

# Van Hove Limit for Infinitely Extended Open Quantum Systems

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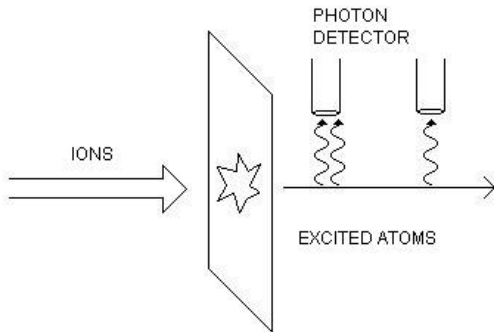
- The Markovian Approach and Davies generators
- Our Generator : Quantum Fokker-Planck Equation
- Example : a Quantum Particle in 3D Space
- Proposal : a Quantum Collisionless Boltzmann Equation
- Outlook on Quantum Brownian Motion
- Conclusions

## Collaborations

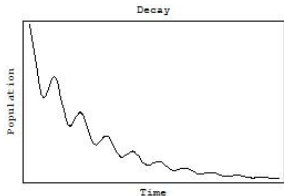
- Prof. F. Rossi (Dip. Fisica, Politecnico di Torino)
- Prof. H. Fujita Yashima (Dip. Mat., Università di Torino)
- Prof. C-A Pillet (CPT - UMR 6207 et Université de Toulon)
- Prof. V. Gritsev (Dép. Phys., Université de Fribourg)

# Beam Foil Spectroscopy

An experiment to start with!



# Need of a Quantum Theory of Relaxation Phenomena



- Coherent superposition of system eigenstates
- ⇒ non-trivial interplay between Coherent Dynamics and Energy-Relaxation/Decoherence

## Contact with microscopic quantum description at large times

- The fundamental equations governing the basic laws of Physics are time reversible and not dissipative.
- Macroscopic irreversible equations obtained through
  - averaging over microscopic degrees of freedom (stochasticity)
  - energy-time scale separation ( $\mu\text{eV}$  versus  $\text{meV}$ , etc.)
  - neglecting recollisions (Markovicity)

# Van Hove Limit in Quantum Open Systems

- $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$        $H_0 = H_S \otimes 1 + 1 \otimes H_B$
- $H' = Q \otimes \Phi$ ,       $H_\lambda = H_0 + \lambda H'$

## System observables in Heisenberg picture

- The state on  $\mathcal{H}$  is  $\rho = \rho_S \otimes \sigma_B$
- At time  $t$ ,  $O^\lambda(t) = e^{iH_\lambda t} O_S \otimes 1 e^{-iH_\lambda t}$
- We measure  $\langle O^\lambda(t) \rangle_\rho = \text{tr}[\rho O^\lambda(t)] = \text{tr}[\rho_S O_S^\lambda(t)]$  where
- $O_S^\lambda(t) = P_0 O^\lambda(t)$  system observable at time  $t$
- $P_0 X \otimes Y = \text{tr}(\sigma_B Y) X \otimes 1$  partial trace projection

## Markovian Approximation in the Van Hove Limit

- Define  $W_t^\lambda O_S := O_S^\lambda(t)$  system evolution superoperator
- Expect  $W_t^\lambda \sim \exp\{\mathbb{L}_\lambda t\}$ ,     $0 \leq t \leq \lambda^{-2}\bar{\tau}$ ,     $\lambda \sim 0$

# Exact System Evolution : the Memory Kernel

## Formulation on operator spaces

- $\mathcal{B} = \mathcal{B}_0 \oplus \mathcal{B}_1$  Banach spaces  $\mathcal{B}_i = P_i(\mathcal{B})$ ,  $P_1 = 1 - P_0$
- $Z O = i[H_0, O]$  and  $A O = i[H', O]$  **Liouvillians**
- $W_t^\lambda = P_0 \exp\{(Z + \lambda A)t\}|_{\mathcal{B}_0}$  **subsystem evolution**

## The Nakajima-Zwanzig master equation

$$W_t^\lambda = X_t^\lambda + \lambda^2 \int_0^t dt_1 \int_0^{t_1} dt_2 X_{t-t_1}^\lambda A_{01} U_{t_1-t_2}^\lambda A_{10} W_{t_2}^\lambda$$

- $A_{ij} = P_i A P_j$  splitted interaction
- $U_t^\lambda = \exp\{(Z + \lambda A_{00} + \lambda A_{11})t\}$ ,  $X_t^\lambda = P_0 U_t^\lambda$

[1] Nakajima, S., Prog. Theor. Phys. **20(6)** 948-959 (1958)

[2] Zwanzig, R, J. Chem. Phys. **33** 1338 (1960)

# The Born-Markov approximation: Davies generator

## Markovian Hypotheses (Bounds on Dyson Expansion)

$$\int_0^{\lambda^{-2\bar{\tau}}} dx \|A_{01} U_x^\lambda A_{10}\| < C, \quad |\lambda| < 1$$

$$\forall \bar{\tau} > 0, \quad \lim_{\lambda \rightarrow 0} \int_0^{\lambda^{-2\bar{\tau}}} dx \|A_{01}(U_x^\lambda - U_x)A_{10}\| = 0$$

## Davies Markovian Approximation Theorem (MAT)

- $\forall \bar{\tau} > 0 \quad \lim_{\lambda \rightarrow 0} \sup_{0 \leq t \leq \lambda^{-2\bar{\tau}}} \|W_t^\lambda - \exp\{\mathbb{L}_\lambda t\}\| = 0$
- with  $\mathbb{L}_\lambda := Z_0 + \lambda A_{00} + \lambda^2 K_D$ , and
- $K_D = \int_0^\infty dr U_{-r} A_{01} U_r A_{10}$  Davies generator
- $K_D$  well defined for arbitrary  $H_S$  spectra

[1] E. B. Davies, *Markovian Master Equations II*, Math. Ann. **219** 147-158 (1976)

# Confined Systems : Davies averaged generator<sup>1</sup>

## Time averaging map $\mathfrak{h}$

$$K^{\mathfrak{h}} = \lim_{T \rightarrow +\infty} \frac{1}{2T} \int_{-T}^T dq U_q K U_{-q}$$

Then  $\mathbb{L}_\lambda = Z_0 + \lambda^2 K_D^{\mathfrak{h}}$

- satisfies MAT iff  $K_D$  does
- incorporates Pauli Master Equation as  $[Z_0, K_D^{\mathfrak{h}}] = 0$
- describes resonances of the Liouvillian (Fermi Golden Rule)<sup>2,3</sup>
- generates a Quantum Dynamical Semigroup

but

- only if  $P_0$  is a partial trace
- only when  $A_{00} = 0$  (no average forces on the system)
- $K^{\mathfrak{h}}$  well defined only if  $Z_0$  has discrete spectrum

[1] E. B. Davies, Commun. Math. Phys. **39** 91-110 (1974)

[2] Jaksic V., Pillet C.-A., Ann. Inst. H. Poincaré Phys. Theor. **67** 425-445 (1997)

[3] Dereziński J., Jaksic V., J. Stat. Phys. **116** 411-423 (2004)



# Infinitely Extended systems : $K_D$ is the only candidate

all of  $\mathbf{R}^3$ . The Markovian limit for systems with an  $H_S$  with a discrete spectrum, is, in essence, understood, whereas the case of an  $H_S$  with a continuous spectrum still presents certain difficulties.

[1] H. Sphon, Rev. Mod. Phys. 53 3 (1980)

$K_D$  employed only under severe restrictions

ABSTRACT. — We consider a non-relativistic quantum mechanical particle in an external potential well, coupled to an infinite free quantum field. We prove rigorously that with certain cut-offs and in the weak coupling limit, the particle decays exponentially between its bound states as predicted by perturbation theory. We also prove the existence of a « dyna-

[2] E.B. Davies, Ann. Inst. Henri Poincaré 28 1 (1978)

## Why $K_D$ is so bad?

- It does not generate a proper QDS

[4] Dümmcke R and Spohn H, Z. Phys. B 34 419 (1979)

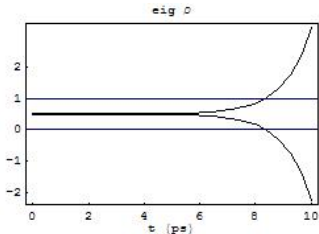
- is it really a big problem after all, or just some transient?

# Failure of $K_D$ approximation at large times

Case of a two-level quantum-dot system in a thermal bosonic environment

## One particle sector

$$\rho = \begin{pmatrix} \langle a|\rho|a\rangle & \langle a|\rho|b\rangle \\ \langle b|\rho|a\rangle & \langle b|\rho|b\rangle \end{pmatrix} = \begin{pmatrix} f_a & p \\ p^* & f_b \end{pmatrix}$$



- Very small perturbation of thermal distribution at  $t = 0$
- Characteristic interlevel splitting: 30 meV
- Very high temperatures!
- Analytically solved: divergences don't come from numerics!
- **Totally unphysical results for large times/steady states**

[1] Taj D., Iotti R.C., Rossi F., Eur. Phys. J. B **72** 3 (2009)

# The main idea : symmetry could recover probabilities

I remember once when I was in Copenhagen, that Bohr asked me what I was working on and I told him I was trying to get a satisfactory relativistic theory of the electron, and Bohr said 'But Klein and Gordon have already done that!' That answer first rather disturbed me. Bohr seemed quite satisfied by Klein's solution, but I was not because of the negative probabilities that it led to. I just kept on with it, worrying about getting a theory which would have only positive probabilities.

Conversation between Dirac and J. Mehra, March 28, 1969, quoted by Mehra in *Aspects of Quantum Theory*, ed. by A. Salam and E. P. Wigner (Cambridge University Press, Cambridge, 1972).

Figure: S. Weinberg "The Quantum Theory of fields", vol 1, Cambridge University Press (1995)

## Probabilities must be positive!

- It could help in getting a good (unique?) evolution equation
- **Hidden time symmetries in the memory kernel could imply positive probabilities!**

# The Van Hove Limit: a new approach

## The Nakajima-Zwanzig master equation

$$W_t^\lambda = X_t^\lambda + \lambda^2 \int_0^t dt_1 \int_0^{t_1} dt_2 X_{t-t_1}^\lambda A_{01} U_{t_1-t_2}^\lambda A_{10} W_{t_2}^\lambda$$

## Davies' change of variable in the integral kernel

$$\begin{pmatrix} \sigma \\ r \end{pmatrix} = \begin{pmatrix} 0 & \lambda^2 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} t_1 \\ t_2 \end{pmatrix}$$

- linear homogeneous
- $\lambda^2$  jacobian

## Our change of variable in the integral kernel

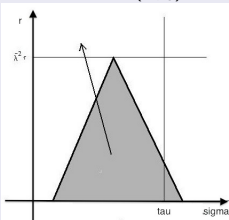
$$\begin{pmatrix} \sigma \\ r \end{pmatrix} = \begin{pmatrix} \lambda^2/2 & \lambda^2/2 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} t_1 \\ t_2 \end{pmatrix} + \begin{pmatrix} \lambda^2 q \\ 0 \end{pmatrix} \text{ for some } q \in \mathbb{R}$$

(we will remove the  $q$ -asymmetry in a second step)

# Dynamical Scattering Time $T_\lambda$

Time rescaled interaction picture:  $W_\tau^{\lambda,i} = X_{-\lambda^{-2}\tau}^\lambda W_{\lambda^{-2}\tau}^\lambda$

$$W_\tau^{\lambda,i} = 1 + \iint_{\mathcal{D}(\lambda,q)} d\sigma dr X_{-\lambda^{-2}\sigma - \frac{r}{2} - q}^\lambda A_{01} U_r^\lambda A_{10} X_{\lambda^{-2}\sigma - \frac{r}{2} + q}^\lambda W_{\sigma + \lambda^2(\frac{r}{2} + q)}^{\lambda,i}$$



- Let  $T_\lambda \approx |\lambda|^{-\xi}$ ,  $\lambda \sim 0$ ,  $0 < \xi < 2$
- e.g.  $T_\lambda = (|\lambda| \|P_0 A^2 P_0\|^{1/2})^{-1}$   
Dynamical Scattering Time

## Memory effects removal under Markovian Hypotheses

- $\xi > 0 \Rightarrow \iint_{\mathcal{D}(\lambda,q)} d\sigma dr \approx \int_0^\tau d\sigma \int_0^\infty dr e^{-(\frac{r}{2})^2 / T_\lambda^2}, \quad \lambda \sim 0$
- $\xi < 2 \Rightarrow W_{\sigma + \lambda^2(\frac{r}{2} + q)}^{\lambda,i} \approx W_\sigma^{\lambda,i}, \quad \lambda \sim 0$

# Averaging with Dynamical Scattering Time

## Averaging among our generators

$$K_{(q,T)} = \int_0^\infty dr e^{-\frac{(r/2)^2}{T^2}} U_{-\frac{r}{2}+q} A_{01} U_r A_{10} U_{\frac{r}{2}-q} = U_q K_{(0,T)} U_{-q}$$

- $\overline{\{K_{(q,T)}\}_{q \in \mathbb{R}}}$  corresponds to  $K_{(0,T)}^\natural$ : use gaussian with  $\sigma = T_\lambda$ !

## Our Dynamical Time averaged generator

$$K_T = P_0 \left\{ \int_{-\infty}^{+\infty} dt_1 \Phi(t_1) \int_{-\infty}^{t_1} dt_2 \Phi(t_2) \right\} P_0$$

$$\Phi(t) = \sqrt{\delta_T}(t) U_{-t}(A - A_{00})U_t, \quad \delta_T(t) = \frac{1}{\sqrt{2\pi}T} e^{-\frac{t^2}{2T^2}}$$

## Results under the same Markovian Hypotheses of Davies

- MAT for  $\mathbb{L}_\lambda = Z_0 + \lambda A_{00} + \lambda^2 K_{T_\lambda}$  ( $0 \leq t \leq \lambda^{-2}\bar{\tau}$ ,  $\lambda \sim 0$ )
- $\mathbb{L}_\lambda$  always well defined  $\forall \lambda \neq 0$ , independently of  $Z_0$  spectrum!
- If  $\|P_0\| = 1$  then  $\exp\{\mathbb{L}_\lambda t\}$  is a contraction!!!
- $\lim_{\bar{\tau} \rightarrow +\infty} K_{|\lambda|^{-1}\bar{\tau}} = K_D^\natural$  when  $\exists$ , recovering Davies

# $K_T$ generates a QDS on Operator Algebras

Let  $\mathcal{B}, \mathcal{B}_0$  be Operator Algebras with identity

- Let  $P_0 : \mathcal{B} \rightarrow \mathcal{B}_0$  Conditional Expectation
- Let  $P_0(i[H_\lambda, \cdot])$  generate automorphisms ( $H_\lambda = H_0 + \lambda H'$ )

"The" Quantum Fokker-Planck Equation

$$\begin{aligned} \partial_t X = & P_0(i[H_\lambda, X]) + \lambda^2 i \left[ \int \frac{d\omega}{2\pi\omega} P_0(\tilde{\mathcal{L}}_{\lambda\omega}^\dagger \tilde{\mathcal{L}}_{\lambda\omega}), X \right] \\ & - \frac{\lambda^2}{2} \{ P_0(\tilde{\mathcal{L}}_\lambda \tilde{\mathcal{L}}_\lambda), X \} + \lambda^2 P_0(\tilde{\mathcal{L}}_\lambda X \tilde{\mathcal{L}}_\lambda) \end{aligned}$$

**Dynamically Averaged Coupling**

$$\mathcal{L}_{\lambda\omega} = \int_{-\infty}^{+\infty} dt \sqrt{\delta_{T_\lambda}(t)} e^{i\omega t} U_t(H') \quad \tilde{\mathcal{L}}_{\lambda\omega} := P_1(\mathcal{L}_{\lambda\omega})$$

# A Free Quantum Particle in 3D Euclidean Space

Inelastically Coupled to a Fermionic Heat Bath

Limit Dynamics for  $H_0 = H_S \otimes 1 + 1 \otimes H_B$ ,  $H' = Q \otimes \Phi$

- $h(t) = \text{tr}[\sigma_\beta \Phi U_t(\Phi)] - \text{tr}[\sigma_\beta \Phi]^2$ , first order corrected!
- $A_{\omega,\lambda} = \int \frac{dt}{\sqrt{2\pi}} \sqrt{\delta T_\lambda}(t) e^{i\omega t} e^{iH_S t} Q e^{-iH_S t}$

$$K_{T(\lambda)} X = -2\pi i \int \frac{d\omega}{\sqrt{2\pi}} s(\omega) [A_{\omega,\lambda}^\dagger A_{\omega,\lambda}, X] \\ + 2\pi \int \frac{d\omega}{\sqrt{2\pi}} \hat{h}(\omega) \left( -\frac{1}{2} \{A_{\omega,\lambda}^\dagger A_{\omega,\lambda}, X\} + A_{\omega,\lambda}^\dagger X A_{\omega,\lambda} \right)$$

- Markovian Hypotheses verified if  $\int dt h(t)(1 + |t|^\epsilon) < \infty$
- For  $H_S = \varepsilon(P) = \frac{P^2}{2}$  in 3D,  $\langle p|Q|p' \rangle = q(\varepsilon_p, \varepsilon_{p'})$ ,  $q \in S(\mathbb{R}^2)$ , there  $\exists L$  s.t.  $\|T(\lambda)K_{T(\lambda)} - L\| \rightarrow 0$ , and  $[Z_0, L] = 0$ .
- Thermal distributions of observables affiliated to  $H_S$  are stationary under  $L$  if furthermore  $\hat{h} \in S(\mathbb{R})$ .
- I found a Pauli Equation with FGR **conditionally on  $\rho_S = \rho_\beta \dots$**



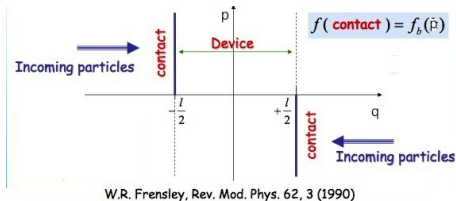
# Summary of this section

**Abstract.** We study the van Hove limit for master equations on a Banach space, and propose a contraction semigroup as limit dynamics. The generator has a Lindblad form if specialized to  $C^*$ -algebras, is always well defined irrespectively of the subsystem spectrum, includes first-order contributions, and returns Davies averaged generator, when the latter is defined. The theory is applied to the case of a free particle in contact with a heat bath.

[1] Taj D., Ann. Henri Poincaré Online First (2010)

# Time Independent Mesoscopic Quantum Transport

A device modelling approach



158 12. Transport in Mesoscopic Semiconductor Structures

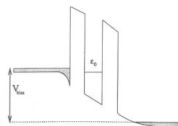


Fig. 12.1. Double-barrier semiconductor heterostructure biased close to resonance, where charge carriers emerging from the source contact are matched to the energy of the quasi-bound state  $\epsilon_0$  in the quantum well. Occupied contact states are shown as hatched, and the band bending is due to charge accumulation or depletion

## Some Existing Models in Perpendicular Quantum Transport

- Landauer-Buttiker<sup>1</sup> : NESS I-V
- Quantum Kinetics (Haug, Jauho) : quantum truncation.
- Lattice models (Datta) : atomistic devices

[1] W. Aschbacher, V. Jaksic, Y. Pautrat, C.-A. Pillet, J. Math. Phys. **48** 032101-032129 (2007)

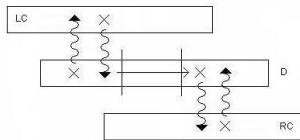
## Want

- Full space and time resolution of charge density in device
- Boltzmann Transport Eq. with Up-wind BC's as  $\hbar \rightarrow 0$

# Quantum Transport: our model (1)

## Physical ideas

- LC, RC, D all infinitely extended: **quantum non-locality**
- LC-D and RC-D **interactions spatially localized**



## Physical Subsystem

- $\mathcal{F} = \mathcal{F}_l \otimes \mathcal{F}_d \otimes \mathcal{F}_r$
- $\langle O_l \otimes O_d \otimes O_r \rangle = \text{Tr}[\bar{\sigma}_l O_l] \text{Tr}[\bar{\sigma}_r O_r] O_d$

## Spatial locality: interaction implemented

- $H'_z = \int C_z(x) \Psi_z^\dagger(x) \Psi_d(x) dx + h.c., \quad (z = l, r)$
- e.g.  $C_l(x) = \theta(-(x + l/2))$ ,  $C_r(x) = \theta(x - l/2)$

# Quantum Transport: our model (2)

## Limit dynamics: the many body equation

$$\partial_t X = i[H_d, X] + \lambda^2 \int dk g_z^\pm(k) \left( i \left[ \int \frac{d\omega}{2\pi\omega} a^\pm(\Psi_{k\omega}^z) a^\mp(\Psi_{k\omega}^z), X \right] - \frac{1}{2} \{ a^\pm(\Psi_k^z) a^\mp(\Psi_k^z), X \} + a^\pm(\Psi_k^z) X a^\mp(\Psi_k^z) \right)$$

- **Fermi-Dirac**  $f_{\beta\mu}^z$ ,  $g_z^+ = f_{\beta\mu}^z$ ,  $g_z^- = 1 - f_{\beta\mu}^z$
- **Scattering probability amplitude**

$$\Psi_{k,\omega}^z(k') = \sqrt{\delta\bar{\omega}_\lambda} (\omega_k^z - \omega_{k'}^d - \omega) \hat{C}_z(k, k')$$

- **Excellent physical interpretation, and exactly solvable!**
- **Gaussian states are invariant**  
 $\omega_G(a^\dagger(f_1) \cdots a^\dagger(f_n) a(g'_n) \cdots a(g_1)) = \delta_{n,n'} \det \langle f_i, G g_j \rangle$
- **G** obeys an associated **closed linear equation**

# A Wigner Transport Equation (WTE) for a free device

## The (improper) Wigner Function on the "classical" phase space

- Classical picture : density  $f(q, p)$
- Quantum picture :  $f(q, p) = \int \frac{dr}{2\pi} e^{ipr} \langle q + \frac{r}{2} | G | q - \frac{r}{2} \rangle$

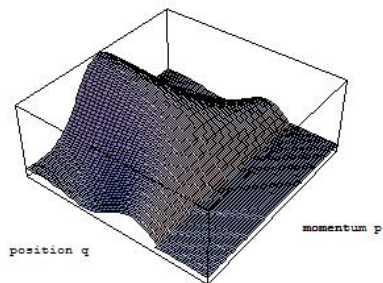
For a free device  $\hbar_d = \frac{p^2}{2m}$ , the Eq. for  $G$  becomes

$$\text{WTE} \quad \partial_t f = -p \partial_q f - \frac{1}{2} \{L^\lambda, f\}_{\star_\hbar} + S^\lambda$$

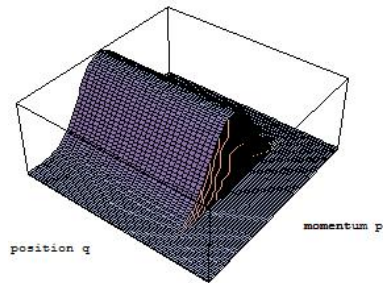
- $L_l^\lambda(q, p) = L_l^\lambda(q) = \sqrt{2\pi}\lambda^2 T(\lambda) \theta[-(q + l/2)]$
- $S_l^\lambda(q, p) = L_l^\lambda(q) \int \frac{dp'}{\pi} f_{\beta\mu}^l(p') \frac{1}{\Delta p(q)} \text{sinc}\left(\frac{p-p'}{\Delta p(q)}\right)$
- $\Delta p(q) = \frac{\hbar}{2|q+l/2|}$ 
  - $\Rightarrow$  classical scheme recovered for  $\hbar \rightarrow 0!$
  - $\Rightarrow$  classical scheme recovered for  $q \rightarrow \pm\infty!$
  - $\Rightarrow$  Heisenberg principle appears very naturally!

# A Wigner Transport Equation (WTE) for a free device

Quantum source



Classical Source



- $S_l^\lambda(q, p) = L_l^\lambda(q) \int \frac{dp'}{\pi} f_{\beta\mu}^l(p') \frac{1}{\Delta p(q)} \text{sinc} \left( \frac{p-p'}{\Delta p(q)} \right)$
- $\Delta p(q) = \frac{\hbar}{2} \frac{1}{|q+l/2|}$ 
  - $\Rightarrow$  classical scheme recovered for  $\hbar \rightarrow 0$ !
  - $\Rightarrow$  classical scheme recovered for  $q \rightarrow \pm\infty$ !
  - $\Rightarrow$  Heisenberg principle appears very naturally!

# Summary of this section

We have proposed a WTE for mesoscopic time independent quantum transport (Quantum Collisionless Boltzmann Equation)

$$\partial_t f = -p \partial_q f - \frac{1}{2} \{L^\lambda, f\}_{\star_\hbar} + S^\lambda$$

Although still preliminary, our WTE

- is physically robust (guarantees positivity at all times)
- it's classical limit is a well known PDE (Collisionless Boltzmann Equation) with appropriate (Up-wind) BC's
- it's a limit dynamics of the exact hamiltonian evolution
- fully embodies quantum uncertainty principles
- the solution offers a full space and time resolution of device
- phonons and nonzero average forces could be accounted for...

# Quantum Brownian Motion

Einstein's kinetic theory of the Brownian motion, based upon light water molecules continuously bombarding a heavy pollen, provided an explanation of diffusion from the Newtonian mechanics. Since the discovery of quantum mechanics it has been a challenge to verify the emergence of diffusion from the Schrödinger equation.

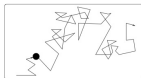


Figure 1: Brown's picture under the microscope

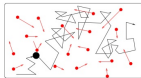


Figure 2: Einstein's explanation to Brown's picture

	CLASSICAL MECHANICS	QUANTUM MECHANICS
Stochastic dynamics (no memory)	Random walk (Wiener)	Random kick model with zero time corr. potential (Pillet, Schenker-Kang)
Hamiltonian particle in a random environment (one body)	Lorentz gas: particle in random scatterers (Kesten-Papanicolaou) (Komorowski-Ryzhik)	Anderson model or quantum Lorentz gas (Spohn, Erdős-Yau, Erdős-Salmhofer-Yau Disertori-Spencer-Zirnbauer)
Hamiltonian particle in a heat bath (randomness in the many-body data)	Einstein's kinetic model (Dürr-Goldstein-Lebowitz)	Electron in phonon or photon bath (Erdős, Erdős-Adami, Spohn-Lukkarinen De Roeck-Fröhlich)
Periodic Lorentz gas (randomness in the one-body initial data)	Sinai billiard (Bunimovich-Sinai)	Ballistic (Bloch waves, easy)
Many-body interacting Hamiltonian	Nonlinear Boltzmann eq (short time: Lanford)	Quantum NL Boltzmann (unsolved)

[1] L. Erdos, Lecture notes on Quantum Brownian Motion, Les Houches Summer School (2010)



# The diffusion constant

Heuristically, for  $N \gg 0$  interactions

- $(\delta x) \sim \sqrt{N}$
- $N \sim t$

$$(\delta x)^2 = D t, \quad t \rightarrow \infty$$

## Low relative momenta

$$\langle X^2 \rangle_\rho(t) = \text{tr}(\rho(t) X^2) = \int dp \partial_r^2 [\rho_r](t)|_{r=0}(p)$$

- $[\rho_r](t)(p) := \langle p - \frac{r}{2} | \rho(t) | p + \frac{r}{2} \rangle$
- $r$ : **relative momentum**

$\Rightarrow$  Only low relative momenta matter : need  $[\rho_r]$  up to  $o(r^2)$

# A Translation Invariant Model

## Model Hamiltonian for a Quantum Particle in $\mathbb{R}^d$

- $H_0 = \epsilon(P) \otimes 1 + 1 \otimes \int dq \, \omega_q b_q^\dagger b_q$
- $H' = \int dp_1 dp_2 dq \, |p_1\rangle\langle p_2| \otimes b_q \, \phi(q) \delta(p_1 - p_2 - q) + h.c.$

## Relative Momenta Fibration of the Limit Dynamics

$$\partial_t[\rho]_r = L_r^\lambda [\rho]_r$$

- $\{f(P)\}$  is **left invariant** under  $K_{T(\lambda)}$
- The zero fiber is the Pauli Equation

$$\partial_t f(p) = \lambda^2 \int dp' \, \{m(p, p') f(p') - m(p', p) f(p)\}$$

- with FGR transition rates

$$\begin{aligned} m(p, p') &= \{ |\phi(p - p')|^2 N_{p-p'} \delta(\epsilon_p - \epsilon_{p'} - \omega_{p-p'}) \\ &\quad + |\phi(p' - p)|^2 (1 + N_{p-p'}) \delta(\epsilon_{p'} - \epsilon_p - \omega_{p'-p}) \} \end{aligned}$$

# Summary and Conclusions

## Generalised Van Hove Limit

We studied weakly perturbed projected one-parameter group of isometries. We have found a generator that

- satisfies MAT in the Van Hove Limit under Davies markovian hypotheses
- is always well defined, independently of subsystems details
- generates contractions and a QDS in operator algebras
- generalizes Davies generator

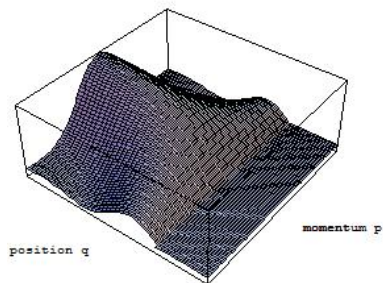
It furnishes a way to understand infinite open systems such as

- A free particle in 3D locally coupled to a fermionic heath bath
- Nanodevices (Quantum Collisionless Boltzmann Equation)
- A free particle in 3D non-locally coupled to bosonic bath?

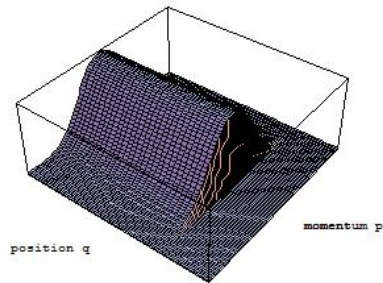


# A Wigner Transport Equation (WTE) for a free device

Quantum source



Classical Source



- $S_l^\lambda(q, p) = L_l^\lambda(q) \int \frac{dp'}{\pi} f_{\beta\mu}^I(p') \frac{1}{\Delta p(q)} \text{sinc} \left( \frac{p-p'}{\Delta p(q)} \right)$
- $\frac{1}{2}(L_l^\lambda \star_{\hbar} f + f \star_{\hbar} L_l^\lambda)(q, p) = L_l^\lambda(q) \int \frac{dp'}{\pi} f(q, p') \frac{1}{\Delta p(q)} \text{sinc} \left( \frac{p-p'}{\Delta p(q)} \right)$

$\Rightarrow$  with only left reservoir, say,  $f(q, p) = f_{\beta\mu}^I$  is stationary!