Max Planck Institute
for the Physics of Complex Systems

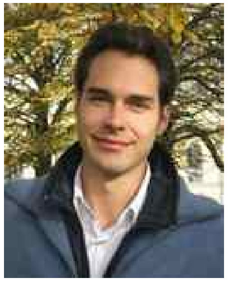
mpi**pks**
Dresden

Klaus Hornberger

Distinction of pointer states in (more) realistic environments

In collaboration with

Johannes Trost & Marc Busse



Pointer states

"Into what mixture does
the wave packet collapse?" (Zurek 1981)

"Predictability sieve" (Zurek, Habib, Paz 1993)

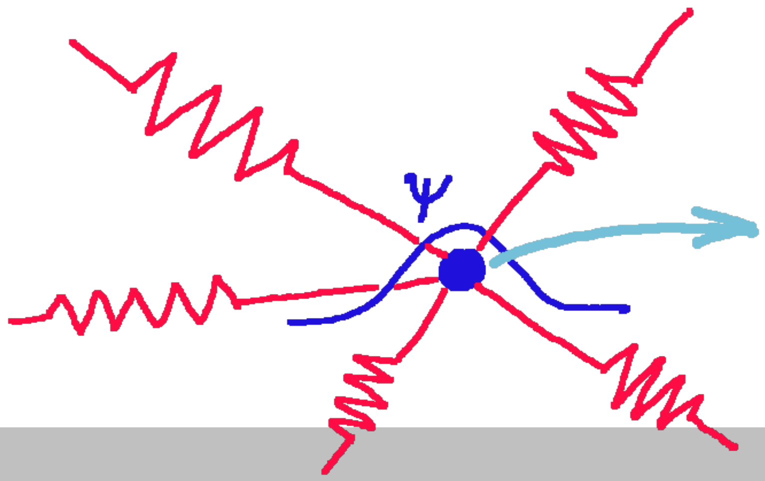
"Hilbert-Schmidt robustness" (Gisin, Rigo 1995,
Diósi, Kiefer 2000)

Pointer states

"Into what mixture does
the wave packet collapse?" (Zurek 1981)

"Predictability sieve" (Zurek, Habib, Paz 1993)

"Hilbert-Schmidt robustness" (Gisin, Rigo 1995,
Diósi, Kiefer 2000)



Pointer states

Given a master equation $\partial_t \rho \;=\; \mathcal{L}\rho$
a set of projectors $\{P_j(t)\}$ may be called *pointer states* of $\mathcal{L}$
provided there is a decoherence time scale t_{dec}
such that for all ρ_0

$$\mathrm{e}^{\mathcal{L}t}\rho_0 \;\cong\; \sum_j \mathrm{Tr}[P_j(0)\,\rho_0]\; P_j(t) \qquad \text{for} \;\; t > t_{\mathrm{dec}}$$

Pointer states

Given a master equation $\partial_t \rho \;=\; \mathcal{L}\rho$
a set of projectors $\{P_j(t)\}$ may be called *pointer states* of $\mathcal{L}$
provided there is a decoherence time scale t_{dec}
such that for all ρ_0

$$\mathrm{e}^{\mathcal{L}t}\rho_0 \;\cong\; \sum_j \mathrm{Tr}[P_j(0)\,\rho_0]\;P_j(t) \qquad \text{for} \;\; t > t_{\mathrm{dec}}$$

How to identify the $\hat{P}_j$ and their equation of motion?

How do the statistical weights emerge?

Klaus Hornberger

Distinction of pointer states in (more) realistic environments

plan of the talk:

- Monitoring approach

  – deriving microscopically realistic master equations –

- Hund's paradox

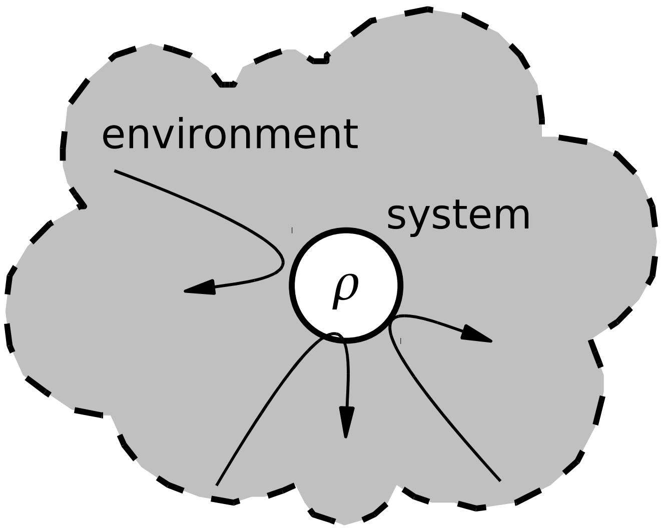
  – super-selecting chiral molecular configuration states –

- Pointer states of motion

  – the pointer basis induced by collisional decoherence –

Monitoring approach

$$\partial_t \rho \;=\; ?$$



How to derive Markovian master equations with microscopically realistic, non-perturbative interactions?

Idea:

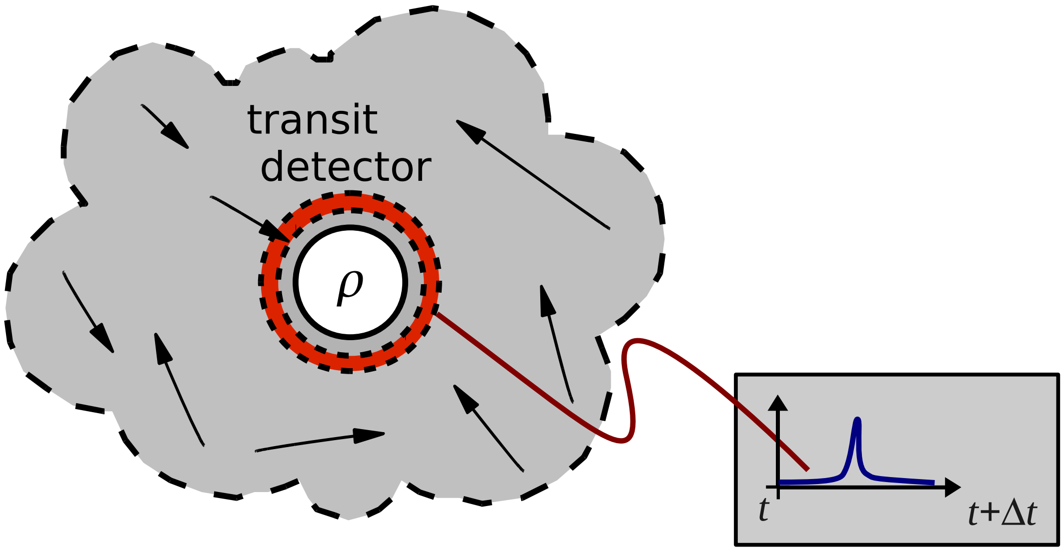
Don't start with the Schrödinger equation for the total system,

but put the Markov assumption (“memory-free environment”)

as the central premise!

Monitoring approach: operators

$$\partial_t \rho \;=\; ?$$



Γ : rate operator (positive)

$$\Pr(\mathrm{C}_{\Delta t}|\rho\otimes\rho_{\mathrm{env}}) \;=\; \mathrm{Tr}(\Gamma[\rho\otimes\rho_{\mathrm{env}}])\,\Delta t \;+\mathcal{O}\big(\Delta t^2\big)$$

probability for single event

S : scattering operator (unitary)

$$\rho' \;=\; \mathrm{Tr}_{\mathrm{env}}\big(S[\rho\otimes\rho_{\mathrm{env}}]S^\dagger\big)$$

effect of a single event

Monitoring master equation

combine time-dependent scattering theory
with the formalism of generalized,
continuous measurements

✔ manifestly markovian
✔ non-perturbative description
✔ rate and scattering operator can be defined microscopically

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\rho \;=\;& \frac{1}{i\hbar}[H,\rho] + i\,\mathrm{Tr}_{\mathrm{env}}\big(\big[\Gamma^{1/2}\mathrm{Re}(T)\Gamma^{1/2}, \rho\otimes\rho_{\mathrm{env}}\big]\big) \\
&+ \mathrm{Tr}_{\mathrm{env}}\big(T\Gamma^{1/2}[\rho\otimes\rho_{\mathrm{env}}]\Gamma^{1/2}T^{\dagger}\big) \\
&- \frac{1}{2}\,\mathrm{Tr}_{\mathrm{env}}\big(\Gamma^{1/2}T^{\dagger}T\,\Gamma^{1/2}[\rho\otimes\rho_{\mathrm{env}}]\big) \\
&- \frac{1}{2}\,\mathrm{Tr}_{\mathrm{env}}\big([\rho\otimes\rho_{\mathrm{env}}]\,\Gamma^{1/2}T^{\dagger}T\,\Gamma^{1/2}\big)
\end{aligned}
$$

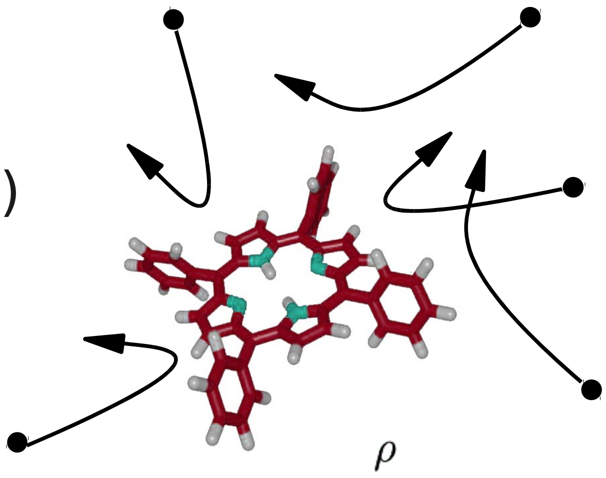
$(S = I + iT)$

Master equation for ro-vibrational dynamics in background gas

microscopically realistic choice

$\Gamma =$ (gas current density) x (cross section)

$S =$ (multi-channel S-Matrix)

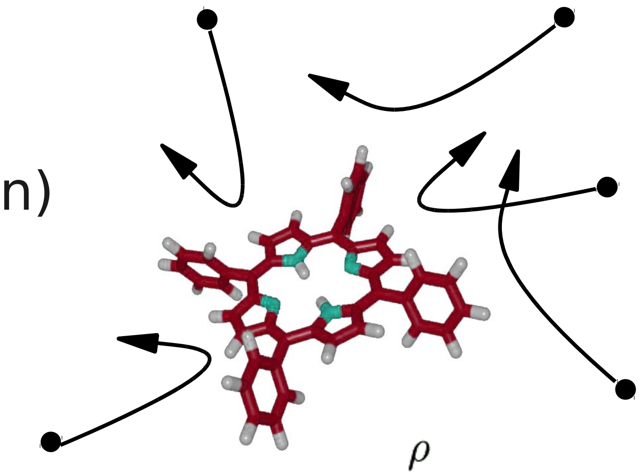


Master equation for ro-vibrational dynamics in background gas

microscopically realistic choice

$\Gamma =$ (gas current density) x (cross section)

$S =$ (multi-channel S-Matrix)



yields:

$$\partial_t \rho_{\alpha\beta} = -i\omega_{\alpha\beta}\rho_{\alpha\beta} + \sum_{\substack{\alpha_0\beta_0 \\ \omega_{\alpha\alpha_0}=\omega_{\beta\beta_0}}} \rho_{\alpha_0\beta_0} M_{\alpha\beta}^{\alpha_0\beta_0} - \frac{1}{2}\sum_{\substack{\alpha_0 \\ \omega_\alpha=\omega_{\alpha_0}}} \rho_{\alpha_0\beta} \sum_\gamma M_{\gamma\gamma}^{\alpha_0\alpha} - \frac{1}{2}\sum_{\substack{\beta_0 \\ \omega_\beta=\omega_{\beta_0}}} \rho_{\alpha\beta_0} \sum_\gamma M_{\gamma\gamma}^{\beta\beta_0}$$

Multi-channel scattering amplitudes

with

$$M_{\alpha\beta}^{\alpha_0\beta_0} = n_{\text{gas}} \int \mathrm{d}\Omega \left\langle v_{\text{out}}\, f_{\alpha\alpha_0}\!\left(\cos\theta; \frac{m}{2}v_{\text{in}}^2\right) f_{\beta\beta_0}^*\!\left(\cos\theta; \frac{m}{2}v_{\text{in}}^2\right)\right\rangle_{v_{\text{in}}}$$

(extends Dümcke 1985)

Klaus Hornberger

Distinction of pointer states in (more) realistic environments

plan of the talk:

- Monitoring approach

  – deriving microscopically realistic master equations –

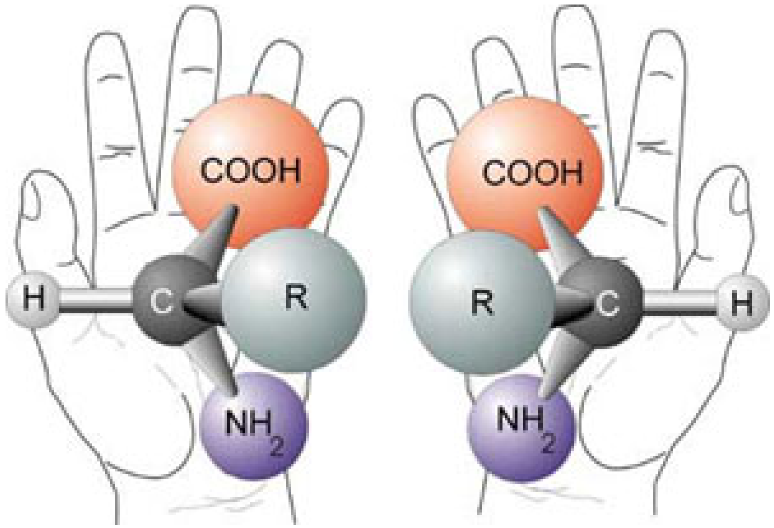
- Hund's paradox

  – super-selecting chiral molecular configuration states –

- Pointer states of motion

  – the pointer basis induced by collisional decoherence –

Hund's paradox of molecular chirality

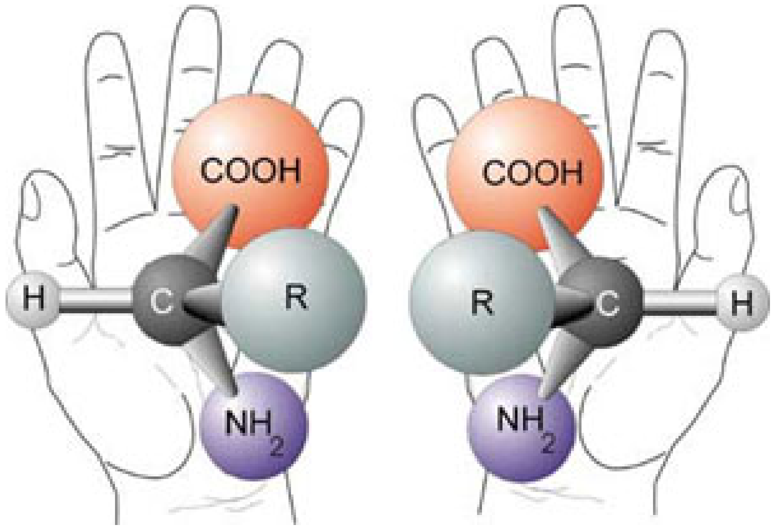


Friedrich Hund (1927)

Why are many molecules found in a chiral configuration?

—in spite of the parity invariance of their hamiltonian?

Hund's paradox of molecular chirality



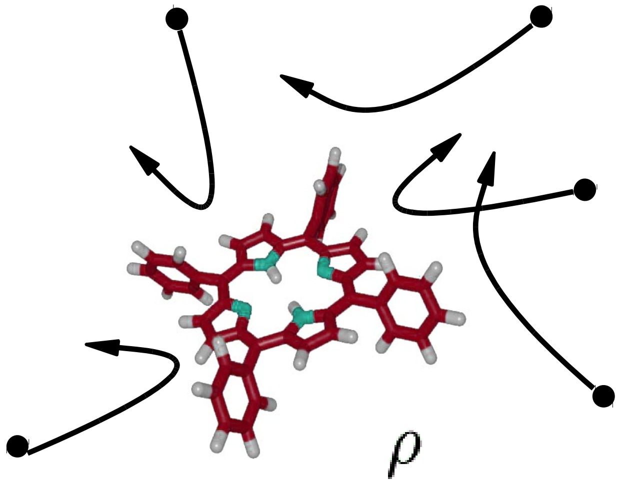
Friedrich Hund (1927)

Why are many molecules found in a chiral configuration?

—in spite of the parity invariance of their hamiltonian?

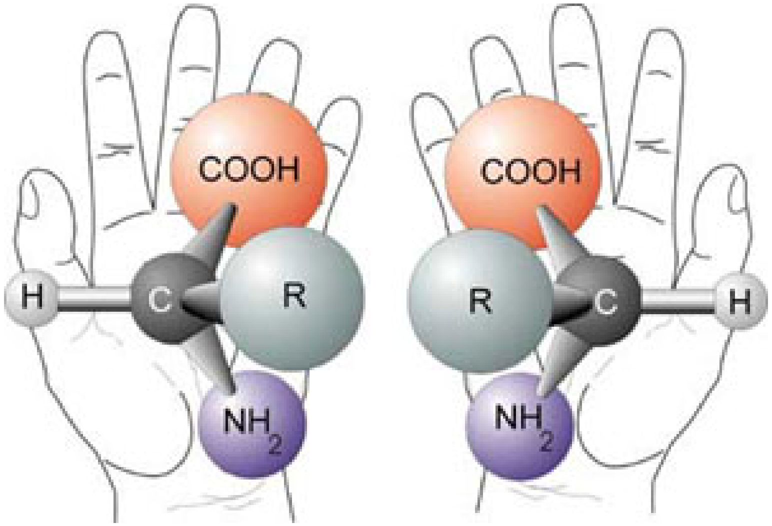
Effect of an *achiral* gas environment on the configuration & orientation state?

realistic master equation required !



Hund's paradox of molecular chirality

Effect of an *achiral* gas environment

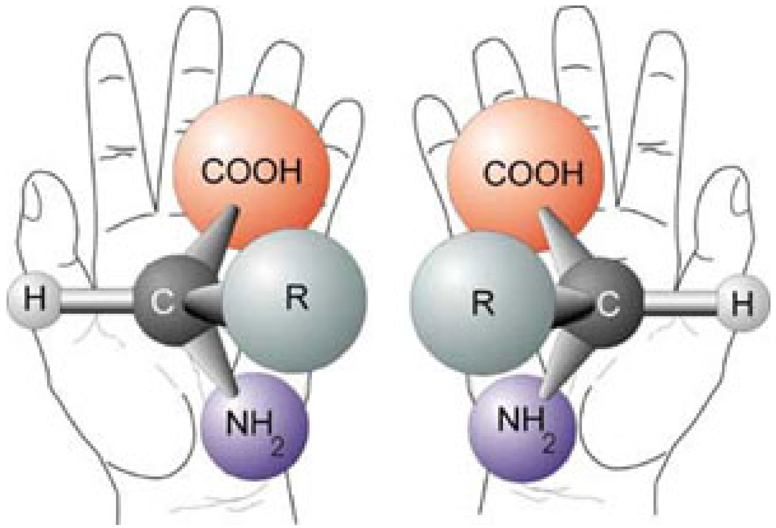


- $|L\rangle + \mathrm{e}^{i\varphi}|R\rangle$ decay with decoherence rate

$$\gamma \;=\; n_{\text{gas}} \left\langle v \underbrace{\int \frac{\mathrm{d}\boldsymbol{n}\,\mathrm{d}\boldsymbol{n}_0}{8\pi} \left| f^{(L)}_{\alpha,\alpha_0}(v\,\boldsymbol{n}, v\,\boldsymbol{n}_0) - f^{(R)}_{\alpha,\alpha_0}(v\,\boldsymbol{n}, v\,\boldsymbol{n}_0) \right|^2}_{\text{“decoherence cross section”}} \right\rangle_{v,\alpha,\alpha_0}$$

Hund's paradox of molecular chirality

Effect of an *achiral* gas environment



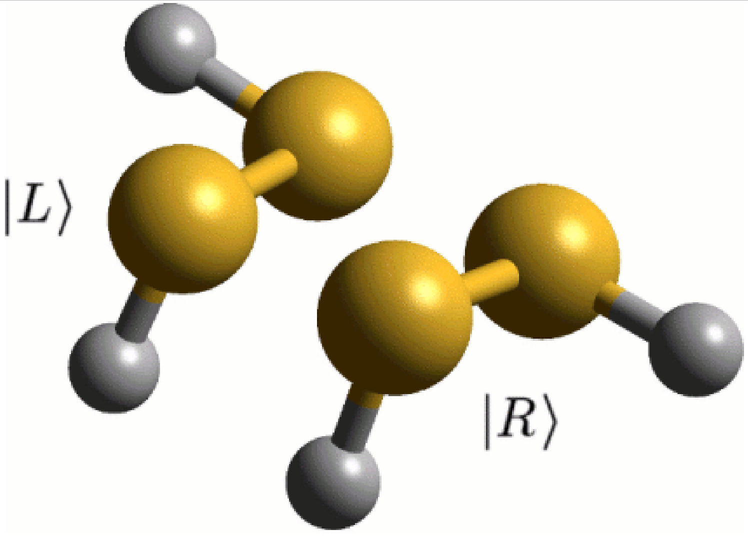
- $|L\rangle + \mathrm{e}^{i\varphi}|R\rangle$ decay with decoherence rate

$$\gamma \;=\; n_{\mathrm{gas}} \left\langle v \int \frac{\mathrm{d}\boldsymbol{n}\,\mathrm{d}\boldsymbol{n}_0}{8\pi} \left| f^{(L)}_{\alpha,\alpha_0}(v\,\boldsymbol{n}, v\,\boldsymbol{n}_0) - f^{(R)}_{\alpha,\alpha_0}(v\,\boldsymbol{n}, v\,\boldsymbol{n}_0) \right|^2 \right\rangle_{v,\alpha,\alpha_0}$$

- *only* the chiral states $|L\rangle$ and $|R\rangle$ exhibit a quantum-Zeno-like stabilization $\sim\omega^2/\gamma$ against tunneling and decay if $\gamma \gg \omega$

Harris, Stodolsky (1978)

Hund's paradox of molecular chirality

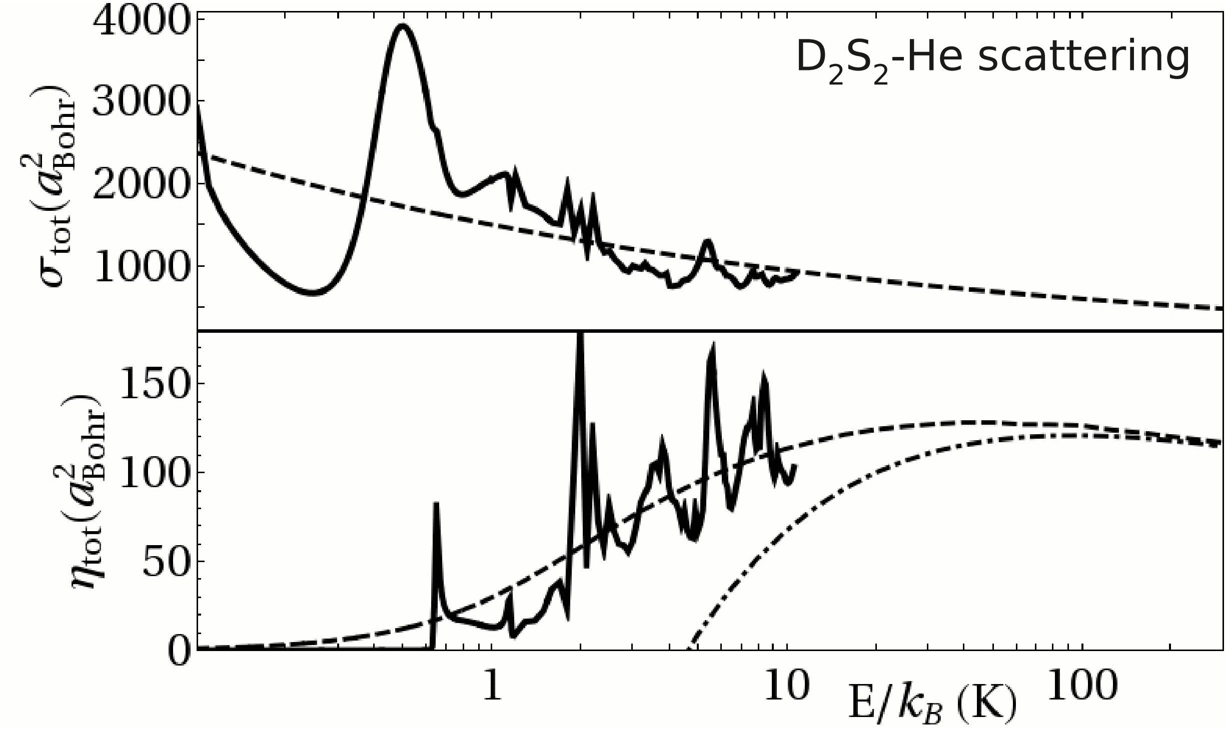


D_2S_2 tunnels with 28 Hz in vacuum

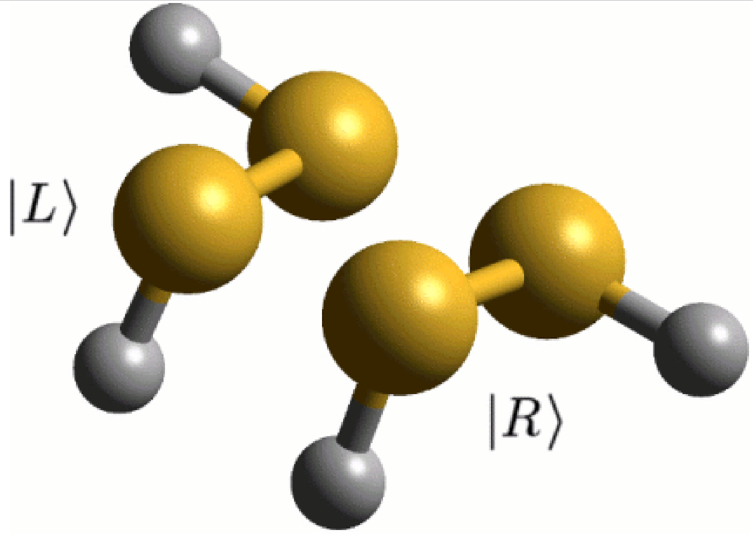
The stabilization effect is dominated by a higher order contribution to the van der Waals interaction described by the EQED tensor $A_{j,k\ell}(i\omega)$

scattering cross section

decoherence cross section



Hund's paradox of molecular chirality



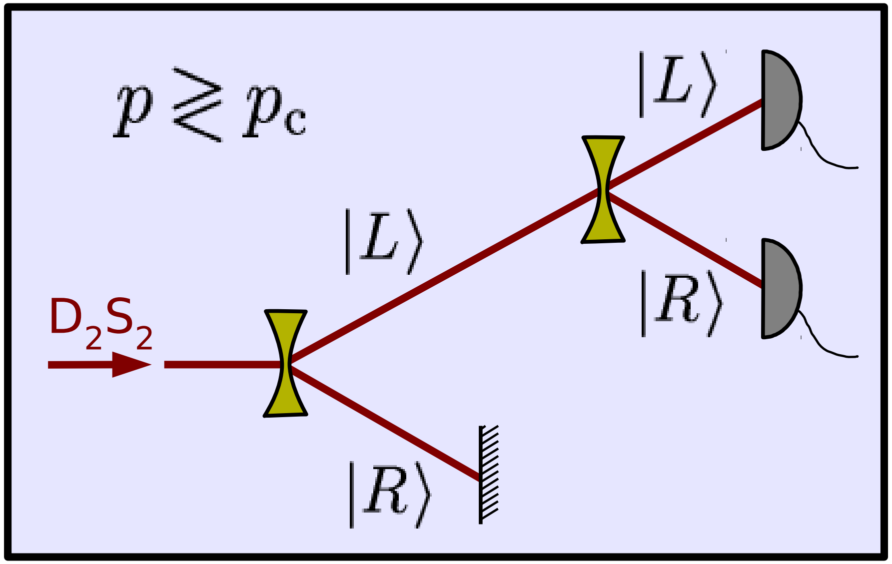
D_2S_2 tunnels with 28 Hz in vacuum

The stabilization effect is dominated by a higher order contribution to the van der Waals interaction described by the EQED tensor $A_{j,k\ell}(i\omega)$

critical pressure in 300K He atmosphere:

$p_c = 1.6 \times 10^{-5}$ mbar

... allows one to observe the chiral stabilization in an optical Stern-Gerlach type setup [e.g. Li, Bruder, Sun: PRL 2007]



Klaus Hornberger

Distinction of pointer states in (more) realistic environments

plan of the talk:

- Monitoring approach

  – deriving microscopically realistic master equations –

- Hund's paradox

  – super-selecting chiral molecular configuration states –

- Pointer states of motion

  – the pointer basis induced by collisional decoherence –

reminder: definition of Pointer states

Given a master equation $\partial_t \rho \;=\; \mathcal{L}\rho$
a set of projectors $P_j(t)$ may be called *pointer states* of $\mathcal{L}$
provided there is a decoherence time scale t_{dec}
such that for all ρ_0

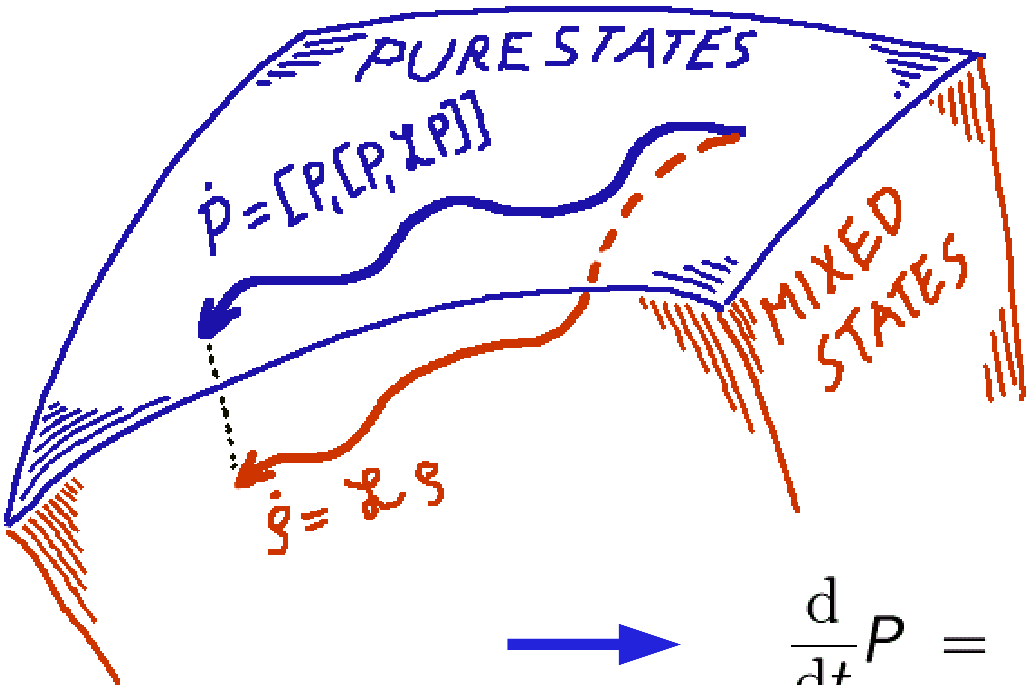
$$\mathrm{e}^{\mathcal{L}t}\rho_0 \;\cong\; \sum_j \mathrm{Tr}[P_j(0)\,\rho_0]\; P_j(t) \qquad \text{for } t > t_{\mathrm{dec}}$$

Continuous variable version

$$\mathrm{e}^{\mathcal{L}t}\rho_0 \;\cong\; \int \mathrm{d}\alpha\; \mathrm{prob}(\alpha\,|\,\rho_0) P_\alpha(t) \qquad \text{for } t > t_{\mathrm{dec}}$$

with $\int \mathrm{d}\alpha\; \mathrm{prob}(\alpha\,|\,\rho_0) = 1$

Nonlinear equation for candidate pointer states



among all e.o.m. propagating P within the manifold of pure states, choose the one minimizing $\| \dot{P} - \mathcal{L} \|^2_{\mathrm{HS}}$

$$\frac{\mathrm{d}}{\mathrm{d}t} P = [P, [P, \mathcal{L}P]]$$

(Rigo&Gisin 1995, Strunz 2002)

corresponds to the deterministic part of a particular unraveling of $\mathcal{L}$

In vector representation $P = |\psi\rangle\langle\psi|$

$$\partial_t |\psi\rangle = \frac{1}{i\hbar}(H - \langle H \rangle_\psi)|\psi\rangle + \sum_k \left\{ \langle L_k^\dagger \rangle_\psi (L - \langle L_k \rangle_\psi) - \frac{1}{2}\Big(L_k^\dagger L_k - \langle L_k^\dagger L_k \rangle_\psi \Big) \right\} |\psi\rangle$$

(Diosi 1986)

Orthogonal unraveling $\rho = \mathbb{E}[|\psi\rangle\langle\psi|]$

piecewise deterministic evolution

$$\partial_t |\psi\rangle \;=\; \frac{1}{i\hbar}(H - \langle H\rangle_\psi)|\psi\rangle + \sum_k \left\{ \langle L_k^\dagger\rangle_\psi (L - \langle L_k\rangle_\psi) - \frac{1}{2}\Big(L_k^\dagger L_k - \langle L_k^\dagger L_k\rangle_\psi \Big) \right\} |\psi\rangle$$

interrupted by orthogonal jumps

$$|\psi\rangle \;\rightarrow\; \frac{1}{\sqrt{r_k}}(L_k - \langle L_k\rangle_\psi)|\psi\rangle$$

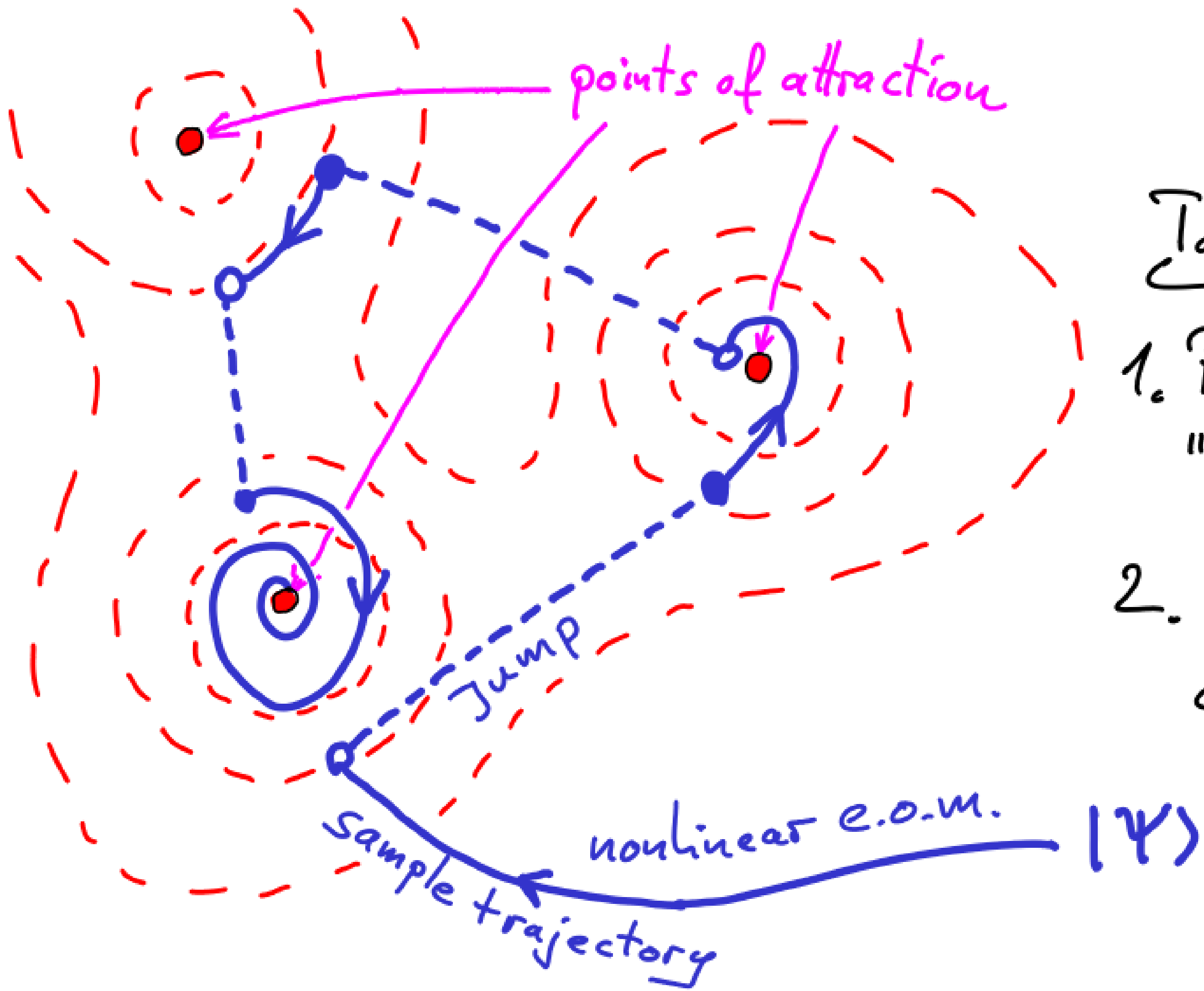
with rate $r_k \;=\; \langle L_k^\dagger L_k\rangle_\psi - \langle L_k^\dagger\rangle_\psi \langle L_k\rangle_\psi$

total jump rate $\sum_k r_k \;=\; -\,\mathrm{Tr}(\rho\,\mathcal{L}\rho)$

entropy production rate!

If there are "points of attraction" with vanishing jump rate, an ensemble of (candidate) pointer states is naturally generated

Orthogonal unraveling – sample trajectory



To be shown:

1. Points of attraction "behave classically"
2. Arrival probabilities are given by Mr. Born

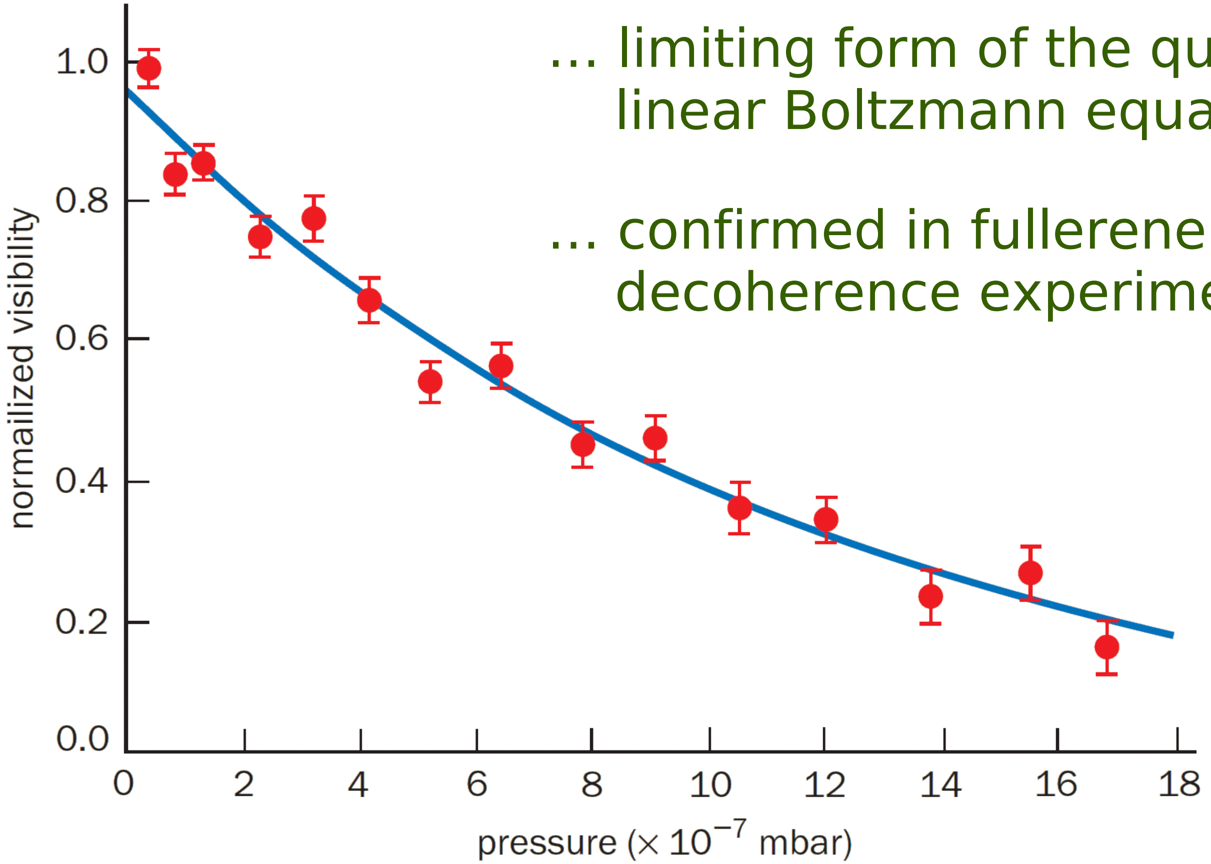
If there are "points of attraction" with vanishing jump rate, an ensemble of (candidate) pointer states is naturally generated

Collisional decoherence master equation

… describes particle "localization" by gas collisions

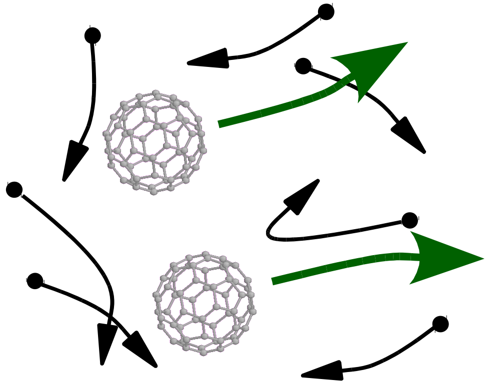
$$\mathcal{L}\rho = \frac{1}{i\hbar}[H,\rho] + \gamma \int \mathrm{d}q\, G(q) \left(\mathrm{e}^{ixq} \rho\, \mathrm{e}^{-ixq} - \rho \right)$$

$G(q)$: momentum exchange distribution



… limiting form of the quantum linear Boltzmann equation (Vacchini & KH, Phys Rep 2009)

… confirmed in fullerene buckyball decoherence experiments (KH,..,& Zeilinger, PRL 2003)



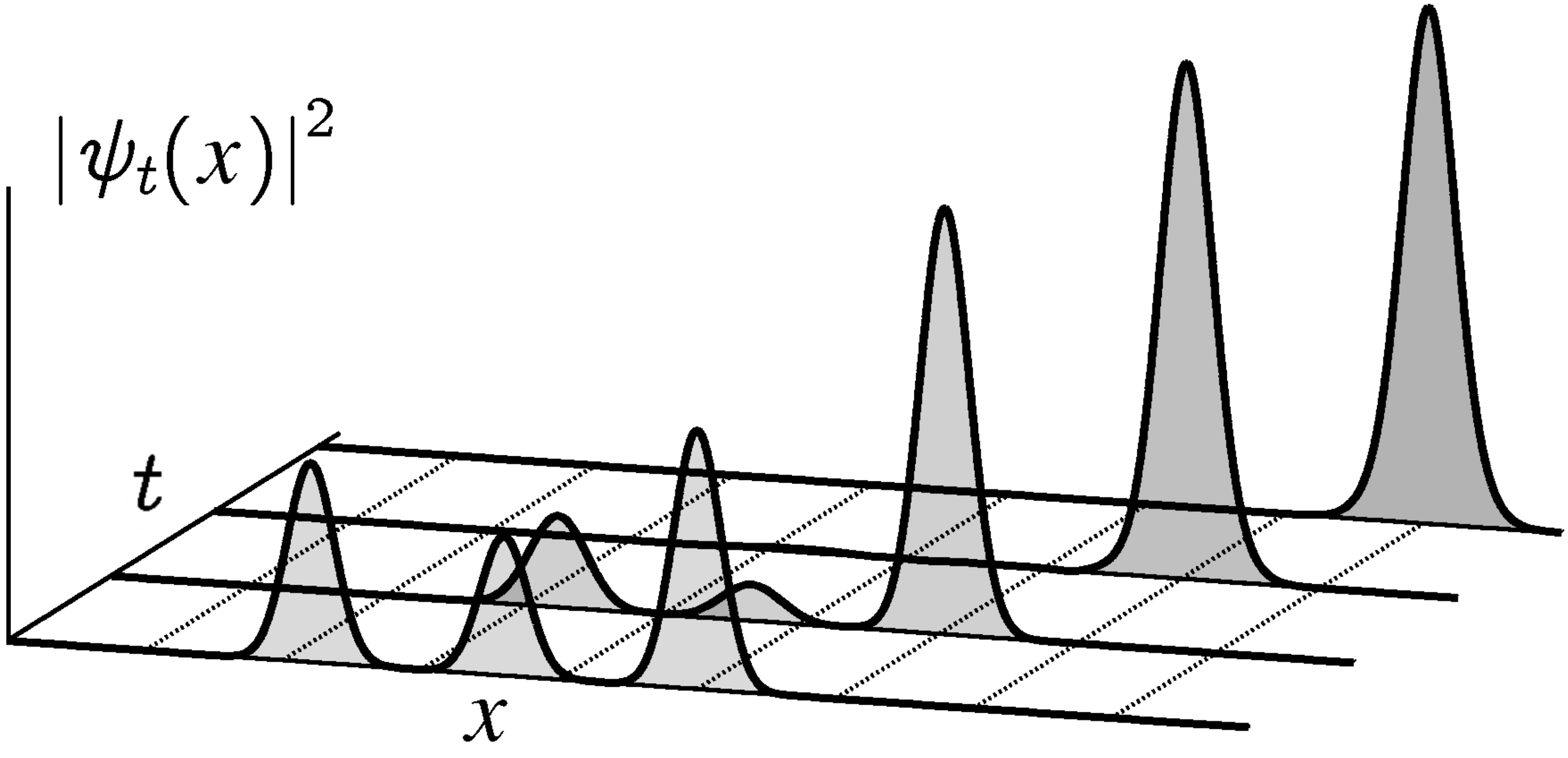
Nonlinear e.o.m. for collisional decoherence

$$\partial_t \psi(x) \;=\; -\frac{\hbar}{2m\,i}\partial_x^2 \psi(x) + \gamma\psi(x)\Big(|\psi|^2 * \tilde{G}(x) - \int \mathrm{d}y\, |\psi(y)|^2 \Big(|\psi|^2 * \tilde{G}\Big)(y)\Big)$$

Nonlinear e.o.m. for collisional decoherence

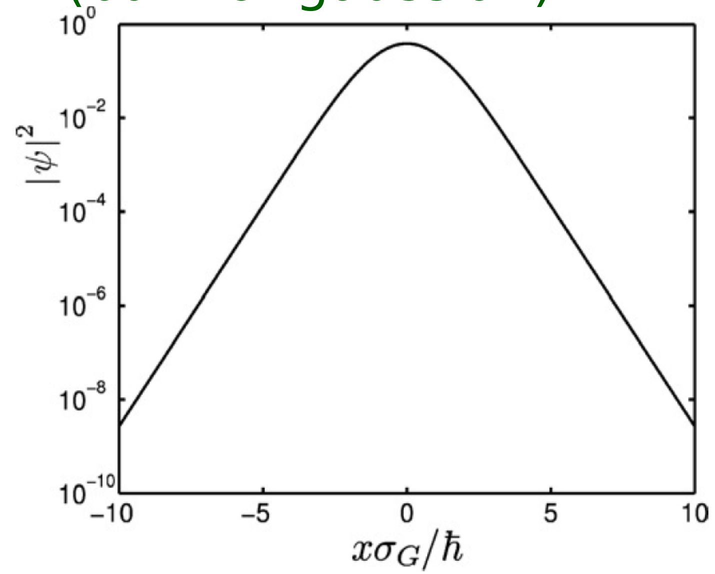
$$\partial_t\psi(x) \;=\; -\frac{\hbar}{2m\,i}\partial_x^2\psi(x)+\gamma\psi(x)\Big(|\psi|^2*\tilde{G}(x)-\int \mathrm{d}y\,|\psi(y)|^2\big(|\psi|^2*\tilde{G}\big)(y)\Big)$$

...exhibits *soliton-like solutions*, our candidate pointer states

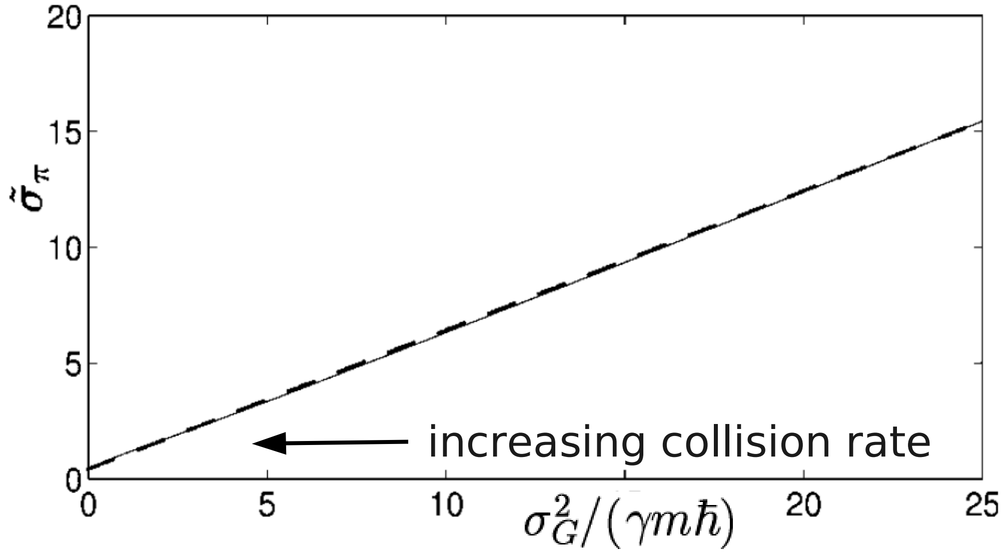


Properties of the (candidate) pointer states

exponentially localized
(but not gaussian)



increasing coupling
decreases their width



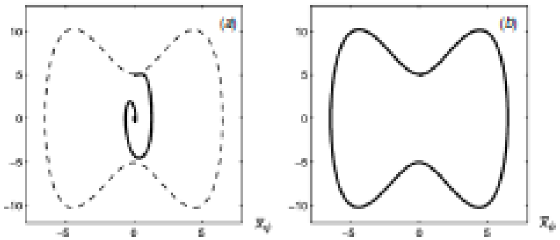
provide an
overcomplete basis

$$\int \mathrm{d}\Gamma\, I(\Gamma)\, P_\Gamma \;=\; I$$

(follows with covariance properties
of master the master equation)

move on the classical
Newtonian trajectories

...in the limit of strong coupling



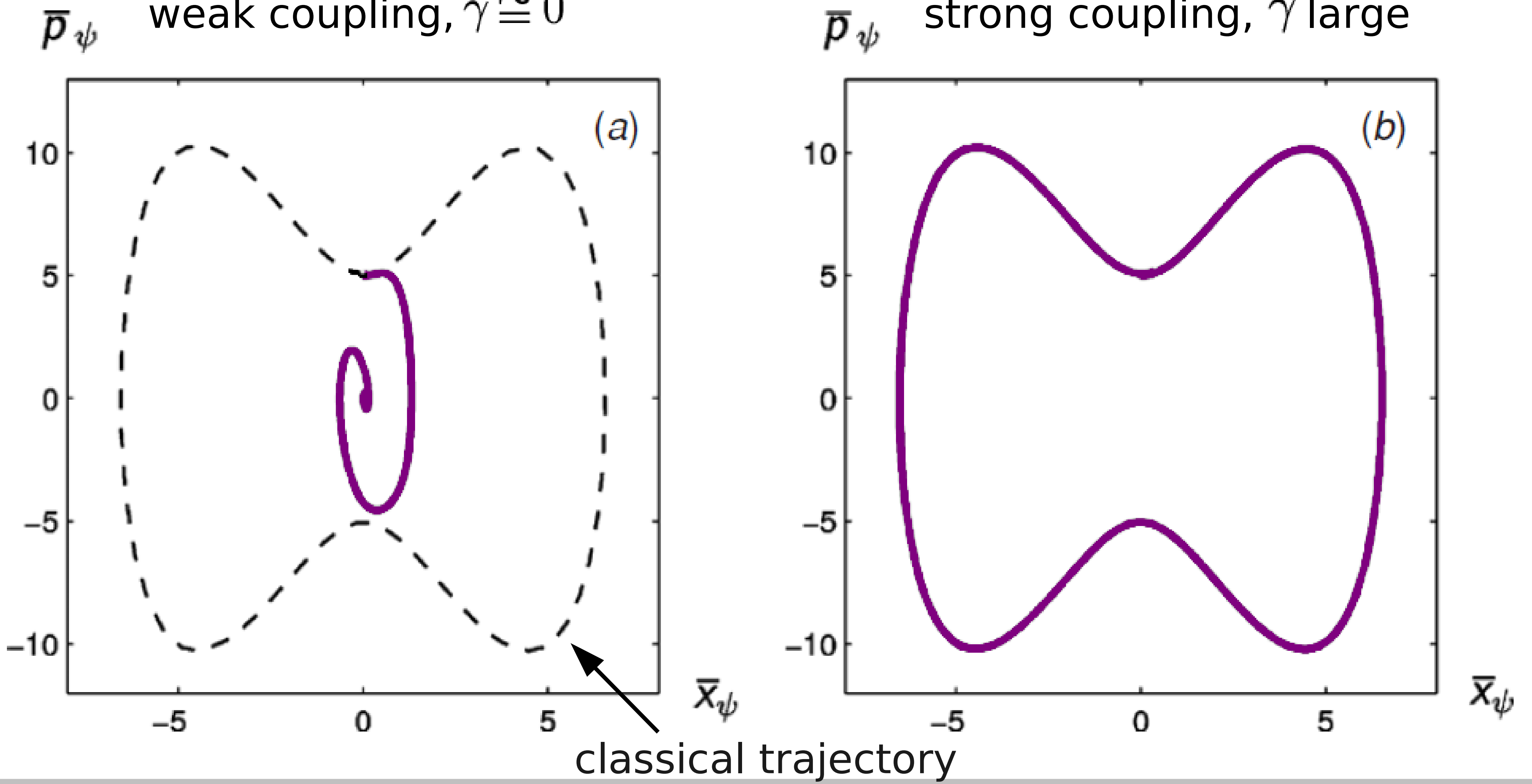
see
next
slide...

Properties of the (candidate) pointer states

phase space dynamics
in a quartic potential

$$V(x) = a\,x^4 + b\,x^2$$

weak coupling, $\gamma \cong 0$ | strong coupling, γ large



The statistical weights

Superposing N spatially non-overlapping wave packtes,

$$|\psi_0\rangle = \sum_{i=1}^{N} c_i |\phi_i\rangle \qquad \phi_i(x)\,\phi^*_{j\neq i}(x) = 0$$

the stochastic process can be mapped to the coefficients $c_1, \ldots, c_N$

deterministic evolution:

$$\frac{\mathrm{d}}{\mathrm{d}t} c_i = -\left(\sum_{j=1}^{N} F_{ij} \, | \, c_j \, |^2 - \sum_{j,k=1}^{N} F_{jk} \, | \, c_j \, |^2 \, | \, c_k \, |^2 \right) c_i$$

with localization rates $F_{ij} = \gamma \left\{ 1 - \tilde{G}\left(\langle x \rangle_{\phi_i} - \langle x \rangle_{\phi_j} \right) \right\}$

The statistical weights

Superposing N spatially non-overlapping wave packtes,

$$|\psi_0\rangle = \sum_{i=1}^{N} c_i |\phi_i\rangle \qquad \phi_i(x)\,\phi^*_{j\neq i}(x) = 0$$

the stochastic process can be mapped to the coefficients $c_1, \ldots, c_N$

deterministic evolution:

$$\frac{\mathrm{d}}{\mathrm{d}t} c_i = -\left(\sum_{j=1}^{N} F_{ij}\,|c_j|^2 - \sum_{j,k=1}^{N} F_{jk}\,|c_j|^2 |c_k|^2 \right) c_i$$

jumps:

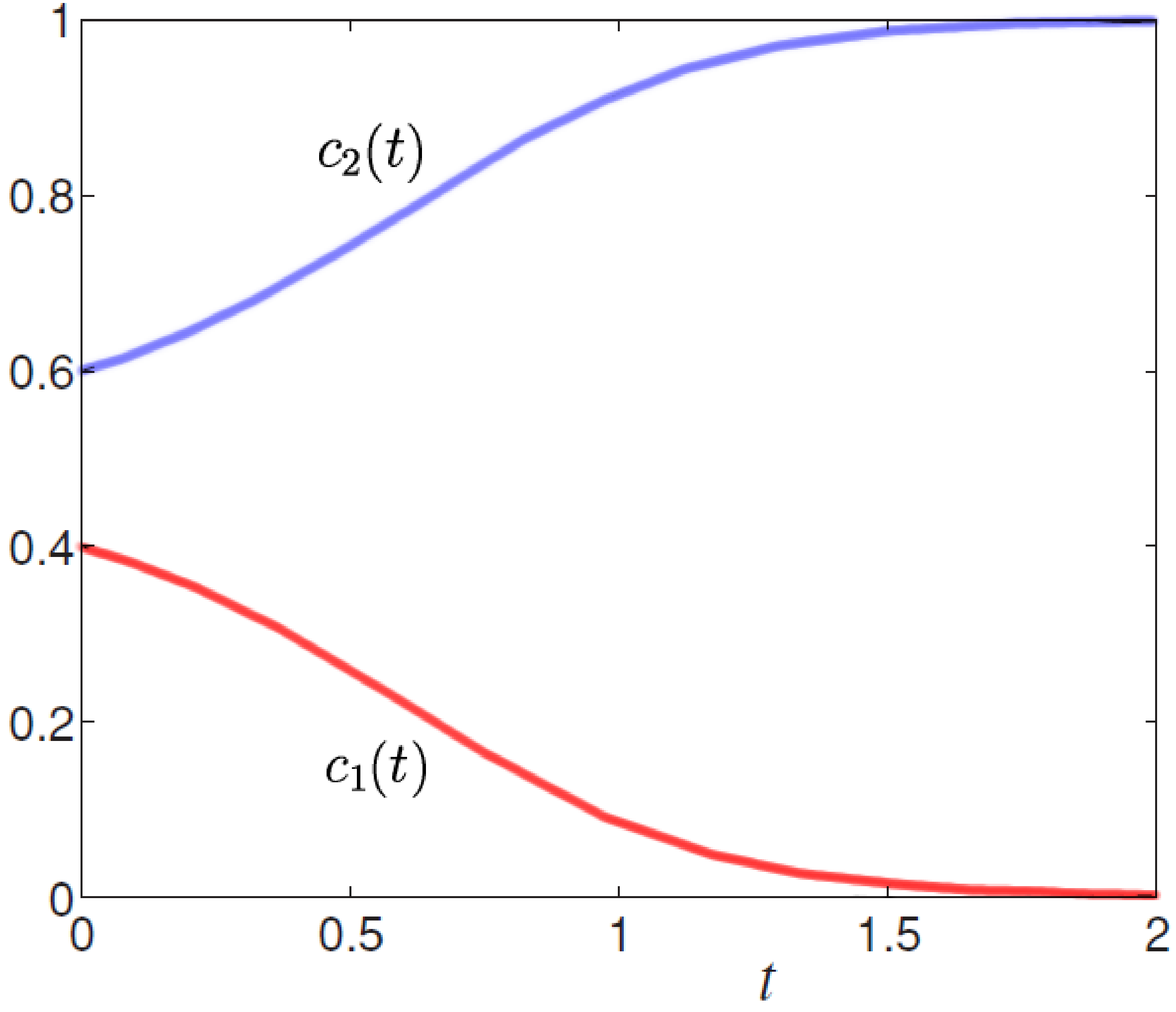
$$c_i^{(q)} \rightarrow \mathcal{N}_q \left(e^{iq\langle \mathsf{x}\rangle_{\phi_i}/\hbar} - \sum_{j=1}^{N} |c_j|^2 e^{iq\langle \mathsf{x}\rangle_{\phi_j}/\hbar} \right) c_i$$

with localization rates $F_{ij} = \gamma \left\{ 1 - \tilde{G}\left(\langle \mathsf{x}\rangle_{\phi_i} - \langle \mathsf{x}\rangle_{\phi_j} \right) \right\}$

and jump rates $r^{(q)} = \gamma\, G(q) \left(1 - \sum_{i,j=1}^{N} |c_i|^2 |c_j|^2 e^{iq\left(\langle \mathsf{x}\rangle_{\phi_i} - \langle \mathsf{x}\rangle_{\phi_j} \right)/\hbar} \right)$

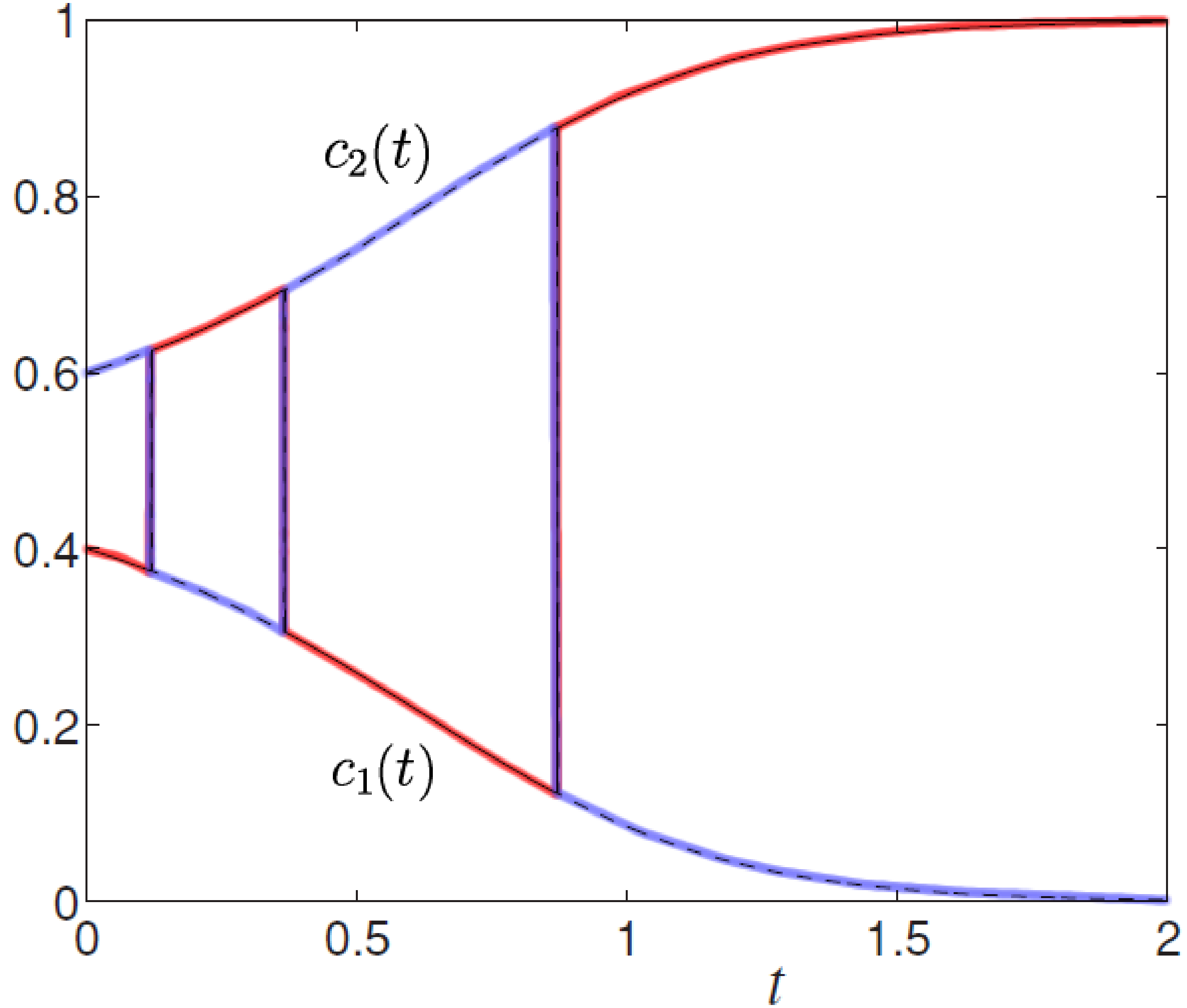
The statistical weights, N=2

deterministic evolution



The statistical weights, N=2

stochastic process analytically tractable

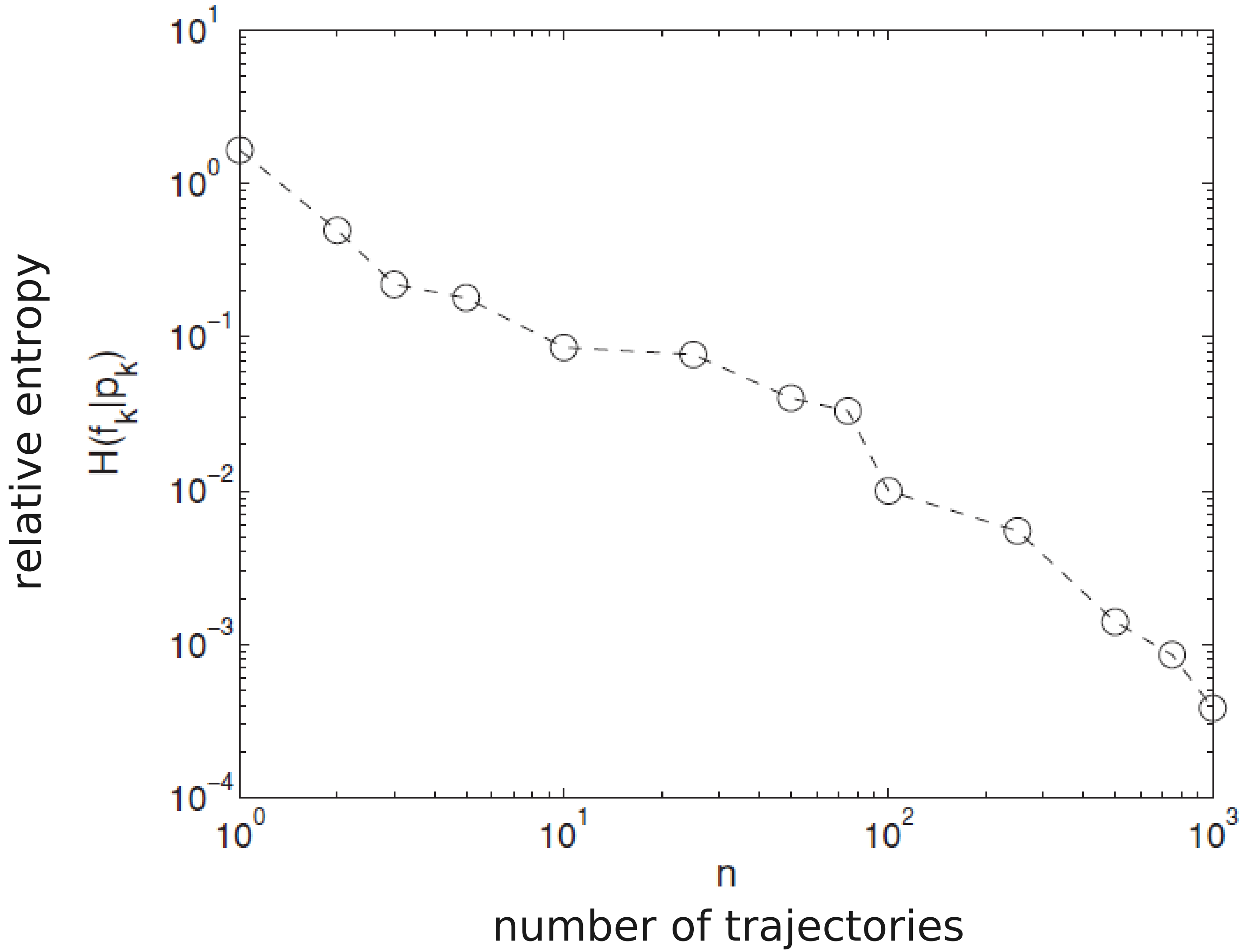


$$\mathrm{Prob}(c_1(\infty)=1)=\mathrm{Prob}(\text{ odd jumps})=1-\frac{1}{2}\exp\left(-2\int_0^\infty \mathrm{d}t\int \mathrm{d}q\; r_t^{(q)}\right)=|c_1(0)|^2$$

✓

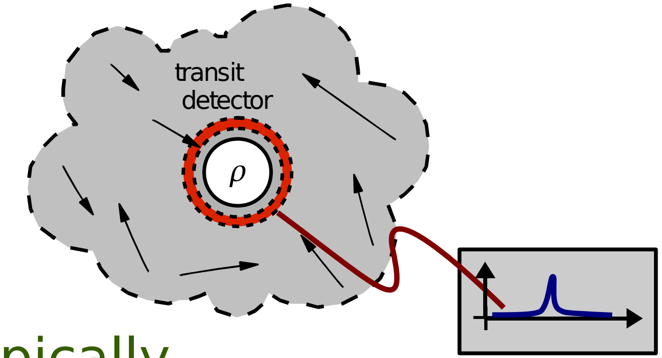
The statistical weights, $N>2$

numerical analysis confirms $\mathrm{Prob}(c_j(\infty)=1) \;=\; |c_j(0)|^2$

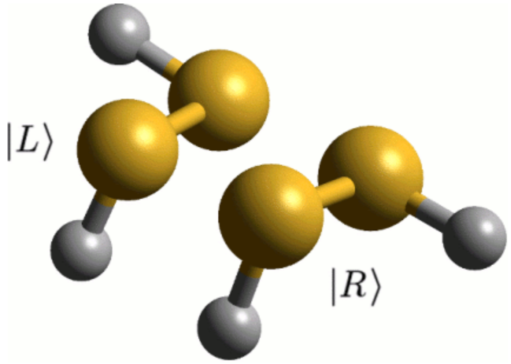


M. Busse & K.H., JPA (2010)

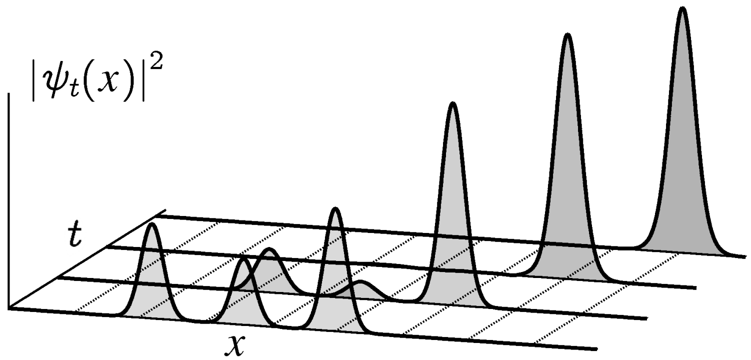
Summary



- Monitoring approach
  - – a method to derive microscopically realistic master equations –



- Hund's paradox
  - – super-selecting chiral molecular configuration states –



- Pointer states of motion
  - – the pointer basis induced by collisional decoherence –