# Nonequilibrium thermal spatial and temporal quantum correlations

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IWQCD1

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Grupo de Física

Materia Condensada

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# Outline

1. Motivation

2. Quantum coherences:
Equilibrium & Nonequilibrium

3. Two-site thermal quantum coherences

4. Two-time thermal quantum coherences

5. Real life systems

6. Conclusions

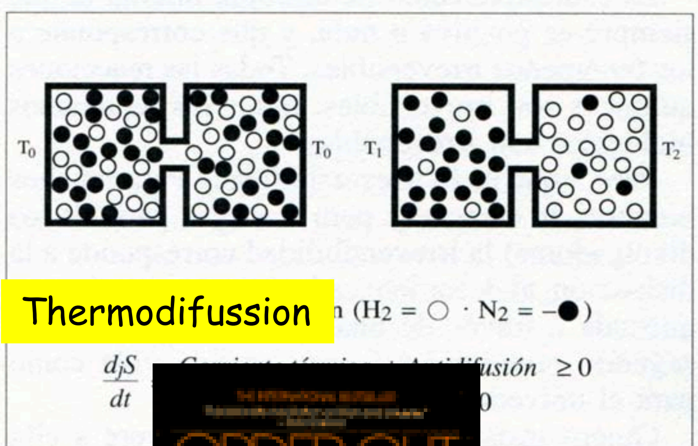
# Nonequilibrium thermal physics...

## Ilya Prigogine

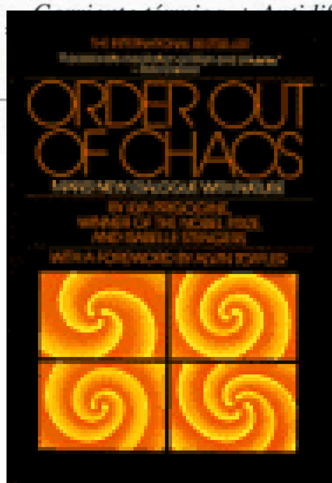
Moscow 1917- Brussels 2003

Chemistry Nobel Prize 1977

## Order out of chaos...




Thermodifussion



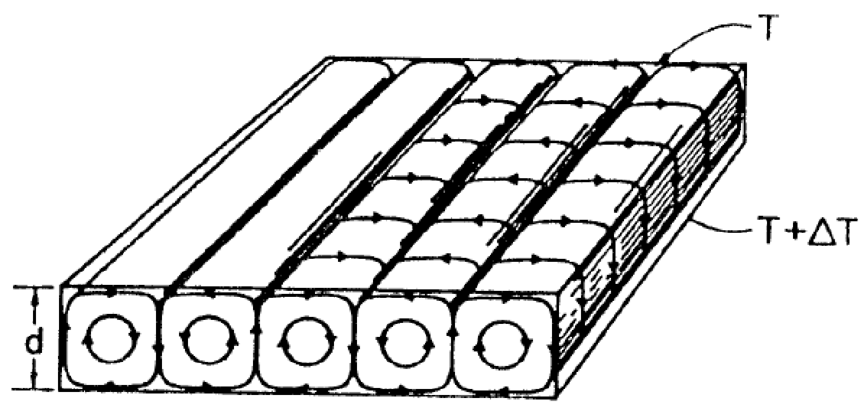




Figure 2: Sketch of parallel convecting rolls in a Rayleigh-Bénard experiment.

# Nonequilibrium Physics = Biological dynamics

# The Biological Frontier of Physics

**Problems at the interface between biology and physics offer unique opportunities for physicists to make quantitative contributions to biology. Equally important, they enrich the discipline of physics by challenging its practitioners to think in new ways.**

Rob Phillips and Stephen R. Quake

38 May 2006 Physics Today

In the introduction to his classic magnetic-monopole pape of 1931, Paul Dirac remarked,

> There are at present fundamental problems in theoretical physics awaiting solution, e.g. the relativistic formulation of quantum mechanics and the nature of atomic nuclei (to be followed by more difficult ones such as the problem of life), the solution of which problems will presumably require a more drastic revision of our fundamental concepts than any that have gone before.[1]

In a deep sense, the problem of the dynamics of macromolecules and their assemblies, of organelles, and of cells themselves strikes right to the heart of just how much physicists will be able to do with systems that are far from equilibrium. Indeed, we believe that biological dynamics is *the* example of nonequilibrium physics. Until now, much of the emphasis in the study of nonequilibrium systems has been on small departures from equilibrium. Furthermore, in many instances the debate that has swirled around questions of nonequilibrium has been philosophical rather than centered on making predictions about specific experimental case studies. Biology, though, may provide the jumping-off point for systematic and predictive ideas on nonequilibrium physics because of the existence of so many manifestly important and well-characterized systems.

# Nonequilibrium thermal physics…

## Order out of chaos…

Some questions arise:

1- Are there corresponding effects in quantum physics?.

2- Is it possible, not only to find but to enhance, quantum coherences by out-of-equilibrium environments?.

# Non-equilibrium Quantum Physics…

PHYSICAL REVIEW E **82**, 021921 (2010)

## Dynamic entanglement in oscillating molecules and potential biological implications

Jianming Cai,[1,2] Sandu Popescu,[3,4] and Hans J. Briegel[1,2]
[1] *Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 25, A-6020 Innsbruck*
[2] *Institut für Quantenoptik und Quanteninformation der Österreichischen Akademie der Wissenschaften, Innsbruck, Austria*
[3] *H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, United Kingdom*
[4] *Hewlett-Packard Laboratories, Stoke Gifford, Bristol BS12 6QZ, United Kingdom*

(Received 8 February 2010; revised manuscript received 14 June 2010; published 25 August 2010)

We demonstrate that entanglement can persistently recur in an oscillating two-spin molecule that is coupled to a hot and noisy environment, in which no static entanglement can survive. The system represents a non-

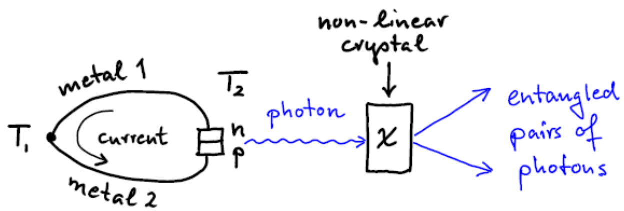



Figure 1: Simple entanglement-generating device (see text).

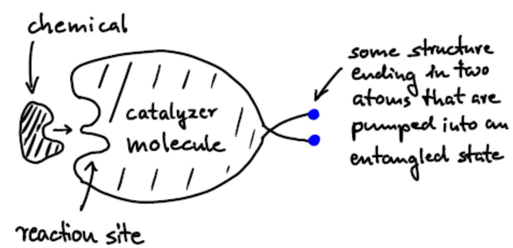



Figure 2: Hypothetical molecular device that is capable of creating entanglement by a molecular pumping process.

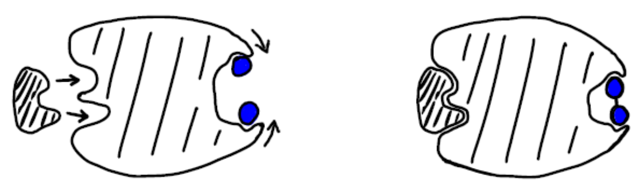
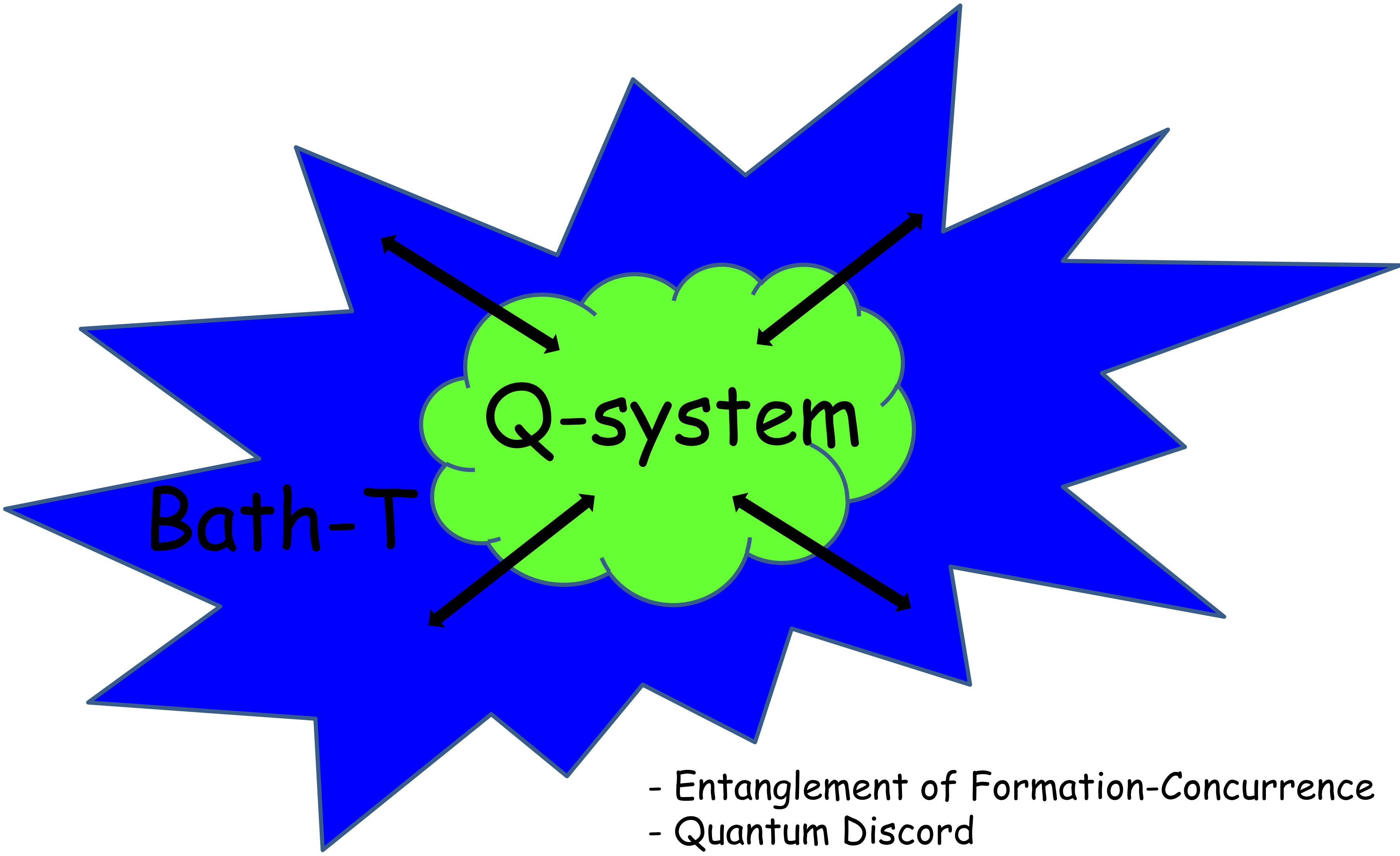


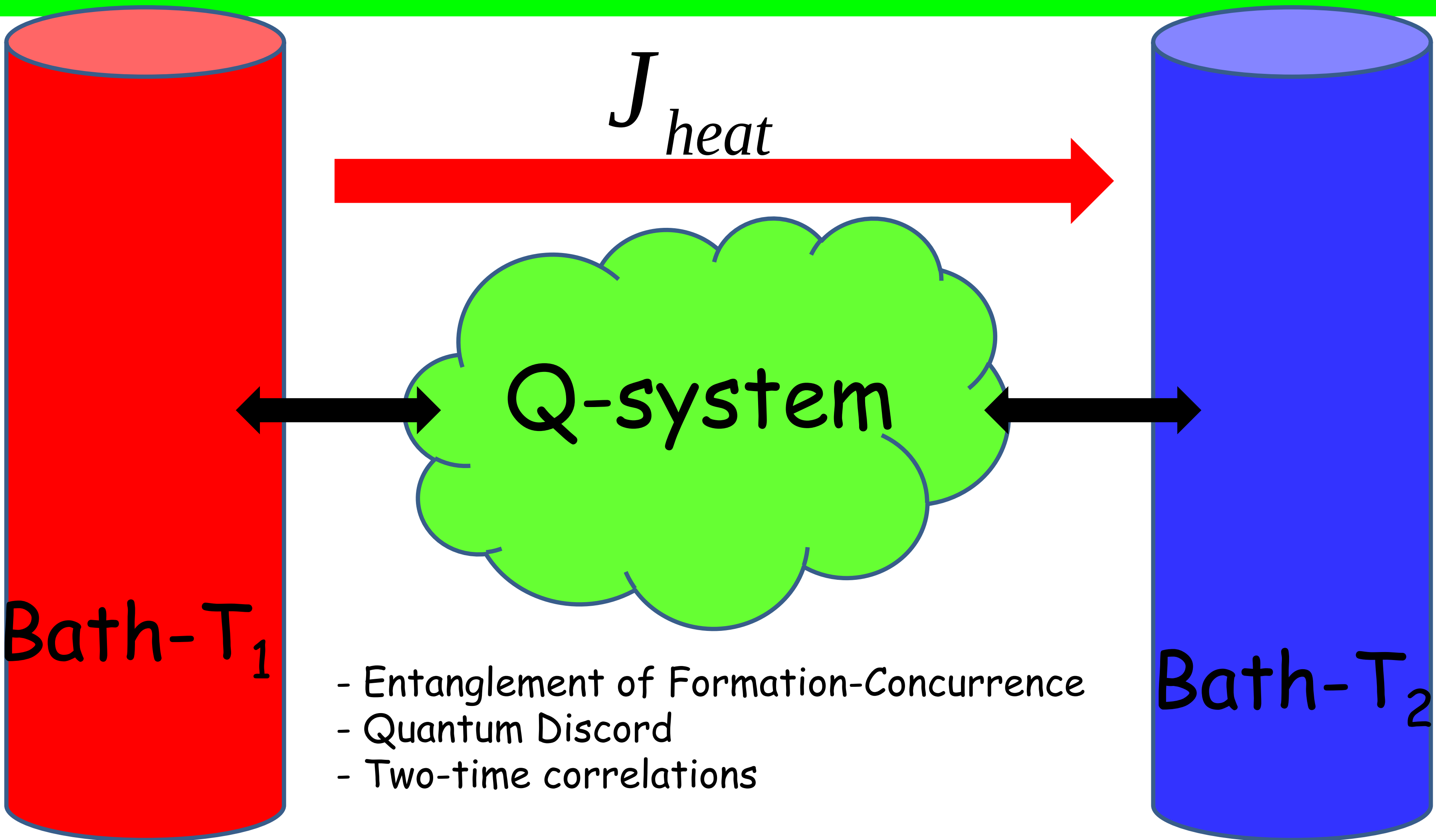
Figure 3: Entanglement of two atoms (blue) in a molecule, induced by a stream of reactant chemicals which dock to the catalyzing molecule, leading to a conformation change (see text).

# Quantum coherences in thermal equilibrium...



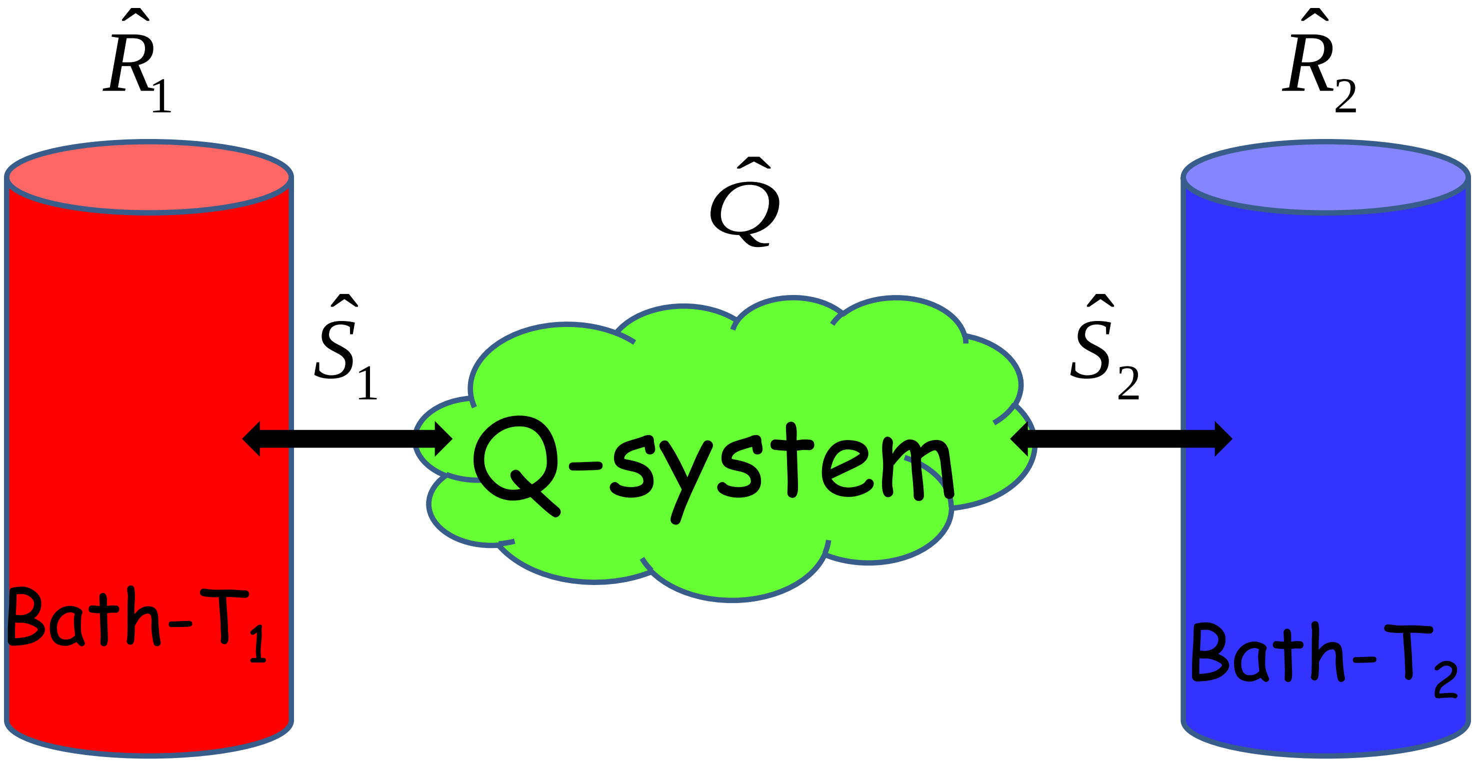

- Entanglement of Formation-Concurrence
- Quantum Discord

# Quantum coherences under nonequilibrium thermal conditions…




- Entanglement of Formation-Concurrence
- Quantum Discord
- Two-time correlations

# Nonequilibrium quantum set up




$$\hat{H} = \hat{Q} + \hat{R}_1 + \hat{R}_2 + \hat{S}_1 + \hat{S}_2$$

$T_1 \geq T_2$

# *General formalism*

$$\frac{d\hat{\gamma}}{dt} = -i\left[\hat{H}, \hat{\gamma}\right]$$

**Liouville-Von Neumann equation**

$$\hat{\gamma}(t) = \hat{\rho}(t)\hat{\rho}_1\hat{\rho}_2$$

**Weak system+bath couplings**

**System's density operator**

$$\hat{\rho}_i = \frac{e^{-\beta_i \hat{R}_i}}{Tr_i\left\{e^{-\beta_i \hat{R}_i}\right\}} \quad , \quad \beta_i = (K_B T_i)^{-1}$$

**Reservoirs in local thermal equilibrium**

# General formalism

## Born-Markov approximation-Lindblad equation

$$\frac{d\hat{\rho}}{dt} = -i\left[\hat{Q}, \hat{\rho}(t)\right] - L_1(\hat{\rho}) - L_2(\hat{\rho})$$

$$L_j(\hat{\rho}) = \sum_\mu J^{(j)}\left(\omega_{j,\mu}\right)\left\{-\hat{V}_{j,\mu}\hat{\rho}\hat{V}^+_{j,\mu} + \hat{\rho}\hat{V}^+_{j,\mu}\hat{V}_{j,\mu} + e^{-\beta_j\omega_{j,\mu}}\left(\hat{V}_{j,\mu}\hat{V}^+_{j,\mu}\hat{\rho} - \hat{V}^+_{j,\mu}\hat{\rho}\hat{V}_{j,\mu}\right)\right\}$$
$$-\sum_\mu J^{(j)}\left(-\omega_{j,\mu}\right)\left\{-\hat{V}^+_{j,\mu}\hat{\rho}\hat{V}_{j,\mu} + \hat{\rho}\hat{V}_{j,\mu}\hat{V}^+_{j,\mu} + e^{-\beta_j\omega_{j,\mu}}\left(\hat{V}^+_{j,\mu}\hat{V}_{j,\mu}\hat{\rho} - \hat{V}_{j,\mu}\hat{\rho}\hat{V}^+_{j,\mu}\right)\right\}$$

M.Goldman, J.Mag.Res. 149, 160 (2001)

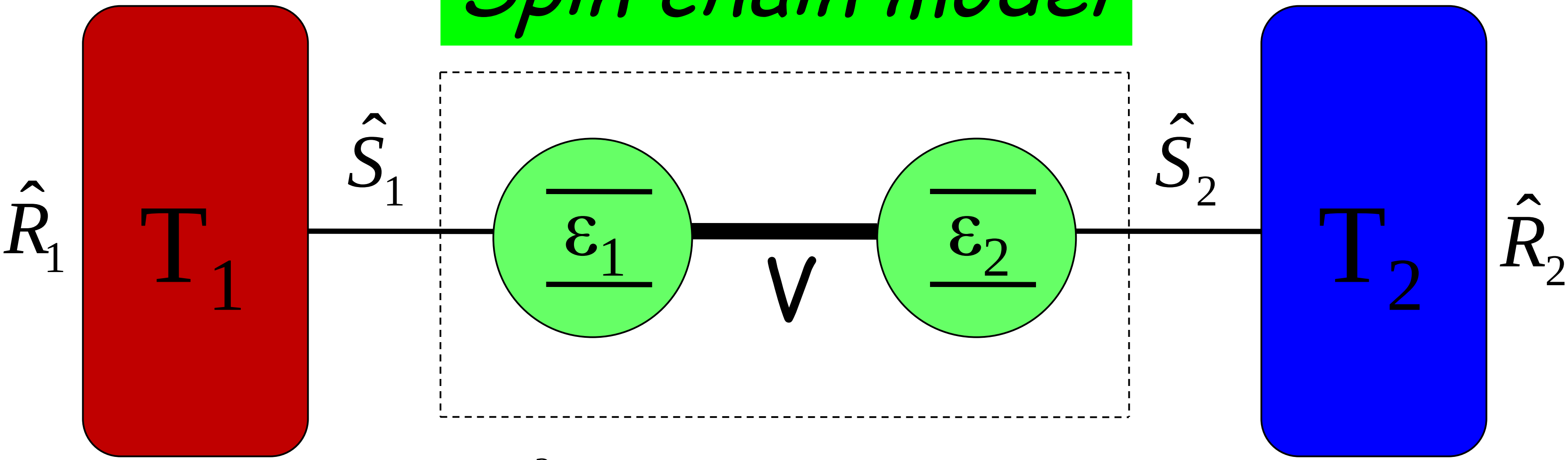
$$\hat{S}_j = \sum_\mu \hat{V}_{j,\mu}\hat{f}_{j,\mu} \quad \text{with} \quad \left[\hat{Q}, \hat{V}_{j,\mu}\right] = \omega_{j,\mu}\hat{V}_{j,\mu}$$

$$J^{(j)}_{\mu,\nu}(\omega_{j,\nu}) = \int_0^\infty d\tau e^{i\omega_{j,\nu}\tau} Tr_j\left\{\hat{\rho}_j \bar{f}^+_{j,\nu}(\tau)\hat{f}_{j,\nu}\right\}$$

j-bath spectral density

Temperature effects

# Spin chain model




$$\hat{Q} = \sum_{\alpha=1}^{2} \frac{\varepsilon_\alpha}{2} \hat{\sigma}_{\alpha,z} + V(\hat{\sigma}_1^+ \hat{\sigma}_2^- + \hat{\sigma}_1^- \hat{\sigma}_2^+)$$

Boson reservoirs: $\hat{R}_j = \sum_n \omega_{n,j} \hat{a}_{n,j}^+ \hat{a}_{n,j}$

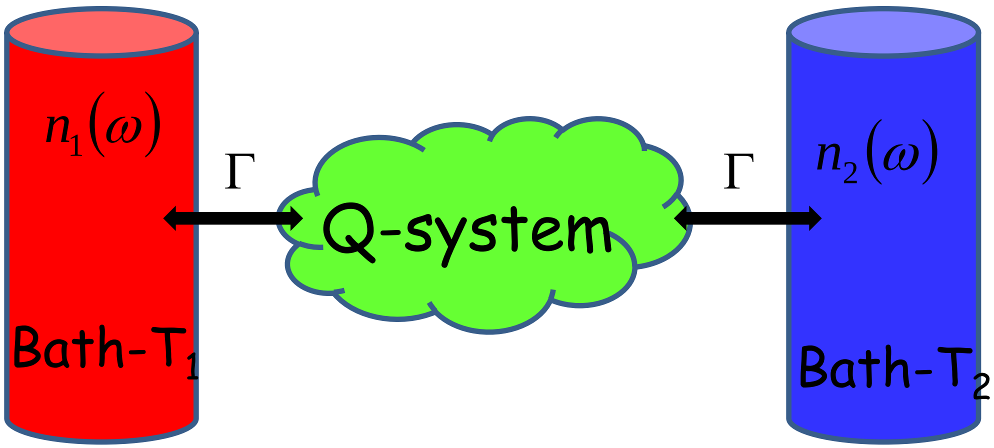
Couplings: $\hat{S}_j = \hat{\sigma}_j^+ \sum_n g_n^{(j)} \hat{a}_{n,j} + \hat{\sigma}_j^- \sum_n g_n^{(j)*} \hat{a}_{n,j}^+$

# Nonequilibrium steady-state solution

$$\frac{d\hat{\rho}_{ss}}{dt} = 0 \quad \Rightarrow \quad i\left[\hat{Q}, \hat{\rho}_{ss}\right] + L_1(\hat{\rho}_{ss}) + L_2(\hat{\rho}_{ss}) = 0$$

$$J^{(j)}(\omega_\mu) = \Gamma_j n_j\left(\omega_\mu\right)$$

Weisskopf-Wigner




$$n_j\left(\omega_\mu\right) = \frac{1}{e^{\beta_j \omega_\mu} - 1}$$

Bose-Einstein occupation

# Results - 1

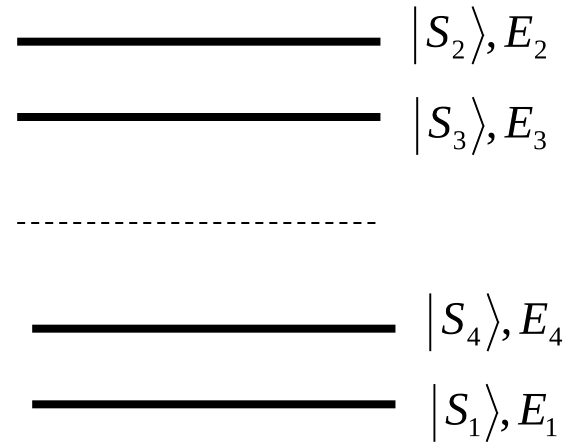
## Two-site quantum coherences

Correlations in states of two spatially separated systems

## Concurrence

# Two-Spin system

$$\hat{Q} = \sum_{\alpha=1}^{2} \frac{\varepsilon_\alpha}{2}\hat{\sigma}_{\alpha,z} + V(\hat{\sigma}_1^{+}\hat{\sigma}_2^{-} + \hat{\sigma}_1^{-}\hat{\sigma}_2^{+})$$




$$|S_1\rangle = |0,0\rangle \rightarrow E_1 = -\frac{\varepsilon_1 + \varepsilon_2}{2}$$

$$|S_2\rangle = |1,1\rangle \rightarrow E_2 = \frac{\varepsilon_1 + \varepsilon_2}{2}$$

$$|S_3\rangle = \cos\left(\frac{\theta}{2}\right)|1,0\rangle + \sin\left(\frac{\theta}{2}\right)|0,1\rangle \rightarrow E_3 = \sqrt{V^2 + \frac{(\varepsilon_1 + \varepsilon_2)^2}{4}}$$

$$|S_4\rangle = -\sin\left(\frac{\theta}{2}\right)|1,0\rangle + \cos\left(\frac{\theta}{2}\right)|0,1\rangle \rightarrow E_4 = -\sqrt{V^2 + \frac{(\varepsilon_1 + \varepsilon_2)^2}{4}}$$

$$Tan(\theta) = \frac{2V}{\varepsilon_1 - \varepsilon_2}$$

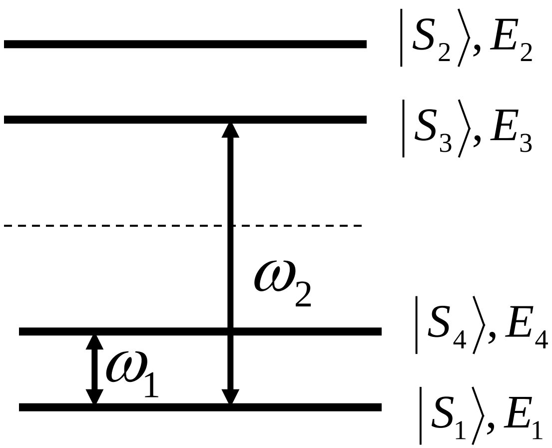
# Symmetric case: $\varepsilon_1 = \varepsilon_2 = \varepsilon$

## Steady-state density matrix in the Q eigenbasis

$$\hat{\rho} = \begin{pmatrix} \frac{e_1}{2}\left(1-\frac{e_2}{2}\right) & 0 & 0 & 0 \\ 0 & \left(1-\frac{e_1}{2}\right)\frac{e_2}{2} & 0 & 0 \\ 0 & 0 & \frac{e_1 e_2}{4} & 0 \\ 0 & 0 & 0 & \left(1-\frac{e_1}{2}\right)\left(1-\frac{e_2}{2}\right) \end{pmatrix}$$

$$e_j = e(\omega_j) = \frac{n_1(\omega_j) + n_2(\omega_j)}{1 + n_1(\omega_j) + n_2(\omega_j)} \leq 1$$

$T_1$     $T_2$



# Results

$$\hbar = 1, K_B = 1$$

$$Spin - spin\ coupling\ : V = 1$$

$$Weak\ spin - spin\ coupling\ : V < \varepsilon$$

$$T_M = \frac{T_1 + T_2}{2}$$ → Mean temperature

$$\Delta T = | T_1 - T_2 |$$ → Temperature gradient

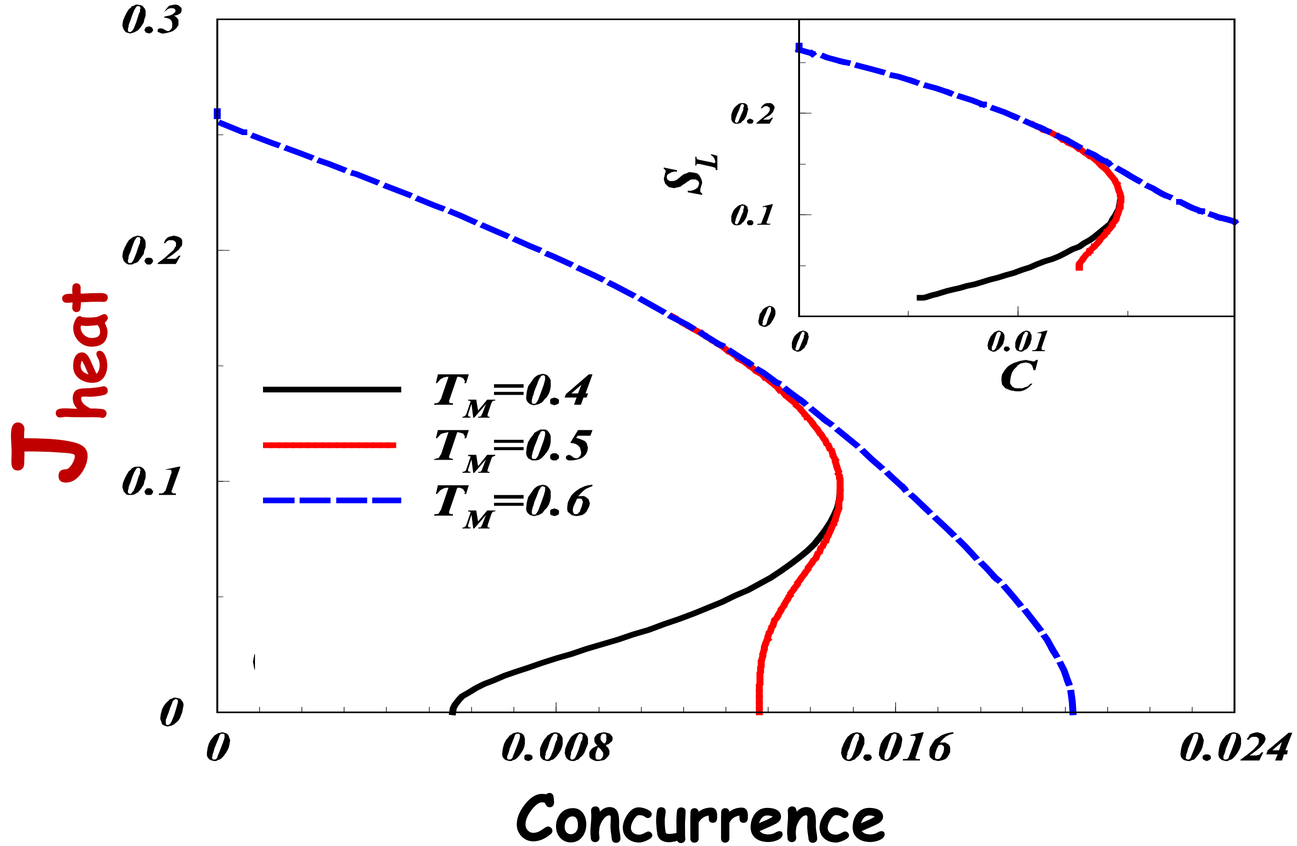
# Entanglement → Concurrence
(W.K.Wooters, PRL 80, 2245 (1998))

$$C = 2Max\left\{0, \frac{|\rho_{3,3} - \rho_{4,4}|}{2} - \sqrt{\rho_{1,1}\rho_{2,2}}\right\}$$

# Equilibrium case: $T_1 = T_2 = T$

$$C_{EQ}(T) = \frac{\sinh\left(\frac{1}{T}\right) - 1}{2\cosh\left(\frac{\omega_1}{2T}\right)\cosh\left(\frac{\omega_2}{2T}\right)} \Rightarrow C_{EQ}(T) = 0 \; if \; T \geq T_c = 1.1346$$

$$J_{heat}(\Delta T) = \frac{\kappa}{\sqrt{\alpha}} |C_{EQ} - C(\Delta T)|^{\frac{1}{2}}$$




$$T_M = \frac{T_1 + T_2}{2}$$ → Mean temperature

$$\Delta T = |T_1 - T_2|$$ → Temperature gradient

L.Quiroga, FJR, MER & RP, Phys.Rev. A75, 032308 (2007)

# Results - 2

## Two-time quantum coherences

Correlations in states of a single system at different points in time

- Two-time correlation
- Leggett-Garg inequality

PHYSICAL REVIEW
LETTERS

VOLUME 54 | 4 MARCH 1985 | NUMBER 9

## Quantum Mechanics versus Macroscopic Realism: Is the Flux There when Nobody Looks?

A. J. Leggett
*Department of Physics,*[a] *University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, and Department of Physics, Harvard University, Cambridge, Massachusetts 02138*

and

Anupam Garg
*University of Illinois at Urbana-Champaign, Urbana, Illinois 61801*
(Received 19 November 1984)

Measurement of a dichotomic observable: $Q \to \pm 1$

Assumptions:

- Macroscopic realism
- Noninvasive measurement=Stationarity

**LGI**

$$F(t_1,t_2,t_3)=C(t_1,t_2)+C(t_2,t_3)-C(t_1,t_3)\leq 1$$

$$C(t_1,t_2) = \langle Q(t_1)Q(t_2) \rangle$$

PHYSICAL REVIEW LETTERS

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# Quantum Mechanics versus Macroscopic Realism: Is the Flux There when Nobody Looks?

A. J. Leggett
*Department of Physics,*[a] *University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, and Department of Physics, Harvard University, Cambridge, Massachusetts 02138*

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(Received 19 November 1984)

## Main message:

LGI provides a criterion to characterize the boundary between the classical and quantum domains and the possible identification of macroscopic quantum coherences.

# Leggett-Garg inequality (LGI)

$$F(t_1,t_2,t_3)=C(t_1,t_2)+C(t_2,t_3)-C(t_1,t_3)\leq 1$$

- LGI can be violated by quantum mechanical unitary dynamics, i.e. Rabi or Larmor.
- For an open quantum system LGI violation can persist depending on the noise strength.
- For Markovian noise, above a certain noise intensity and after a certain time, LGI is not more violated, i.e. classical behavior.

# Leggett-Garg inequality (LGI)

$$F(t_1,t_2,t_3)=C(t_1,t_2)+C(t_2,t_3)-C(t_1,t_3)\leq 1$$

## Technical details:

$$C(t_1,t_2)=p(^+t_1)q(^+t_2|^+t_1)+p(^-t_1)q(^-t_2|^-t_1)-p(^+t_1)q(^-t_2|^+t_1)-p(^-t_1)q(^+t_2|^-t_1)$$

$p(^it)$: Probability of measuring Q with result i at time t

$q(^it_1|^jt_2)$: Conditional probability of measurements of $Q$ at $t_1$ and $t_2$

## Kraus operators:

$$\hat{\rho}(t)=\sum_{m=1}^{N}\hat{K}_m(t)\hat{\rho}(0)\hat{K}_m^{+}(t)$$

J.C.Castillo, FJR & LQ, in preparation

# Leggett-Garg inequality (LGI)

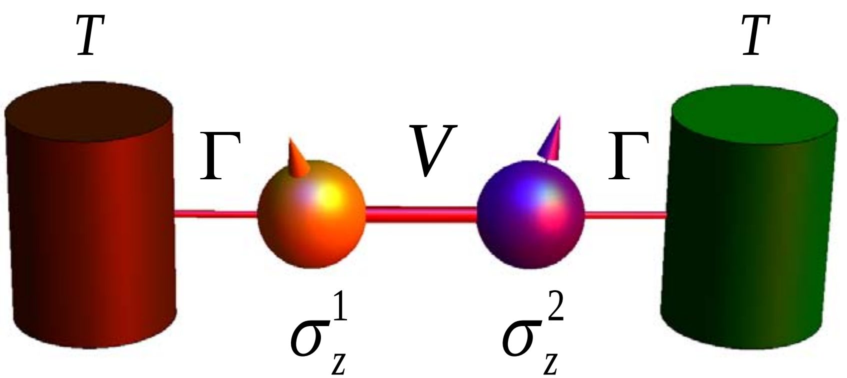
$$F(t_1,t_2,t_3)=C(t_1,t_2)+C(t_2,t_3)-C(t_1,t_3)\leq 1$$

$$Q=\sigma_z^1$$

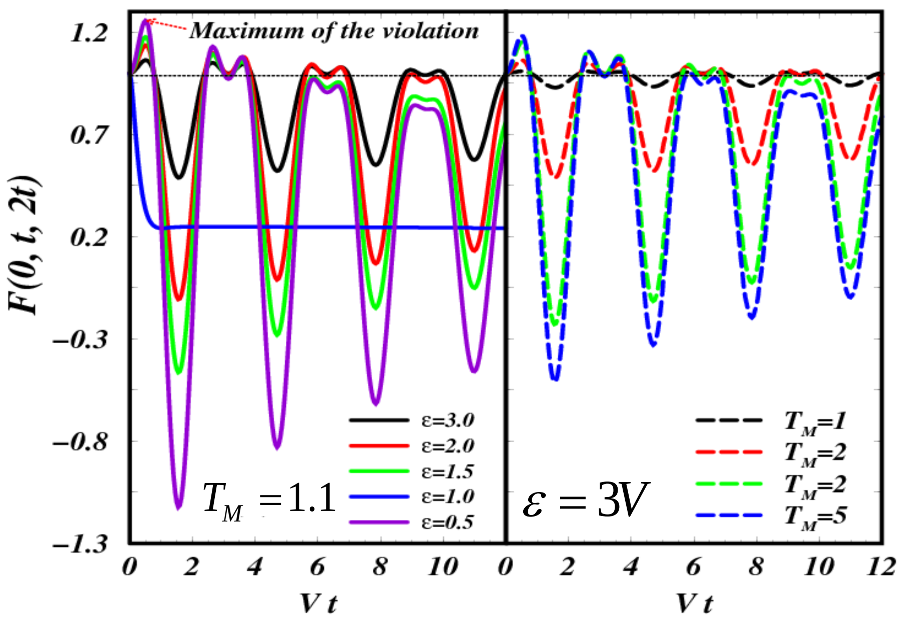
$$C(t_1,t_2)=<\sigma_z^1(t_1)\sigma_z^1(t_2)>$$

$\rho_{ss}$ : Steady-state

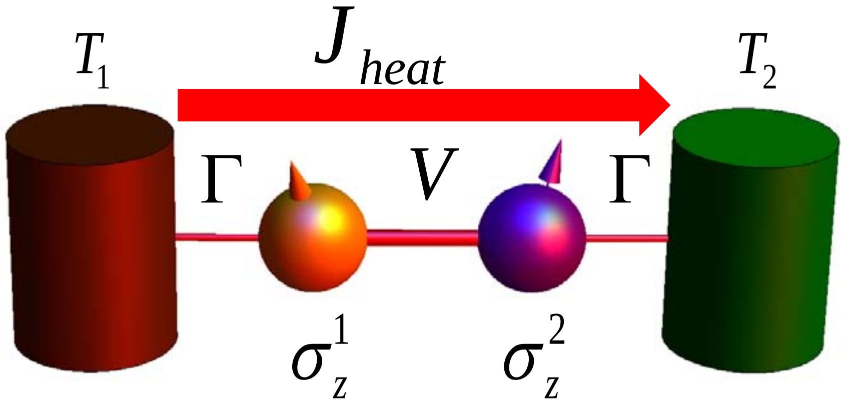
$$\Gamma=0.01V$$



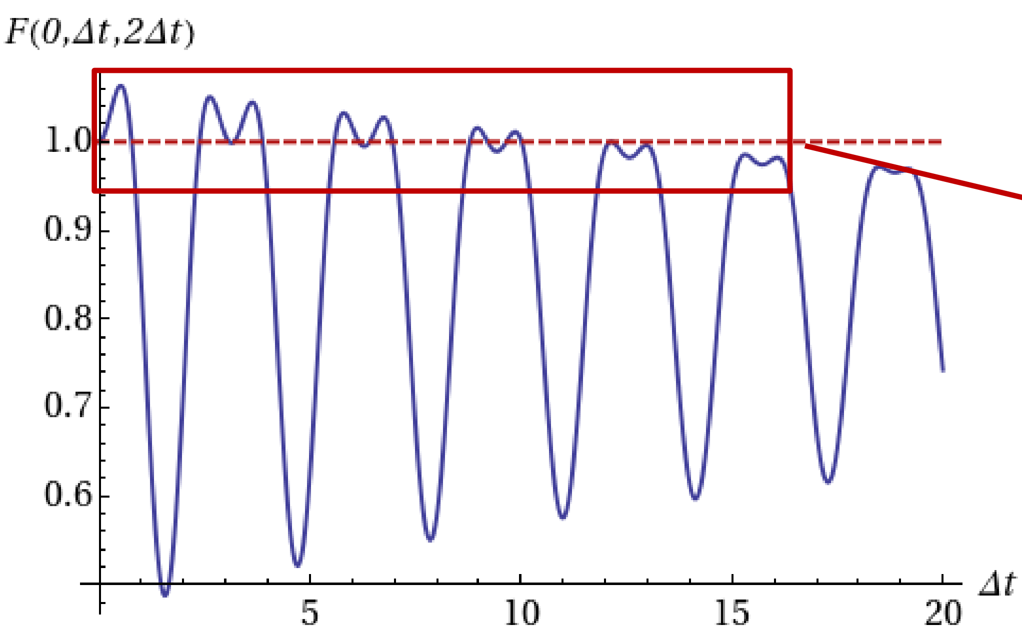

## Thermal equilibrium LGI
## ΔT=0

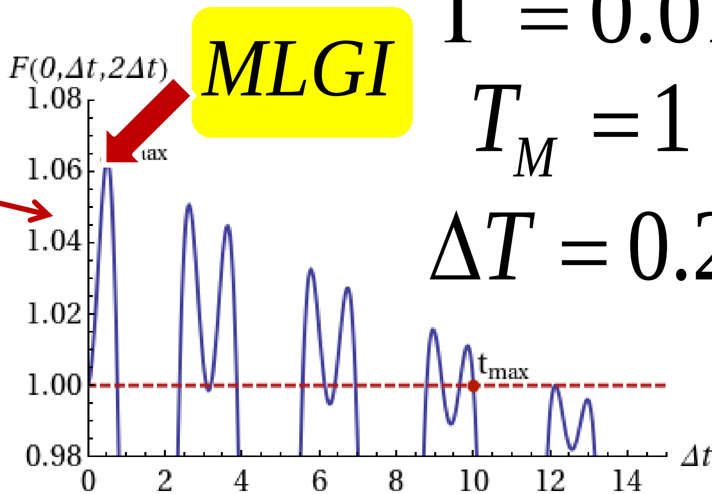


# Nonequilibrium thermal LGI
# ΔT≠0

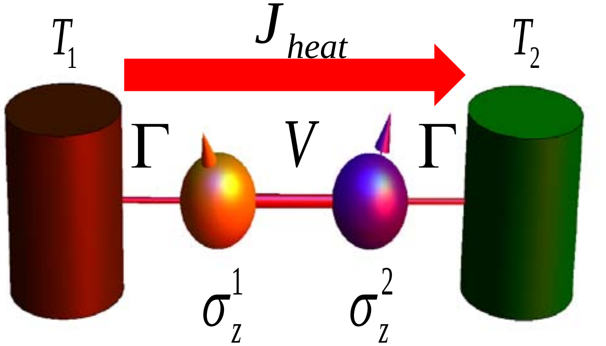



$$\varepsilon = 3V$$
$$\Gamma = 0.01V$$
$$T_M = 1$$
$$\Delta T = 0.2$$

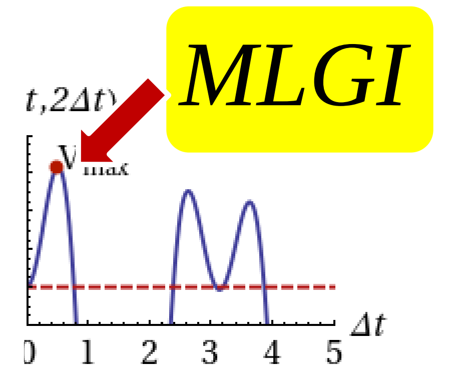


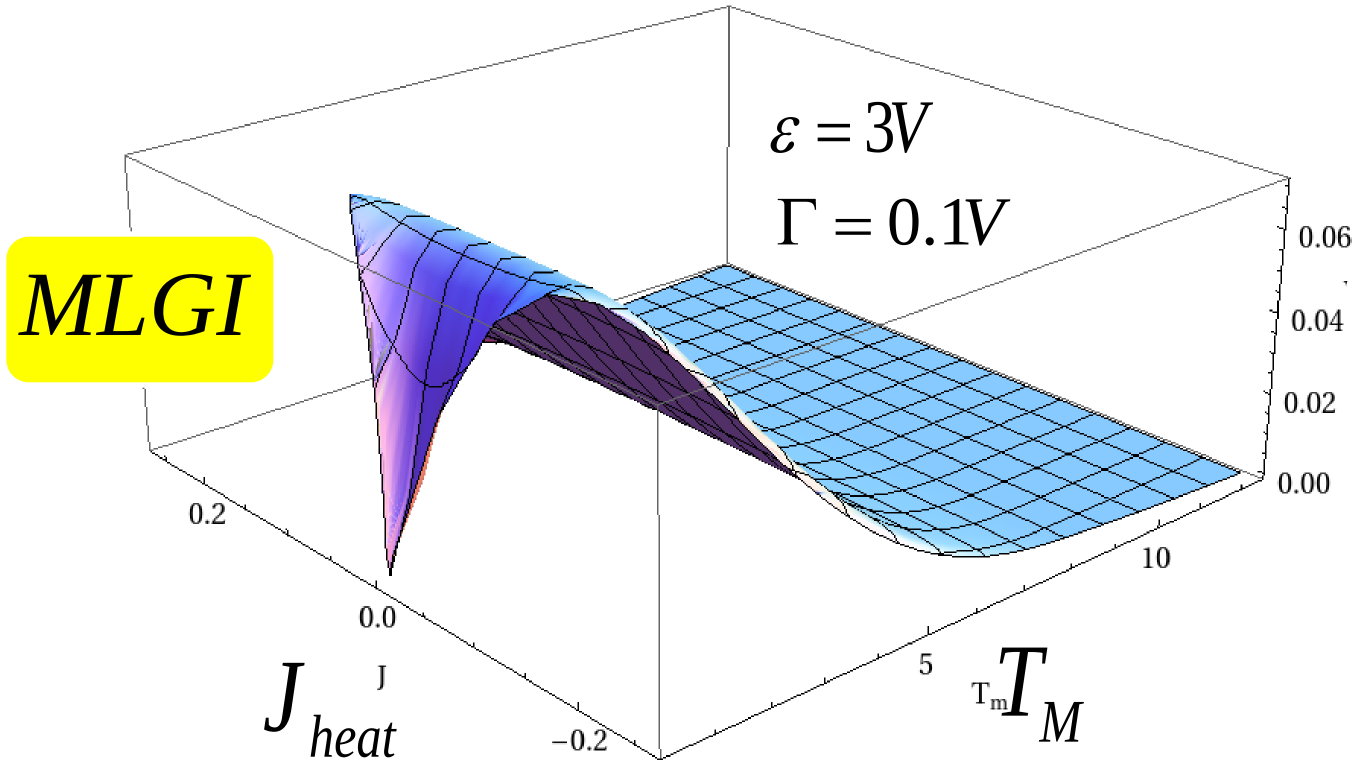



# Nonequilibrium thermal LGI
# ΔT≠0

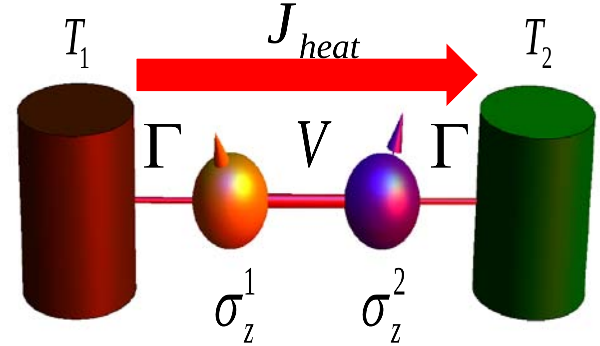



$$J_{heat} = Tr\left\{\hat{Q}L(\hat{\rho})\right\} \Rightarrow J_{heat} \propto \Delta T$$



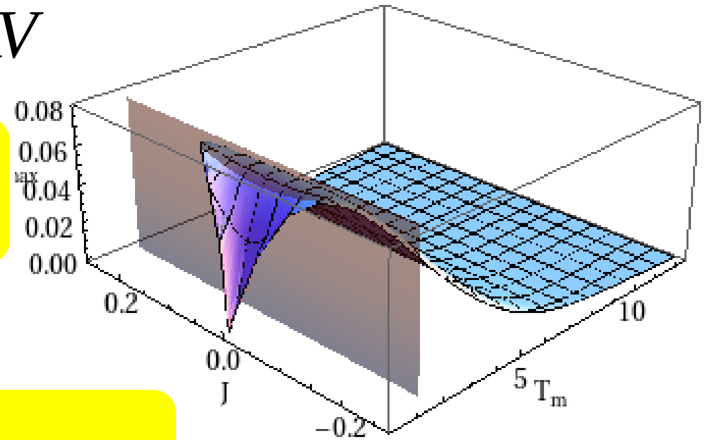



# Nonequilibrium thermal LGI
# ΔT≠0

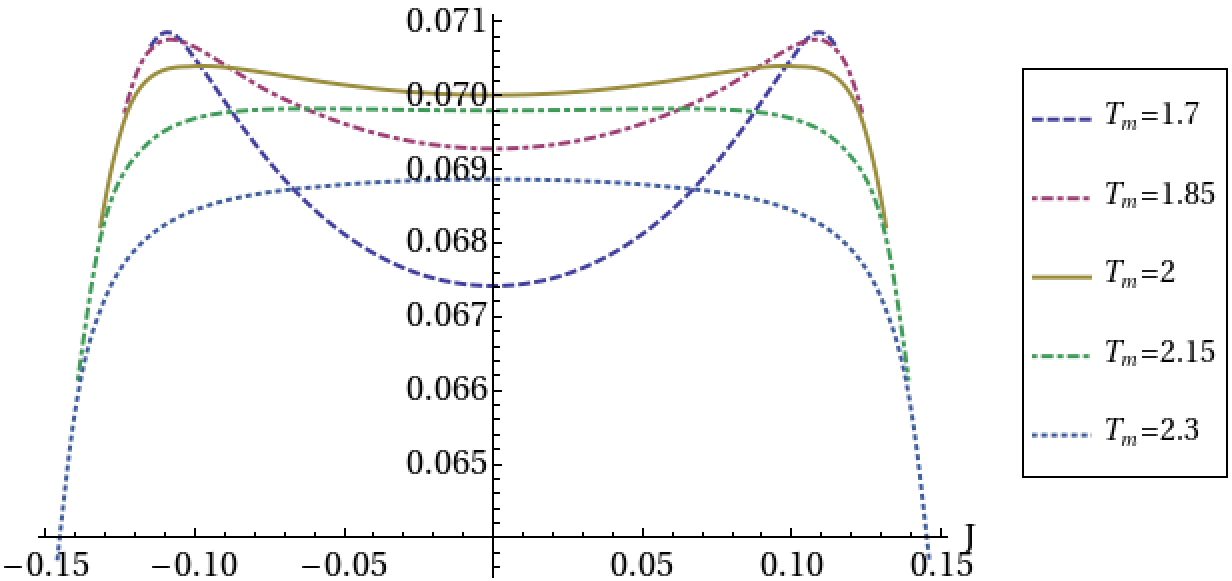



$\varepsilon = 3V \quad \Gamma = 0.1V$

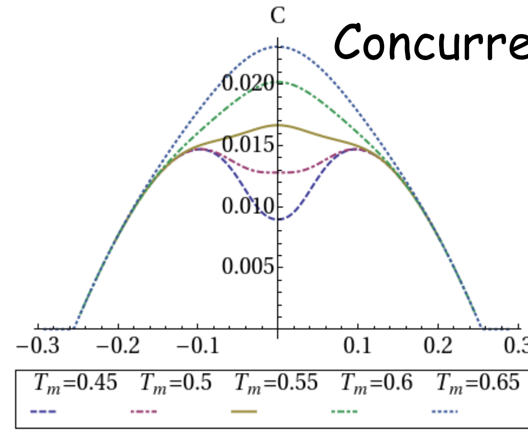
**MLGI**



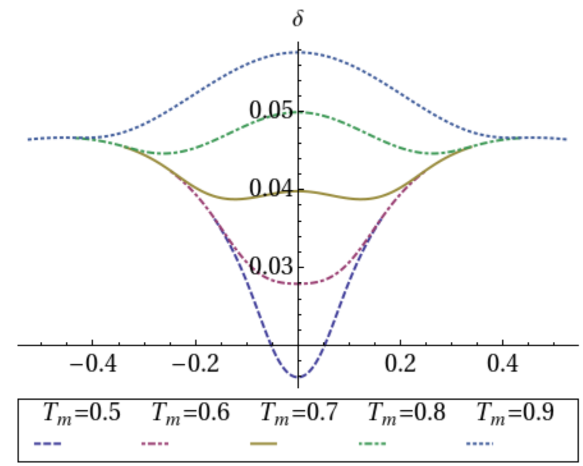

**MLGI**




Concurrence

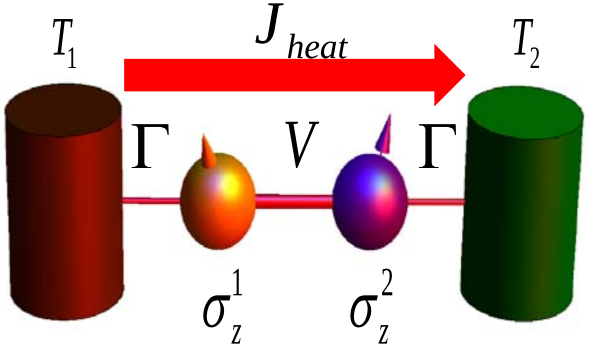


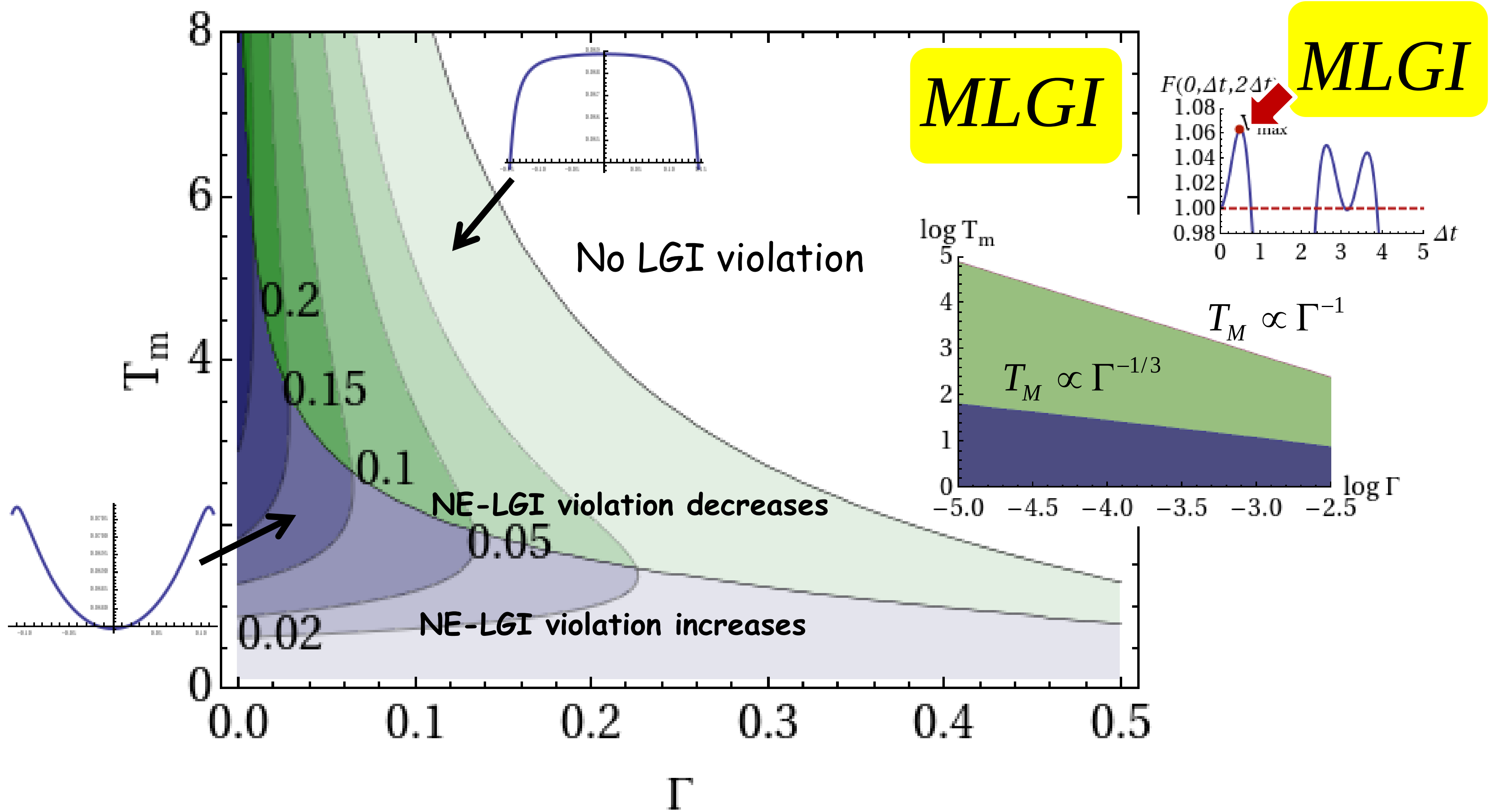

Quantum Discord



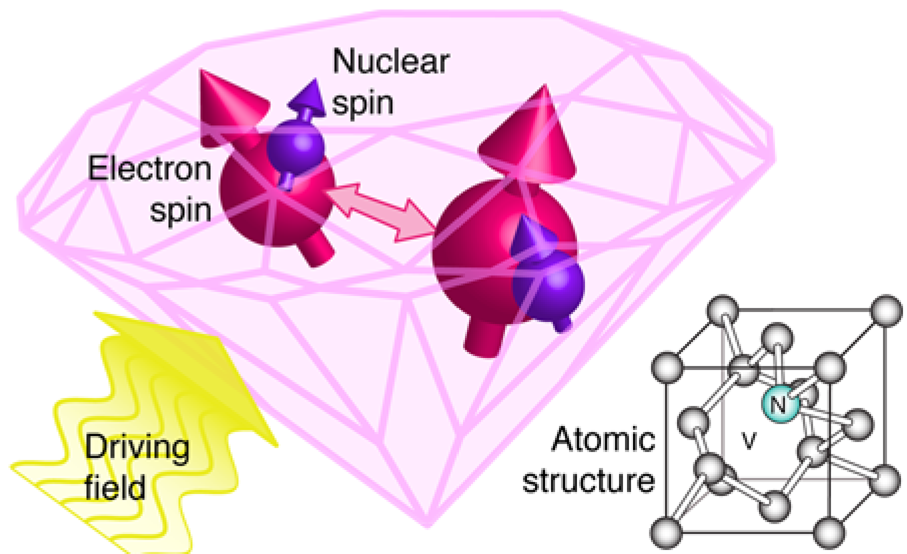
# Nonequilibrium thermal LGI
# ΔT≠0

J.C.Castillo, FJR & LQ, AIP Proc. (in press, 2012)



# Real life system:
# NV centers in diamond…




Physics 4, 78 (2011) DOI: 10.1103/Physics.4.78

**Driving a Hard Bargain with Diamond Qubits**

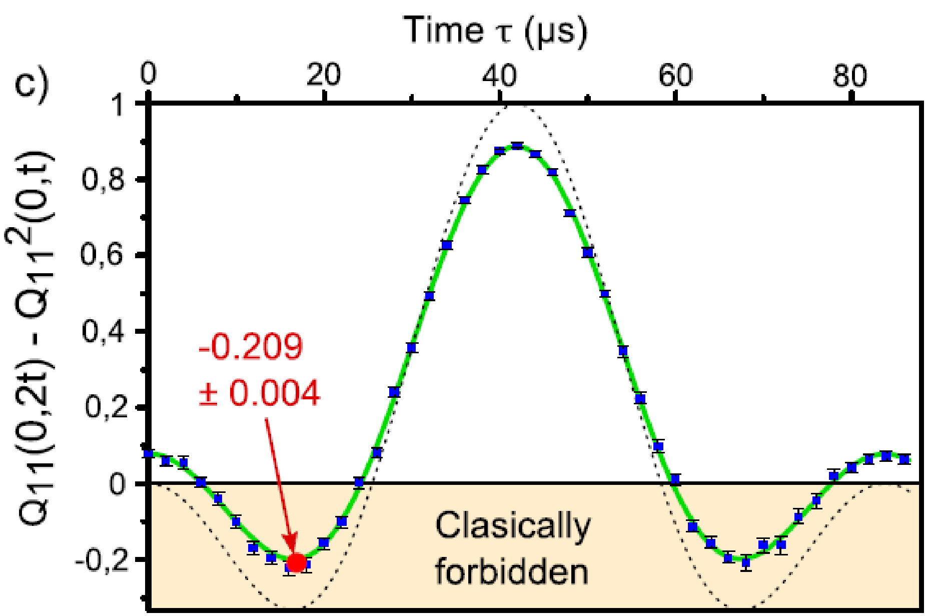
APS/S. Benjamin and J. Smith

# Real life system:
# NV centers in diamond…

PRL 107, 090401 (2011) PHYSICAL REVIEW LETTERS week ending 26 AUGUST 2011

**Violation of a Temporal Bell Inequality for Single Spins in a Diamond Defect Center**

G. Waldherr,[1,*] P. Neumann,[1] S. F. Huelga,[2] F. Jelezko,[1,3] and J. Wrachtrup[1]
[1]*3. Physikalisches Institut and Research Center SCOPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany*
[2]*Institut für Theoretische Physik, Universität Ulm, Ulm D-89073, Germany*
[3]*Institut für Quantenoptik, Universität Ulm, Ulm D-89073, Germany*
(Received 25 March 2011; published 24 August 2011; publisher error corrected 26 August 2011)



# Conclusions

## Two-site quantum coherences

1- Nontrivial dependence of the heat current on the entanglement (concurrence) for two-qubit systems.

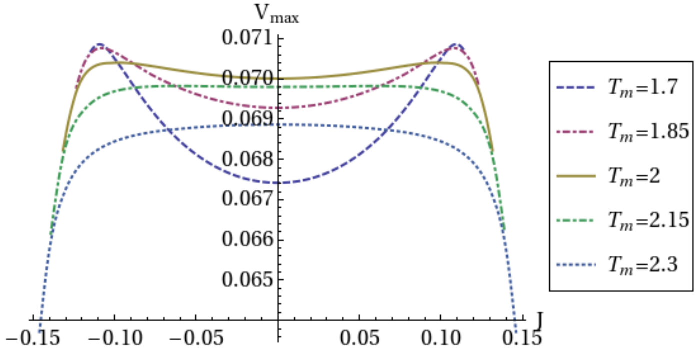
2- It may be quite useful in the context of NV centers in diamond, quantum dot and superconductor qubit systems.

L.Quiroga et al., PRA 75, 032308 (2007); cond-mat/0612046

# Conclusions

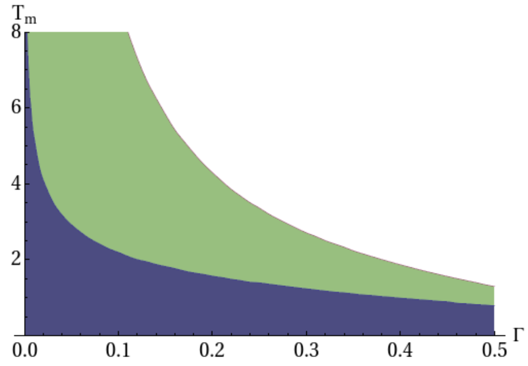
## Two-time quantum coherences

- At low temperatures: Going away from equilibrium increases violation of LGI




- Robust result: wide range of coupling strength

- LGI violation agrees with the result for entanglement and quantum discord
  - Measures of quantumness, but different types of correlations




- Experimental implementation

J.C.Castillo et al., AIP Proc. (in press, 2012)

# Conclusions

Time-dependent & nonequilibrium quantum phenomena
in condensed matter environments
can be of interest for…

1- Quantum information hardware
2- Nonequilibrium quantum thermodynamics
3- Matter-radiation quantum interfaces
4- Biological systems (Photosynthesis?)
5- …

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