Quantum dynamics of strongly-coupled electron-nuclear systems

Bill Coish

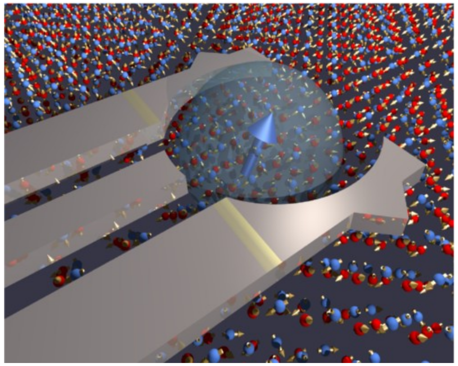
Department of Physics, McGill University, Montréal, Québec

QCPS-III, Orlando, Florida 19 December 2010

WAC, J. Fischer, D. Loss, Phys. Rev. B 81, 165315 (2010)

Collaborators:

Basel, Switzerland: D. Loss, J. Fischer, D. Klauser
Waterloo: F. Qassemi, J. Gambetta, F. Wilhelm
Oslo, Norway: J. Bergli
Innsbruck, Austria: T. Monz, R. Blatt, …

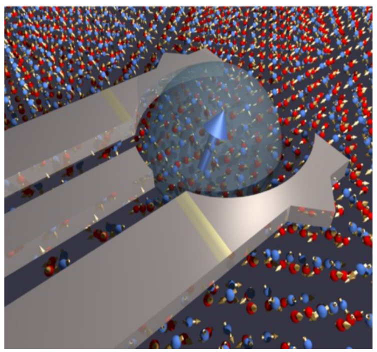


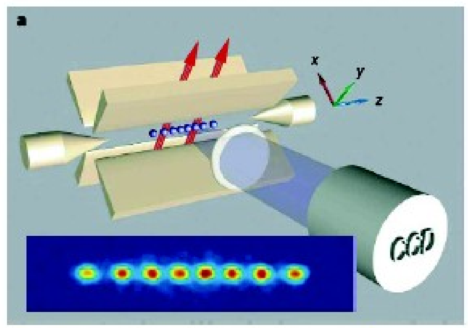
RQMP

INTRIQ

Directions

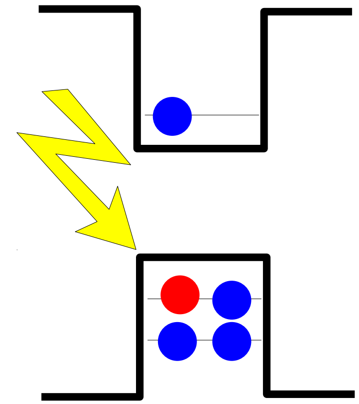
Quantum coherence/decoherence





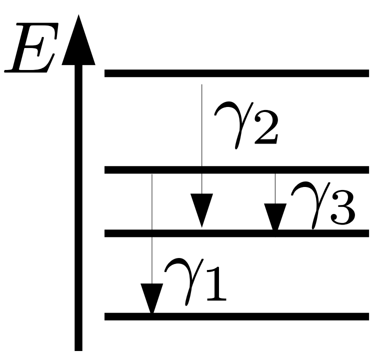
WAC and J. Baugh, Phys. Stat. Solidi B (2009)
WAC, J. Fischer, D. Loss, PRB (2010)
T. Monz, ... WAC, ... R. Blatt arXiv:1009.6126

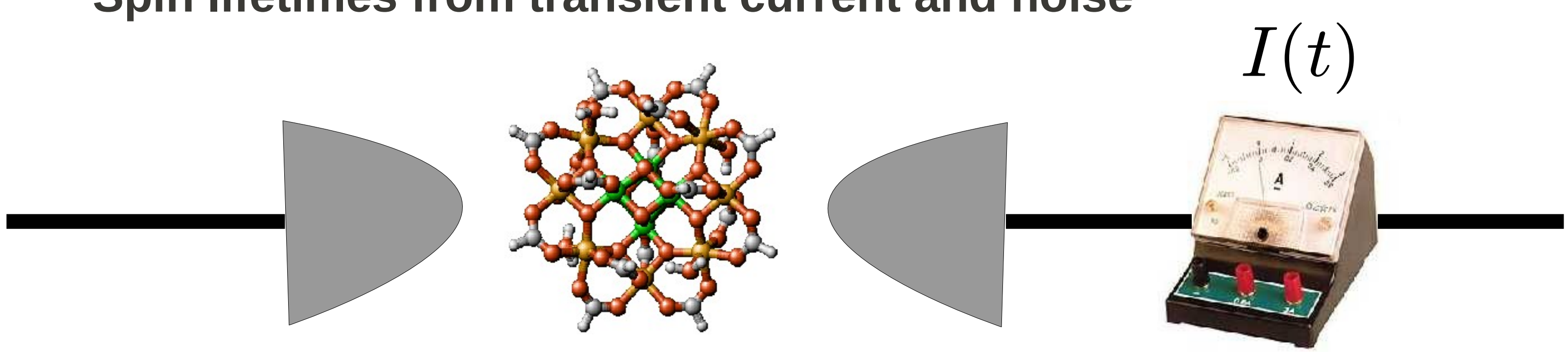
Light-matter interactions;
Coupling optical, vibrational modes



WAC and J. M. Gambetta, PRB (R) (2009)
First expt.: M. Metcalfe et al. (NIST), PRL (2010)

Spin-dependent transport;
Spin lifetimes from transient current and noise



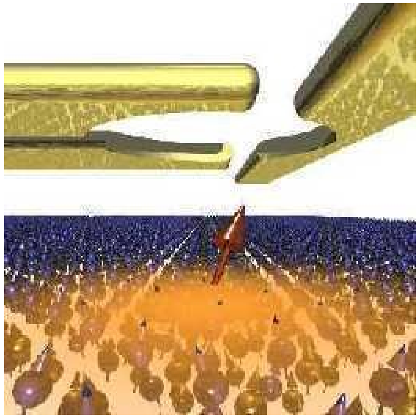


F. Qassemi, WAC, F. K. Wilhelm, PRL (2009)

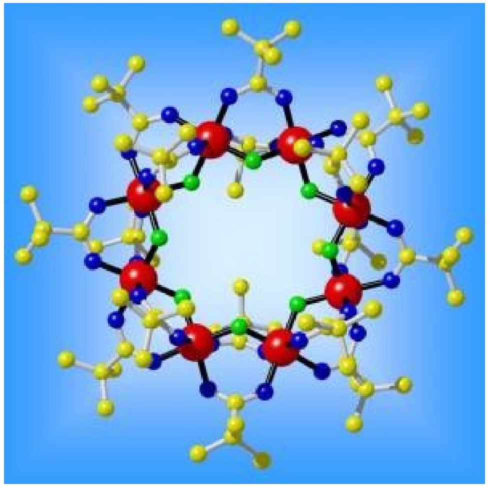
Nuclear spins are (almost) everywhere...

NV centers in diamond

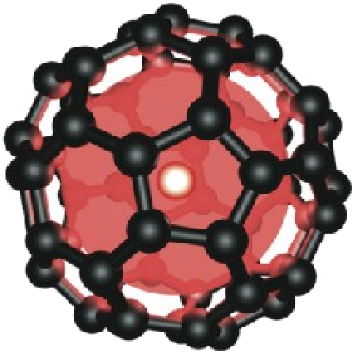
Quantum dots



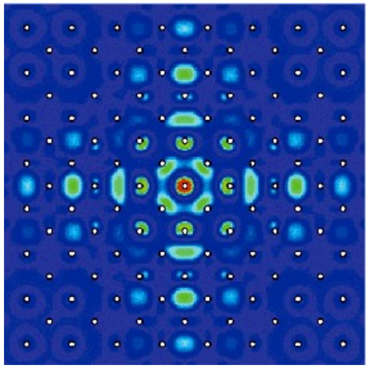
Molecular Magnets



N@C_{60}

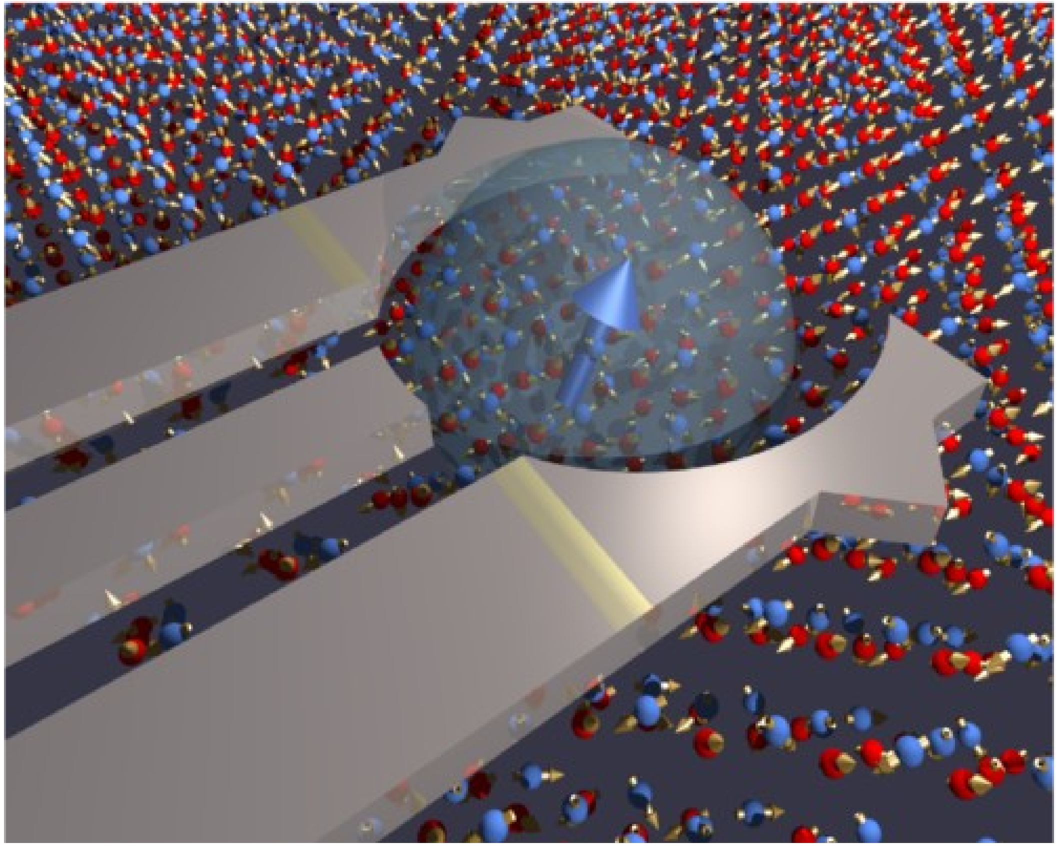


Phosphorus donors



Coherence

Problem: One spin sees many

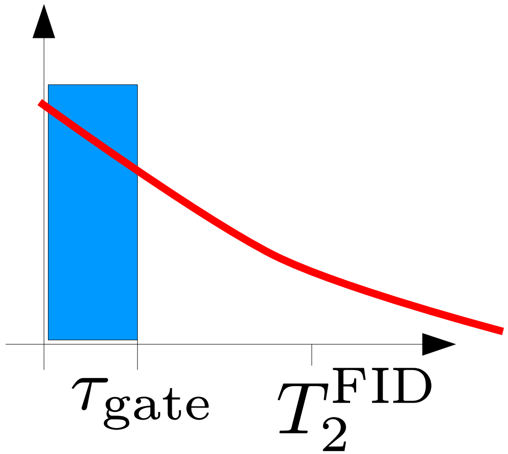


$N \sim 10^6$

nuclei

WAC and J. Baugh, `Nuclear spins in nanostructures',
Phys. Stat. Solidi B (2009)

Free-induction vs. Echoes

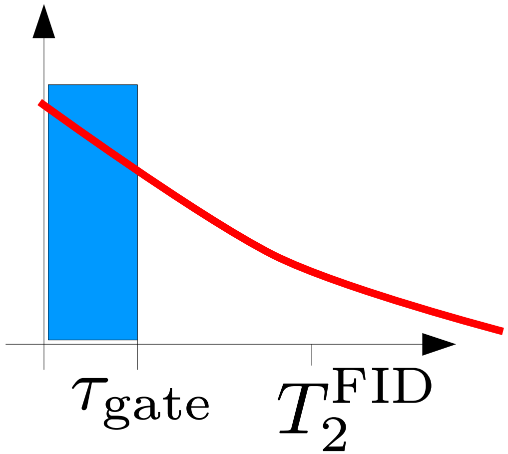


Free-induction decay - approximate error rate?:

$$\eta \sim \tau_{\rm gate}/T_2^{\rm FID}$$

$$S_x(t) \propto e^{-t/T_2}$$

Free-induction vs. Echoes



Free-induction decay - approximate error rate?:

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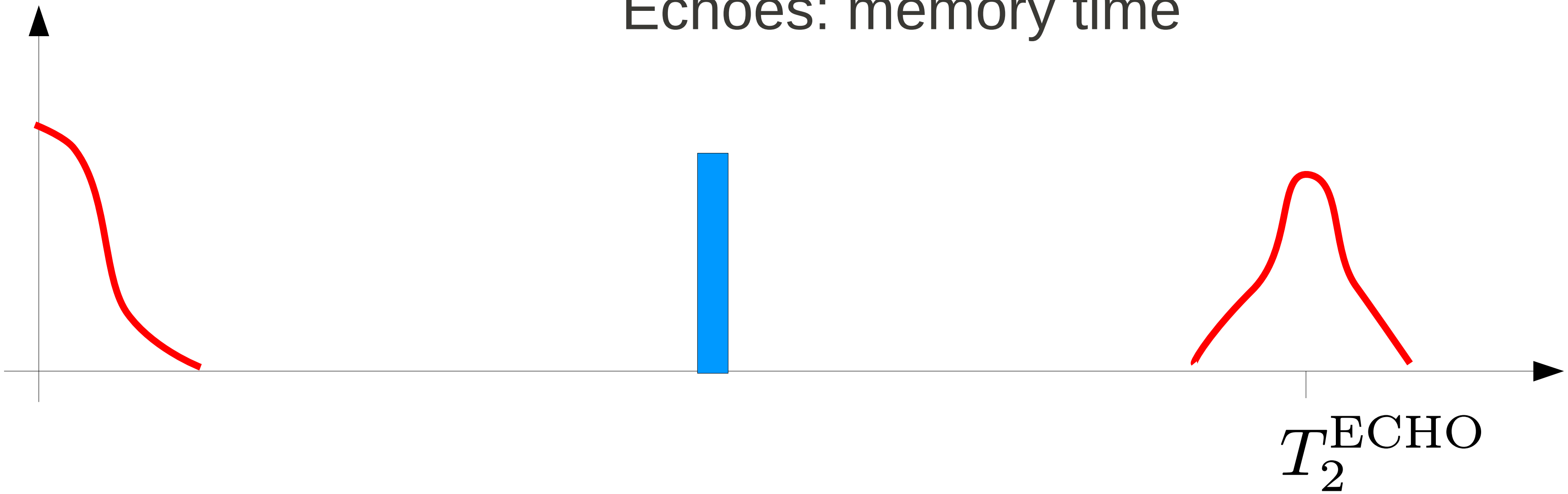
$$S_x(t) \propto e^{-t/T_2}$$

Echoes: memory time



In general, even for a single spin: $T_2^{\text{FID}} \neq T_2^{\text{ECHO}}$

Hyperfine Hamiltonian

$$H_{\mathrm{hf}} = bS^z + \mathsf{h} \cdot \mathsf{S}$$

Electron Zeeman energy

Coupling to nuclear field

$$\mathsf{h} = \sum_k A_k \mathsf{I}_k$$

$$A = \sum_k A_k$$

Hyperfine Hamiltonian

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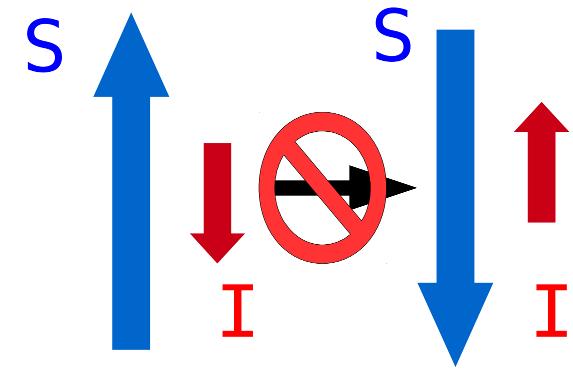
$$\mathsf{h}\cdot\mathsf{S} = h^z S^z + \frac{1}{2}\left(h^+ S^- + h^- S^+\right)$$

V_{ff} does not conserve energy for large b



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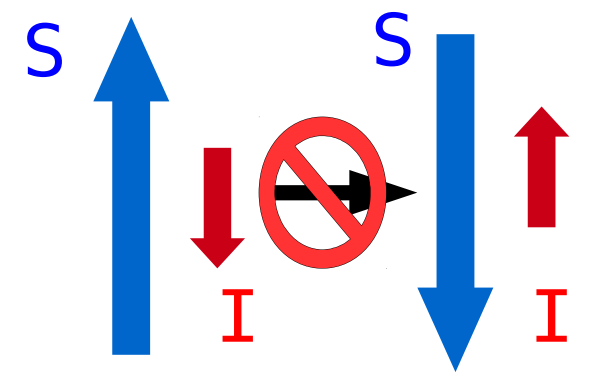
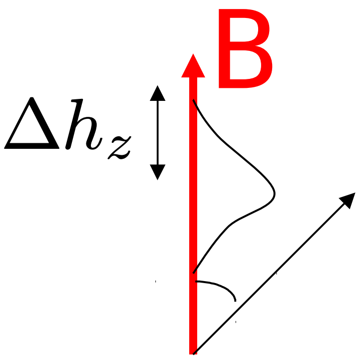


$V_{\rm ff}$ does not conserve energy for large b

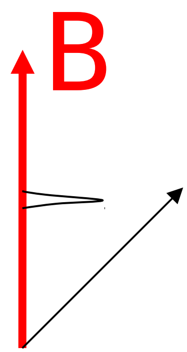
Perturbation theory in $\frac{A}{b} \ll 1$ $\quad b/g^*\mu_B \gtrsim 3.5\,\mathrm{T}\ (\mathrm{GaAs})$

Nuclear-spin bath preparation



$$h \Rightarrow \langle S_x \rangle_t \propto e^{-(t/\tau)^2} \quad \tau \sim \mathrm{ns}$$

measurement



$$h \Rightarrow \langle S_x \rangle_t \propto e^{i\omega t}$$

(narrowed state)

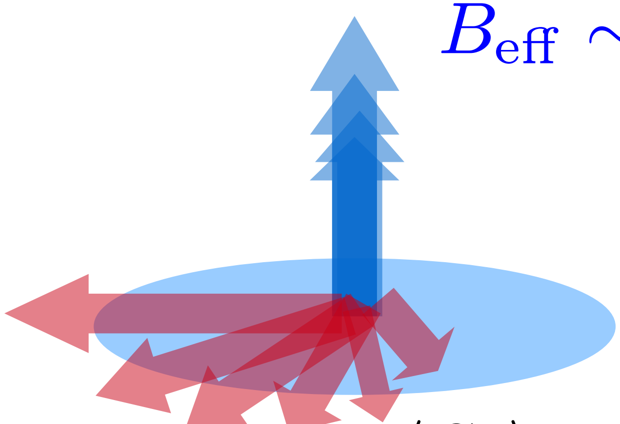
Theory: WAC and Loss, PRB (2004), Klauser, WAC and Loss, PRB (2006,2008),
Stepanenko et al., PRL (2006), Giedke et al., PRA (2006),
Ribeiro and Burkard, PRL (2009),

Expt.: Greilich et al., Science (2006), (2007), Reilly et al., Science (2008),
Xu et al., Nature (2009), Vink et al., Nat. Phys. (2009), Latta et al., Nat. Phys. (2009)

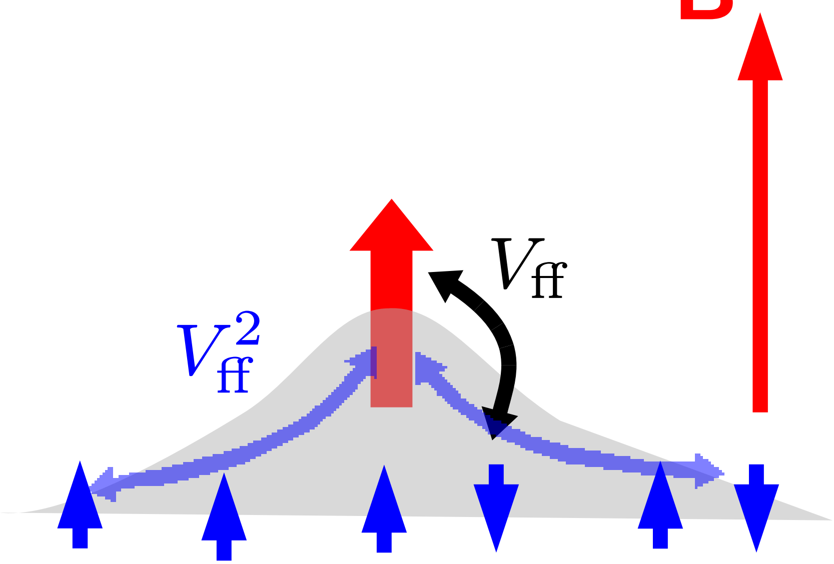
After Narrowing...

Dynamics in nuclear-spin system lead to decay

$$B_{\text{ff}} \sim B + B_N(t)$$



$$\langle S_x \rangle_t \propto e^{-t/T_2}$$



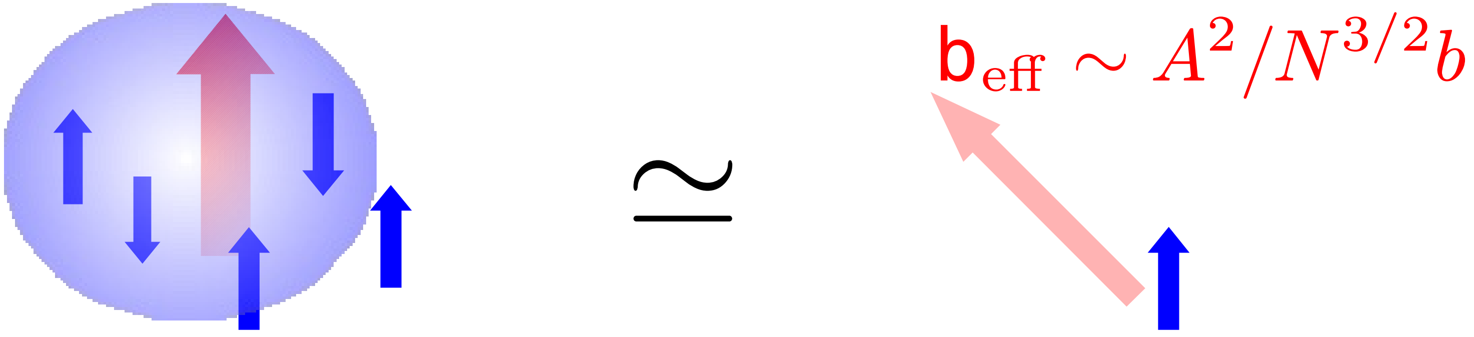
$$V_{\text{ff}} = \frac{1}{2}\left(h^+ S^- + h^- S^+\right)$$

Nuclear-spin dynamics

D. Klauser, WAC, D. Loss, PRB (2008)

Short time:

$$\langle h_z(t) \rangle \simeq \langle h_z(0) \rangle \left(1 - \left(\frac{t}{\tau_n} \right)^2 + \mathcal{O}(t^3) \right) \qquad \tau_n \sim \frac{N^{3/2} b}{A^2} \sim 10^{-4}\,\mathrm{s}$$



Nuclear-spin dynamics

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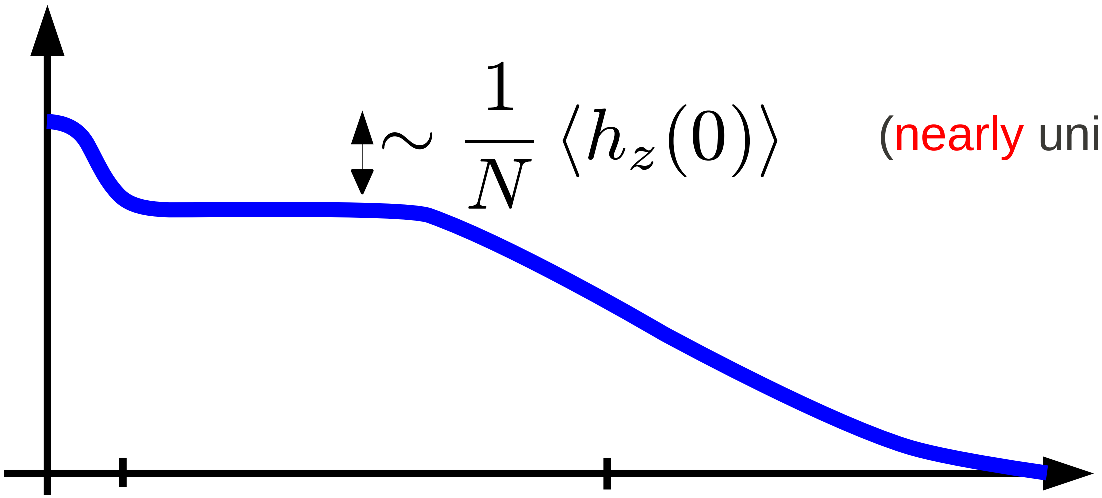
Beyond short time (generalized master equation):



$\langle h_z(t)\rangle$

$\sim \frac{1}{N}\langle h_z(0)\rangle$ (nearly uniform polarization)

$\tau_c \sim \frac{N}{A} \sim 10^{-6}\,\mathrm{s}$ (Nuclear correlation time)

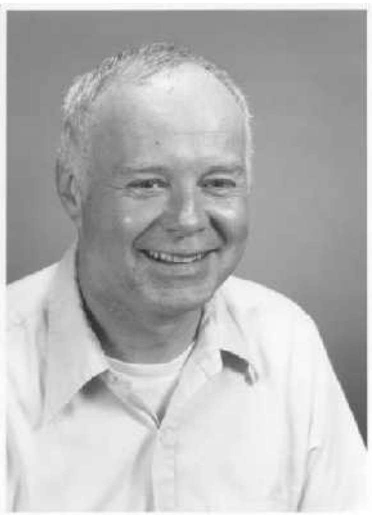
$\tau_{\mathrm{diff}} \gtrsim 1 - 10\,\mathrm{s}$ (Dipolar spin diffusion)

PHYSICAL REVIEW VOLUME 125, NUMBER 3 FEBRUARY 1, 1962

Spectral Diffusion Decay in Spin Resonance Experiments

J. R. Klauder and P. W. Anderson
Bell Telephone Laboratories, Murray Hill, New Jersey

(Received September 1, 1961)



. While some progress has been made in solving, under rather restricted circumstances and with assumptions which are not by any means always valid, the exact quantum-mechanical equations of motion,[2] there is little hope of real progress in that direction on such immensely complicated questions as spectral diffusion.

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Spectral Diffusion Decay in Spin Resonance Experiments

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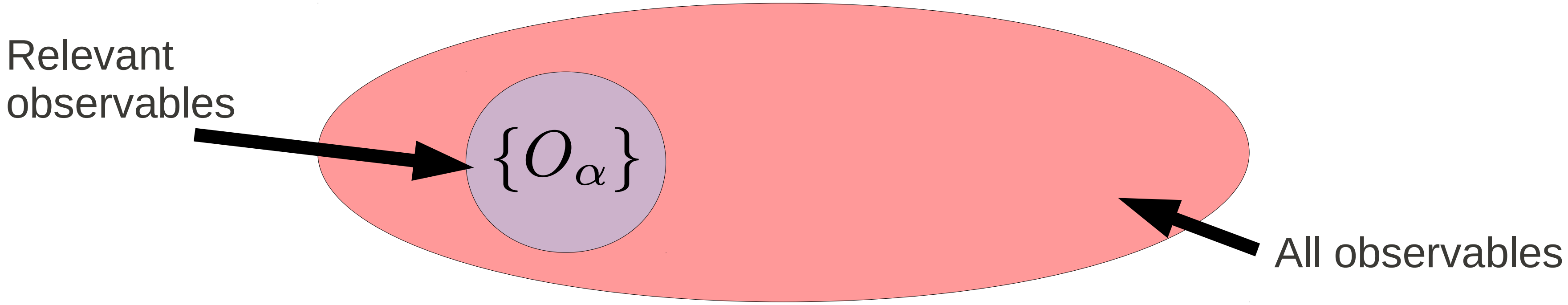
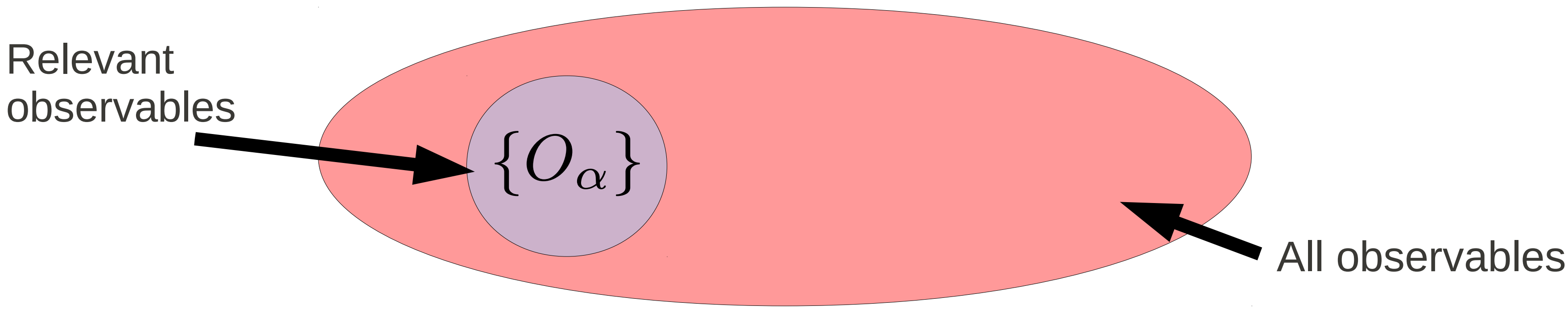
Not an 'easy' problem!

New approach: A general theory of coherent quantum dynamics



Von Neumann: $\dot{\rho} = -i\,[H, \rho]$ $\qquad \langle O_\alpha \rangle_t = \mathrm{Tr}\,\{\mathrm{O}\rho(\mathrm{t})\}$

New approach: A general theory of coherent quantum dynamics



Von Neumann: $\dot{\rho} = -i\left[H, \rho\right]$ $\quad \left\langle O_\alpha \right\rangle_t = \mathrm{Tr}\left\{\mathrm{O}\rho(\mathrm{t})\right\}$

Nakajima-Zwanzig Generalized Master Equation

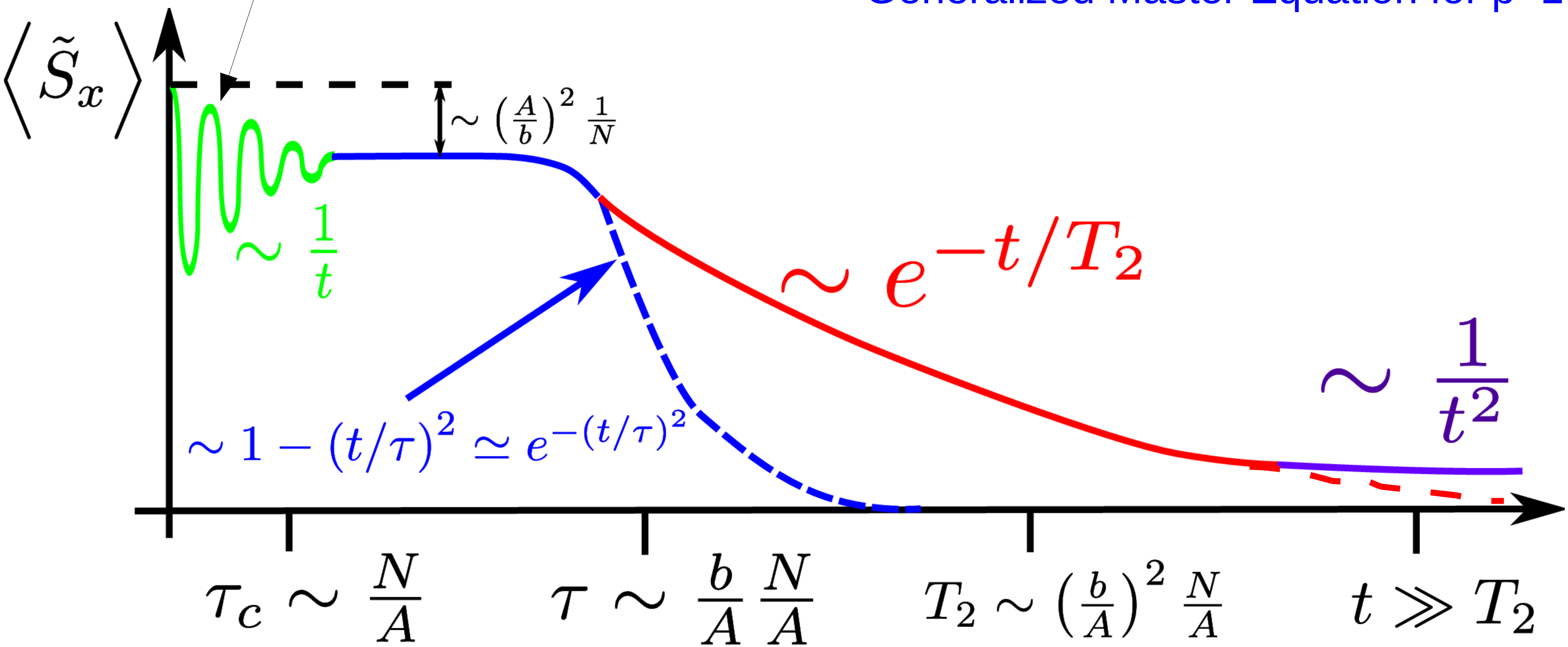
$$\left\langle \dot{O}_\alpha \right\rangle_t = -i \sum_\beta \omega_{\alpha\beta} \left\langle O_\beta \right\rangle_t - i \sum_\beta \int_0^t dt' \Sigma_{\alpha\beta}(t - t') \left\langle O_\beta \right\rangle_{t'}$$

$$H = H_0 + V \qquad \Sigma(t) = \sum_n \Sigma^{(n)}(t) \qquad \Sigma^{(n)}(t) = O\left(V^n\right)$$

Free-induction decay: history

Khaetskii, Loss, Glazman, PRL (2002), PRB (2003)
WAC and Loss, PRB (2004)

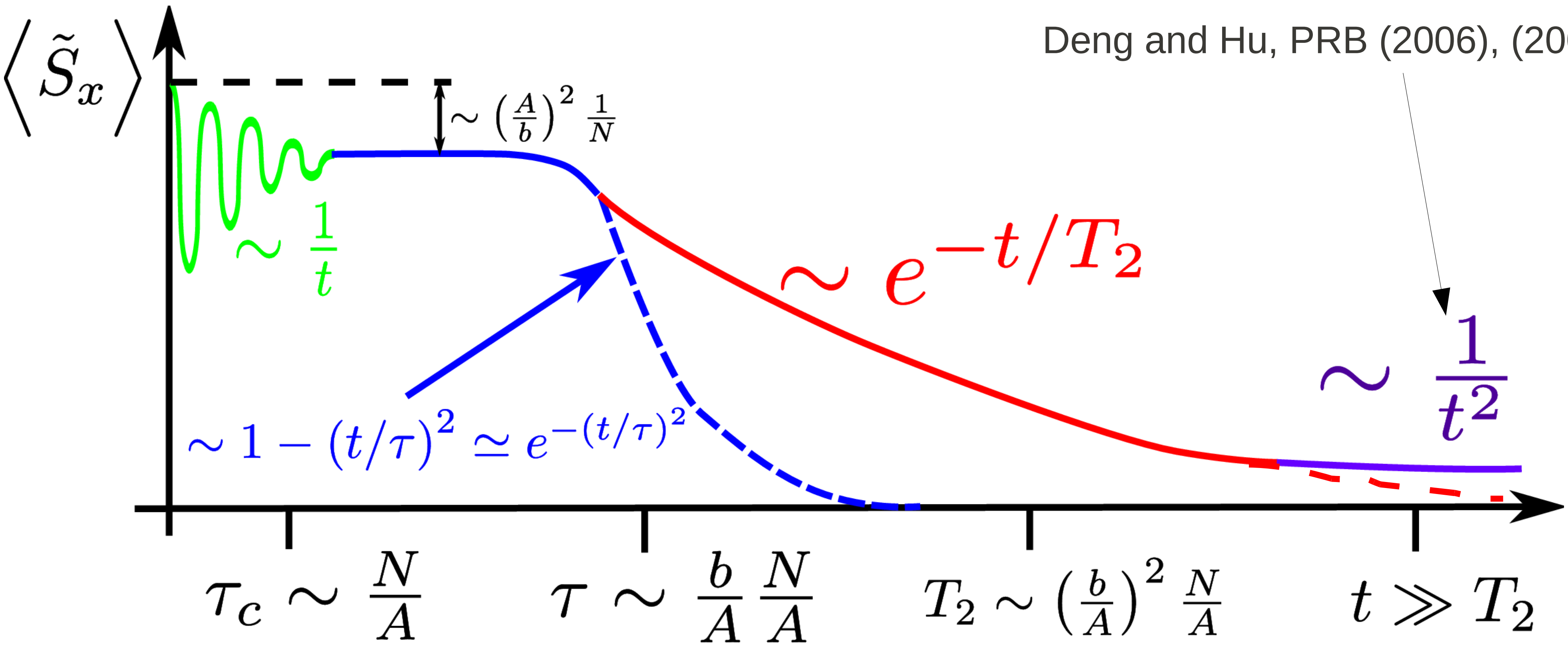
Exact solution for p=1,
Generalized Master Equation for p<1.



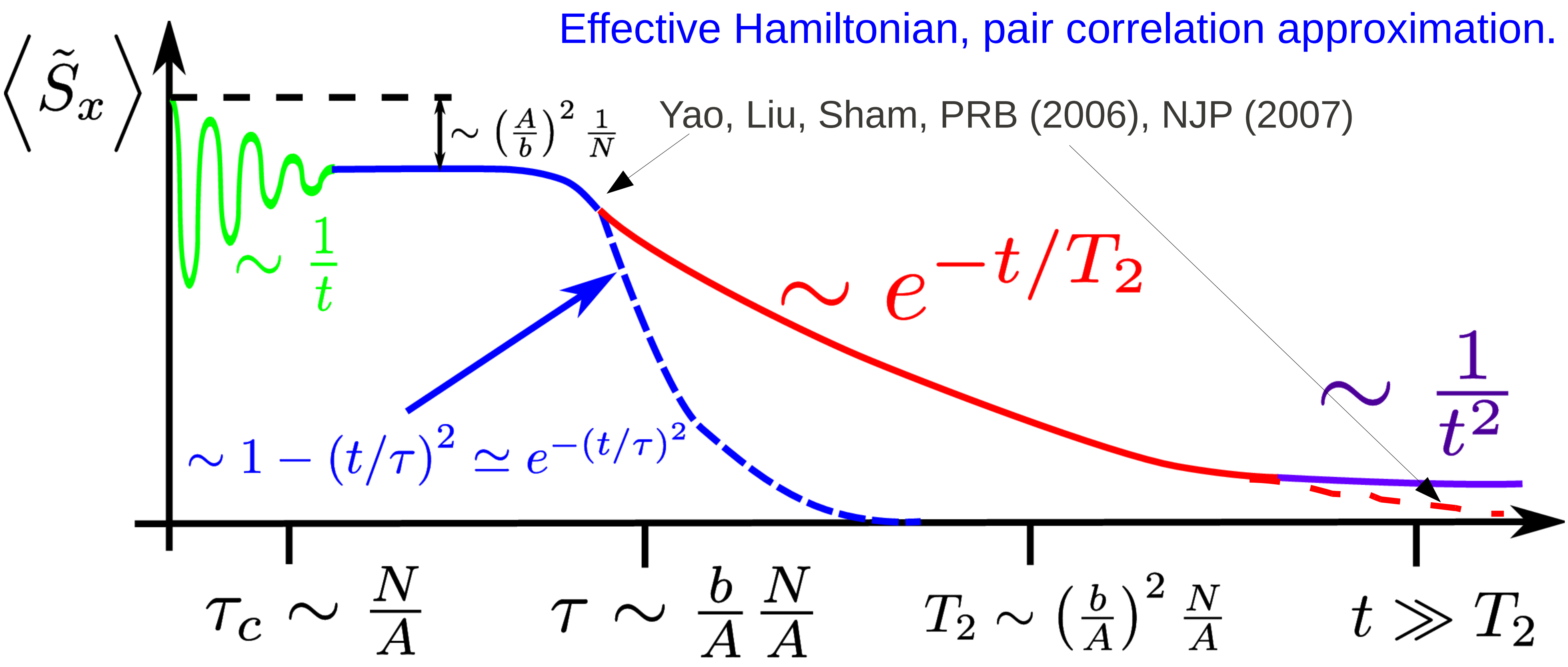
Free-induction decay: history

Equation-of-motion method.

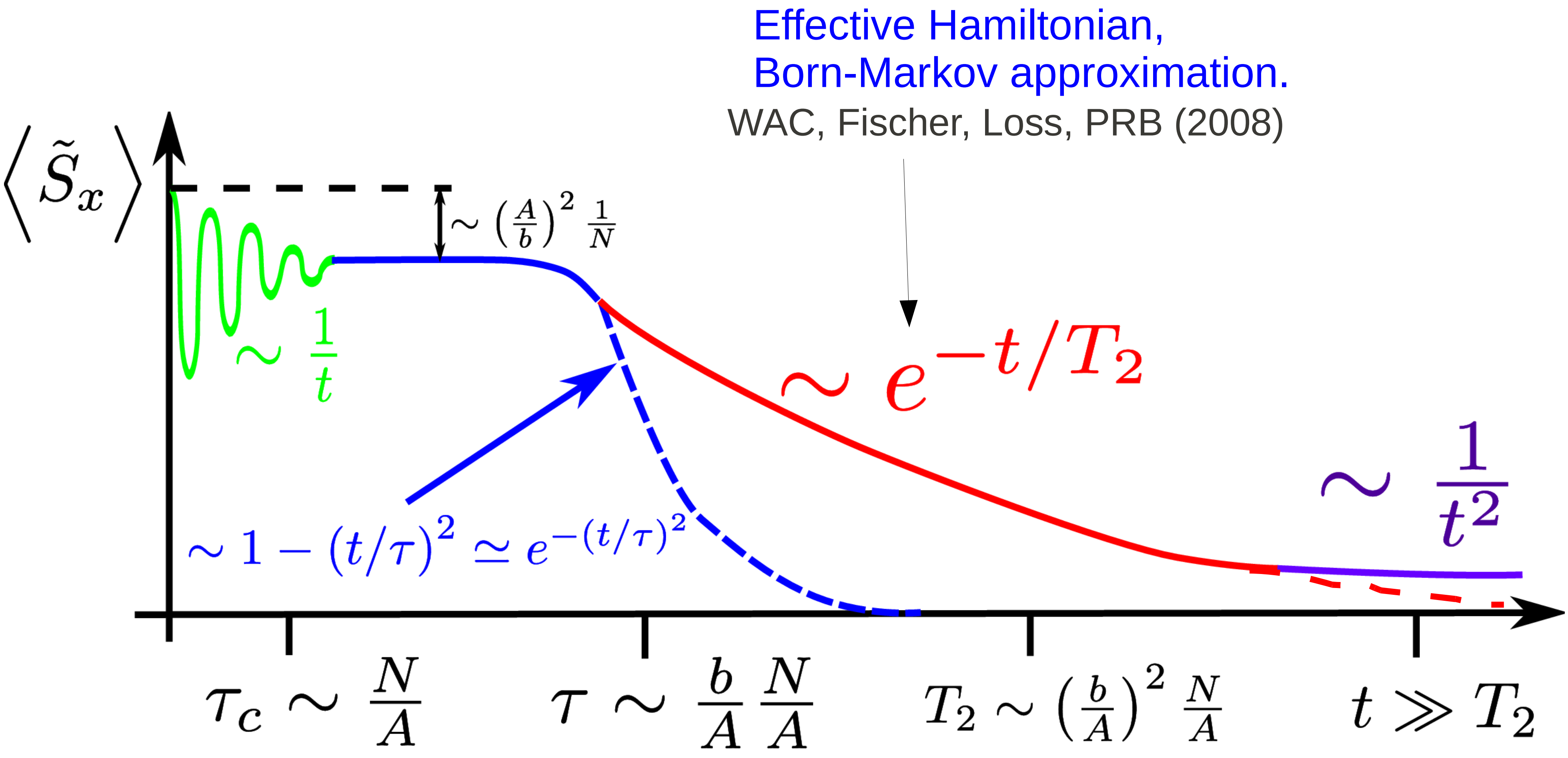
Deng and Hu, PRB (2006), (2008)



Free-induction decay: history



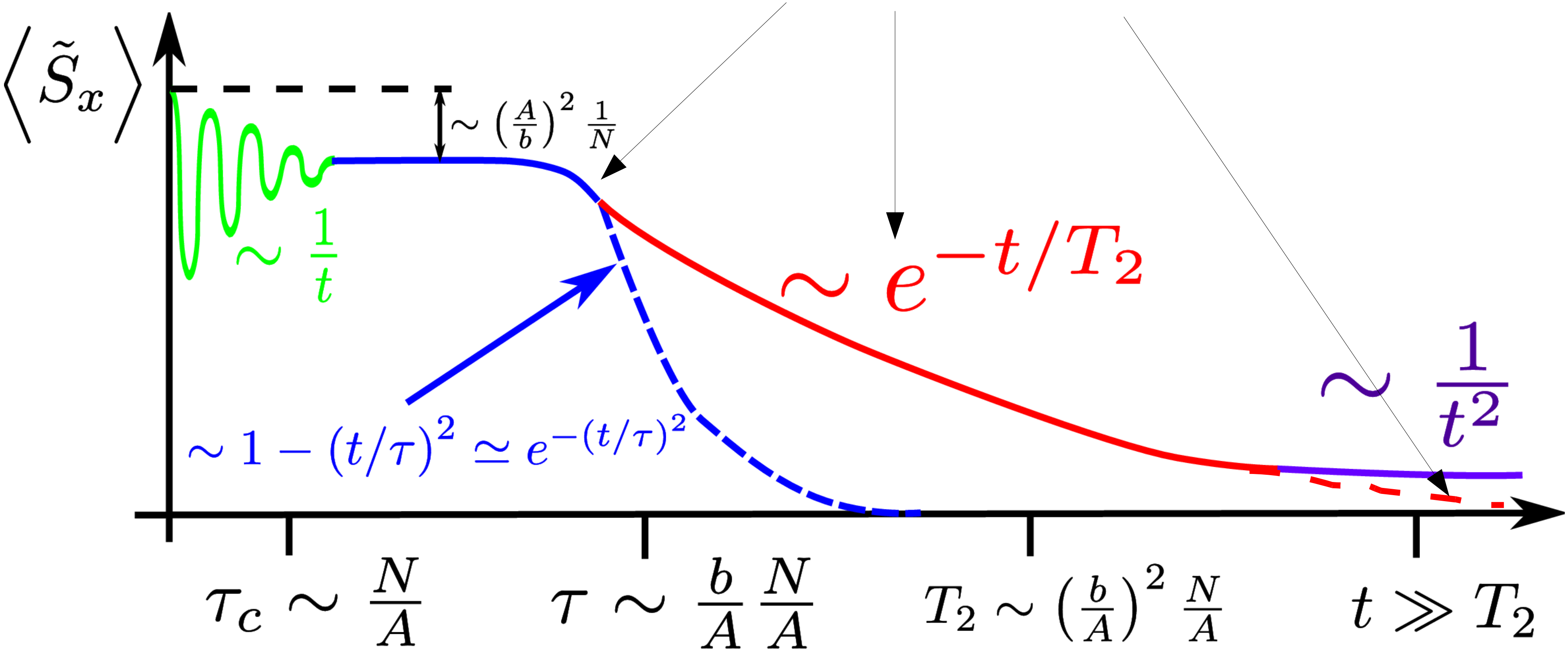
Free-induction decay: history



Free-induction decay: history

Effective Hamiltonian,
High-order resummation, low b-field.

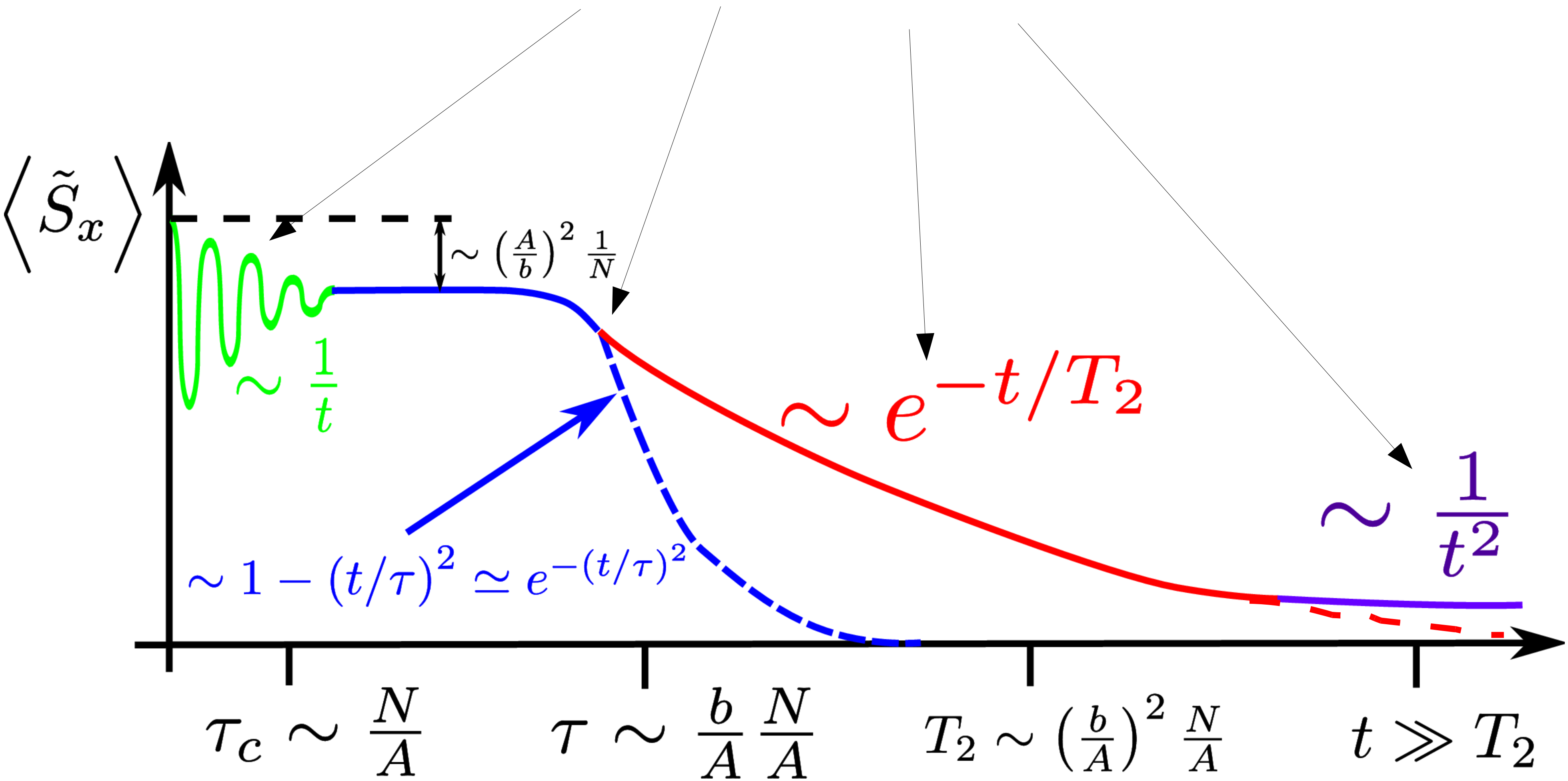
Cywinski, Witzel, Das Sarma, PRL (2009), PRB (2009)



Free-induction decay: history

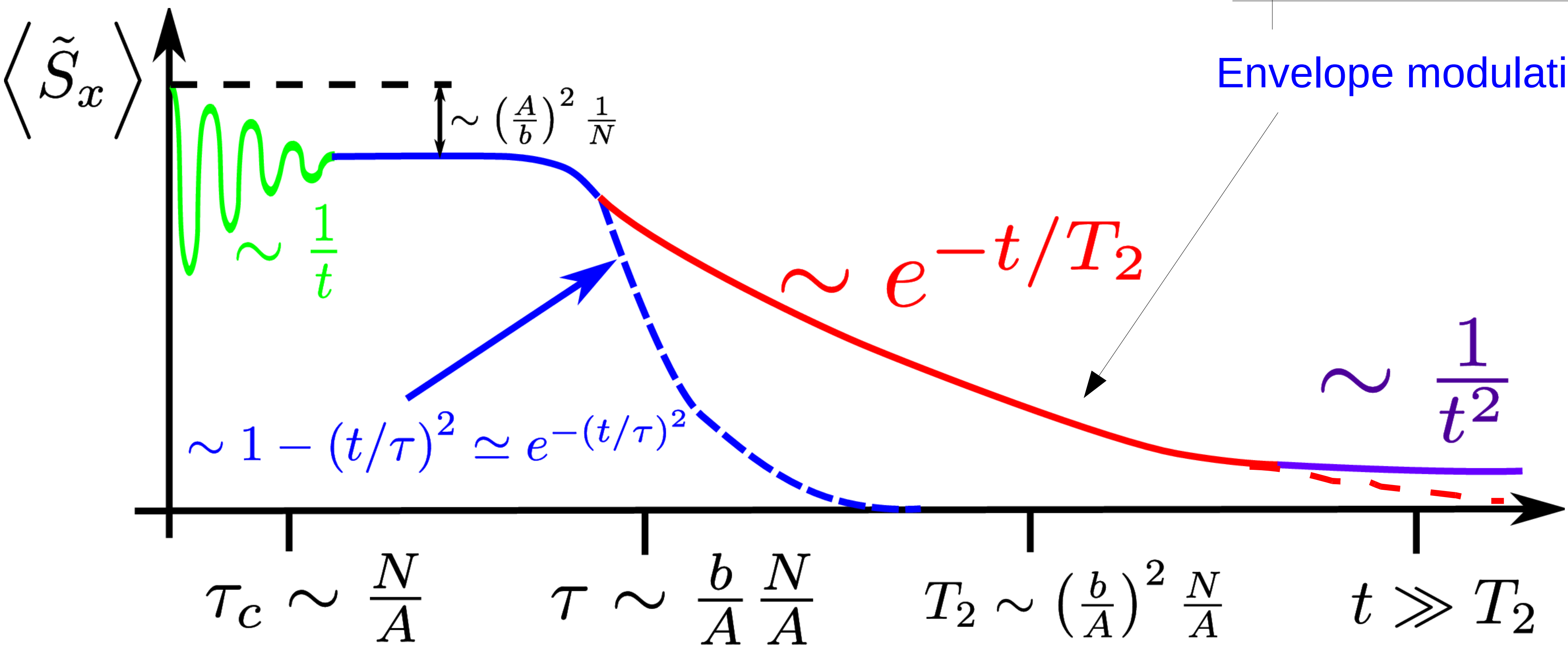
Generalized Master Equation, Higher order.

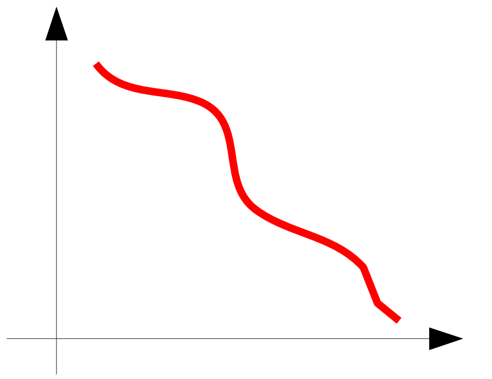
WAC, Fischer, Loss, PRB (2010)



Free-induction decay: history

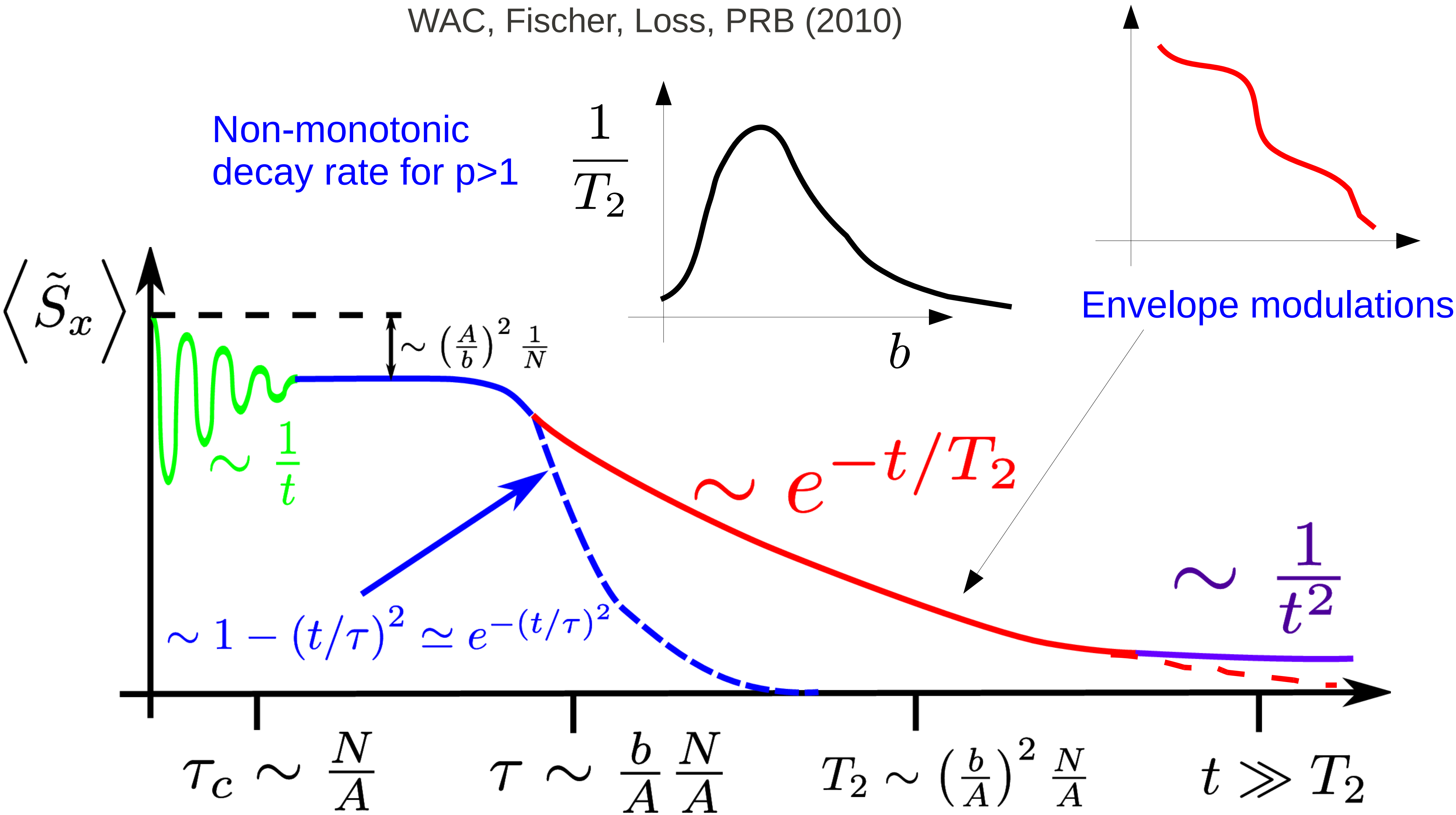
WAC, Fischer, Loss, PRB (2010)





Free-induction decay: history

WAC, Fischer, Loss, PRB (2010)



Solve the problem in two ways:

$$\langle \mathcal{O} \rangle_t = \langle \psi(0) | \, e^{iHt} \mathcal{O} e^{-iHt} \, | \psi(0) \rangle$$

$$H = H_0 + V_{\mathrm{ff}}$$

(1) Effective Hamiltonian

$$\tilde{H} = e^{S} H e^{-S} = H_0 + V_{\mathrm{eff}} + O\left(V_{\mathrm{ff}}^3\right)$$

$$\left| \tilde{\psi}(0) \right\rangle = e^{S} \, | \psi(0) \rangle = | \psi(0) \rangle + O\left(V_{\mathrm{ff}}\right)$$

neglected

Expand in powers of $V_{\mathrm{eff}} \sim O\left(V_{\mathrm{ff}}^2\right) \sim O\left(\frac{A}{b}\right)$

(2) Work directly with the 'real' Hamiltonian

Expand in powers of V_{ff}

Initial conditions

Fast initialization:

$$\rho(0) = \rho_S(0) \otimes \rho_I(0)$$

Sufficient condition: $\tau_{\mathrm{init}} \lesssim 1/A \simeq 50\,\mathrm{ps}$

Narrowed bath:

$$\rho_I(0) = \sum_i \rho_{ii} \left|n_i\right\rangle \left\langle n_i\right| \qquad \omega \left|n_i\right\rangle = \omega_n \left|n_i\right\rangle$$

Generalized Master Equation (GME)

Coherence factor: $$x_t = 2e^{-i(\omega_n + \Delta\omega)t} \langle S_+ \rangle_t$$

GME: $$\dot{x}_t = -i\Delta\omega x_t - i \int_0^t dt' \tilde{\Sigma}(t-t') x_{t'}$$

Lamb shift: $$\Delta\omega = -\mathrm{Re} \int_0^\infty dt \tilde{\Sigma}(t)$$

Markov: $$\frac{1}{T_2} = -\mathrm{Im} \int_0^\infty dt \tilde{\Sigma}(t)$$ $$x_t \simeq x_0 e^{-t/T_2}$$

Direct expansion vs. effective H

$$\Sigma(s) = \int_0^\infty e^{-st}\Sigma(t)$$

Expanding in $V_{\rm ff}$

$$\tilde{\Sigma} \simeq \tilde{\Sigma}^{(2)} + \tilde{\Sigma}^{(4)} + O\left(V_{\rm ff}^6\right)$$

$$\Delta\omega \simeq -{\rm Re}\tilde{\Sigma}^{(2)}(s=0^+) = O(V_{\rm ff}^2)$$

$$\frac{1}{T_2} \simeq -{\rm Im}\tilde{\Sigma}^{(4)}(s=0^+)$$

Expanding in $V_{\rm eff} \sim V_{\rm ff}^2$

$$\tilde{\Sigma}_{\rm eff} = \tilde{\Sigma}_{\rm eff}^{(2)} + O\left(V_{\rm ff}^8\right)$$

$$\Delta\omega_{\rm eff} \simeq -{\rm Re}\tilde{\Sigma}_{\rm eff}^{(2)}(s=0^+) = O(V_{\rm ff}^4)$$

$$\frac{1}{T_2} \simeq -{\rm Im}\tilde{\Sigma}_{\rm eff}^{(2)}(s=0^+)$$

For one isotope: $\tilde{\Sigma}^{(4)} = \tilde{\Sigma}_{\rm eff}^{(2)}$ (with 1/N corrections)

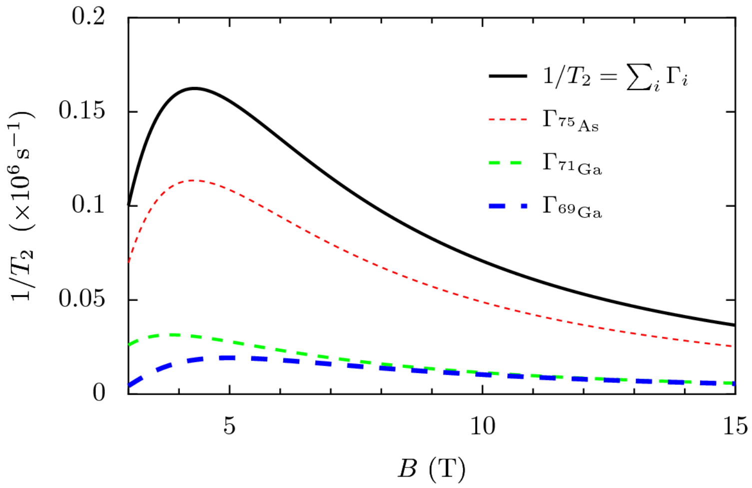
Multiple isotopes: $\tilde{\Sigma}^{(4)} \neq \tilde{\Sigma}_{\rm eff}^{(2)}$

Non-monotonic decoherence Rate!

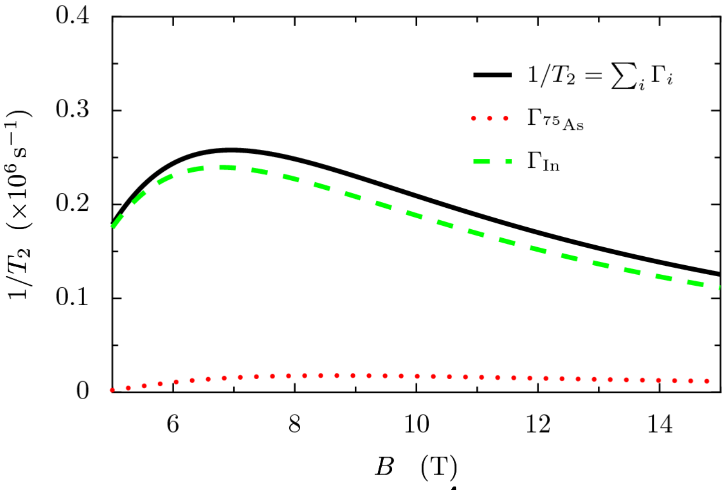
$$\frac{1}{T_2} \simeq -\mathrm{Im}\tilde{\Sigma}^{(4)}(s=0^+) \propto \frac{1}{b^2}\sum_{k,k'} A_k^2 A_{k'}^2 \delta(A_k - A_{k'} - \Delta\omega)$$

$$A_k \leq A/N \qquad \Delta\omega \propto \frac{1}{b}$$

GaAs



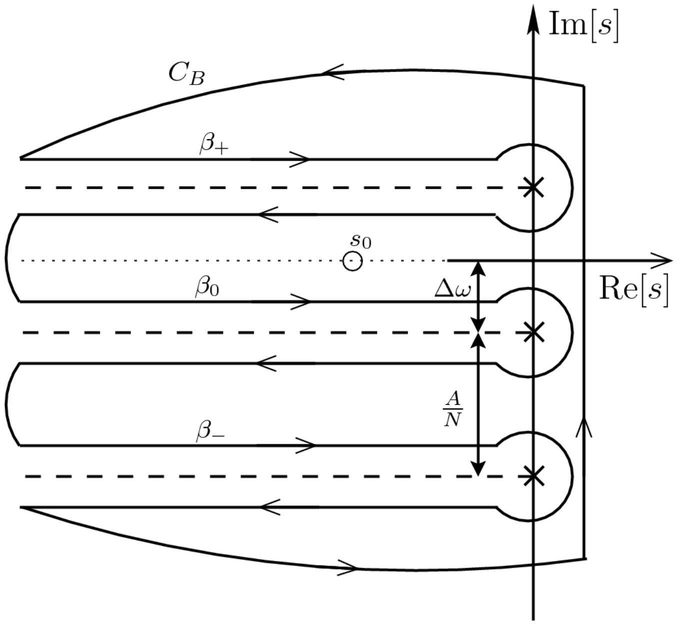
InGaAs



Qualitative behavior (maximum) is controlled by $\left(1-p^2\right)\frac{A}{b} < 1$

Full non-Markovian time dependence

$$x(s) = \frac{x_0}{s - i\Delta\omega - i\tilde{\Sigma}(s)}$$



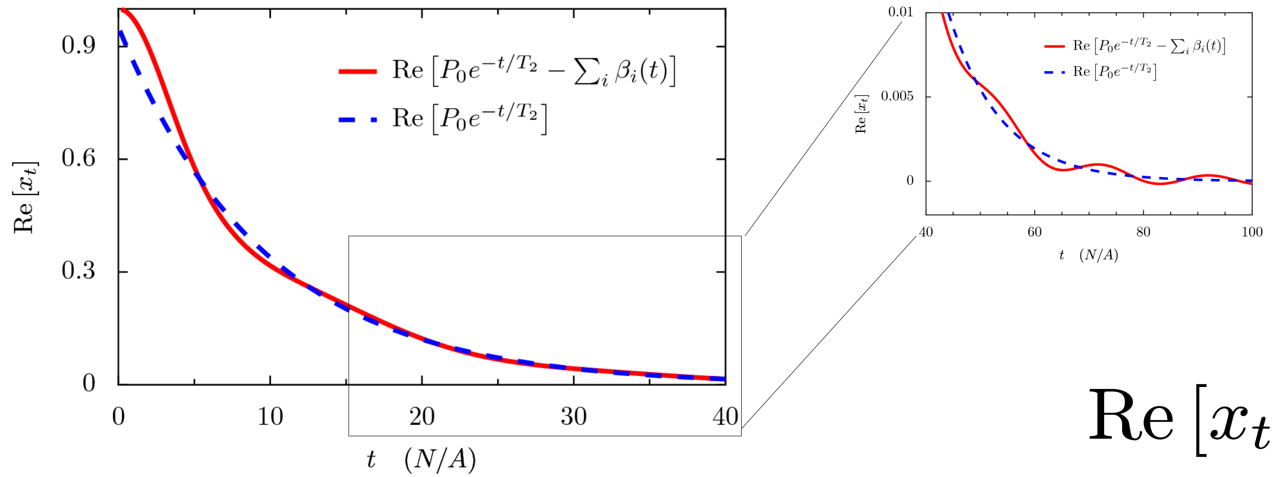
$$x_t = \lim_{\gamma\to 0} \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} e^{st} x(s)$$

$$= \sum_i \mathrm{Res}[e^{st} x(s), x = s_i] - \sum_\alpha \beta_\alpha(t)$$

Exponential decay or sustained oscillations

Power-law decay

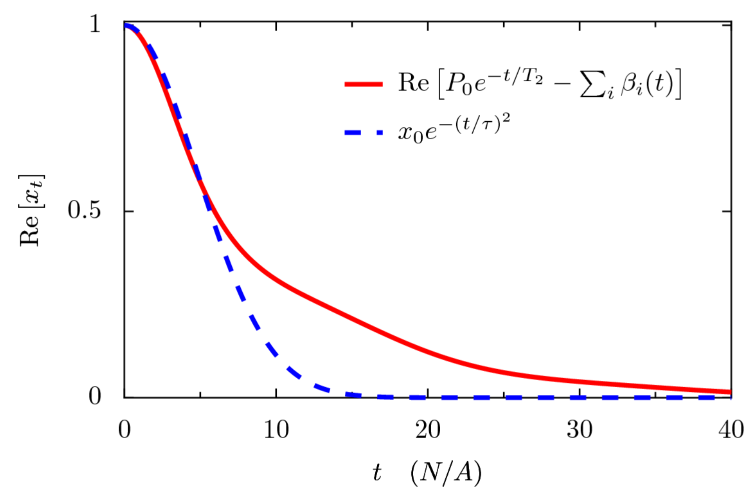
$A/b = \frac{1}{3}$ Envelope modulations!



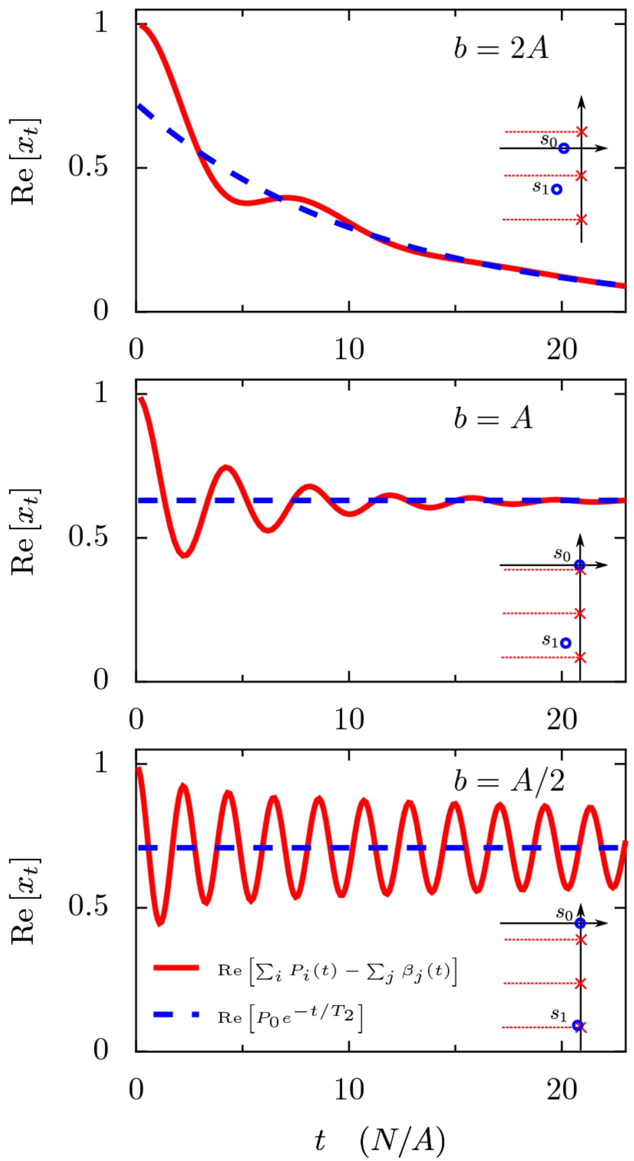
$$t \gg \frac{1}{\Delta\omega}$$

$$\mathrm{Re}\,[x_t] \sim \frac{C\cos\left(\Delta\omega t + \phi\right)}{t^2}$$

Short time: $t < \tau$



Non-perturbative regime b~A



Biexponential decay, strong modulations

Higher-order corrections needed

Conclusions

New envelope modulations of the free-induction decay envelope (distinct from ESEEM)

In general, non-monotonic dependence of $1/T_2$ on magnetic field (reaches a maximum!)

Neither of these result is recovered correctly from the leading-order effective Hamiltonian.