When ExaBytes are not Enough: An Efficient Quantum Algorithm for Dynamics of a Spin System Coupled to Specific Spin Baths

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2012 Landau Days

# How **Big/Small is an Exabyte?**



#### Quantum Statistical Mechanics

•Discrete quantum system can be thermalized by a finite bath ♦ Glemer and Michel, Europhysics Letters 2006 Prove reaction actuilibrium is a universal protection of quantum systems: almost any subsystem in interaction with a large enough bath will reach an equilibrium state and remain close to it for almost all times Linden, Popescu, Short, Winger, PRE 2009 For sufficiently large times the ensemble is for all practical purpose indistinguishable from a canonical density operator Reimann, New J. Physics 2010 Different processes coupled to the same noise source can have different decoherence rates (stronger noise can have faster decoherence) \*7hos, Hung, Liu, Mys. Kev. Lett. 2011 \* As long as finite bath drives system toward a quantum-typicality state, decoherence for spin  $\frac{1}{2}$  bath goes as  $\sigma \approx 2^{-Nbath/2}$ \*JIII, D. Boodt Novotny Michielsen Mivachite, to or submitted



# Are All Baths Equal?



# MOTIVATION : PHYSICS

# Locking electron spins into magnetic resonance by electron-nuclear feedback

Ivo T Vink, Katja C Nowack, Frank H L Koppens, Jeroen Danon, Yuli V Nazarov and Lieven M K Vandersypen Nat Phys 5(10):764–768 (2009)



# **MOTIVATION :** *Computational Science*

 $|\Psi(t)\rangle = e^{-itH}|\Psi(0)\rangle$ 

 $\hbar =$ 

*2 difficulties: Minus sign problem (phase) Size of vector* 2<sup>M+N</sup>

M spins spin bath (N)

#### **MOTIVATION :**

Exascale Supercomputers

 $|\Psi(t)\rangle = \mathrm{e}^{-\mathrm{i}tH}|\Psi(0)\rangle$ 



M spins

spin bath (N)

*2 difficulties: Minus sign problem (phase) Size of matrix 2<sup>M+N</sup>*

 2011
 1 PB
 M+N=50

 2015
 5 PB
 M+N=52

 2018
 16 PB
 M+N=54

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#### Approach to Equilibrium in Nano-scale Systems at Finite Temperature

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10<sup>90</sup>

10<sup>85</sup>

10<sup>80</sup>

10<sup>75</sup>

**10**<sup>70</sup>

10<sup>65</sup>

10<sup>60</sup>

) 10<sup>55</sup>

10<sup>50</sup>

10<sup>45</sup>

**10**<sup>40</sup>

10<sup>35</sup>

10<sup>30</sup>

10<sup>25</sup>

10<sup>20</sup>

**10**<sup>15</sup>

**10**<sup>10</sup>

10<sup>5</sup>

- Motivation
  - Desire for real-time simulations of quantum syst
- Method
- Efficient real-time dynamic algorithm for spin sys

   V.V. Dobrovitski and H. De Raedt, Phys. Rev. E 67, 08

   Measure expectation values of spin comp

   Measure quantum purity: P(t) = Tr(ρ<sup>2</sup>)
   Measure entropy: S(t)=-ρ(t) lnρ(t)
   Measure thermalization: σ(t)=|<sub>1</sub> = 2<sup>128</sup>

   Spin ½ coupled to special spin batts

   New algorithm

Exabyte =  $2^{60}$ 

# Spin-1/2 coupled to spin bath

 $\mathcal{H}=\mathcal{H}_S+\mathcal{H}_B+\mathcal{H}_{SB},$ 

$$\mathcal{H}_S = \omega_0 S_0^z,$$

$$\mathcal{H} |\Psi(t)\rangle = -\frac{\hbar}{i} \frac{\partial}{\partial t} |\Psi(t)\rangle$$

$$|\Psi(t)\rangle = \exp\left(-\frac{i\mathcal{H}t}{\hbar}\right)|\Psi(0)\rangle$$

$$\rho(t) = \mathrm{Tr}_{B}\left[\rho_{S+B}(t)\right],$$

$$\left< S_0^{\ell}(t) \right> = \mathrm{Tr} \left[ s^{\ell} \rho(t) \right]$$

$$\begin{split} \textbf{Method: Set up} \\ S_m^{\ell} &= I_2 \otimes I_2 \otimes \cdots \otimes I_2 \otimes s^{\ell} \otimes I_2 \otimes \cdots \otimes I_2 \quad |\Psi(t)\rangle = e^{-itH} |\Psi(0)\rangle \\ \ell \in \{x, y, z\} \\ \mathcal{H} &= \omega_0 S_{N_n+N_n+1}^* \left[ \sum_{i_1 \in 0}^{1} \sum_{i_2 = 0}^{1} \cdots \sum_{i_{N_n = 0}}^{1} J_{i_1,i_2,\cdots,i_{N_n}}(S_1^n)^{i_1}(S_2^n)^{i_2} \cdots (S_{N_n}^n)^{i_{N_n}} \right] \\ &+ \sum_{i_1 \in 0}^{1} \sum_{i_2 = 0}^{1} \cdots \sum_{i_{N_n = 0}}^{1} J_{i_1,i_2,\cdots,i_{N_n}}(S_1^n)^{i_1}(S_2^n)^{i_2} \cdots (S_{N_n}^n)^{i_{N_n}} \\ &+ S_{N_n+N_n+1}^n \left[ \sum_{j_1 = 0}^{1} \sum_{j_2 = 0}^{1} \cdots \sum_{j_{N_n = 0}}^{1} K_{j_1,j_2,\cdots,j_{N_n}}(S_{N_n+1}^n)^{j_1}(S_{N_n+2}^n)^{j_{N_n}} \cdots (S_{N_n+N_n}^n)^{j_{N_n}} \right] \\ &+ \sum_{i_1 = 0}^{1} \sum_{j_2 = 0}^{1} \cdots \sum_{j_{N_n = 0}}^{1} K_{j_1,j_2,\cdots,j_{N_n}}(S_{N_n+1}^n)^{j_1}(S_{N_n+2}^n)^{j_{N_n}} \cdots (S_{N_n+N_n}^n)^{j_{N_n}} \right] \\ & \mathbf{M} = 1 \text{ spins} \\ \text{ spin bath } (N) \end{split}$$



$$\begin{split} & \mathcal{M}\text{ethod: Block Diagonalize} \\ & |\Psi(t)\rangle = e^{-itH}|\Psi(0)\rangle \\ & \tilde{\mathcal{H}} = \omega_0 S_{N_x+N_y+1}^z \\ & + S_{N_x+N_y+1}^z \left[\sum_{i_1=0}^{1} \sum_{i_2=0}^{1} \cdots \sum_{i_{N_x=0}}^{1} J_{i_1,i_2,\cdots,i_{N_x}}(S_1^z)^{i_1} (S_2^z)^{i_2} \cdots (S_{N_x}^z)^{i_{N_x}}\right] \\ & + \sum_{i_1=0}^{1} \sum_{i_2=0}^{1} \cdots \sum_{i_{N_x=0}}^{1} \tilde{J}_{i_1,i_2,\cdots,i_{N_x}}(S_1^z)^{i_1} (S_2^z)^{i_2} \cdots (S_{N_x}^z)^{i_{N_x}}\right] \\ & + S_{N_x+N_y+1}^y \left[\sum_{j_1=0}^{1} \sum_{j_2=0}^{1} \cdots \sum_{j_{N_y=0}=0}^{1} K_{j_1,j_2,\cdots,j_{N_y}} (S_{N_x+1}^z)^{j_1} (S_{N_x+2}^x)^{j_2} \cdots (S_{N_x+N_y}^z)^{j_{N_y}}\right] \\ & + \sum_{j_1=0}^{1} \sum_{j_2=0}^{1} \cdots \sum_{j_{N_x=0}=0}^{1} K_{j_1,j_2,\cdots,j_{N_y}} (S_{N_x+1}^z)^{j_1} (S_{N_x+2}^x)^{j_2} \cdots (S_{N_x+N_y}^z)^{j_{N_y}}\right] \\ & \tilde{\mathcal{H}}_{\text{B}} = \begin{pmatrix} \Omega_x + \omega_0 \ \Omega_x - i\Omega_y \\ \Omega_x + i\Omega_y \ \Omega_z - \omega_0 \end{pmatrix} \\ \\ & \text{Block} \\ & \text{Diagonal} \\ \end{array}$$

# Bring together spin-1/2 and bath at t=0

$$\psi(0)\rangle = \begin{pmatrix} \sin \alpha_0 \\ \cos \alpha_0 \end{pmatrix} \qquad \qquad |\widetilde{\Phi}(0)\rangle = \sum_{j=1}^{2^{N_B}} c_j |\varphi_j\rangle \qquad \text{with}$$

$$|\Psi(0)\rangle = |\Phi(0)\rangle \otimes |\psi(0)\rangle$$

$$\begin{split} \rho(t) &= \operatorname{Tr}_{B} \left[ e^{-i\mathcal{H}t} \left( \rho(0) \otimes \rho_{B}(0) \right) e^{i\mathcal{H}t} \right] \\ &= \operatorname{Tr}_{B} \left[ P_{p} e^{-i\widetilde{\mathcal{H}}t} P_{p}^{\dagger} \left( \rho(0) \otimes \rho_{B}(0) \right) P_{p} e^{i\widetilde{\mathcal{H}}t} P_{p}^{\dagger} \right] \\ &= \operatorname{Tr}_{B} \left[ e^{-i\widetilde{\mathcal{H}}t} \left( \rho(0) \otimes \widetilde{\rho}_{B}(0) \right) e^{i\widetilde{\mathcal{H}}t} \right] . \end{split}$$

$$\begin{split} \rho(t) &= \left( |c_1|^2 \, e^{-i\widetilde{\mathcal{H}}_1 t} \rho(0) e^{i\widetilde{\mathcal{H}}_1 t} \right) + \left( |c_2|^2 \, e^{-i\widetilde{\mathcal{H}}_2 t} \rho(0) e^{i\widetilde{\mathcal{H}}_2 t} \right) + \dots + \left( |c_{2^{N_B}}|^2 \, e^{-i\widetilde{\mathcal{H}}_{2^{N_B}} t} \rho(0) e^{i\widetilde{\mathcal{H}}_{2^{N_B}} t} \right) \\ &= |c_1|^2 \, \rho_1(t) + |c_2|^2 \, \rho_2(t) + \dots + |c_{2^{N_B}}|^2 \, \rho_{2^{N_B}}(t) \, . \end{split}$$

 $\sum_{j=1}^{2^{N_B}} \left| c_j \right|^2 = 1,$ 

# **Main Equations**

$$\begin{split} \rho(t) &= \left( |c_1|^2 e^{-i\widetilde{\mathcal{H}}_1 t} \rho(0) e^{i\widetilde{\mathcal{H}}_1 t} \right) + \left( |c_2|^2 e^{-i\widetilde{\mathcal{H}}_2 t} \rho(0) e^{i\widetilde{\mathcal{H}}_2 t} \right) + \dots + \left( |c_{2^{N_B}}|^2 e^{-i\widetilde{\mathcal{H}}_{2^{N_B}} t} \rho(0) e^{i\widetilde{\mathcal{H}}_{2^{N_B}} t} \right) \\ &= |c_1|^2 \rho_1(t) + |c_2|^2 \rho_2(t) + \dots + |c_{2^{N_B}}|^2 \rho_{2^{N_B}}(t) \,. \end{split}$$

$$\left\langle S_{0}^{\ell}(t)\right\rangle = \sum_{j=1}^{2^{N_{B}}} \left|c_{j}\right|^{2} \operatorname{Tr}\left[s^{\ell} \rho_{j}(t)\right]$$

> Only requires storage for  $2x^2$  matrices, for any  $N_B$ 

 $\triangleright$  Requires solution of  $2^{N_B}$  different TDSE to get solution

# **Main Equations**

$$\begin{split} \rho(t) &= \left( |c_1|^2 e^{-i\widetilde{\mathcal{H}}_1 t} \rho(0) e^{i\widetilde{\mathcal{H}}_1 t} \right) + \left( |c_2|^2 e^{-i\widetilde{\mathcal{H}}_2 t} \rho(0) e^{i\widetilde{\mathcal{H}}_2 t} \right) + \dots + \left( |c_{2^{N_B}}|^2 e^{-i\widetilde{\mathcal{H}}_{2^{N_B}} t} \rho(0) e^{i\widetilde{\mathcal{H}}_{2^{N_B}} t} \right) \\ &= |c_1|^2 \rho_1(t) + |c_2|^2 \rho_2(t) + \dots + |c_{2^{N_B}}|^2 \rho_{2^{N_B}}(t) \,. \end{split}$$

$$\left\langle S_0^{\ell}(t) \right\rangle = \sum_{j=1}^{2^{N_B}} \left| c_j \right|^2 \mathrm{Tr} \left[ s^{\ell} \rho_j(t) \right]$$

If symmetry in Hamiltonian (not necessiaryly in initial bath vector)

$$\rho_j(t)$$
 are identical for  $j \in \{i, \dots, i+k\}$ 

$$\left\langle S_0^{\ell}(t) \right\rangle = \dots + \left\{ \left( \sum_{j=i}^{i+k} \left| c_j \right|^2 \right) \operatorname{Tr} \left[ s^{\ell} \rho_{\operatorname{sym}}(t) \right] \right\} + \dots$$

### If all interactions identical and 2-body only

$$\Omega_{m_x m_y} = \sqrt{m_x^2 J_2^2 + m_y^2 K_2^2 + \omega_0^2}$$

$$\lambda_{N_x,m_x} = \begin{pmatrix} N_x \\ N_x/2 - m_x \end{pmatrix} = \frac{N_x!}{(N_x/2 - m_x)! (N_x/2 + m_x)!}$$

 $\vec{\Omega}_{m_xm_y} = \left(m_x J_2, \ m_y K_2, \ \omega_0\right),$ 

$$\begin{pmatrix} 0 & 1 \end{pmatrix} \exp\left[i\widetilde{\mathcal{H}}_{j}t\right] \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \exp\left[-i\widetilde{\mathcal{H}}_{j}t\right] \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{2} \frac{\omega_{0}^{2} + \left(\Omega_{xj}^{2} + \Omega_{yj}^{2}\right) \cos\left[\sqrt{\Omega_{xj}^{2} + \Omega_{yj}^{2} + \omega_{0}^{2}}t\right]}{\Omega_{xj}^{2} + \Omega_{yj}^{2} + \omega_{0}^{2}}$$

$$\left\langle S_{0}^{z}(t) \right\rangle = \frac{1}{2^{N_{x}+N_{y}+1}} \sum_{m_{x}=-N_{x}/2}^{N_{x}/2} \sum_{m_{y}=-N_{y}/2}^{N_{y}/2} \lambda_{N_{x},m_{x}} \lambda_{N_{y},m_{y}} \frac{\left[ \left(m_{x}^{2} J_{2}^{2} + m_{y}^{2} K_{2}^{2} \right) \cos\left(\Omega_{m_{x}m_{y}}t\right) \right] + \omega_{0}^{2}}{\Omega_{m_{x}m_{y}}^{2}}$$

Sum only over  $N_h+1$  for each x-bath or y-bath

#### Theory: no interactions among bath spins; all spins start down $H = H_{\rm S} + H_{\rm SB}$ , **New Journal of Physics** (1)The open-access journal for physics $H_{\rm S} = \omega_0 S^z$ , (2) $H_{\rm SB} = g_1 S^{x} \sum_{k=1}^{N} I_k^{x} + g_2 S^{y} \sum_{k=1}^{N} J_l^{y},$ (3)Quantum frustration of dissipation by a spin bath D D Bhaktavatsala Rao<sup>1</sup>, Heiner Kohler<sup>2</sup> No bath dynamics: and Fernando Sols<sup>3</sup> <sup>1</sup> Department of Physics, Indian Institute of Technology Kanpur, Kanpur 208016, India $_{\rm rot}$ and J<sup>2</sup> Department of Physics, University of Duisburg-Essen, D-47057 Duisburg, Germany <sup>3</sup> Departamento de Física de Materiales, Universidad Complutense de Madrid, conserved E-28040 Madrid, Spain E-mail: f.sols@fis.ucm.es New Journal of Physics 10 (2008) 115017 (17pp) $\rho(t) = \bigoplus_{m_1, m_2 = -N/2}^{N/2} \rho_{m_1 m_2}(t)$ $= \mathrm{Tr}\rho^2$ Final result $\mathcal{P}(t) - \frac{1}{2} = \frac{1}{2} \exp(-Ng^2 t^2/8)$ ne Bath **Two Baths**





## 1-bath: x-bath



#### small t One Bath: Exponential







/



# **Summary and Conclusion**

Different baths (any interactions) have different asymptotic forms for the quantum purity

 One –bath : exponential in N<sub>bath</sub> t<sup>2</sup>
 Two-baths : power law in N<sub>bath</sub> t<sup>2</sup>

 Algorithm requires storage 2<sup>M</sup>, rather than 2<sup>M+N</sup> (sum over 2<sup>N</sup> different 2<sup>M</sup> systems)

 All Baths are NOT the same

$$\left\langle S_{0}^{\ell}(t)\right\rangle = \sum_{j=1}^{2^{N_{B}}} \left|c_{j}\right|^{2} \operatorname{Tr}\left[s^{\ell} \rho_{j}(t)\right]$$





