}{\sqrt{\pi}} \frac{\sigma}{2} e^{-\frac{\sigma^2}{4}(x-x_k)^2 + i p_j (x-x_k)} \end{aligned}$$

$$c_{j,k} = \frac{\sqrt{\Delta x}}{(\alpha\pi)^{1/4}} \frac{1}{S} \sqrt{\frac{\sigma^2 \alpha}{2\alpha + \sigma^2}} e^{-\frac{(p_j - p_0)^2}{(2\alpha+\sigma^2)}} e^{-\frac{\alpha\sigma^2 (x_0 - x_k)^2}{2(2\alpha+\sigma^2)}} e^{-i(x_0 - x_k)\frac{(2\alpha p_j + \sigma^2 p_0)}{(2\alpha+\sigma^2)}}$$

Heller, E. J. Time-Dependent Approach to Semiclassical Dynamics. *J. Chem. Phys.* (1975) ***62***: 1544–1555.

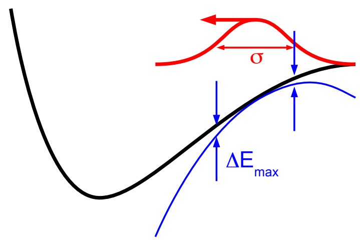
Thawed Gaussian Propagation

Solving time-dependent Schrödinger equation with numerically exact methods requires computational effort that scales exponentially with dimensionality of the system. This problem can be avoided by employing a representation of the wave functions in non-orthogonal narrow Gaussians

$$\Psi(\mathbf{x}, t=0) = \sum_j c_j G_j(\mathbf{x})$$

$$G(\mathbf{x}_j) = e^{i[(\mathbf{x}-\mathbf{x}_j)\mathbf{A}_j(\mathbf{x}-\mathbf{x}_j)+\mathbf{p}_j(\mathbf{x}-\mathbf{x}_j)+\gamma_j]}$$

that validate the local harmonic approximation.



$$V = V_0(\mathbf{x}_j) + \mathbf{V}_1 \cdot (\mathbf{x}-\mathbf{x}_j) + \frac{1}{2}(\mathbf{x}-\mathbf{x}_j)\cdot \mathbf{V}_2 \cdot (\mathbf{x}-\mathbf{x}_j)$$

With the local harmonic approximation, time-dependent Schrödinger equation for a basis Gaussian

$$i\hbar \frac{\partial G(\mathbf{x})}{\partial t} = [\hat{V} - \sum_{k=1}^{D} \frac{\partial^2_{x_k}}{2m_k}] G(\mathbf{x})$$

can be solved by comparing terms of the same orders

$$\dot{\mathbf{x}}_j = \mathbf{p}_j \cdot \mathbf{m}^{-1}$$

$$\dot{\mathbf{p}}_j = -\mathbf{V}_1$$

$$\dot{\mathbf{A}}_j = -2\mathbf{A}_j \cdot \mathbf{m}^{-1}\mathbf{A}_j - \mathbf{V}_2/2$$

$$\dot{\gamma}_j = itr[\mathbf{A}_j \cdot \mathbf{m}^{-1}] + \frac{1}{2}\mathbf{p}_j \cdot \mathbf{m}^{-1} \cdot \mathbf{p}_j - V_0$$

Gaussian Beam Thawed Gaussian Propagation
Hermite Gaussian Basis

$$\phi_{i,k}(x) = \frac{\sqrt{\Delta x}}{\sqrt{2\pi Q_k}} e^{-\frac{P_k}{2Q_k}(x-x_k)^2+\imath p_k(x-x_k)+\imath S_k}$$

$$\dot{x}_k = \frac{p_k}{m},$$

$$\dot{p}_k = -V'(x_k),$$

$$\dot{S}_k = p\dot{x}_k - \left(V(x_k) + \frac{p_k^2}{2m}\right)$$

$$\dot{Q}_k = \imath\frac{P_k}{m},$$

$$\dot{P}_k = \imath V''(x_k)Q_k,$$

Hagedorn, G. A.: Raising and lowering operators for semiclassical wave packets. *Ann. Phys.* **269**: 77-104 (1998)] and [Faou, E.,Gradinaru, V.; Lubich, C: Computing Semiclassical Quantum Dynamics with Hagedorn Wavepackets. *SIAM J. Sci. Comput.* **31**: 3027-3041 (2009)]:

Time Sliced Thawed Gaussian Propagation Method

Kong, X.; Markmann, A.; Batista, V.S., A Time-Sliced Thawed Gaussian Propagation Method for Simulations of Quantum Dynamics. *J. Phys. Chem.* A 120: 3260-3269(2016).

Lagrangian propagation

HT

$$\Psi(x) = \sum_{j,k} c_{j,k} \phi_{j,k}(x) \qquad \phi_{j,k}(x,\tau) = \sum_{j',k'} \tilde{c}^{j,k}_{j',k'}(\tau)\phi_{j',k'}(x,0)$$

$$\tilde{c}^{j,k}_{j',k'}(\tau) = \frac{\Delta x}{S\sqrt{2\pi}}\sqrt{\frac{\gamma_\tau \gamma}{(\gamma_\tau + \gamma)}} e^{-\frac{1}{2(\gamma_\tau+\gamma)}\left[\left(p_{j'} - p_j(\tau;k)\right)^2 + \gamma_\tau\gamma(x_k(\tau;j) - x_{k'})^2\right]} \times e^{i\left(S^{j,k}_\tau - (x_k(\tau;j)-x_{k'})\frac{\left(\gamma_\tau p_{j'} + \gamma p_j(\tau;k)\right)}{(\gamma_\tau+\gamma)}\right)}$$

$$\Psi(x,\tau) = \sum_{j,k} c_{j,k}\left(\sum_{j',k'} \tilde{c}^{j,k}_{j',k'}(\tau)\phi_{j',k'}(x)\right)$$

$$= \sum_{j',k'} c_{j',k'}(\tau)\phi_{j',k'}(x),$$

Eulerian propagation

$$c_{j',k'}(\tau) = \sum_{j,k} c_{j,k}\tilde{c}^{j,k}_{j',k'}(\tau)$$

Time Sliced Thawed Gaussian Propagation Method

n-dimensional implementation

Kong, X.; Markmann, A.; Batista, V.S., A Time-Sliced Thawed Gaussian Propagation Method for Simulations of Quantum Dynamics. *J. Phys. Chem.* A 120: 3260-3269(2016).

$$\Psi(\mathbf{x}) = \sum_{\mathbf{i},\mathbf{k}} c_{\mathbf{i},\mathbf{k}} \phi_{\mathbf{i},\mathbf{k}}(\mathbf{x})$$

$$\phi_{\mathbf{i},\mathbf{k}}(\mathbf{x}) = \prod_{d=1}^{n} \phi_{i_d,k_d}(x_d)$$

$$c_{\mathbf{i},\mathbf{k}} = \int dx_1 \cdots dx_n \prod_{d=1}^{n} \psi^*_{i_d,k_d}(x_d) \Psi(x_1, \cdots x_n)$$

$$\psi_{i_d,k_d}(x_d) = \frac{1}{S_d} \frac{\sqrt{\Delta x_d}}{\sqrt{2\pi}} \sqrt{\frac{\sigma_d^2}{2}} e^{-\frac{\sigma_d^2}{4}(x_d - x_{kd})^2 + \imath p_d (x_d - x_{kd})}$$

$$\Psi(\mathbf{x}) = e^{\imath[(\mathbf{x}-\mathbf{x}_0)\cdot\mathbf{A}_0\cdot(\mathbf{x}-\mathbf{x}_0)+\mathbf{p}_0\cdot(\mathbf{x}-\mathbf{x}_0)+\gamma_0]}$$

Time Sliced Thawed Gaussian Propagation Method

n-dimensional implementation

Kong, X.; Markmann, A.; Batista, V.S., A Time-Sliced Thawed Gaussian Propagation Method for Simulations of Quantum Dynamics. *J. Phys. Chem.* A 120: 3260-3269(2016).

$$c_{\mathbf{i},\mathbf{k}} = \int dx_1 \cdots dx_n \left(\prod_{d=1}^{n} \frac{\sigma_d \sqrt{\Delta x_d}}{2 S_d \sqrt{\pi}} \right)$$

$$\times\, e^{-(x_1 - x_{k1}, \ldots, x_n - x_{kn}) \begin{pmatrix} \frac{\sigma_1^2}{4} & & 0 \\ & \ddots & \\ 0 & & \frac{\sigma_n^2}{4} \end{pmatrix} \begin{pmatrix} x_1 - x_{k1} \\ \vdots \\ x_n - x_{kn} \end{pmatrix} - \imath (p_{i1}, \ldots, p_{in}) \begin{pmatrix} x_1 - x_{k1} \\ \vdots \\ x_n - x_{kn} \end{pmatrix}}$$

$$\times\, e^{\imath \left[(x_1 - x_{01}, \ldots, x_n - x_{0n}) \begin{pmatrix} A_{011} & \ldots & A_{01n} \\ \vdots & \ddots & \vdots \\ A_{0n1} & \ldots & A_{0nn} \end{pmatrix} \begin{pmatrix} x_1 - x_{01} \\ \vdots \\ x_n - x_{0n} \end{pmatrix} + (p_{01}, \ldots, p_{0n}) \begin{pmatrix} x_1 - x_{01} \\ \vdots \\ x_n - x_{0n} \end{pmatrix} + \gamma_0 \right]}$$

$$= N_c \int dx_1 \cdots dx_n \exp \left[-(x_1 - x_{01}, \ldots, x_n - x_{0n})\, \mathbf{A}_0' \begin{pmatrix} x_1 - x_{01} \\ \vdots \\ x_N - x_{0n} \end{pmatrix} + \mathbf{B} \begin{pmatrix} x_1 - x_{01} \\ \vdots \\ x_n - x_{0n} \end{pmatrix} + \gamma \right]$$

Time Sliced Thawed Gaussian Propagation Method

n-dimensional implementation

Kong, X.; Markmann, A.; Batista, V.S., A Time-Sliced Thawed Gaussian Propagation Method for Simulations of Quantum Dynamics. *J. Phys. Chem.* A 120: 3260-3269(2016).

$$c_{\mathbf{i},\mathbf{k}} = N_c \int dx_1 \cdots dx_n \; e^{-(x_1-x_{01},\ldots,x_n-x_{0n})\mathbf{A}_0' \begin{pmatrix} x_1 - x_{01} \\ \vdots \\ x_n - x_{0n} \end{pmatrix} + \mathbf{B} \begin{pmatrix} x_1 - x_{01} \\ \vdots \\ x_n - x_{0n} \end{pmatrix} + \gamma},$$

$$= N_c \left| \frac{\partial(x_1,\ldots,x_n)}{\partial(\xi_1,\ldots,\xi_n)} \right| \int d\xi_1 \cdots d\xi_n \; e^{-(\xi_1,\ldots,\xi_n) \begin{pmatrix} a_1 & & 0 \\ & \ddots & \\ 0 & & a_3 \end{pmatrix} \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_n \end{pmatrix} + (b_1,\ldots,b_n) \begin{pmatrix} \xi_1 \\ \vdots \\ \xi_n \end{pmatrix} + \gamma};$$

$$= N_c \, \pi^{n/2} \, e^{\gamma} \prod_{d=1}^{n} a_d^{-1/2} e^{\frac{b_d^2}{4a_d}},$$

Time Sliced Thawed Gaussian Propagation Method

n-dimensional propagation

Kong, X.; Markmann, A.; Batista, V.S., A Time-Sliced Thawed Gaussian Propagation Method for Simulations of Quantum Dynamics. *J. Phys. Chem.* A 120: 3260-3269(2016).

$$\phi_{\mathbf{i},\mathbf{k}}(\mathbf{x}) = e^{\imath[(\mathbf{x}-\mathbf{x}_k)\mathbf{A}(\mathbf{x}-\mathbf{x}_k)+\mathbf{p}_i(\mathbf{x}-\mathbf{x}_k)+\gamma]}$$

$$\mathbf{A} = \begin{pmatrix} \frac{\sigma_1^2}{4} & & 0 \\ & \ddots & \\ 0 & & \frac{\sigma_n^2}{4} \end{pmatrix},$$

$$\mathbf{p}_i = (p_{i_1}, p_{i_2}, \ldots, p_{i_n}),$$

$$\mathbf{x}_k = (x_{k_1}, x_{k_2}, \ldots, x_{k_n}),$$

$$\gamma = -\imath \sum_{d=1}^{n} \ln\left(\frac{\sigma_d\sqrt{\Delta x_d}}{2\sqrt{\pi}}\right).$$

$$\dot{\mathbf{x}}_k = \mathbf{p}_i \cdot \mathbf{m}^{-1},$$

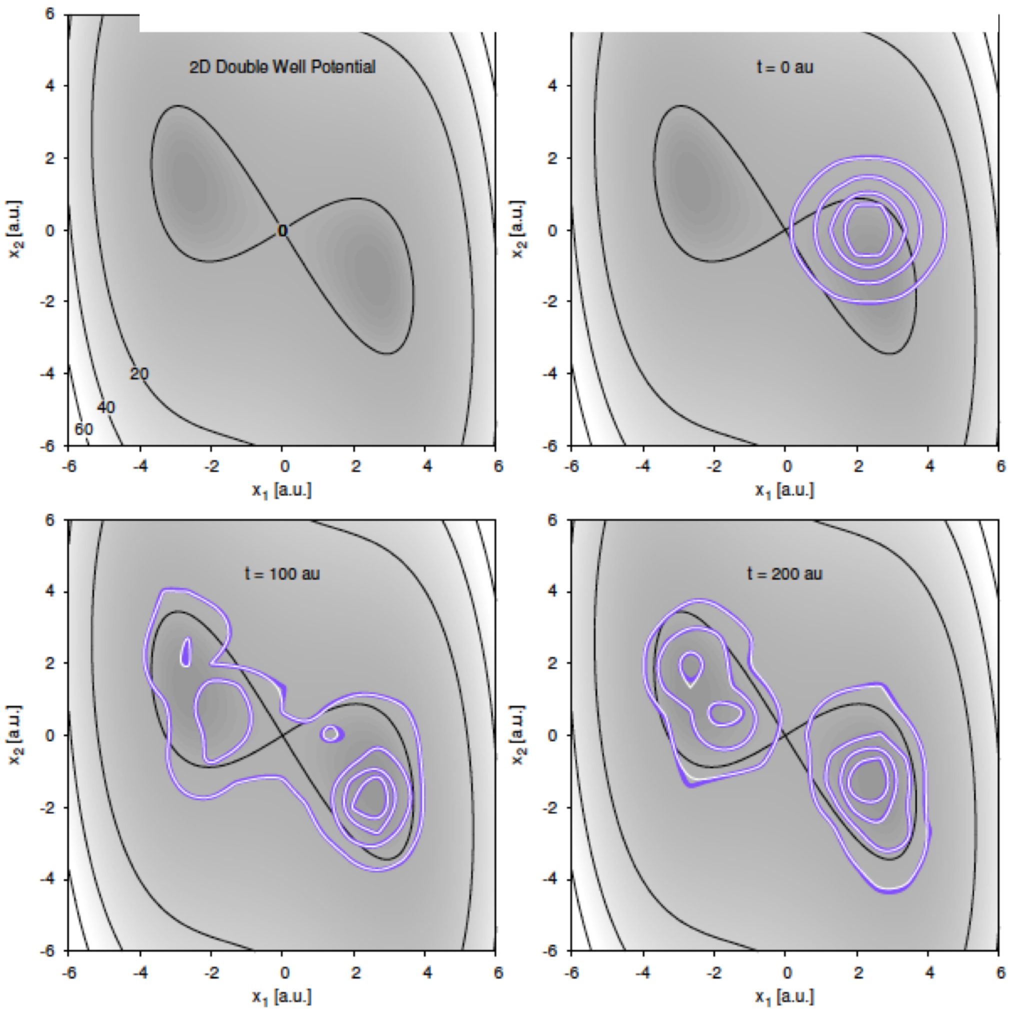
$$\dot{\mathbf{p}}_i = -\mathbf{V}'_k,$$

$$\dot{\mathbf{A}} = -2\mathbf{A}\mathbf{m}^{-1}\mathbf{A} - \frac{1}{2}\mathbf{V}''_k,$$

$$\dot{\gamma} = \imath Tr[\mathbf{A}\mathbf{m}^{-1}] + \frac{1}{2}\mathbf{p}_i\mathbf{m}^{-1}\mathbf{p}_i - V_k,$$

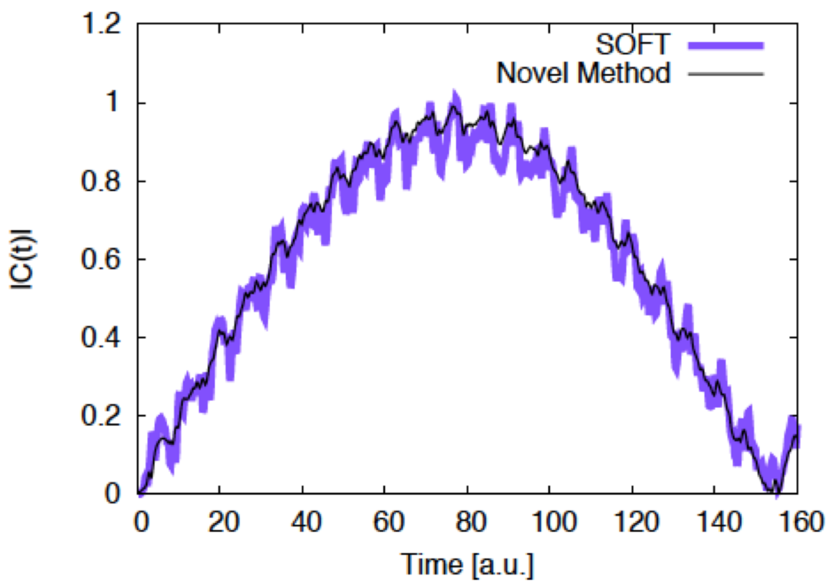
Benchmark Calculations: Comparison with SOFT

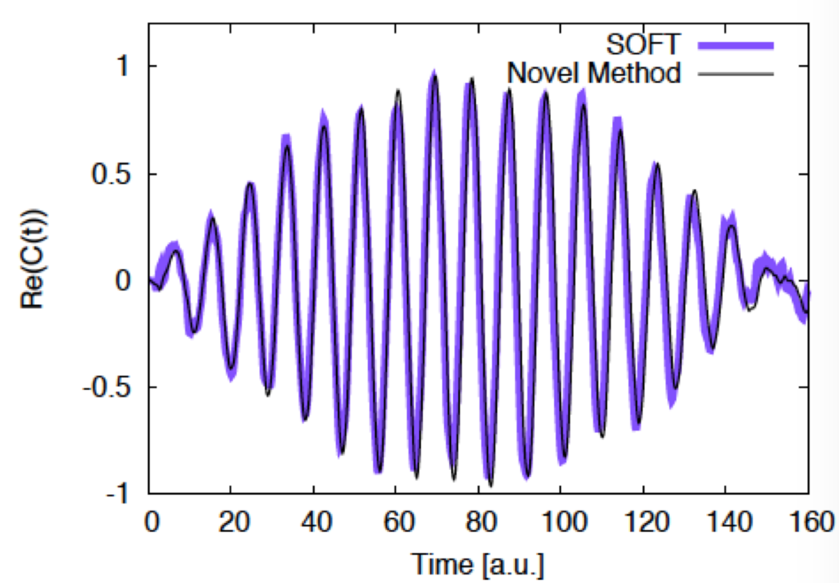
$$V(x_1, x_2) = \frac{x_1^4}{16\eta} - \frac{x_1^2}{2} + \frac{x_2^2}{2} + \frac{x_1 x_2}{2}$$



Benchmark Calculations: Comparison with SOFT

$$C(t) = \int dx \Psi^*(-x, 0)\Psi(x, t)$$



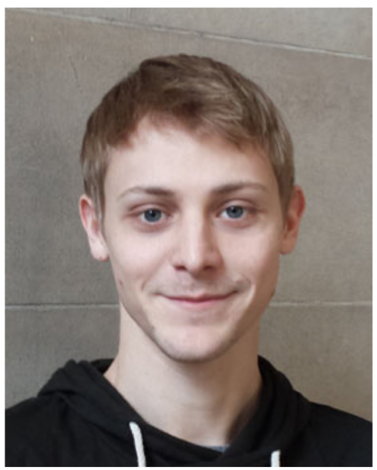


A New Bosonization Technique

The Single Boson Representation

Kenneth Jung, Xin Chen and Victor S. Batista

Department of Chemistry, Yale University



Kenneth Jung

Xin Chen

Holstein-Primakoff Representation

Spin-Boson Hamiltonian

$$\hat{H} = \frac{2}{\hbar}\left[\epsilon\hat{S}_z + J\hat{S}_x + \hat{S}_z \times f(\mathbf{y})\right] + H_b(\mathbf{y}, \mathbf{p}_y),$$

$$\hat{S}^- = \hat{a}^\dagger \hbar \sqrt{2S - \hat{N}} \qquad \hat{S}^+ = \hbar\sqrt{2S - \hat{N}}\hat{a}$$

$$\hat{S}_x = \frac{1}{2}\left[\hat{S}^+ + \hat{S}^-\right] = \frac{\hbar}{2}\left[\sqrt{2S - \hat{N}}\hat{a} + \hat{a}^\dagger\sqrt{2S - \hat{N}}\right] \qquad \hat{S}_z = \hbar(S - \hat{N})$$

$$[\hat{a}, \hat{a}^\dagger] = 1 \longrightarrow [\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z \qquad \hat{S}^2|\chi_+\rangle = \hbar^2 S(S+1)|\chi_+\rangle$$

$$\tilde{x} + i\tilde{p} = \sqrt{2}\hat{a} \qquad \tilde{x} - i\tilde{p} = \sqrt{2}\hat{a}^\dagger$$

$$\hat{H} = H_b(\mathbf{y}, \mathbf{p}_y) + (\epsilon + f(\mathbf{y}))(2S - (\tilde{x}^2 + \tilde{p}^2 - 1)) + J\tilde{x}\sqrt{4S - (\tilde{x}^2 + \tilde{p}^2 - 1)}$$

[T. Holstein and H. Primakoff *Phys. Rev.* **58**, 1098-1113 (1940)]

Schwinger-Bosonization

Schwinger-Jordan Transform

$$\hat{S}^+ = \hbar \hat{b}^\dagger \hat{a},$$

$$\hat{S}^- = \hbar \hat{a}^\dagger \hat{b},$$

$$\hat{S}_z = \frac{1}{2}\left[\hat{S}^+, \hat{S}^-\right] = \frac{\hbar}{2}\left(\hat{b}^\dagger \hat{b} - \hat{a}^\dagger \hat{a}\right),$$

$$\hat{S}_x = \frac{1}{2}\left(\hat{S}^+ + \hat{S}^-\right) = \frac{\hbar}{2}\left(\hat{b}^\dagger \hat{a} + \hat{a}^\dagger \hat{b}\right),$$

$$\hat{S}_y = \frac{1}{2i}\left(\hat{S}^+ - \hat{S}^-\right) = \frac{\hbar}{2i}\left(\hat{b}^\dagger \hat{a} - \hat{a}^\dagger \hat{b}\right)$$

[P. Jordan, *Z. Phys.* **94**, 531 (1935)]

[J. Schwinger, in *Quantum Theory of Angular Momentum*, edited by L. C. Biedenharn and H. V. Dam Academic, New York (1965)]

Schwinger-Jordan Representation

Jordan-Schwinger Transform

$$[\hat{a}, \hat{a}^\dagger] = 1 \longrightarrow [\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z$$

Constraint:

$$\hat{S}^2|\chi_+\rangle = \hbar^2 S(S+1)|\chi_+\rangle \longrightarrow S = \frac{1}{2}(\hat{b}^\dagger\hat{b} + \hat{a}^\dagger\hat{a})$$

[P. Jordan, *Z. Phys.* **94**, 531 (1935)]

[J. Schwinger, in *Quantum Theory of Angular Momentum*, edited by L. C. Biedenharn and H. V. Dam Academic, New York (1965)]

Schwinger-Jordan Representation

Spin-Boson Hamiltonian

$$\hat{H} = \frac{2}{\hbar}\left[\epsilon \hat{S}_z + J\hat{S}_x + \hat{S}_z \times f(\mathbf{y})\right] + H_b(\mathbf{y}, \mathbf{p}_y),$$

$$\hat{H} = (\epsilon + f(\mathbf{y}))\left(\hat{b}^\dagger \hat{b} - \hat{a}^\dagger \hat{a}\right) + J\left(\hat{b}^\dagger \hat{a} + \hat{a}^\dagger \hat{b}\right) + H_b(\mathbf{y}, \mathbf{p}_y),$$

$$\hat{H} = H_b(\mathbf{y}, \mathbf{p}_y) + (\epsilon + f(\mathbf{y}))\left[(\tilde{x}_{\nu_1}^2 + \tilde{p}_{\nu_1}^2 - 1) - (\tilde{x}_{\nu_2}^2 + \tilde{p}_{\nu_2}^2 - 1)\right] + J\left(\tilde{x}_{\nu_1}\tilde{x}_{\nu_2} + \tilde{p}_{\nu_1}\tilde{p}_{\nu_2}\right)$$

$$\hat{b}_{\nu_j}^\dagger = \frac{1}{\sqrt{2}}\left[\tilde{x}_{\nu_j} - i\tilde{p}_{\nu_j}\right]$$

$$\hat{b}_{\nu_j} = \frac{1}{\sqrt{2}}\left[\tilde{x}_{\nu_j} + i\tilde{p}_{\nu_j}\right]$$

$$[\tilde{x}_j, \tilde{p}_k] = i\delta_{j\,k} \qquad \hat{a} = \hat{b}_{\nu_2} \qquad \hat{b} = \hat{b}_{\nu_1}$$

$$S = \frac{1}{4}\left[(\tilde{x}_{\nu_1}^2 + \tilde{p}_{\nu_1}^2 - 1) + (\tilde{x}_{\nu_2}^2 + \tilde{p}_{\nu_2}^2 - 1)\right]$$

[P. Jordan, *Z. Phys.* **94**, 531 (1935); J. Schwinger, in *Quantum Theory of Angular Momentum*, edited by L. C. Biedenharn and H. V. Dam Academic, New York (1965)]

Schwinger-Jordan Representation

N-Level Hamiltonian

$$\hat{H} = \sum_{j=1}^{N} \sum_{k=1}^{N} H_{jk} |j\rangle\langle k|,$$

$$= \sum_{j=1}^{N} \sum_{k=1}^{N} H_{jk} \hat{a}_j^{\dagger} \hat{a}_k,$$

$$\hat{H} = \frac{1}{2} \sum_{j=1}^{N} \sum_{k=1}^{N} H_{jk} (\tilde{x}_j - i\tilde{p}_j)(\tilde{x}_k + i\tilde{p}_k),$$

$$= \frac{1}{2} \sum_{j=1}^{N} \sum_{k=1}^{N} H_{jk} (\tilde{x}_j \tilde{x}_k + \tilde{p}_j \tilde{p}_k - \delta_{jk}).$$

[H.-D. Meyer and W. H. Miller *J. Chem. Phys.* (1979) **70**, 3214; M. Thoss and G. Stock *Phys. Rev. Lett.* **78**, 578 (1997); V.S. Batista and W. H. Miller *J. Chem. Phys.* **108**, 498 (1998)]

Harmonic Basis Set

$$H_j = \frac{\hat{p_j}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}_j^2,$$
$$= \frac{\tilde{p_j}^2}{2m}m\omega\hbar + \frac{1}{2}m\omega^2\frac{\hbar}{m\omega}\tilde{x_j}^2,$$
$$= \frac{\hbar\omega}{2}\left[\tilde{p}_j^2 + \tilde{x}_j^2\right].$$

$$\tilde{x}_j = \hat{x}_j\sqrt{\frac{m\omega}{\hbar}},$$
$$\tilde{p}_j = \hat{p}_j\sqrt{\frac{1}{m\omega\hbar}},$$
$$\tilde{x}_j = \frac{1}{\sqrt{2}}[\hat{a}_j^\dagger + \hat{a}_j]$$
$$\tilde{p}_j = \frac{i}{\sqrt{2}}[\hat{b}_j^\dagger - \hat{b}_j],$$

$$H_j = \hbar\omega\left(\hat{n}_j + \frac{1}{2}\right)$$

$$\hat{n}_j = \hat{a}_j^\dagger\hat{a}_j,$$
$$= \frac{1}{2}(\tilde{x}_j - i\tilde{p}_j)(\tilde{x}_j + i\tilde{p}_j),$$
$$= \frac{1}{2}(\tilde{x}_j^2 + i[\tilde{x}_j, \tilde{p}_j] + \tilde{p}_j^2),$$
$$= \frac{1}{2}(\tilde{x}_j^2 + \tilde{p}_j^2 - 1),$$

$$|0\rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\exp\left(-\frac{m\omega}{2\hbar}x^2\right),$$
$$|\nu + 1\rangle = \frac{1}{\sqrt{\nu + 1}}\hat{a}^\dagger|\nu\rangle,$$

$$\langle\mu|a_j^\dagger|\nu\rangle = \sqrt{\nu + 1}\delta_{\mu,\nu+1}$$

Matrix Representation of Boson Operators

$$a^\dagger = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{5} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{7} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2\sqrt{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 \end{pmatrix}$$

$$\langle \mu | a_j^\dagger | \nu \rangle = \sqrt{\nu + 1}\delta_{\mu,\nu+1}$$

$$\langle \nu | a | \mu \rangle = \langle \mu | a^\dagger | \nu \rangle$$

$$a = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{6} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \sqrt{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2\sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$N = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 7 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9 \end{pmatrix}$$

Single Boson Representation of P_{jk}= |j><k| Operators

6-level System: Single Boson Representation

$$\hat{S}^{+} = \hbar\sqrt{2S - \hat{N}}\,\hat{a}$$

$$\hat{\Gamma} = (5 - \hat{N})\,\hat{a} = 5\hat{a} - \hat{a}^{\dagger}\hat{a}^{2}$$

$$\Gamma = \begin{pmatrix} 0 & 5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4\sqrt{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3\sqrt{3} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{5} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\sqrt{7} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -4\sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -9 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\hat{P}_{1,6} = |1\rangle\langle 6| = \frac{1}{5!\sqrt{5!}}\hat{\Gamma}^{5}$$

$$P_{1,6} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & & & & & & \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\hat{P}_{n,m} = \frac{1}{\sqrt{n-1}}\hat{a}^{\dagger}\hat{P}_{n-1,m}$$

Single Boson Representation of P_{jk}= |j><k| Operators

6-level System: Single Boson Representation

$$\frac{1}{5!\sqrt{4!}}\Gamma^4 = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{5}} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Single Boson Representation of P_{jk}= |j><k| Operators

6-level System: Single Boson Representation

Recurrence Relation: $\hat{P}_{n,m} = \frac{1}{\sqrt{n-1}} \hat{a}^{\dagger} \hat{P}_{n-1,m}$

$$\hat{P}_{1,5} = \frac{1}{5!\sqrt{4!}} \hat{\Gamma}^4 - \frac{1}{\sqrt{5}} \hat{P}_{2,6},$$

$$= \frac{1}{5!\sqrt{4!}} (5\hat{a} - \hat{a}^{\dagger}\hat{a}^2)^4 - \frac{1}{\sqrt{5}} \hat{a}^{\dagger} \frac{1}{5!\sqrt{5!}} (5\hat{a} - \hat{a}^{\dagger}\hat{a}^2)^5$$

$$\hat{P}_{1,4} = \Gamma^3 \frac{2}{5!\sqrt{3!}} - \hat{P}_{3,6} \frac{1}{\sqrt{10}} - \hat{P}_{2,5} \frac{4}{5},$$

$$= (5a - a^{\dagger}a^2)^3 \frac{2}{5!\sqrt{3!}} - \frac{1}{\sqrt{2}} (a^{\dagger})^2 \frac{1}{5!\sqrt{5!}} (5a - a^{\dagger}a^2)^5 \frac{1}{\sqrt{10}} - \hat{a}^{\dagger} \hat{P}_{1,5} \frac{4}{5},$$

$$\hat{P}_{1,3} = \Gamma^2/(20\sqrt{2}) - \hat{P}_{4,6}/\sqrt{10} - \hat{P}_{3,5} 3\sqrt{3}/(5\sqrt{2}) - \hat{P}_{2,4} 3\sqrt{3}/5,$$

$$\hat{P}_{1,2} = \Gamma/5 - \hat{P}_{5,6}/\sqrt{5} - 4\hat{P}_{4,5}/5 - 3\sqrt{3}\hat{P}_{3,4}/5 - 4\sqrt{2}\hat{P}_{2,3}/5,$$

$$\hat{P}_{1,1} = \hat{I} - \hat{N}/5 - 4\hat{P}_{2,2}/5 - 3\hat{P}_{3,3}/5 - 2\hat{P}_{4,4}/5 - \hat{P}_{5,5}/5.$$

N-level System: Single Boson Representation

$$\hat{H} = \sum_{j,k=1}^{N} H_{jk} P_{j,k}(\hat{a}, \hat{a}^\dagger),$$

N-level System: Jordan-Schwinger Representation

$$\hat{H} = \sum_{j,k=1}^{N} H_{jk} \hat{a}_j^\dagger \hat{a}_k,$$

Two-level Systems: Single Boson Representation

$$\hat{\Gamma} = (1-\hat{N})\,\hat{a} = \hat{a}-\hat{a}^{\dagger}\hat{a}^{2}.$$

$$\hat{P}_{1,2} = a - a^{\dagger}a^{2},$$

$$\hat{P}_{2,2} = a^{\dagger}a - (a^{\dagger})^{2}a^{2},$$

$$\hat{P}_{1,1} = 1 - a^{\dagger}a,$$

$$\hat{P}_{2,1} = a^{\dagger} - (a^{\dagger})^{2}a.$$

$$\hat{H} = \sum_{j,k=1}^{2} H_{jk}\hat{P}_{j,k},$$

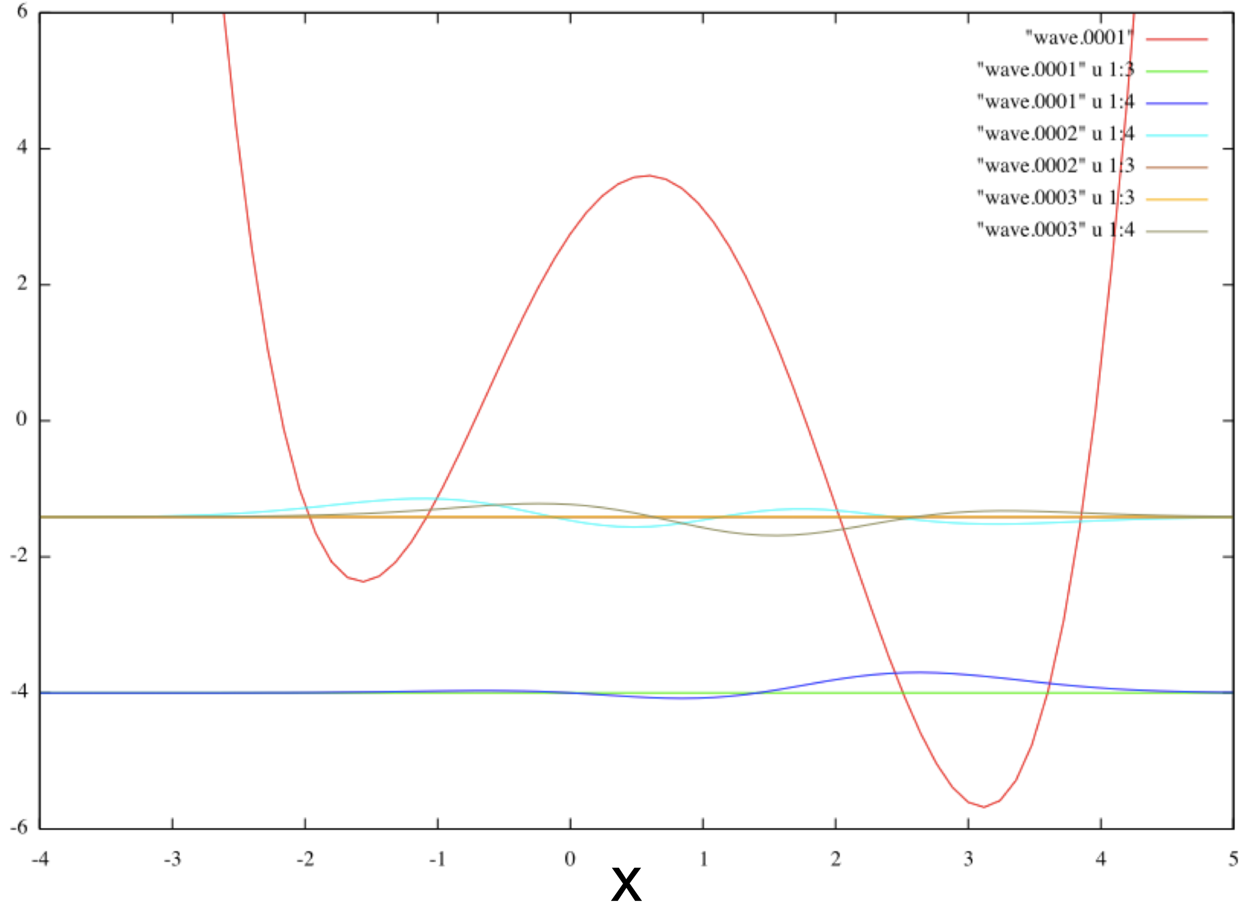
Two-level Systems: Single Boson Representation

$$\hat{H} = H_{11}(1-\hat{N}) + H_{12}((1-\hat{N})\hat{a} + \hat{a}^{\dagger}(1-\hat{N})) + H_{22}\hat{N}(2-\hat{N}).$$

$$\begin{aligned}\hat{H} = &\frac{H_{11}}{2}\left(3 - \tilde{x}^2 - \tilde{p}^2\right) \\ &+ \frac{H_{12}}{\sqrt{2}}\left(4\tilde{x} - \tilde{x}^3 - \frac{1}{2}\tilde{p}^2\tilde{x} - \frac{1}{2}\tilde{x}\tilde{p}^2\right) \\ &+ \frac{H_{22}}{2}\left(3(\tilde{x}^2 + \tilde{p}^2) - \frac{1}{2}(\tilde{x}^2 + \tilde{p}^2)^2 - \frac{5}{2}\right).\end{aligned}$$

Single Boson DVR Hamiltonian

H(x, p=0)



Single Boson DVR Hamiltonian

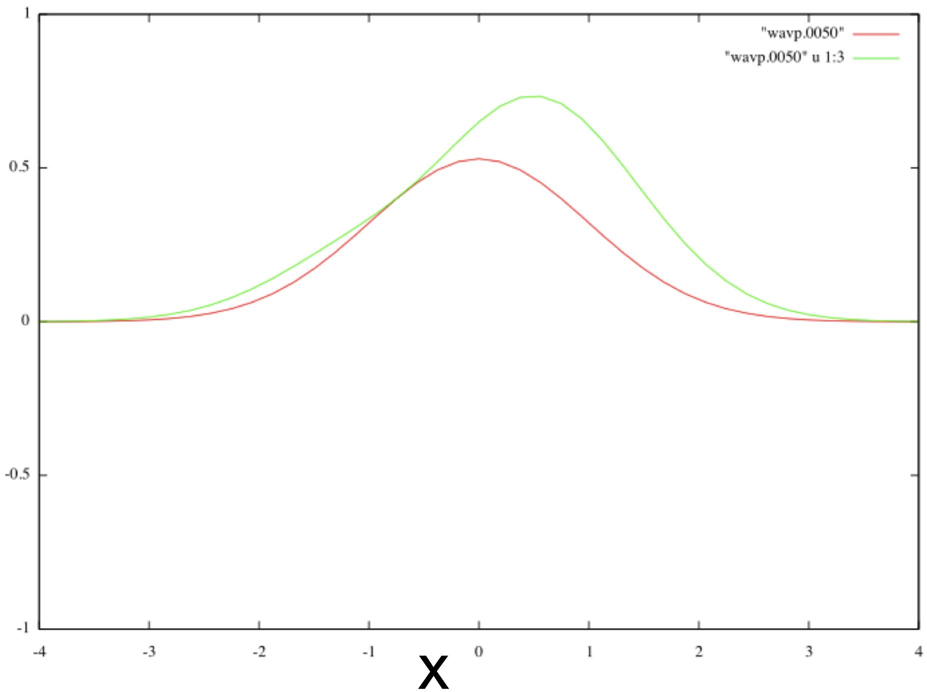
$$H_{j,j'} = \left(\frac{H_{11}}{2}\left(3 - x_j^2\right) + \frac{H_{12}}{\sqrt{2}}\left(4x_j - x_j^3\right) + \frac{H_{22}}{2}\left(3x_j^2 - \frac{5}{2} - \frac{1}{2}x_j^4\right)\right)\delta_{jj'}$$
$$+ \left(\frac{3}{2}H_{22} - \frac{1}{2}H_{11} - \frac{H_{12}}{\sqrt{8}}\left(x_{j'} + x_j\right) - \frac{H_{22}}{4}(x_j^2 + x_{j'}^2)\right)\frac{\Delta x \Delta p}{2\pi\hbar}\sum_{k=1}^{n_p} e^{\frac{i}{\hbar}(x_{j'} - x_j)p_k} p_k^2$$
$$- \frac{H_{22}}{4}\frac{\Delta x \Delta p}{2\pi\hbar}\sum_{k=1}^{n_p} e^{\frac{i}{\hbar}(x_{j'} - x_j)p_k} p_k^4,$$

$$\Delta_x = (x_{max} - x_{min})/n_x \qquad x_j = (j - n_x/2)\Delta_x$$
$$\Delta p = 2\pi/(x_{max} - x_{min}) \qquad p_k = \Delta p(k - n_p/2)$$

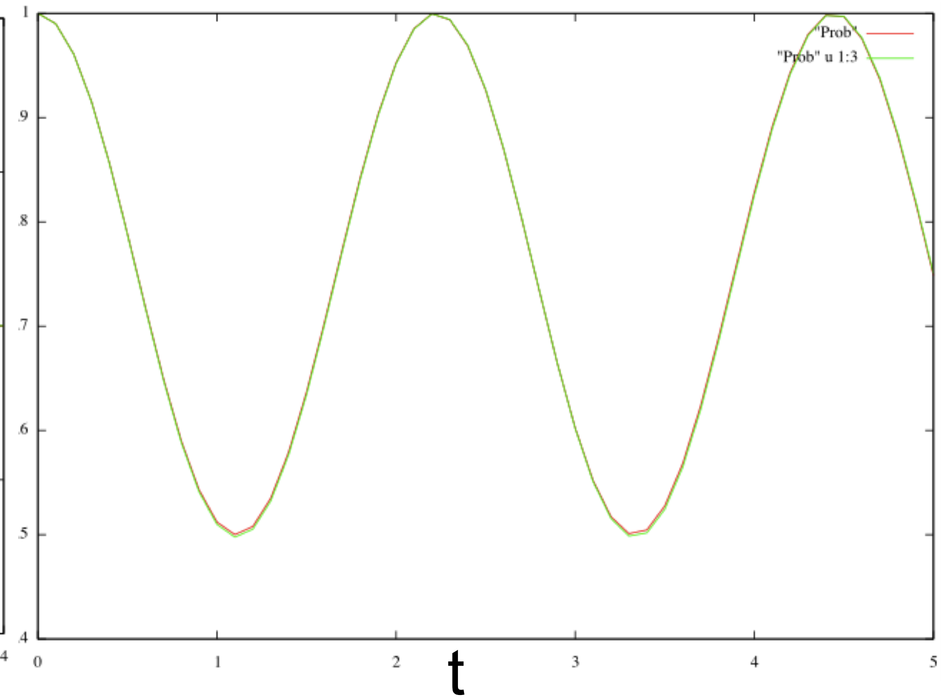
$$\psi(x;t) = e^{-\frac{i}{\hbar}\hat{H}t}\psi(x;0).$$
$$\psi(x;0) = c_0(0)\langle x|0\rangle + c_1(0)\langle x|1\rangle$$

Single Boson DVR Hamiltonian

|Ψ(x)|, Re[Ψ(x)]



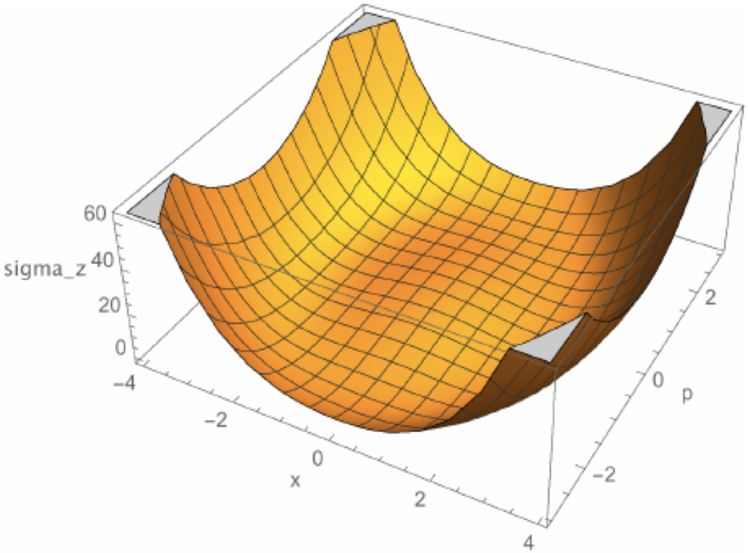
P(t)

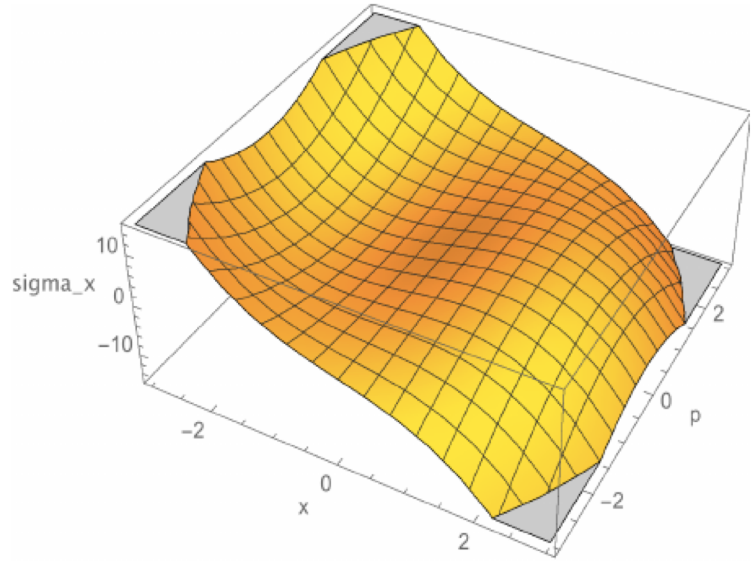


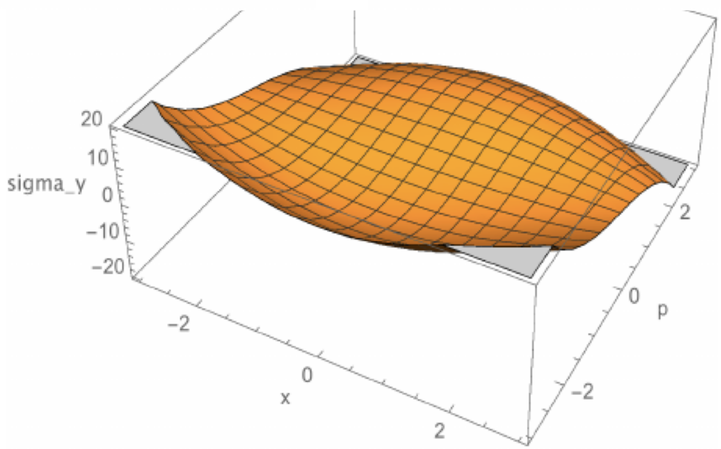
Single Boson Representation of Pauli Matrices

$$\begin{aligned}
\hat{\sigma}_z &= (1-\hat{N}) - \hat{N}(2-\hat{N}) \\
&= \frac{11}{4} - 2(\tilde{x}^2+\tilde{p}^2) + \frac{1}{4}(\tilde{x}^2+\tilde{p}^2)^2 \\
\hat{\sigma}_x &= (1-\hat{N})\hat{a} + \hat{a}^\dagger(1-\hat{N}) \\
&= \frac{1}{\sqrt{8}}\left(8\tilde{x} - 2\tilde{x}^3 - \tilde{p}^2\tilde{x} - \tilde{x}\tilde{p}^2\right) \\
\hat{\sigma}_y &= -i(1-\hat{N})\hat{a} + i\hat{a}^\dagger(1-\hat{N}) \\
&= \frac{i}{2\sqrt{2}}\left(-i6\tilde{p} + \tilde{p}^2\tilde{x} - \tilde{x}\tilde{p}^2 + i(\tilde{p}\tilde{x}^2 + \tilde{x}^2\tilde{p}) + 2i\tilde{p}^3\right) \\
&= \frac{1}{\sqrt{8}}\left(6\tilde{p} + i\tilde{p}^2\tilde{x} - i\tilde{x}\tilde{p}^2 - (\tilde{p}\tilde{x}^2 + \tilde{x}^2\tilde{p}) - 2\tilde{p}^3\right),
\end{aligned}$$

Single Boson Representation of Pauli Matrices







Single Boson Representation of Pauli Matrices

$$\hat{\sigma}^{+} = \frac{1}{2}(\hat{\sigma}_x + i\hat{\sigma}_y) = (1-\hat{N})\hat{a},$$
$$= \frac{1}{\sqrt{8}}\left(5\tilde{x} - \tilde{x}^3 - \tilde{p}^2\tilde{x}\right) + \frac{i}{\sqrt{8}}\left(3\tilde{p} - \tilde{p}^3 - \tilde{p}\tilde{x}^2\right),$$

$$\hat{\sigma}^{-} = \frac{1}{2}(\hat{\sigma}_x - i\hat{\sigma}_y) = \hat{a}^{\dagger}(1-\hat{N}),$$
$$= \frac{1}{\sqrt{8}}\left(3\tilde{x} - \tilde{x}^3 - \tilde{x}\tilde{p}^2\right) - \frac{i}{\sqrt{8}}\left(3\tilde{p} - \tilde{p}^3 - \tilde{p}\tilde{x}^2\right).$$

Single Boson Representation of Pauli Matrices