Heavy flavor transport in heavy-ion collisions

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Heavy-ion collisions: a cartoon of space-time evolution



- Soft probes (low-p_T hadrons): collective behavior of the medium;
- Hard probes (high-p_T particles, heavy quarks, quarkonia): produced in hard pQCD processes in the initial stage, allow to perform a tomography of the medium

A medium displaying a collective behavior



$$(\epsilon + P)\frac{dv^{i}}{dt} \underset{v \ll c}{=} -\frac{\partial P}{\partial x^{i}}$$

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NB picture relying on the condition $\lambda_{
m mfp} \ll L$

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A medium inducing energy-loss to colored probes



Strong unbalance of di-jet events, visible at the level of the event-display itself, without any analysis: jet-quenching

Little Bang vs Big Bang



Both systems undergo a sort of Hubble-law expansion, BUT compare the expansion rates:

• Radiation-dominated universe

$$a \sim t^{1/2} \longrightarrow \dot{a} \sim \frac{1}{2} a^{-1/2} \quad H \equiv \frac{\dot{a}}{a} = \frac{1}{2t} \sim 10^6 \, \mathrm{s}^{-1}$$

• QGP in HIC's undergoing longitudinal expansion $v^z = z/t$

$$heta \equiv \partial_\mu u^\mu \mathop{\sim}\limits_{z
ightarrow 0} rac{1}{t} \sim 10^{22}\,{
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- Description of jet-quenching based on energy-degradation of external probes (high-p_T partons): opacity of the medium;
- Description of heavy-flavour observables requires to employ/develop a setup (transport theory) allowing to deal with more general situations and in particular to describe how particles would (asymptotically) approach equilibrium.

A realistic study requires developing *a multi-step setup*:

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 - However, a source of systematic uncertainty for studies of parton-medium interaction;
- Hadronic rescattering (e.g. Dπ → Dπ), from effective Lagrangians, but no experimental data the on relevant cross-sections

The initial hard production and the pp baseline



- A convenient automated tool to simulate the initial QQ production (the POWHEG-BOX package¹) interfaces the output of a NLO event-generator for the hard process with a parton-shower describing the Initial and Final State Radiation and modeling other non-perturbative processes (intrinsic k_T, MPI, hadronization)
- This provides a fully exclusive information on the final state

¹Alioli et al., JHEP 1006 (2010) 043

pp collisions: just a no final-state effect baseline?



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A pp collision involves multiple partonic interactions:

- No rescattering?
- No closer opposite color-charge to recombine with?

The rate of approach of HQ's to chemical equilibrium is given $\ensuremath{\text{by}}^2$

$$\Gamma_{\rm chem} \underset{M \gg T}{\approx} \frac{g^4 C_F}{8\pi M^2} \left(2C_F - \frac{N_c}{2} + N_f \right) \left(\frac{MT}{2\pi} \right)^{3/2} e^{-M/T}$$

At the initial $T_0 \approx 0.5$ GeV one gets for charm $\Gamma_{\rm chem} \approx 0.015$ fm⁻¹, i.e. $\tau_{\rm chem} \approx 65$ fm/c,

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$$H = 1/2t \approx 10^{-18} \text{fm}^{-1} \longrightarrow \Gamma_{\text{chem}} \gg H$$

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HQ's, in chemical equilibrium in the plasma filling the early universe, are out of chemical equilibrium in HIC's.

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Employing as an estimate for the temperature evolution the Bjorken-flow result

$$T(\tau) = T_0 \left(\frac{\tau_0}{\tau}\right)^{1/3}$$

one gets that $\Gamma_{\rm chem} \ll \Gamma_{\rm exp}$ during the whole fireball evolution

Rapidity density of $Q\overline{Q}$ pairs in AA collisions estimated rescaling the pp result by the number of binary nucleon-nucleon collisions



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For 0-5% most central Pb-Pb collisions at the LHC one gets³



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$$\frac{dN^{QQ}}{dy} = \underbrace{\langle N_{\rm coll} \rangle}_{\rm Glauber} \underbrace{\frac{1}{\sigma^{\rm in}} \frac{d\sigma^{QQ}}{dy}}_{\rm pQCD}$$

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$$\left. \frac{dN^{c\overline{c}}}{dy} \right|_{y=0} \approx 12.3 \quad \text{and} \quad \left. \frac{dN^{b\overline{b}}}{dy} \right|_{y=0} \approx 0.79$$

The initial ($\tau_0 \approx 0.5 \text{ fm/c}$, $T_0 \approx 0.5 \text{ GeV}$) density given by pQCD and at equilibium is ($d\vec{x} = d\vec{x}_{\perp}\tau_0 dy$)

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$$n_{\rm pQCD}^{c\overline{c}} \approx 0.179 \,\text{fm}^{-3} \quad \text{vs} \quad n_{\rm therm}^{c\overline{c}} \approx 1.539 \,\text{fm}^{-3}$$
$$n_{\rm pQCD}^{b\overline{b}} \approx 0.011, \,\text{fm}^{-3} \quad \text{vs} \quad n_{\rm therm}^{c\overline{c}} \approx 0.012 \,\text{fm}^{-3}$$

One has:

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HQ number is conserved during the evolution: at hadronization charm is overpopulated with respect to the other hadrons at chemical equilibrium (figure from A. Andronic et al., Phys.Lett. B797 (2019) 134836), although at the beginning it is underpopulated

Theory and experimental verification of brownian motion by Einstein (1905) and Perrin (1909) From the vertical distribution of an emulsion

$$n(z) = n_0 e^{-(M^*g/K_BT)z}$$



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imposing the balance between gravity current (from top to bottom)

$$j^{z}_{
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 $D_s = \frac{K_B T}{6\pi a \eta}$

One gets an expression for the diffusion coefficient





From the random walk of the emulsion particles (follow the motion along one direction!) one extracts the diffusion coefficient

$$\langle x^2
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and from Einstein formula one estimates the Avogadro number:

$$\mathcal{N}_A K_B \equiv \mathcal{R} \longrightarrow \mathcal{N}_A = \frac{\mathcal{R} T}{6\pi a \eta D_s}$$

Perrin obtained the values $N_A \approx 5.5 - 7.2 \cdot 10^{23}$.
What do we want to learn? A bit of history...



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Perrin obtained the values $N_A \approx 5.5 - 7.2 \cdot 10^{23}$. We would like to derive HQ transport coefficients in the QGP with a comparable precision and accuracy!

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Hydrodynamic (macroscopic) approach to diffusion

Combining Fick's law and particle-number conservation one gets the diffusion equation

$$\vec{j} = -D_s \vec{\nabla} n, \quad \partial_t n + \vec{\nabla} \cdot \vec{j} = 0 \quad \longrightarrow \quad \partial_t n - D_s \nabla^2 n = 0$$

It is convenient to solve the equation in Fourier space, where

$$n(t,x) = \int \frac{dk}{2\pi} e^{ikx} \tilde{n}(t,k) \longrightarrow \partial_t \tilde{n}(t,k) + D_s k^2 \tilde{n}(t,k) = 0$$

whose solution is

$$\tilde{n}(t,k) = \tilde{n}(0,k)e^{-D_sk^2t}$$

Assuming all particles initially at the origin, $n(0,x) = N_0\delta(x) \longrightarrow \tilde{n}(0,k) = N_0$, one gets

$$n(t,x) = N_0 \int \frac{dk}{2\pi} e^{ikx} e^{-D_s k^2 t} \quad \longrightarrow \quad \left| n(t,x) = N_0 \left(\frac{1}{4\pi D_s t} \right)^{1/2} e^{-x^2/4D_s t} \right|$$

from which it follows that $\langle x^2 \rangle = 2D_s t$

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We do not have a microscope!



Transport coefficients can be accessed indirectly, comparing transport predictions with different values of momentum broadenig

$$c = \frac{2T^2}{D_s}$$

with experimental results for momentum (left) and angular (right) HF particle distributions



Still far from accuracy and precision of Perrin result for \mathcal{N}_A ...

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- hadronization (impossible to neglect)
 - source of systematic uncertainty in extracting transport coefficients;
 - an issue of interest in itself: how quark \rightarrow hadron transition changes in the presence of a medium (addressed in the following)

Transport (microscopic) approach to diffusion: Boltzmann equation

Time evolution of HQ phase-space distribution $f_Q(t, x, p)$:

 $\frac{d}{dt}f_Q(t, \boldsymbol{x}, \boldsymbol{p}) = C[f_Q]$

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• Total derivative along particle trajectory

$$\frac{d}{dt} \equiv \frac{\partial}{\partial t} + \mathbf{v} \frac{\partial}{\partial \mathbf{x}} + \mathbf{F} \frac{\partial}{\partial \mathbf{p}}$$

Neglecting *x*-dependence and mean fields: $\partial_t f_Q(t, \mathbf{p}) = C[f_Q]$

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• Collision integral:

$$C[f_Q] = \int d\mathbf{k} [\underbrace{w(\mathbf{p} + \mathbf{k}, \mathbf{k}) f_Q(\mathbf{p} + \mathbf{k})}_{\text{gain term}} - \underbrace{w(\mathbf{p}, \mathbf{k}) f_Q(\mathbf{p})}_{\text{loss term}}]$$

 $w(\pmb{p}, \pmb{k})$: HQ transition rate $\pmb{p} \rightarrow \pmb{p} - \pmb{k}$

From Boltzmann to Fokker-Planck

Expanding the collision integral for *small momentum exchange*⁴ (Landau)

$$C[f_Q] \approx \int d\mathbf{k} \left[k^i \frac{\partial}{\partial p^i} + \frac{1}{2} k^i k^j \frac{\partial^2}{\partial p^i \partial p^j} \right] [w(\mathbf{p}, \mathbf{k}) f_Q(t, \mathbf{p})]$$

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$$\frac{\partial}{\partial t}f_{Q}(t,\boldsymbol{p})=\frac{\partial}{\partial p^{i}}\left\{A^{i}(\boldsymbol{p})f_{Q}(t,\boldsymbol{p})+\frac{\partial}{\partial p^{j}}[B^{ij}(\boldsymbol{p})f_{Q}(t,\boldsymbol{p})]\right\}$$

where

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Problem reduced to the *evaluation of three transport coefficients*, directly derived from the scattering matrix

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Approach to equilibrium in the FP equation

The FP equation can be viewed as a continuity equation for the phase-space distribution of the kind $\partial_t \rho(t, \vec{p}) + \vec{\nabla}_{\rho} \cdot \vec{J}(t, \vec{p}) = 0$

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admitting a steady solution $f_{eq}(p) \equiv e^{-E_p/T}$ when the current vanishes:

$$\mathcal{A}^i(ec{p}) f_{ ext{eq}}(p) = -rac{\partial B^{ij}(ec{p})}{\partial p^j} f_{ ext{eq}}(p) - B^{ij}(oldsymbol{p}) rac{\partial f_{ ext{eq}}(p)}{\partial p^j}.$$

Approach to equilibrium in the FP equation

The FP equation can be viewed as a continuity equation for the phase-space distribution of the kind $\partial_t \rho(t, \vec{p}) + \vec{\nabla}_{\rho} \cdot \vec{J}(t, \vec{p}) = 0$

$$\frac{\partial}{\partial t}\underbrace{f_Q(t,\boldsymbol{p})}_{\equiv\rho(t,\vec{p})} = \frac{\partial}{\partial \boldsymbol{p}^i}\underbrace{\left\{A^i(\boldsymbol{p})f_Q(t,\boldsymbol{p}) + \frac{\partial}{\partial \boldsymbol{p}^j}[B^{ij}(\boldsymbol{p})f_Q(t,\boldsymbol{p})]\right\}}_{\equiv -J^i(t,\vec{p})}$$

admitting a steady solution $f_{eq}(p) \equiv e^{-E_p/T}$ when the current vanishes:

$$\mathcal{A}^i(ec{p}) f_{ ext{eq}}(p) = -rac{\partial B^{ij}(ec{p})}{\partial p^j} f_{ ext{eq}}(p) - B^{ij}(oldsymbol{p}) rac{\partial f_{ ext{eq}}(p)}{\partial p^j}.$$

One gets

$$A(p)p^{i}=rac{B_{1}(p)}{TE_{p}}p^{i}-rac{\partial}{\partial p^{j}}\left[\delta^{ij}B_{0}(p)+\hat{p}^{i}\hat{
ho}^{j}(B_{1}(p)-B_{0}(p))
ight],$$

leading to the relativistic generalization of the Einstein fluctuation-dissipation relation

$$A(p) = \frac{B_1(p)}{TE_p} - \left[\frac{1}{p}\frac{\partial B_1(p)}{\partial p} + \frac{d-1}{p^2}(B_1(p) - B_0(p))\right],$$

quite involved due to the *momentum dependence* of the transport coefficients (*measured* HQ's are relativistic particles!)

Fokker-Planck equation: non-relativistic solution

• Ignoring the momentum dependence of the transport coefficients $\gamma \equiv A(p)$ and $D \equiv B_0(p) = B_1(p)$ the FP equation reduces to

$$\frac{\partial}{\partial t}f_Q(t,\boldsymbol{p}) = \gamma \frac{\partial}{\partial p^i}[p^i f_Q(t,\boldsymbol{p})] + D \nabla_p^2 f_Q(t,\boldsymbol{p})$$

• Starting from the *initial condition* $f_Q(t=0, \mathbf{p}) = \delta(\mathbf{p} - \mathbf{p}_0)$ one gets

$$f_Q(t, \boldsymbol{p}) = \left(\frac{\gamma}{2\pi D[1 - \exp(-2\gamma t)]}\right)^{3/2} \exp\left[-\frac{\gamma}{2D} \frac{[\boldsymbol{p} - \boldsymbol{p}_0 \exp(-\gamma t)]^2}{1 - \exp(-2\gamma t)}\right]$$

• Asymptotically the solution *forgets about the initial condition* and tends to a thermal distribution

$$f_Q(t, \boldsymbol{p}) \underset{t \to \infty}{\sim} \left(rac{\gamma}{2\pi D}
ight)^{3/2} \exp \left[- \left(rac{\gamma M_Q}{D}
ight) rac{\boldsymbol{p}^2}{2M_Q}
ight]$$

 $\longrightarrow D = M_Q \gamma T$: Einstein fluctuation-dissipation relation

Fokker-Planck solution: physical meaning

$$f_Q(t, \boldsymbol{p}) = \left(\frac{\gamma}{2\pi D[1 - \exp(-2\gamma t)]}\right)^{3/2} \exp\left[-\frac{\gamma}{2D} \frac{[\boldsymbol{p} - \boldsymbol{p}_0 \exp(-\gamma t)]^2}{1 - \exp(-2\gamma t)}\right]$$

From the first moments of the momentum distribution...

$$\langle {m
ho}(t)
angle = {m
ho}_0 \, e^{-{m \gamma} t}$$

 $\gamma:$ friction coefficient

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 $\langle \boldsymbol{p}^2(t) \rangle - \langle \boldsymbol{p}(t) \rangle^2 = rac{3D}{\gamma} \left(1 - e^{-2\gamma t} \right) \underset{t \to 0}{\sim} 6Dt$ $\sim t \to \infty 3MT$ equipartition theorem

D: momentum-diffusion coefficient

Ex: derive the above results. Trivial, after setting

$$\boldsymbol{p} = \left(\boldsymbol{p} - \boldsymbol{p}_0 e^{-\gamma t}\right) + \boldsymbol{p}_0 e^{-\gamma t}$$

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The relativistic Langevin equation

The Fokker-Planck equation can be recast into a form suitable to follow the dynamics of each individual quark arising from the pQCD Monte Carlo simulation of the initial $Q\overline{Q}$ production: the Langevin equation



with the properties of the noise encoded in

$$\langle \xi^{i}(\boldsymbol{p}_{t}) \rangle = 0 \quad \langle \xi^{i}(\boldsymbol{p}_{t}) \xi^{j}(\boldsymbol{p}_{t'}) \rangle = b^{ij}(\boldsymbol{p}) \frac{\delta_{tt'}}{\Delta t} \quad b^{ij}(\boldsymbol{p}) \equiv \kappa_{L}(p) \hat{p}^{i} \hat{p}^{j} + \kappa_{T}(p) (\delta^{ij} - \hat{p}^{i} \hat{p}^{j})$$

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Transport coefficients related to the FP ones (derivation in the following slides):

• Momentum diffusion:

$$\kappa_{T}(p) = 2B_{0}(p) = \frac{1}{2} \frac{\langle \Delta p_{T}^{2} \rangle}{\Delta t} \quad \text{and} \quad \kappa_{L}(p) = 2B_{1}(p) = \frac{\langle \Delta p_{L}^{2} \rangle}{\Delta t}$$

• Friction term, in the Ito pre-point discretization scheme,

$$\eta_D^{\mathrm{Ito}}(p) = A(p) = \frac{B_1(p)}{TE_p} - \left[\frac{1}{p}\frac{\partial B_1(p)}{\partial p} + \frac{d-1}{p^2}(B_1(p) - B_0(p))\right]_{\text{constrained}} = 0$$

Numerical implementation

Introduce the tensor

$$\begin{array}{lll} C^{ij}(\boldsymbol{p}) &\equiv& \sqrt{\kappa_L(\boldsymbol{p})}\hat{\boldsymbol{p}}^i\hat{\boldsymbol{p}}^j + \sqrt{\kappa_T(\boldsymbol{p})}(\delta^{ij} - \hat{\boldsymbol{p}}^i\hat{\boldsymbol{p}}^j) \\ &\equiv& \sqrt{\kappa_L(\boldsymbol{p})}P_L^{ij} + \sqrt{\kappa_T(\boldsymbol{p})}P_T^{ij} \end{array}$$

and redefine the noise variable as

$$\xi^i \equiv C^{ik}(\boldsymbol{p}) rac{1}{\sqrt{\Delta t}} \zeta^k \quad ext{with} \quad \langle \zeta^k(t_n)
angle = 0 \quad ext{and} \quad \langle \zeta^k(t_n) \zeta^l(t_m)
angle = \delta_{mn} \delta^{kl}.$$

The Langevin equation becomes then

$$\Delta p^{i} = -\eta_{D}(p)p^{i}\Delta t + C^{ik}(p + \xi \Delta p)\sqrt{\Delta t} \zeta^{k},$$

where, for the sake of generality, the argument of the strength of the noise term can be evaluated ($\xi \in [0, 1]$) at any point in the interval $[\mathbf{p}, \mathbf{p} + \Delta \mathbf{p}]$. In the following we will consider the cases $\xi = 0$ (Ito *pre-point* scheme) and $\xi = 1$ (*post-point* scheme).

The link with the Fokker-Plank equation

Consider an arbitrary function of the HQ momentum $g(\mathbf{p})$ and take the expectation value over the thermal ensemble of its variation, keeping only terms up to order Δt :

$$\langle g(\boldsymbol{p} + \Delta \boldsymbol{p}) - g(\boldsymbol{p}) \rangle = \left\langle \frac{\partial g}{\partial p^i} \Delta p^i + \frac{1}{2} \frac{\partial^2 g}{\partial p^i \partial p^j} \Delta p^i \Delta p^j \right\rangle + \dots$$

From

$$\Delta p^{i} = -\eta_{D}(p)p^{i}\Delta t + C^{ik}(p + \xi \Delta p)\sqrt{\Delta t} \zeta^{k}, \quad \langle \zeta^{k}
angle = 0, \quad \langle \zeta^{k} \zeta^{l}
angle = \delta^{kl}$$

one gets:

$$\langle g(\boldsymbol{p} + \Delta \boldsymbol{p}) - g(\boldsymbol{p}) \rangle = \left\langle \frac{\partial g}{\partial p^{i}} \left(-\eta_{D} \boldsymbol{p}^{i} + \xi \frac{\partial C^{ik}}{\partial p^{j}} C^{jk} \right) + \frac{1}{2} \frac{\partial^{2} g}{\partial p^{i} \partial p^{j}} C^{ik} C^{jk} \right\rangle \Delta t + \dots$$

In the above the expectation value is taken accorrding to the HQ phase-space distribution

$$\langle g(\boldsymbol{p})
angle_t \equiv \int d\boldsymbol{p} \, g(\boldsymbol{p}) f(t, \boldsymbol{p})$$

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The link with the Fokker-Plank equation

Time evolution given be the differential equation

$$\frac{d}{dt}\langle g(\boldsymbol{p})\rangle_t \equiv \int d\boldsymbol{p} g(\boldsymbol{p}) \frac{\partial}{\partial t} f(t, \boldsymbol{p})$$

Integrating by parts:

$$LHS = \int d\mathbf{p} \, \mathbf{g}(\mathbf{p}) \left\{ \frac{\partial}{\partial p^{i}} \left[\left(\eta_{D} p^{i} - \xi \frac{\partial C^{ik}}{\partial p^{j}} C^{jk} \right) f(t, \mathbf{p}) \right] + \frac{1}{2} \frac{\partial^{2}}{\partial p^{i} \partial p^{j}} \left[\left(C^{ik} C^{jk} \right) f(t, \mathbf{p}) \right] \right]$$

Comparing with the FP equation

$$\frac{\partial}{\partial t}f_{Q}(t,\boldsymbol{p})=\frac{\partial}{\partial p^{i}}\left[A^{i}(\boldsymbol{p})f_{Q}(t,\boldsymbol{p})\right]+\frac{\partial}{\partial p^{i}\partial p^{j}}\left[B^{ij}(\boldsymbol{p})f_{Q}(t,\boldsymbol{p})\right]$$

one gets

$$\begin{aligned} A^{i}(\boldsymbol{p}) &\equiv A(\boldsymbol{p})\boldsymbol{p}^{i} = \eta_{D}\boldsymbol{p}^{i} - \xi \frac{\partial C^{ik}}{\partial \boldsymbol{p}^{j}} C^{jk} \\ C^{ij}(\boldsymbol{p}) &\equiv \sqrt{\kappa_{L}(\boldsymbol{p})} P_{L}^{ij} + \sqrt{\kappa_{T}(\boldsymbol{p})} P_{T}^{ij} = \sqrt{2B_{1}(\boldsymbol{p})} P_{L}^{ij} + \sqrt{2B_{0}(\boldsymbol{p})} P_{T}^{ij} \end{aligned}$$

The transport coefficients describing momentum-diffusion in the Langevin equation *always* coincide with the corresponding ones in the Fokker-Planck equation, no matter which discretization scheme is employed. In general, this is not the case for the friction term. From

$$\eta_D(p)p^i = A(p)p^i + \frac{\xi}{\partial p^i}C^{jk}$$

one gets

$$\eta_D(p) = A(p) + \frac{\xi}{p} \left[\frac{1}{p} \frac{\partial B_1}{\partial p} + \frac{d-1}{p^2} \sqrt{2B_0(p)} (\sqrt{2B_1(p)} - \sqrt{2B_0(p)}) \right]$$

where, furthermore, A(p), $B_0(p)$ and $B_1(p)$ are related by the Einstein relation.

Actually, in the Ito *pre-point* scheme $\xi = 0$, so that the friction coefficients appearing in the FP and Langevin equations are the same: $A(p) = \eta_D^{\text{pre}}(p)$. Furthermore, in order to approach thermal equilibrium, the Einstein relation must be satisfied:

$$\eta_D^{\text{pre}}(p) = \mathcal{A}(p) = \frac{B_1(p)}{TE_p} - \left[\frac{1}{p}\frac{\partial B_1(p)}{\partial p} + \frac{d-1}{p^2}(B_1(p) - B_0(p))\right]$$

NB: A(p), $B_0(p)$ and $B_1(p)$ can be calculated from the scattering matrix. However, since the Einstein relation must satisfied, one has to calculate only two of them and fix the last one through the above equation

Asymptotic approach to thermalization



Validation of the model (figures adapted from Federica Capellino master thesis):

- Left panel: evolution in a static medium
- Right panel: decoupling from expanding medium at $T_{\rm FO}\!=\!160$ MeV

For late times or very large transport coefficients HQ's approach local kinetic equilibrium with the medium. For an expanding medium high- p_T tail remains off equilibrium.

From momentum broadening to spatial diffusion (I)

Start from the NR Langevin equation along x-direction

$$x_{t+1} = x_t + \frac{p_t}{M} \Delta t , \quad p_{t+1} = p_t - \eta_D p_t \Delta t + \xi_t \Delta t , \quad \langle \xi_t \xi_{t'} \rangle = \frac{\delta_{tt'}}{\Delta t} \kappa$$

From momentum broadening to spatial diffusion (I)

Start from the NR Langevin equation along x-direction

$$x_{t+1} = x_t + \frac{p_t}{M} \Delta t$$
, $p_{t+1} = p_t - \eta_D p_t \Delta t + \xi_t \Delta t$, $\langle \xi_t \xi_{t'} \rangle = \frac{\delta_{tt'}}{\Delta t} \kappa$

Study how a local excess of particles diffuses after N time-steps Δt :

$$P(\Delta x, N\Delta t) = \int \prod_{i=0}^{N} dp_i W[p_0, p_1, ..., p_N] \delta\left(\Delta x - \sum_{i=0}^{N-1} \frac{p_i}{M} \Delta t\right)$$

From momentum broadening to spatial diffusion (I)

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$$x_{t+1} = x_t + \frac{p_t}{M} \Delta t$$
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Probability for the sequence of momenta $[p_0, p_1, ..., p_N]$ obtained from the product of conditional probabilities, i.e.

$$W[p_0, p_1] = P(p_1|p_0)P(p_0),$$

where, the noise following a Gaussian distribution,

$$P(p_{0}) = \frac{e^{-p_{0}^{2}/2MT}}{(2\pi MT)^{1/2}}, \quad P(p_{1}|p_{0}) = \int d\xi \underbrace{\delta[p_{1} - (p_{0} - \eta_{D}p_{0}\Delta t + \xi\Delta t)]}_{\frac{1}{\Delta t}\delta[\xi - (\underbrace{(p_{-}p_{0})/\Delta t}_{\equiv \dot{p}_{0}} + \eta_{D}p_{0})]} \left(\frac{\Delta t}{2\pi\kappa}\right)^{1/2} \exp\left[-\frac{\Delta t}{2\kappa}\xi^{2}\right]$$

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From momentum broadening to spatial diffusion (II)

Hence one gets:

$$W[p_0, p_1, ..., p_N] = \frac{e^{-p_0^2/2MT}}{(2\pi MT)^{1/2}} \left(\frac{1}{2\pi\kappa\Delta t}\right)^{N/2} \exp\left[-\sum_{i=0}^{N-1} \frac{\Delta t}{2\kappa} (\dot{p}_i + \eta_D p_i)^2\right]$$

One writes the Dirac delta as

$$\delta\left(\Delta x - \sum_{i=0}^{N-1} \frac{p_i}{M} \Delta t\right) = \int \frac{dq}{2\pi} \exp\left[iq\left(\Delta x - \sum_{i=0}^{N-1} \frac{p_i}{M} \Delta t\right)\right]$$

From momentum broadening to spatial diffusion (II)

Hence one gets:

$$W[p_0, p_1, ..., p_N] = \frac{e^{-p_0^2/2MT}}{(2\pi MT)^{1/2}} \left(\frac{1}{2\pi\kappa\Delta t}\right)^{N/2} \exp\left[-\sum_{i=0}^{N-1} \frac{\Delta t}{2\kappa} (\dot{p}_i + \eta_D p_i)^2\right]$$

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All integrals over $p_N, ... p_1, p_0, q$ are Gaussian. One gets $(t \equiv N \Delta t)$:

$$P(\Delta x, t) = \frac{1}{(2\pi\sigma^2)^{1/2}} e^{-(\Delta x)^2/2\sigma^2} \quad \text{with} \quad \left[\sigma^2 = \frac{T}{M} l_1^2 + \frac{\kappa}{M^2} l_2 \right] \quad \text{where}$$

$$l_1 \equiv \int_0^t dt' e^{-\eta_D(t-t')} = \frac{1}{\eta_D} \left[1 - e^{-\eta_D t} \right] \quad l_2 = \frac{1}{\eta_D^2} t - \frac{2}{\eta_D^3} (1 - e^{-\eta_D t}) + \frac{1}{2\eta_D^3} (1 - e^{-2\eta_D t})$$

From momentum broadening to spatial diffusion (III)

Exploting the Einstein relation $\eta_D = \kappa/2MT$ one gest

$$\sigma^{2}(t) = 2\left(\frac{T}{M\eta_{D}}\right)t - 2\left(\frac{T}{M\eta_{D}}\right)\frac{1}{\eta_{D}}(1 - e^{-\eta_{D}t}),$$

from which one can identify

$$D_s \equiv \frac{T}{M\eta_D} = \frac{2T^2}{\kappa}$$

In the two opposite limits one gets:

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$$\sigma^2 \underset{t \to \infty}{\sim} 2 D_S t$$
 diffusive behavior

The stronger the interaction, the slower the spatial diffusion!

$$\sigma^2 \underset{t \to 0}{\sim} D_s \eta_D t^2 = \frac{2T^2}{\kappa} \frac{\kappa}{2MT} t^2 = \frac{T}{M} t^2 = \langle v_x^2 \rangle t^2$$
 free streaming

For details: P. Petreczky and D. Teaney, PRD 73 (2006) 014508.

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HQ transport coefficients: non-perturbative definition

One consider the non-relativistic limit of the Langevin equation for a HQ

$$rac{dm{p}'}{dt}=-\eta_Dm{p}^i+\xi^i(t), \quad ext{with} \quad \langle\xi^i(t)\xi^j(t')
angle=\delta^{ij}\delta(t-t')\kappa$$

in which the strength of the noise is given by a single number, the momentum-diffusion coefficient κ . Hence, in the $p \rightarrow 0$ limit:

$$\kappa = rac{1}{3} \int_{-\infty}^{+\infty} dt \langle \xi^i(t) \xi^i(0)
angle_{\mathrm{HQ}} pprox rac{1}{3} \int_{-\infty}^{+\infty} dt \underbrace{\langle F^i(t) F^i(0)
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$$\kappa = \frac{1}{3} \int_{-\infty}^{+\infty} dt \langle \xi^i(t) \xi^i(0) \rangle_{\mathrm{HQ}} \approx \frac{1}{3} \int_{-\infty}^{+\infty} dt \underbrace{\langle F^i(t) F^i(0) \rangle_{\mathrm{HQ}}}_{\equiv D^{>}(t)},$$

For a static ($M = \infty$) HQ the force is due to the color-electric field:

$$F(t) = \int dx \ Q^{\dagger}(t,x) t^{*} Q(t,x) E^{*}(t,x)$$

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For a static ($M = \infty$) HQ the force is due to the color-electric field:

$$F(t) = \int dx \ Q^{\dagger}(t,x) t^{a} Q(t,x) E^{a}(t,x)$$

The above non-perturbative definition, referring to the $M \to \infty$ limit, is the starting point for a thermal-field-theory evaluation based on

- weak-coupling calculations (up to NLO);
- gauge-gravity duality ($\mathcal{N} = 4$ SYM, Solana and Teaney PRD 74 (2006) 085012)
- lattice-QCD simulations

HQ momentum diffusion: weak-coupling calculation



• HQ momentum diffusion due to scattering with light quarks and gluons
HQ momentum diffusion: weak-coupling calculation



- HQ momentum diffusion due to scattering with light quarks and gluons
- Already the tree-level result actually contains higher-order (all order!) corrections due to the screening of the interaction

$$rac{1}{ec q^2} \longrightarrow rac{1}{ec q^2+m_D^2} \quad ext{with} \quad m_D \sim gT$$

HQ momentum diffusion: weak-coupling calculation



- HQ momentum diffusion due to scattering with light quarks and gluons
- Already the tree-level result actually contains higher-order (all order!) corrections due to the screening of the interaction

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m with} \quad m_D \sim g T$$

• Further $\mathcal{O}(g)$ corrections to κ arise from overlapping scatterings. Having a total scattering rate $\sim g^2 T$ and the duration of a single scattering $\sim 1/q \sim 1/gT$ entails that a fraction $\mathcal{O}(g)$ of scattering events overlap with each other (see diagrams)

HQ momentum diffusion: weak-coupling calculation



One gets, for $N_f = N_c = 3$ (S. Caron-Huot and G⁹.D. Moore, JHEP 0802 (2008) 081),

$$\kappa = \frac{16\pi}{3} \alpha_s^2 T^3 \left(\ln \frac{1}{g} + 0.07428 + 1.9026g + \mathcal{O}(g^2) \right)$$

- For realistic values of the coupling $\alpha_s \sim$ 0.3 NLO corrections to κ are large!
- NLO result limited to the $M = \infty$ case

Getting the HQ momentum-diffusion coefficient requires to evaluate

$$\kappa = \frac{1}{3} \int_{-\infty}^{+\infty} dt \langle \xi^{i}(t) \xi^{i}(0) \rangle_{\mathrm{HQ}} = \frac{1}{3} \int_{-\infty}^{+\infty} dt \underbrace{\langle F^{i}(t) F^{i}(0) \rangle_{\mathrm{HQ}}}_{\equiv D^{>}(t)}$$
where $F(t) = \int dx \, Q^{\dagger}(t, x) t^{\vartheta} Q(t, x) E^{\vartheta}(t, x)$

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where $F(t) = \int dx \ Q^{\dagger}(t,x)t^{a}Q(t,x)E^{a}(t,x)$

From the lattice one can get only the euclidean correlator (t=-i au)

$$\mathcal{D}_{\mathcal{E}}(au) = -rac{\langle \operatorname{Re}\operatorname{Tr}[\mathcal{U}(eta, au) g \mathcal{E}^i(au,0) \mathcal{U}(au,0) g \mathcal{E}^i(0,0)]
angle}{\langle \operatorname{Re}\operatorname{Tr}[\mathcal{U}(eta,0)]
angle}$$

How to proceed?

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$$\kappa = rac{1}{3} \int_{-\infty}^{+\infty} dt \langle \xi^i(t) \xi^i(0)
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angle}{\langle \operatorname{Re}\operatorname{Tr}[m{U}(eta,0)]
angle}$$

How to proceed? κ comes from the $\omega \to 0$ limit of the FT of $D^>$. In a thermal ensemble $\sigma(\omega) \equiv D^>(\omega) - D^<(\omega) = (1 - e^{-\beta\omega})D^>(\omega)$, so that

$$\kappa \equiv \lim_{\omega \to 0} \frac{D^{>}(\omega)}{3} = \lim_{\omega \to 0} \frac{1}{3} \frac{\sigma(\omega)}{1 - e^{-\beta \omega}} \underset{\omega \to 0}{\sim} \frac{1}{3} \frac{T}{\omega} \sigma(\omega)$$

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Getting the HQ momentum-diffusion coefficient requires to evaluate

$$\kappa = \frac{1}{3} \int_{-\infty}^{+\infty} dt \langle \xi^{i}(t) \xi^{i}(0) \rangle_{\mathrm{HQ}} = \frac{1}{3} \int_{-\infty}^{+\infty} dt \underbrace{\langle F^{i}(t) F^{i}(0) \rangle_{\mathrm{HQ}}}_{\equiv D^{>}(t)}$$

where $F(t) = \int dx \ Q^{\dagger}(t,x) t^{a} Q(t,x) E^{a}(t,x)$

From the lattice one can get only the euclidean correlator (t=-i au)

$$D_{E}(\tau) = -\frac{\langle \operatorname{Re}\operatorname{Tr}[U(\beta,\tau)gE^{i}(\tau,0)U(\tau,0)gE^{i}(0,0)]\rangle}{\langle \operatorname{Re}\operatorname{Tr}[U(\beta,0)]\rangle}$$

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$$\kappa \equiv \lim_{\omega \to 0} \frac{D^{>}(\omega)}{3} = \lim_{\omega \to 0} \frac{1}{3} \frac{\sigma(\omega)}{1 - e^{-\beta\omega}} \underset{\omega \to 0}{\sim} \frac{1}{3} \frac{T}{\omega} \sigma(\omega)$$

From $D_E(\tau)$ one extracts the spectral density according to

$$D_E(\tau) = \int_0^{+\infty} \frac{d\omega}{2\pi} \frac{\cosh(\tau - \beta/2)}{\sinh(\beta\omega/2)} \sigma(\omega)$$

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The direct extraction of the spectral density from the euclidean correlator

$$D_{E}(\tau) = \int_{0}^{+\infty} \frac{d\omega}{2\pi} \frac{\cosh(\tau - \beta/2)}{\sinh(\beta\omega/2)} \sigma(\omega)$$

is a ill-posed problem, since the latter is known for a limited set (~ 20) of points $D_E(\tau_i)$, and one wishes to obtain a fine scan of the the spectral function $\sigma(\omega_i)$. A direct χ^2 -fit is not applicable.

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Momentum broadening in the non-static case

In the case of experimental interest HQ's have a large but finite mass and most of the p_T -bins for which data are available refer to quite fast, or even relativistic, HF hadrons: extending the estimates for the HQ transport coefficients to finite momentum is mandatory to provide theoretical predictions relevant for the experiment.

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For the same hydro background, simulations with momentum dependent transport coefficients $\kappa_{T/L}$ (left panel: weak-coupling HTL calculation) leads to quite different D-meson p_T -distributions wrt to the static lattice-QCD results (A.B. *et al.*, JHEP 1802 (2018) 043).

Theory-to-data comparison: a snapshot of recent results



In spite of their large mass, also the D-mesons turn out to be quenched and to have a sizable v_2 . Does also charm reach local thermal equilibrium? Transport calculations are challenged to consistently reproduce this rich phenomenology.

Some recent developments

- Event-by-event fluctuations: odd harmonics (*v*₃) and elliptic flow in central collisions;
- Modification of HF hadrochemistry in AA and pp collisions

Event-by-event fluctuations



• The random distribution of nucleons can lead to different geometric deformations (elliptic, triangular...) for the same impact parameter. Odd anisotropies (triangular, pentagonal...) can only arise from EBE fluctuations;

Event-by-event fluctuations



- The random distribution of nucleons can lead to different geometric deformations (elliptic, triangular...) for the same impact parameter. Odd anisotropies (triangular, pentagonal...) can only arise from EBE fluctuations;
- One observes, for *light hadrons*, that ν_n ~ ε_n for n=2,3: anisotropy of particle distribution proportional to geometric eccentricity.

The study of odd flow-harmonics (v_3, v_5) in AA collisions requires a modeling of initial-state event-by-event fluctuations. We perform a Glauber-MC sampling of the initial conditions, each one characterized by a *complex eccentricity*

$$s(\mathbf{x}) = \frac{K}{2\pi\sigma^2} \sum_{i=1}^{N_{\text{coll}}} \exp\left[-\frac{(\mathbf{x} - \mathbf{x}_i)^2}{2\sigma^2}\right] \longrightarrow \epsilon_m e^{im\Psi_m} \equiv -\frac{\{r^2 e^{im\phi}\}}{\{r^2\}}$$

with orientation and modulus given by

$$\Psi_{m} = \frac{1}{m} \operatorname{atan2} \left(-\{r^{2} \sin(m\phi)\}, -\{r^{2} \cos(m\phi)\} \right)$$
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Exploiting the fact that, on an event-by-event basis, for $m = 2, 3 v_m \sim \epsilon_m$ one can again consider an *average background* obtained summing all the events of a given centrality class, each one rotated by its *event-plane* angle ψ_m , depending on the harmonic one is considering.









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 Recombination with light quarks at hadronization provides a relevant contribution to the D-meson v_n;

HF hadronization: experimental findings



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- pattern similar to light hadrons
- baryon enhancement observed also in *pp* collisions: is a dense medium formed also there? Breaking of factorization description in *pp* collisions

Once a *c* quarks reaches a fluid cell at $T_H = 155$ MeV recombined it with a light antiquark or diquark, assumed to be thermally distributed (for more details see A.B. et al., 2202.08732 [hep-ph]).

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Extract the medium particle species according to its thermal weight

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 - Light clusters ($M_C < M_{max}$) undergo isotropic two-body decay in their own rest frame, as in HERWIG;
 - Heavier clusters $(M_C > M_{max})$ undergo string fragmentation into N hadrons, as in PYTHIA.

A simple cartoon



Local color-neutralization mechanism via recombination with the closest nearby opposite color-charge
Results in AA: charmed-hadron p_T -distributions



Charmed hadron p_T -spectra normalized to integrated D^0 -yield per event. At high p_T better agreement with experimental data for curves including momentum dependence of the transport coefficients (HTL curves). NB: IQCD results referring to $N_f = 0$ (gluon plasma).

Results in AA: hadron ratios



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- Mild dependence on the transport coefficients, i.e. on the dynamics in the deconfined phase

How much flow acquired at hadronization?



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Big enhancement of charmed hadron production at intermediate p_T

- Local color-neutralization via recombination efficient mechanism to transfer flow from the fireball to the charmed hadrons;
- stronger effect for charmed baryons due to the larger radial flow of diquarks (mass ordering)

Addressing pp collisions...



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- Perfect correlation between initial entropy (dS/dy) and final particle multiplicity $(dN_{\rm ch}/d\eta)$, $S \approx 7.2N_{\rm ch}$
- Samples of 10³ minimum-bias ($\langle dS/dy \rangle_{mb} \approx 37.6$) and high-multiplicity ($\langle dS/dy \rangle_{0-1\%} \approx 187.5$) events used to simulate HQ transport and hadronization

Results in pp: particle ratios



Premilinary results⁵:

- Enhancement of charmed baryon/meson ratio qualitatively reproduced
- Multiplicity dependence of the radial-flow peak position observed (just a reshuffling of the momentum, without affecting the yields)

⁵In collaboration with D. Pablos, A. De Pace, F. Prino et al.

Results in pp: elliptic flow



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- D-meson v_2 in high-multiplicity pp in agreement with CMS results
- Sizable fraction of v_2 acquired at hadronization

Relevance for the R_{AA} in nuclear collisions



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Relevance for the R_{AA} in nuclear collisions



- Slope of the spectra in pp better described including medium effects
- Inclusion of medium effects in minimum-bias pp benchmark fundamental to better describe charmed hadron R_{AA} (left panel vs magenta curve in the right panel), both the radial-flow peak and the species dependence

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- This mismatch will disappear once measurements of beauty at low *p_T* will become available, allowing a more solid extraction of HF transport coefficient;
- The major novelty is perhaps represented by the recent non-trivial measurements in pp and pA, suggesting the formation of a hot fireball also in these small systems.