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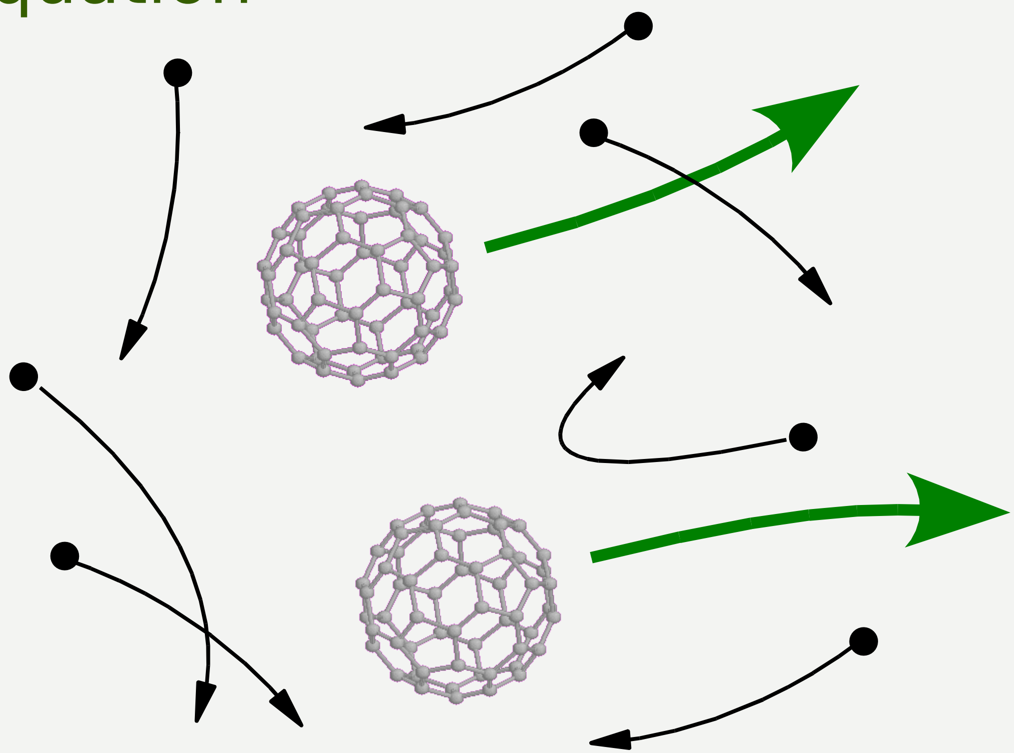
Monitoring approach to the quantum linear Boltzmann equation



Outline

1. Monitoring approach to open quantum dynamics

   —scattering theory meets the theory of measurement—

2. A first application: Internal molecular states

   —wave packet evaluation and the low density limit—

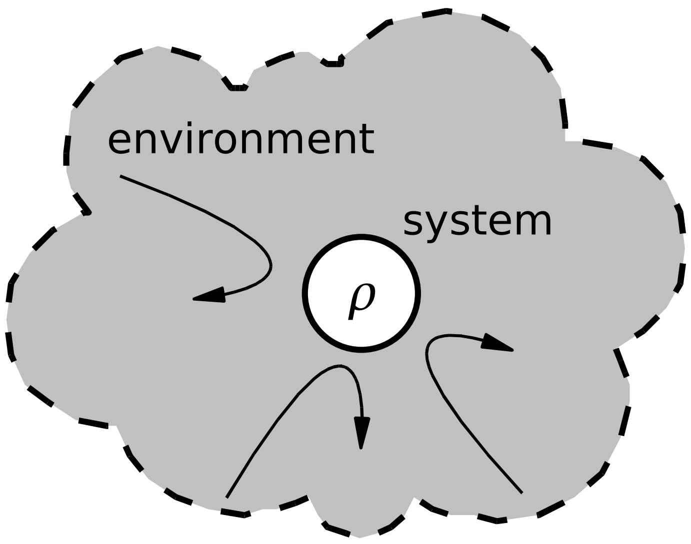
3. The quantum linear Boltzmann equation

   —operator form, limiting cases, momentum representation—

4. Conclusions

Time-local master equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \mathcal{L}\rho$$



Monitoring approach:

crucial assumption:

- single (quasi-)particles interact each at a time, i.e.,
  - the *rate* of collisions and
  - the *effect* of a single collision is separately well defined

advantages:

- Markovian by construction
- microscopically realistic environmental interaction
- non-perturbative treatment

Two basic operators

Γ : rate operator (positive)

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

collision probability

S : scattering operator (unitary)

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

effect of single collision

Two basic operators ... naïvely implemented

Γ: rate operator (positive)

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

collision probability

S: scattering operator (unitary)

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

effect of single collision

naïve implementation ...

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho \;\stackrel{?}{=}\; \mathrm{Tr}_{\mathrm{env}}(\Gamma[\rho\otimes\rho_{\mathrm{env}}])\left\{\mathrm{Tr}_{\mathrm{env}}\big(S[\rho\otimes\rho_{\mathrm{env}}]S^\dagger\big)-\rho\right\}$$

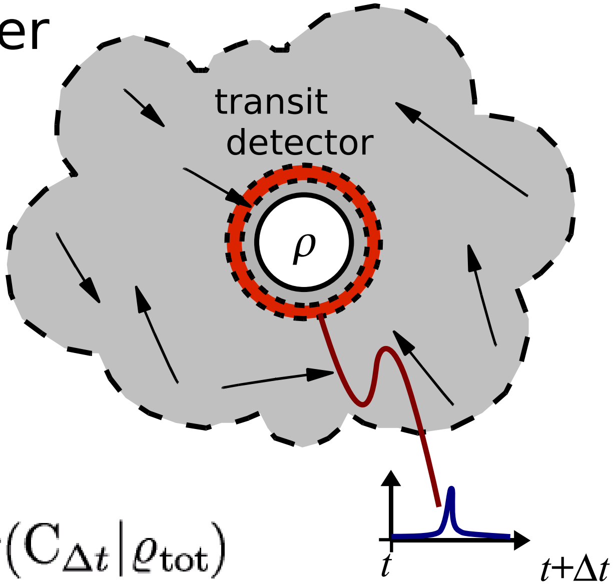
...would lead to a nonlinear equation

Monitoring approach: environment as a probe

a hypothetical, minimally invasive "transit detector"
tells whether system and probe are going to scatter

$$\Pr(\mathrm{C}_{\Delta t}|\varrho_{\mathrm{tot}}) = \mathrm{Tr}(\Gamma\varrho_{\mathrm{tot}})\,\Delta t$$

time resolution



conditioned on transit event:

$$\varrho_{\mathrm{tot}}^{\mathrm{c}} = \frac{\mathcal{M}(\varrho_{\mathrm{tot}}|\mathrm{C}_{\Delta t})}{\mathrm{Tr}\mathcal{M}(\varrho_{\mathrm{tot}}|\mathrm{C}_{\Delta t})}$$

with
$$\mathrm{Tr}\mathcal{M}(\varrho_{\mathrm{tot}}|\mathrm{C}_{\Delta t}) = \Pr(\mathrm{C}_{\Delta t}|\varrho_{\mathrm{tot}})$$

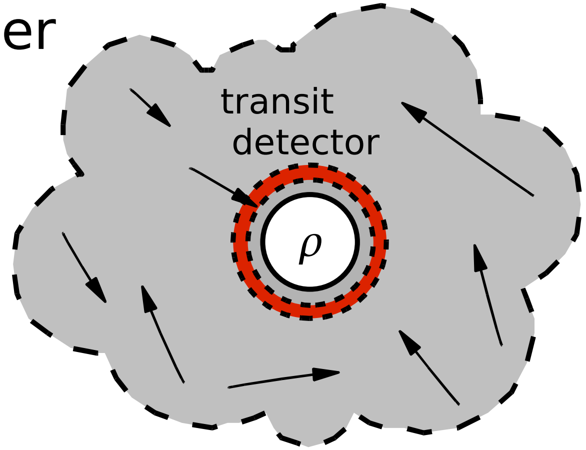
conditioned on null event:

$$\varrho_{\mathrm{tot}}^{\bar{\mathrm{c}}} = \frac{\mathcal{M}(\varrho_{\mathrm{tot}}|\bar{\mathrm{C}}_{\Delta t})}{\mathrm{Tr}\mathcal{M}(\varrho_{\mathrm{tot}}|\bar{\mathrm{C}}_{\Delta t})}$$

with
$$\mathrm{Tr}\mathcal{M}(\varrho_{\mathrm{tot}}|\bar{\mathrm{C}}_{\Delta t}) = 1 - \Pr(\mathrm{C}_{\Delta t}|\varrho_{\mathrm{tot}})$$

Monitoring approach: environment as a probe

a hypothetical, minimally invasive “transit detector” tells whether system and probe are going to scatter



$$\mathrm{Pr}(\mathrm{C}_{\Delta t}|\varrho_{\mathrm{tot}}) = \mathrm{Tr}(\Gamma \varrho_{\mathrm{tot}})\,\Delta t$$

time resolution

measurement transformations:

- efficient $$\mathcal{M}(\varrho_{\mathrm{tot}}|\mathrm{C}_{\Delta t}) = M\varrho_{\mathrm{tot}}M^\dagger \quad \text{with } M^\dagger M = \Delta t\,\Gamma$$

  no additional uncertainty

- minimally invasive $$\mathcal{M}(\varrho_{\mathrm{tot}}|\mathrm{C}_{\Delta t}) = \Gamma^{1/2}\varrho_{\mathrm{tot}}\Gamma^{1/2}\,\Delta t$$

  no reversible back action

- complementary map $$\mathcal{M}\left(\varrho_{\mathrm{tot}}|\bar{\mathrm{C}}_{\Delta t}\right) = \varrho_{\mathrm{tot}} - \mathcal{M}(\varrho_{\mathrm{tot}}|\mathrm{C}_{\Delta t})$$

  no change if outcome disregarded (not CP)

Monitoring master equation

disregarding the transit information...

$$\varrho_{\text{tot}}(\Delta t) = \Pr(\mathrm{C}_{\Delta t}|\varrho_{\text{tot}}) S \frac{\mathcal{M}(\varrho_{\text{tot}}|\mathrm{C}_{\Delta t})}{\mathrm{Tr}\mathcal{M}(\varrho_{\text{tot}}|\mathrm{C}_{\Delta t})} S^\dagger + \Pr\left(\bar{\mathrm{C}}_{\Delta t}|\varrho_{\text{tot}}\right) \frac{\mathcal{M}\left(\varrho_{\text{tot}}|\bar{\mathrm{C}}_{\Delta t}\right)}{\mathrm{Tr}\mathcal{M}\left(\varrho_{\text{tot}}|\bar{\mathrm{C}}_{\Delta t}\right)}$$

$$= S\Gamma^{1/2}\varrho_{\text{tot}}\Gamma^{1/2}S^\dagger\Delta t + \varrho_{\text{tot}} - \Gamma^{1/2}\varrho_{\text{tot}}\Gamma^{1/2}\Delta t$$

...yields the equation:

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho = \lim_{\Delta t \to 0} \frac{\mathrm{Tr}_{\text{env}}(\varrho_{\text{tot}}(\Delta t)) - \rho}{\Delta t}$$

with

$$\varrho_{\text{tot}}(0) = \rho \otimes \rho_{\text{env}}$$

Monitoring master equation

disregarding the transit information...

$$\varrho_{\text{tot}}(\Delta t) = \Pr(\mathrm{C}_{\Delta t}|\varrho_{\text{tot}}) S \frac{\mathcal{M}(\varrho_{\text{tot}}|\mathrm{C}_{\Delta t})}{\mathrm{Tr}\mathcal{M}(\varrho_{\text{tot}}|\mathrm{C}_{\Delta t})} S^\dagger + \Pr\left(\bar{\mathrm{C}}_{\Delta t}|\varrho_{\text{tot}}\right) \frac{\mathcal{M}\left(\varrho_{\text{tot}}|\bar{\mathrm{C}}_{\Delta t}\right)}{\mathrm{Tr}\mathcal{M}\left(\varrho_{\text{tot}}|\bar{\mathrm{C}}_{\Delta t}\right)}$$

$$= S\Gamma^{1/2}\varrho_{\text{tot}}\Gamma^{1/2}S^\dagger \Delta t + \varrho_{\text{tot}} - \Gamma^{1/2}\varrho_{\text{tot}}\Gamma^{1/2}\Delta t$$

...yields the equation:

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

... by using the unitarity of $S = I + i\,T$, i.e., $\mathrm{Im}(T) = \frac{1}{2}T^\dagger T$

Monitoring master equation

restores
complete positivity

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

... by using the unitarity of $S = I + i\,T$, i.e., $\mathrm{Im}(T) = \frac{1}{2}T^{\dagger}T$

Monitoring master equation

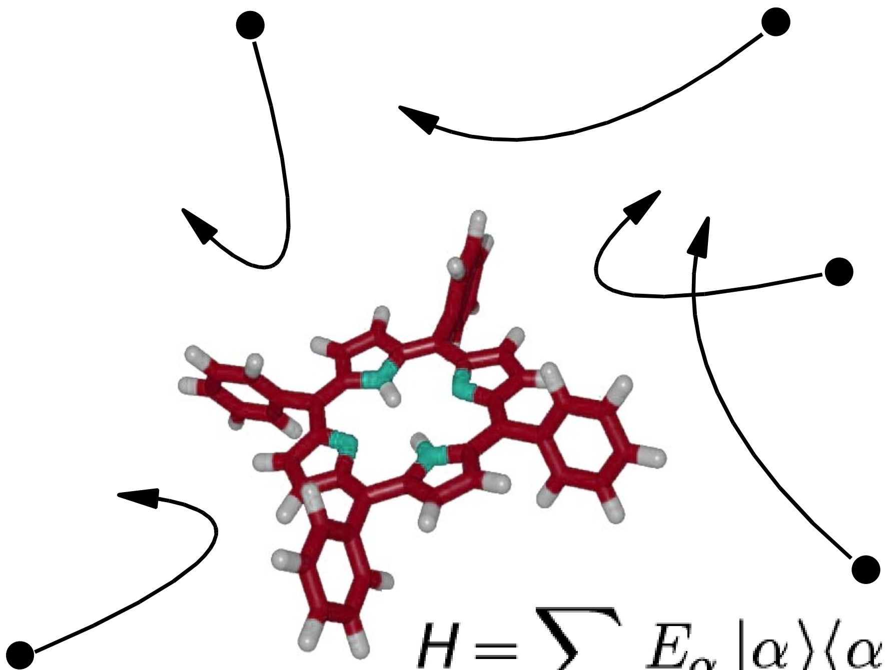
in the Schrödinger picture..

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

K.H., EPL 77 (2007) 50007

Application: Immobile system in gas

microscopic operators:



- collision probability determined by

$$\Gamma = \sum_\alpha |\alpha\rangle\langle\alpha| \otimes n_{\mathrm{gas}} \frac{|\mathbf{p}|}{m} \sigma(\mathbf{p}, \alpha)$$

but the projection to the subspace of incoming wave packets still lacking

$$H = \sum_\alpha E_\alpha |\alpha\rangle\langle\alpha|$$

vibrations, rotations, ...

- $S = I + i\,T$ characterized by multichannel scattering amplitudes

$$\langle\alpha_f|\langle\mathbf{p}_f|T|\alpha_i\rangle|\mathbf{p}_i\rangle = \frac{f_{\alpha\alpha_0}(\mathbf{p}_f, \mathbf{p}_i)}{2\pi\hbar\, m} \delta\left(\frac{p_f^2 - p_i^2}{2m} + E_{\alpha_f} - E_{\alpha_i}\right)$$

motion in the channel basis

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

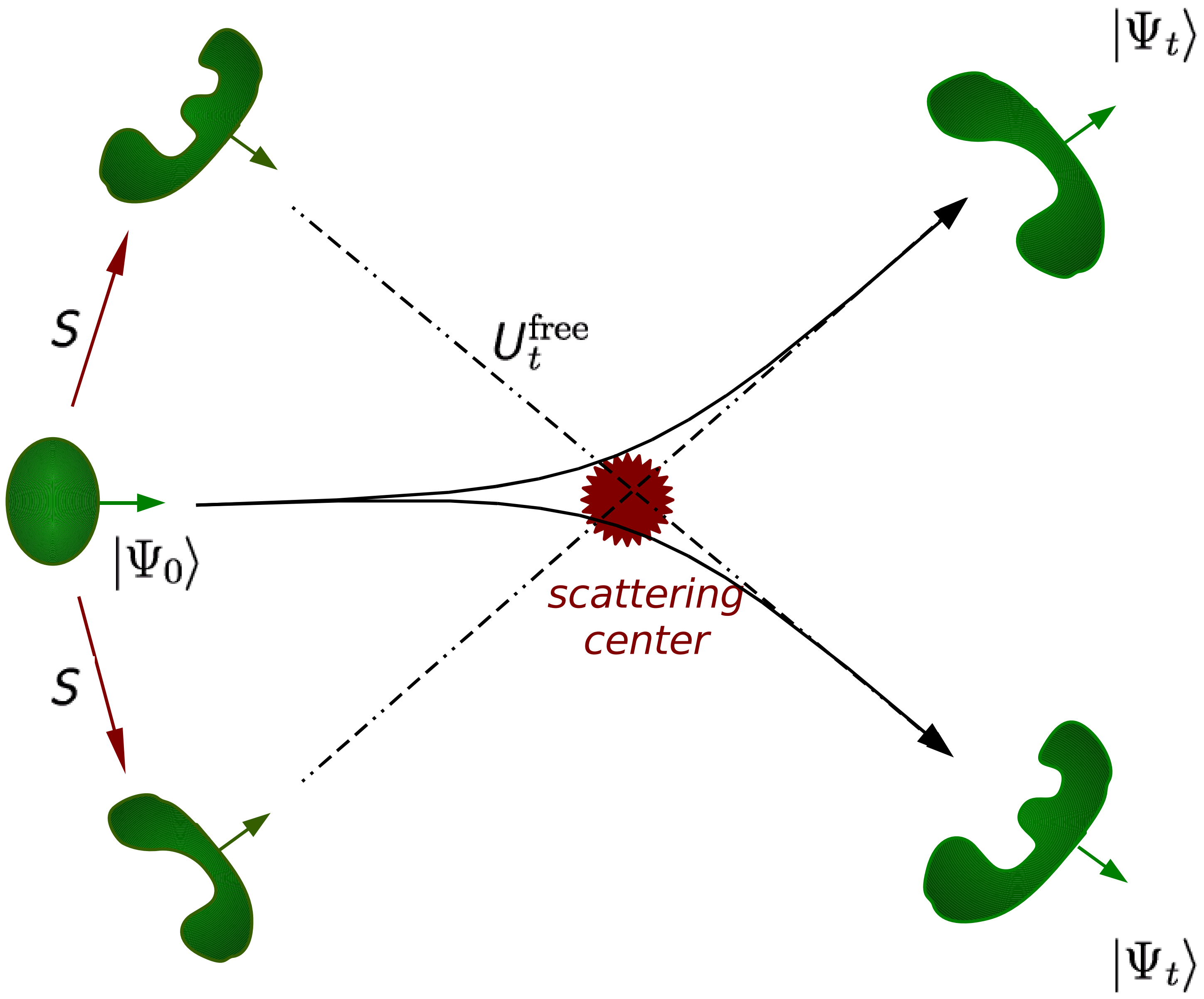
with real energy shifts ε_α

and complex rate coefficients

$$M_{\alpha\beta}^{\alpha_0\beta_0} = \langle\alpha|\mathrm{Tr}_{\mathrm{env}}\left(T\Gamma^{1/2}[|\alpha_0\rangle\langle\beta_0| \otimes \rho_{\mathrm{env}}]\Gamma^{1/2}T^\dagger\right)|\beta\rangle$$

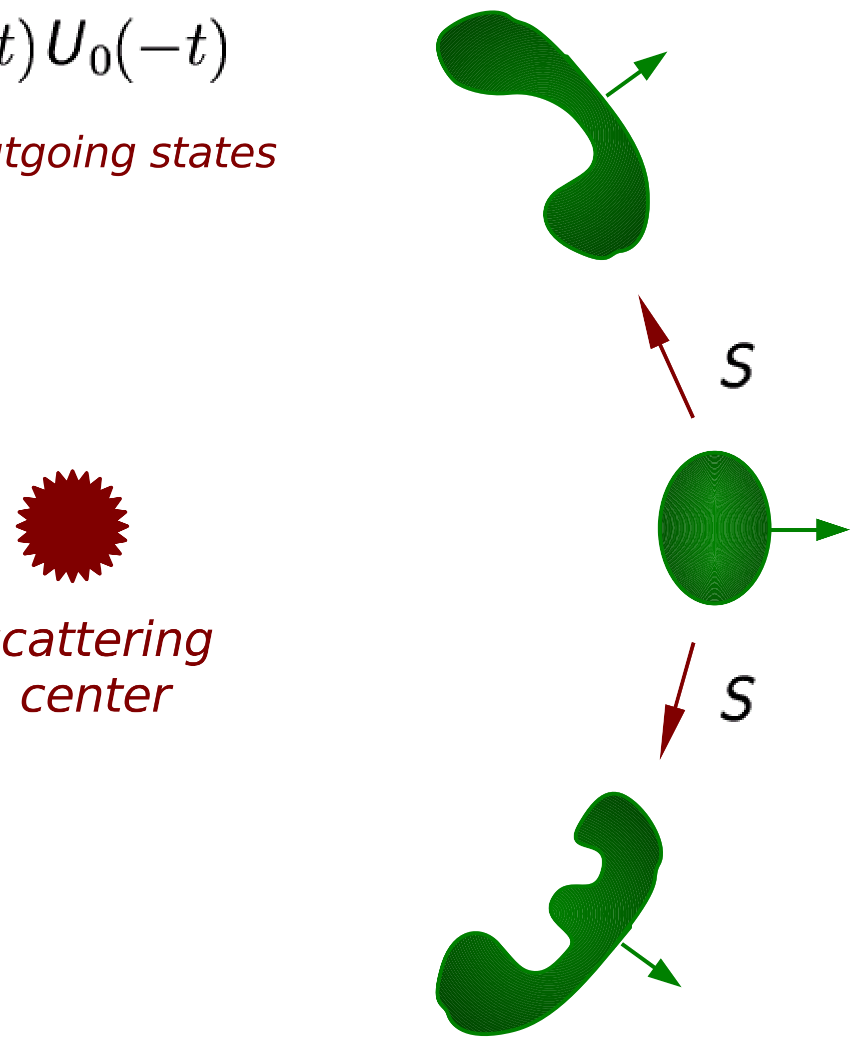
what's $S = I + iT$
actually doing?

Intermission: The S matrix—a pictorial view



$$S = \Omega_-^\dagger \Omega_+ = \lim_{t\to\infty} U_0(-t)\,U(2t)\,U_0(-t)$$

...”unintentionally” transforms outgoing states



motion in the channel basis

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

with real energy shifts ε_α

and complex rate coefficients

$$M_{\alpha\beta}^{\alpha_0\beta_0} = \langle\alpha|\mathrm{Tr}_{\mathrm{env}}\big(T\Gamma^{1/2}[|\alpha_0\rangle\langle\beta_0| \otimes \rho_{\mathrm{env}}]\Gamma^{1/2}T^\dagger\big)|\beta\rangle$$

how to enforce the restriction to incoming wave packets?

wave packet evaluation of the rate coefficients

decomposing ρ_{env} into wave packets

$$\rho_{\text{env}} = \frac{\lambda_{\text{th}}^3}{\Omega} \exp\left(-\frac{\beta\, \boldsymbol{p}^2}{2m} \right) = \int \mathrm{d}\boldsymbol{p}_0\, \hat{\mu}(\boldsymbol{p}_0) \int_\Omega \frac{\mathrm{d}\boldsymbol{r}_0}{\Omega} |\psi_{\boldsymbol{r}_0 \boldsymbol{p}_0}\rangle\langle\psi_{\boldsymbol{r}_0 \boldsymbol{p}_0}|$$

wave packet evaluation of the rate coefficients

decomposing ρ_{env} into wave packets ...

$$\rho_{\text{env}} = \frac{\lambda_{\text{th}}^3}{\Omega} \exp\left(-\frac{\beta\, \boldsymbol{p}^2}{2m} \right) = \int \mathrm{d}\boldsymbol{p}_0\, \hat{\mu}(\boldsymbol{p}_0) \int_\Omega \frac{\mathrm{d}\boldsymbol{r}_0}{\Omega} |\psi_{\boldsymbol{r}_0 \boldsymbol{p}_0}\rangle\langle\psi_{\boldsymbol{r}_0 \boldsymbol{p}_0}|$$

... admits phase space restriction
to proper incoming states

$$M_{\alpha\beta}^{\alpha_0\beta_0} = \int \mathrm{d}\boldsymbol{p}_0\, \hat{\mu}(\boldsymbol{p}_0) \underbrace{\int_\Omega \frac{\mathrm{d}\boldsymbol{r}_0}{\Omega}}\, m_{\alpha\beta}^{\alpha_0\beta_0}(\boldsymbol{r}_0, \boldsymbol{p}_0)$$

“average” over all positions $\boldsymbol{r}_0$

with $m_{\alpha\beta}^{\alpha_0\beta_0}(\boldsymbol{r}_0, \boldsymbol{p}_0) := \int \mathrm{d}\boldsymbol{p}\, \langle\alpha\, |\langle\boldsymbol{p}|\, T\, \Gamma^{1/2} |\alpha_0\rangle |\psi_{\boldsymbol{r}_0 \boldsymbol{p}_0}\rangle \langle\beta_0| \langle\psi_{\boldsymbol{r}_0 \boldsymbol{p}_0}| \Gamma^{1/2}\, T^\dagger |\beta\rangle |\boldsymbol{p}\rangle$

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... admits phase space restriction
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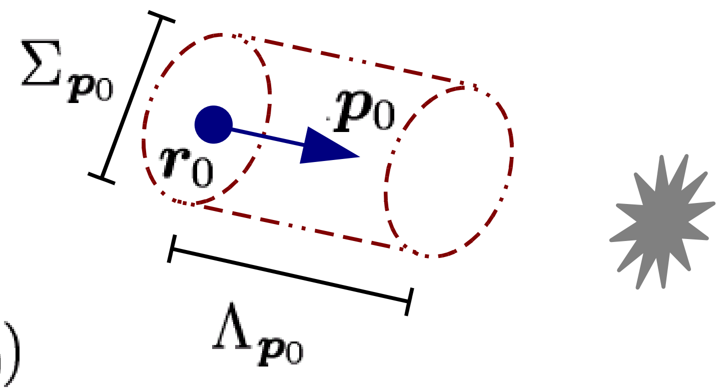


$$M_{\alpha\beta}^{\alpha_0\beta_0} = \int \mathrm{d}\boldsymbol{p}_0\, \hat{\mu}(\boldsymbol{p}_0) \int_\Omega \frac{\mathrm{d}\boldsymbol{r}_0}{\Omega} m_{\alpha\beta}^{\alpha_0\beta_0}(\boldsymbol{r}_0, \boldsymbol{p}_0)$$

$$\rightarrow \int \mathrm{d}\boldsymbol{p}_0\, \hat{\mu}(\boldsymbol{p}_0) \int_{\Lambda_{\boldsymbol{p}_0}} \frac{\mathrm{d}\boldsymbol{r}_{\parallel \boldsymbol{p}_0}}{\Lambda_{\boldsymbol{p}_0}} \int_{\Sigma_{\boldsymbol{p}_0}} \frac{\mathrm{d}\boldsymbol{r}_{\perp \boldsymbol{p}_0}}{\Sigma_{\boldsymbol{p}_0}} m_{\alpha\beta}^{\alpha_0\beta_0}(\boldsymbol{r}_{\parallel \boldsymbol{p}_0} + \boldsymbol{r}_{\perp \boldsymbol{p}_0}, \boldsymbol{p}_0)$$

with $m_{\alpha\beta}^{\alpha_0\beta_0}(\boldsymbol{r}_0, \boldsymbol{p}_0) := \int \mathrm{d}\boldsymbol{p}\, \langle\alpha\, |\langle\boldsymbol{p}| \mathsf{T}\, \Gamma^{1/2} |\alpha_0\rangle |\psi_{\boldsymbol{r}_0 \boldsymbol{p}_0}\rangle \langle\beta_0| \langle\psi_{\boldsymbol{r}_0 \boldsymbol{p}_0}| \Gamma^{1/2}\, \mathsf{T}^\dagger |\beta\rangle |\boldsymbol{p}\rangle$

wave packet evaluation: result

in the limit of delocalized wave packets, $\bar{\beta} \to \infty, \hat{\beta} \to \beta$,
the dependence on $\Lambda_{\boldsymbol{p}_0}$ vanishes and one obtains...

- complex rate coefficients:

$$M_{\alpha\beta}^{\alpha_0\beta_0} = \chi_{\alpha\beta}^{\alpha_0\beta_0} n_{\text{gas}} \int_0^\infty \mathrm{d}v \; \nu(v)\, v_{\text{out}}(v) \times 2\pi \int_{-1}^{1} \mathrm{d}(\cos\theta)\, f_{\alpha\alpha_0}\Big(\cos\theta; \frac{m}{2}v^2\Big)\, f^*_{\beta\beta_0}\Big(\cos\theta; \frac{m}{2}v^2\Big)$$

$$v_{\text{out}}^2 = v^2 - 2\,\frac{E_\alpha - E_{\alpha_0}}{m}$$

outgoing velocity

$$\chi_{\alpha\beta}^{\alpha_0\beta_0} = \begin{cases} 1 & \text{if } E_\alpha - E_{\alpha_0} = E_\beta - E_{\beta_0} \\ 0 & \text{otherwise.} \end{cases}$$

... provided we identify the phase space cross section with the *geometric mean* of the involved microscopic cross sections,

$$\Sigma_{\boldsymbol{p}_0} = \sqrt{\sigma(\boldsymbol{p}_0; \alpha_0)\, \sigma(\boldsymbol{p}_0; \beta_0)}$$

wave packet evaluation: result

in the limit of delocalized wave packets
the dependence on $\Lambda_{\boldsymbol{p}_0}$ vanishes and one obtains...

- complex rate coefficients:

$$M_{\alpha\beta}^{\alpha_0\beta_0} = \chi_{\alpha\beta}^{\alpha_0\beta_0} n_{\text{gas}} \int_0^\infty \mathrm{d}v\ \nu(v)\, v_{\text{out}}(v) \times 2\pi \int_{-1}^{1} \mathrm{d}(\cos\theta)\, f_{\alpha\alpha_0}\Big(\cos\theta; \frac{m}{2}v^2\Big)\, f^*_{\beta\beta_0}\Big(\cos\theta; \frac{m}{2}v^2\Big)$$

- energy shifts:

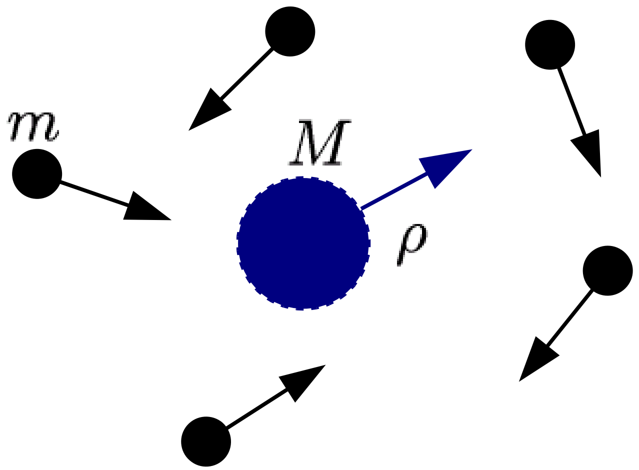
$$\varepsilon_\alpha = -2\pi\hbar^2 \frac{n_{\text{gas}}}{m} \int_0^\infty \mathrm{d}v\ \nu(v)\, \mathrm{Re}\Big[f_{\alpha\alpha}\Big(0; \frac{m}{2}v^2\Big)\Big]$$

- equal to “low density limit” result Dümcke (1985), Alicki&Lendi (1987)
  for $|M_{\alpha\beta}^{\alpha_0\beta_0}| \ll \Delta E/\hbar$ and $H_{\text{int}} = A \otimes B_{\text{env}}$

K.H., EPL 77 (2007) 50007

The quantum linear Boltzmann equation

Distinguished Brownian particle
in an ideal gas



The quantum linear Boltzmann equation

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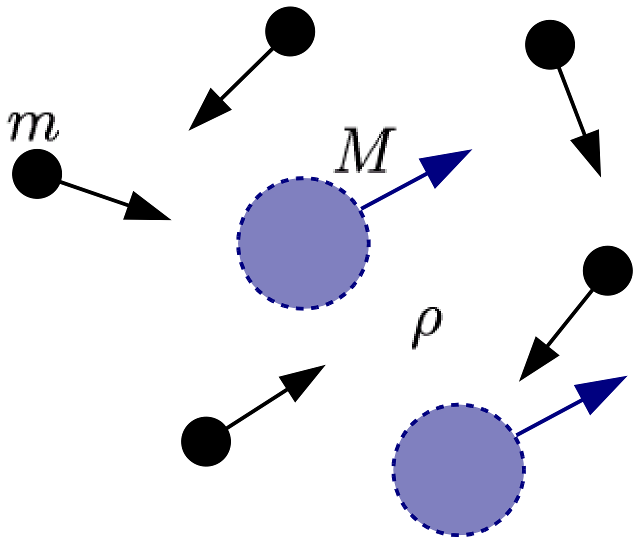


previous work:

$m \lll M$

Joos & Zeh (1985)
Gallis & Fleming (1990)

Alicki (2002)
K.H. & Sipe (2003)

exp: K.H.,...& Zeilinger (2003)

pure decoherence, no dissipation

$m \lesssim M$

Diosi (1995)

Vacchini (2000,2001)
Dodd & Halliwell (2003)

interplay of decoherence and thermalization

K.H., PRL 97, 060601 (2006)

Quantum linear Boltzmann equation: Calculation

rate operator

relative velocity

$$\Gamma = n_{\text{gas}} \frac{|\text{rel}(\mathsf{p}, \mathsf{P})|}{m_*} \sigma(\text{rel}(\mathsf{p}, \mathsf{P}))$$

relative momentum

$$\text{rel}(\boldsymbol{p}, \boldsymbol{P}) = \frac{m_*}{m}\boldsymbol{p} - \frac{m_*}{M}\boldsymbol{P}$$

using again...

- *the general master equation*

$$\begin{aligned}\mathcal{L}^{\mathrm{B}}\rho &= \text{tr}_{\text{gas}}\Big(\mathsf{T}\,\Gamma^{1/2}[\rho \otimes \rho_{\text{gas}}]\,\Gamma^{1/2}\mathsf{T}^\dagger \Big) \\ &\quad - \frac{1}{2}\text{tr}_{\text{gas}}\Big(\Gamma^{1/2}\mathsf{T}^\dagger\mathsf{T}\,\Gamma^{1/2}[\rho \otimes \rho_{\text{gas}}] \Big) \\ &\quad - \frac{1}{2}\text{tr}_{\text{gas}}\Big([\rho \otimes \rho_{\text{gas}}]\Gamma^{1/2}\mathsf{T}^\dagger\mathsf{T}\,\Gamma^{1/2} \Big)\end{aligned}$$

- *an ideal, stationary gas*
- *wave packet decomposition for in-state restriction*

Quantum linear Boltzmann equation: Operator form

leads to...

$$\mathcal{L}^{\mathrm{B}}\rho = \int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}^{\perp}} \mathrm{d}\boldsymbol{K} \left\{ \mathsf{L}_{\boldsymbol{Q},\boldsymbol{K}}\,\rho\,\mathsf{L}^{\dagger}_{\boldsymbol{Q},\boldsymbol{K}} - \frac{1}{2}\rho\,\mathsf{L}^{\dagger}_{\boldsymbol{Q},\boldsymbol{K}}\mathsf{L}_{\boldsymbol{Q},\boldsymbol{K}} - \frac{1}{2}\mathsf{L}^{\dagger}_{\boldsymbol{Q},\boldsymbol{K}}\mathsf{L}_{\boldsymbol{Q},\boldsymbol{K}}\,\rho \right\}$$

with jump operators $\mathsf{L}_{\boldsymbol{Q},\boldsymbol{K}} = \mathrm{e}^{i\mathsf{X}\cdot\boldsymbol{Q}/\hbar}\, L(\boldsymbol{K}, \mathsf{P}; \boldsymbol{Q})$

determined by:

$$L(\boldsymbol{K}, \boldsymbol{P}; \boldsymbol{Q}) = \sqrt{\frac{n_{\mathrm{gas}}\, m}{m_* Q}}\, \mu\left(\boldsymbol{K}_{\perp\boldsymbol{Q}} + \left(1 + \frac{m}{M}\right)\frac{\boldsymbol{Q}}{2} + \frac{m}{M}\boldsymbol{P}_{\parallel\boldsymbol{Q}}\right)^{1/2}$$
$$\times f\left(\mathrm{rel}(\boldsymbol{K}_{\perp\boldsymbol{Q}}, \boldsymbol{P}_{\perp\boldsymbol{Q}}) - \frac{\boldsymbol{Q}}{2}, \mathrm{rel}(\boldsymbol{K}_{\perp\boldsymbol{Q}}, \boldsymbol{P}_{\perp\boldsymbol{Q}}) + \frac{\boldsymbol{Q}}{2}\right)$$

where $\boldsymbol{P}_{\parallel\boldsymbol{Q}} = \frac{(\boldsymbol{P}\cdot \boldsymbol{Q})\boldsymbol{Q}}{Q^2}$ and $\boldsymbol{P}_{\perp\boldsymbol{Q}} = \boldsymbol{P} - \boldsymbol{P}_{\parallel\boldsymbol{Q}}$

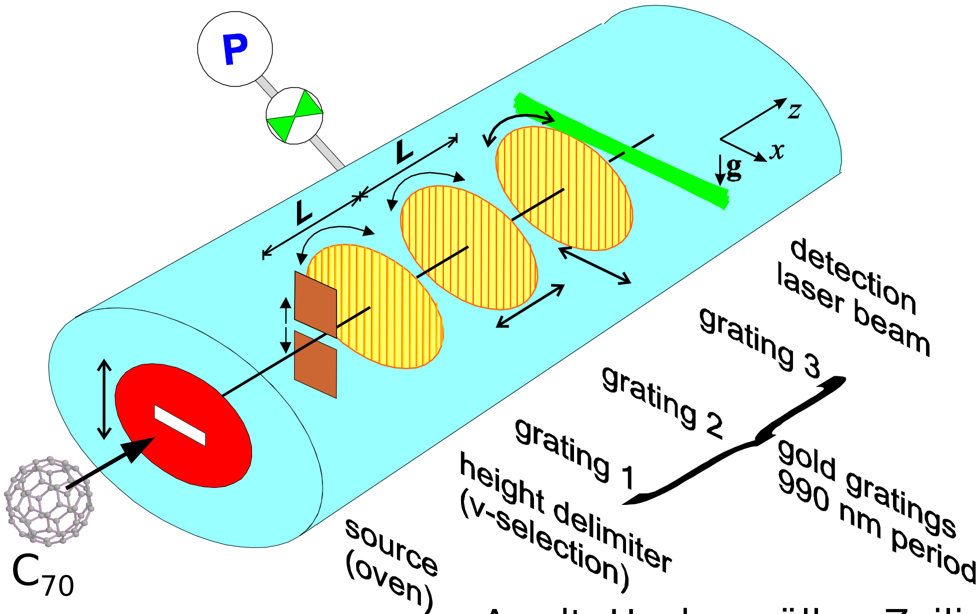
K.H., PRL 97, 060601 (2006)

... fits general form of translation invariant master equation (Holevo 1996)

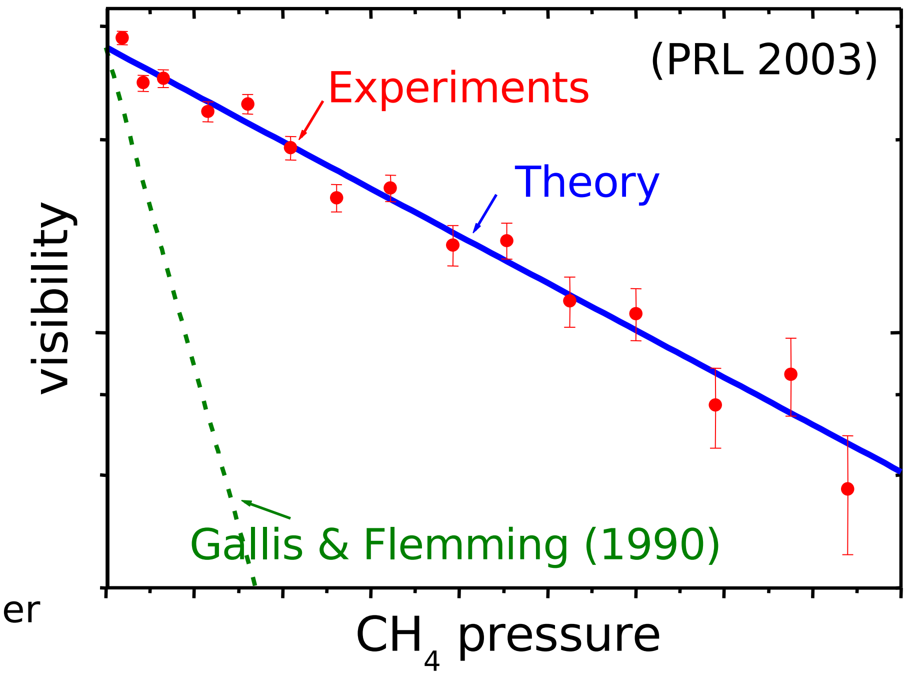
1. Pure decoherence

$$M \gg m \;\Rightarrow\; L_{\boldsymbol{Q},\boldsymbol{K}} \;=\; \mathrm{e}^{iX\cdot Q/\hbar} L(\boldsymbol{K}, \cancel{\boldsymbol{P}}; \boldsymbol{Q})$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \boldsymbol{X}|\tilde{\rho}|\boldsymbol{X}'\rangle \;=\; -F(\boldsymbol{X}-\boldsymbol{X}')\,\langle \boldsymbol{X}|\tilde{\rho}|\boldsymbol{X}'\rangle$$



Arndt, Hackermüller, Zeilinger



$$F(\boldsymbol{x}) = \int_0^\infty \mathrm{d}v\, \nu(v) n_{\mathrm{gas}}\, v \left\{ \sigma(m\,v) - 2\pi \int_{-1}^{1} \mathrm{d}(\cos\theta) \left| f\left(\cos\theta; \frac{m}{2}v^2\right)\right|^2 \mathrm{sinc}\left(2\sin\left(\frac{\theta}{2}\right)\frac{m\,v\,|\boldsymbol{x}|}{\hbar}\right)\right\}$$

(PRA 2003)

2. Diffusive “limit”

The expansion

$$\mathrm{e}^{i\mathsf{X}\cdot\boldsymbol{Q}/\hbar} L(\boldsymbol{K}, \mathsf{P}; \boldsymbol{Q}) \cong \left(1 + i\frac{\mathsf{X}\cdot\boldsymbol{Q}}{\hbar}\right)\left(1 - \beta\frac{\mathsf{P}\cdot\boldsymbol{Q}}{4m}\right) L(\boldsymbol{K}, 0; \boldsymbol{Q})$$

leads to Caldeira-Leggett form *“plus minimal extension”*

$$\mathcal{L}\rho \;=\; -\eta \sum_{j=x,y,z} \left\{ \frac{i}{2\hbar}[\mathsf{X}_j, \{\mathsf{P}_j, \rho\}_+] + \frac{M}{\beta\hbar^2}[\mathsf{X}_j, [\mathsf{X}_j, \rho]] + \frac{\beta}{16M}[\mathsf{P}_j, [\mathsf{P}_j, \rho]] \right\}$$

with microscopically defined friction coefficient

$$\eta \;=\; c_\beta \int_0^\infty \mathrm{d}k_i\, k_i^5 \exp\left(-\beta\frac{k_i^2}{2m}\right) \int \mathrm{d}\cos\Theta\ \sin^2\left(\frac{\Theta}{2}\right) \left| f_{\mathrm{sc}}\left(\cos\Theta; \frac{m_*}{2m^2}k_i^2\right)\right|^2$$

where $c_\beta \;=\; \frac{8}{3}\frac{n_{\mathrm{gas}}\, m_*^2\, \beta^2}{m^4 M}\left(\frac{2\pi\beta}{m}\right)^{1/2}$

Caldeira&Leggett (1983), Diosi (1995)

3. Weak coupling expression

Replacing the exact scattering amplitude by its Born approximation...

$$f\left(\mathrm{rel}(\boldsymbol{K}_{\perp\boldsymbol{Q}}, P_{\perp\boldsymbol{Q}}) + \frac{\boldsymbol{Q}}{2}, \mathrm{rel}(\boldsymbol{K}_{\perp\boldsymbol{Q}}, P_{\perp\boldsymbol{Q}}) - \frac{\boldsymbol{Q}}{2}\right) \rightarrow f_{\mathrm{Born}}(\boldsymbol{Q}) \propto \langle 0|H_{\mathrm{int}}|\boldsymbol{Q}\rangle$$

leads to

$$\int \mathrm{d}\boldsymbol{Q} \int_{\boldsymbol{Q}^\perp} \mathrm{d}\boldsymbol{K} \left\{ L_{\boldsymbol{Q},\boldsymbol{K}} \rho L^\dagger_{\boldsymbol{Q},\boldsymbol{K}} - \ldots \right\} \rightarrow \int \mathrm{d}\boldsymbol{Q} \left\{ \tilde{L}_{\boldsymbol{Q}} \rho \tilde{L}^\dagger_{\boldsymbol{Q}} - \ldots \right\}$$

and one obtains Vacchini's form of the master equation

Vacchini (2000—2002)

Momentum basis:

$$\langle \boldsymbol{P}|\mathcal{L}^{\mathrm{B}}\rho|\boldsymbol{P}'\rangle = \int \mathrm{d}\boldsymbol{Q}\, M_{\mathrm{in}}(\boldsymbol{P},\boldsymbol{P}';\boldsymbol{Q})\,\langle \boldsymbol{P}-\boldsymbol{Q}|\rho|\boldsymbol{P}'-\boldsymbol{Q}\rangle - \frac{1}{2}\left[M_{\mathrm{out}}^{\mathrm{cl}}(\boldsymbol{P}) + M_{\mathrm{out}}^{\mathrm{cl}}(\boldsymbol{P}')\right]\langle \boldsymbol{P}|\rho|\boldsymbol{P}'\rangle$$

where

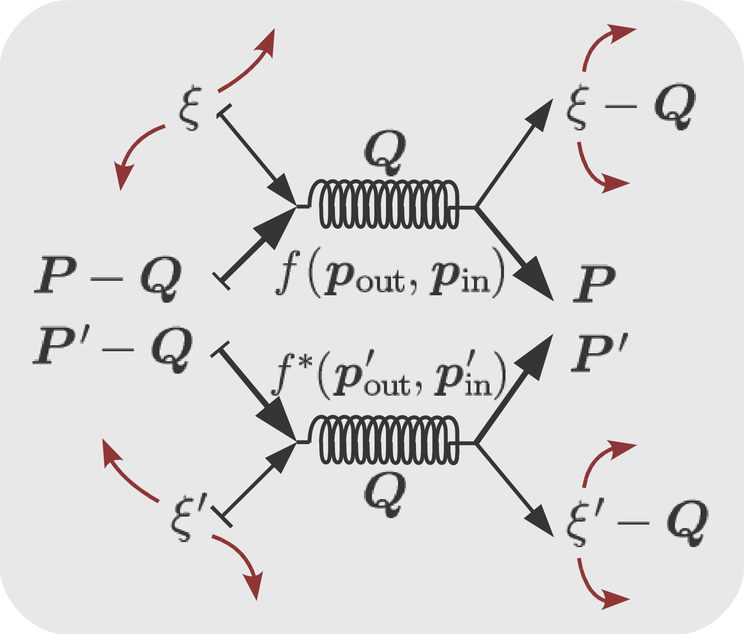
$$M_{\mathrm{out}}^{\mathrm{cl}}(\boldsymbol{P}) = \int \mathrm{d}\boldsymbol{Q}\, M_{\mathrm{in}}(\boldsymbol{P}+\boldsymbol{Q},\boldsymbol{P}+\boldsymbol{Q};\boldsymbol{Q}) =: \int \mathrm{d}\boldsymbol{Q}\, M_{\mathrm{in}}^{\mathrm{cl}}(\boldsymbol{P}+\boldsymbol{Q};\boldsymbol{Q})$$

“classical” scattering rate

and

$$M_{\mathrm{in}}(\boldsymbol{P},\boldsymbol{P}';\boldsymbol{Q}) = \int_{\boldsymbol{Q}^{\perp}} \mathrm{d}\boldsymbol{K}\, L(\boldsymbol{K},\boldsymbol{P}-\boldsymbol{Q};\boldsymbol{Q}) \times L^{*}(\boldsymbol{K},\boldsymbol{P}'-\boldsymbol{Q};\boldsymbol{Q})$$

all permitted pairs of two-particle trajectories weighted by the gas distribution



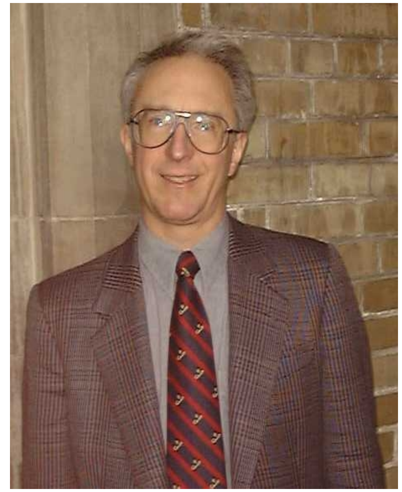
Momentum basis:

$$\langle \boldsymbol{P}|\mathcal{L}^{\mathrm{B}}\rho|\boldsymbol{P}'\rangle = \int \mathrm{d}\boldsymbol{Q}\, M_{\mathrm{in}}(\boldsymbol{P},\boldsymbol{P}';\boldsymbol{Q})\,\langle \boldsymbol{P}-\boldsymbol{Q}|\rho|\boldsymbol{P}'-\boldsymbol{Q}\rangle - \frac{1}{2}\left[M_{\mathrm{out}}^{\mathrm{cl}}(\boldsymbol{P})+M_{\mathrm{out}}^{\mathrm{cl}}(\boldsymbol{P}')\right]\langle \boldsymbol{P}|\rho|\boldsymbol{P}'\rangle$$

- ✔ *form of* M_{in} *has basic interpretation*
- ✔ *QLBE reduces to Boltzmann's classical equation for* $\boldsymbol{P}=\boldsymbol{P}'$
- ✔ *correct limiting form for* $m \lll M$, *in the diffusive, and weak coupling limit (Vacchini)*

The end

Many thanks to...



John E. Sipe
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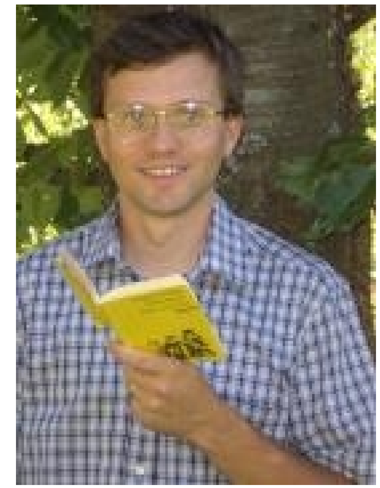

Bassano Vacchini
U Milano

preprints & references available at

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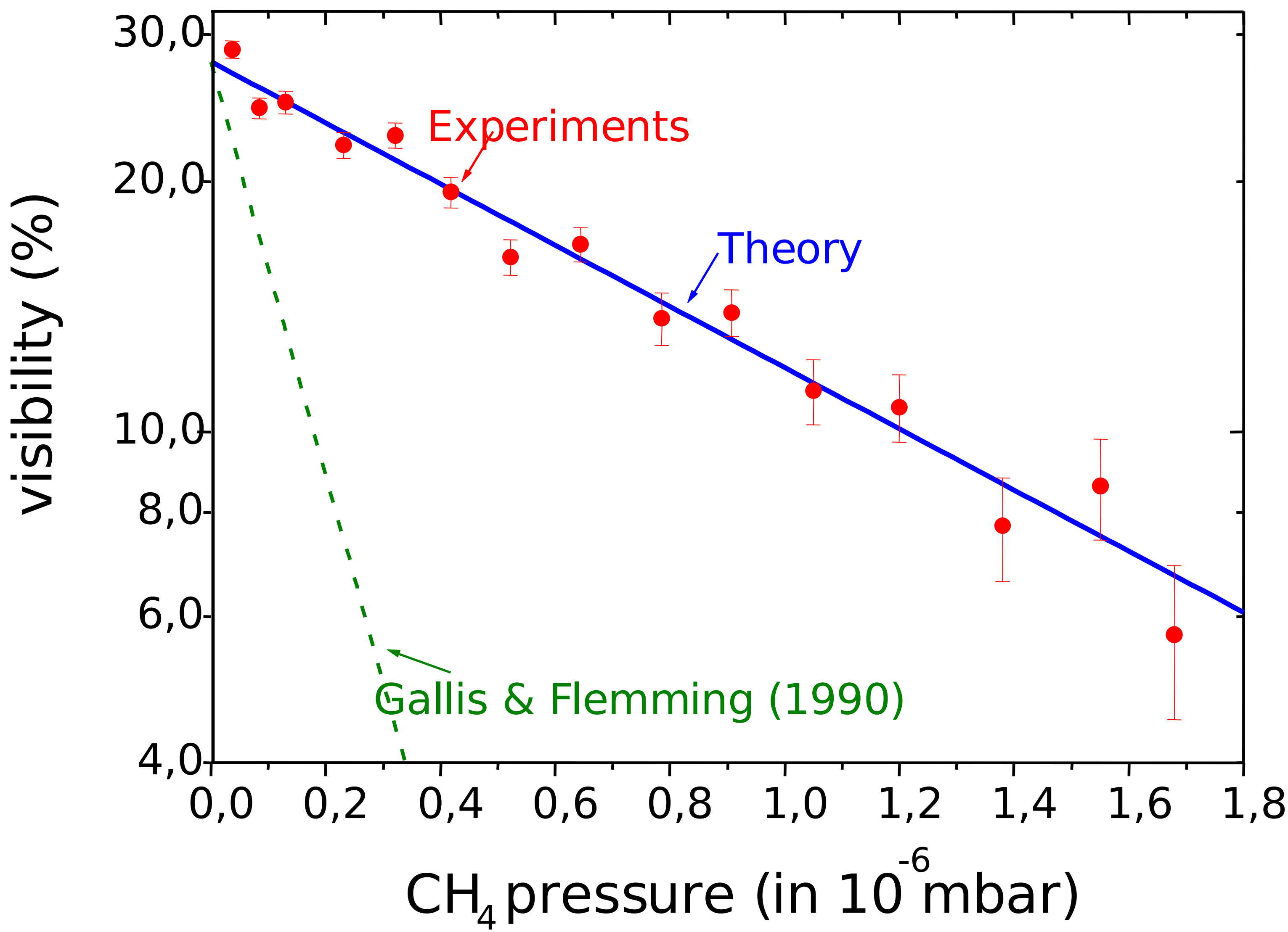
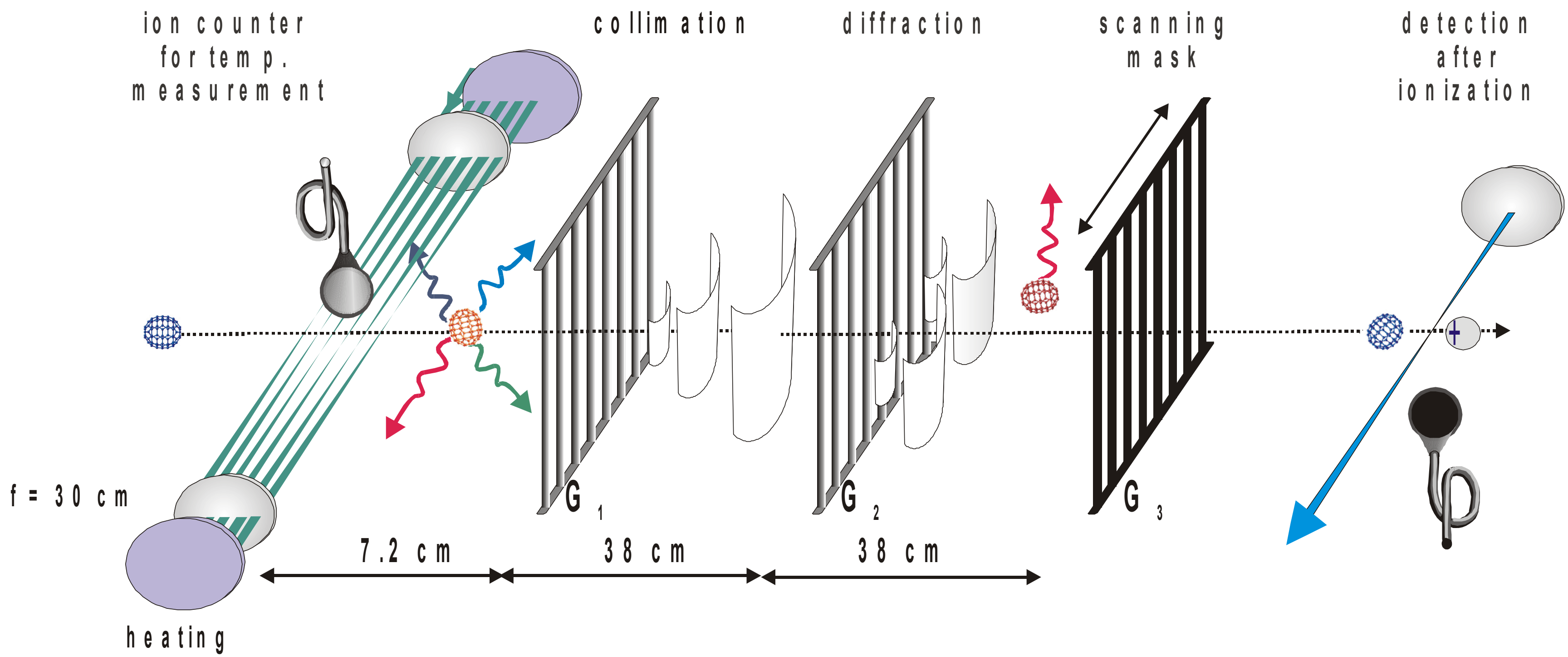
collisional decoherence: decay of visibility with gas pressure



K.H. *et al.*, PRL **90**, 160401 (2003)


ion counter
for temp.
measurement
collimation
diffraction
scanning
mask
detection
after
ionization
f = 30 cm
heating
7.2 cm
38 cm
38 cm
G 1
G 2
G 3
+

$$M_{\rm in}(\boldsymbol{P},\boldsymbol{P}';\boldsymbol{Q}) \;=\; \frac{n_{\rm gas}}{m_*}\int {\rm d}\boldsymbol{p}_0\,\mu(\boldsymbol{p}_0)\;\delta\!\left(\frac{\boldsymbol{p}_f^2-\boldsymbol{p}_i^2}{2}\right) f\,(\boldsymbol{p}_f+\boldsymbol{q}_\perp,\boldsymbol{p}_i+\boldsymbol{q}_\perp)$$
$$\times\; f^*(\boldsymbol{p}_f-\boldsymbol{q}_\perp,\boldsymbol{p}_i-\boldsymbol{q}_\perp)$$

with

$$\boldsymbol{p}_f \;=\; {\rm rel}\!\left(\boldsymbol{p}_0,\frac{\boldsymbol{P}+\boldsymbol{P}'}{2}-\boldsymbol{Q}\right) \;=\; \boldsymbol{p}_i-\boldsymbol{Q}$$
$$\boldsymbol{q} \;=\; {\rm rel}\!\left(0,\frac{\boldsymbol{P}-\boldsymbol{P}'}{2}\right)$$
$$\boldsymbol{q}_\perp \;\equiv\; \boldsymbol{q}_{\perp(\boldsymbol{p}_f-\boldsymbol{p}_i)}$$

evaluation with the diagonal representation

Alternatively, stick to the diagonal representation of $\rho_{\text{env}} = \int \mathrm{d}\boldsymbol{p}_0 \; \mu(\boldsymbol{p}_0) \, |\boldsymbol{p}_0\rangle\langle\boldsymbol{p}_0|$

but modify *S* such that outgoing states are kept invariant

- since momentum states are not of incoming type...

$$\frac{(2\pi\hbar)^3}{\Omega} \langle\alpha \,|\langle\boldsymbol{p}_1| T \,|\alpha_0\,\rangle|\boldsymbol{p}_0\rangle\langle\beta_0|\langle\,\boldsymbol{p}_0| T^\dagger|\beta\,\rangle|\boldsymbol{p}_1\rangle$$

contains square of energy conserving delta functions

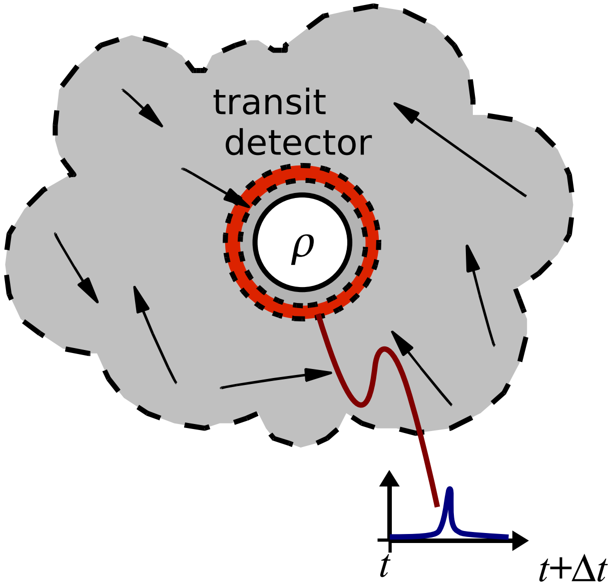
...is ill-defined and must be replaced by

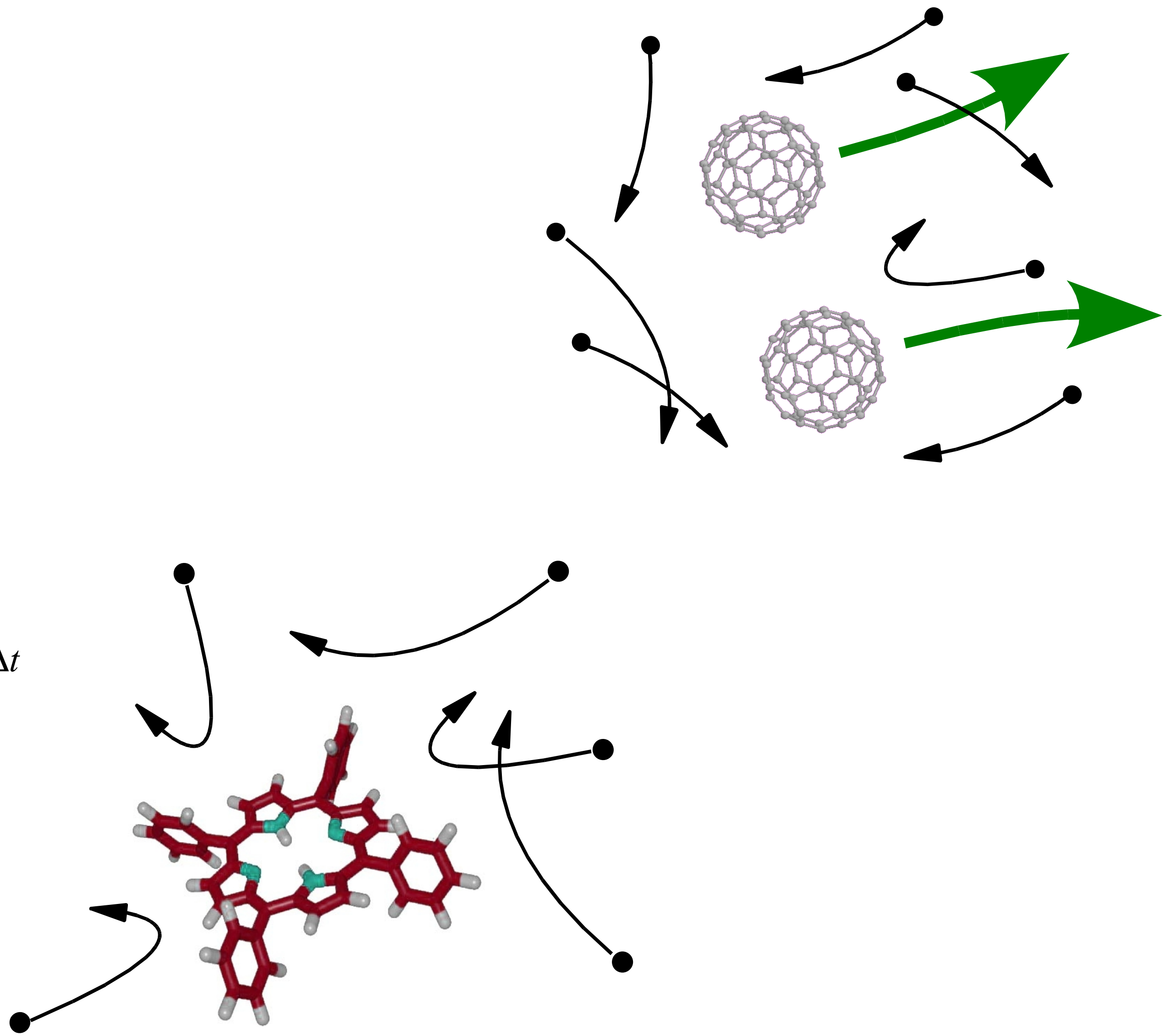
$$\rightarrow \quad \chi_{\alpha\beta}^{\alpha_0\beta_0} \frac{\delta(E_{\alpha p} - E_{\alpha_0 p_0})}{p_0 m} \frac{f_{\alpha\alpha_0}(\boldsymbol{p},\boldsymbol{p}_0)\; f^*_{\beta\beta_0}(\boldsymbol{p},\boldsymbol{p}_0)}{\sqrt{\sigma(p_0;\alpha_0)\sigma(p_0;\beta_0)}}$$

This is the continuum manifestation of the requirement of probability current conservation in the discrete momentum basis.

It yields the same master equation immediately—but slightly less solidly.

summary





Disclaimer

mathematicians, watch out(!)...

Not mathematically rigorous!

Physical argumentation involved!

Only aim: Find the appropriate equation of motion