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Heavy quark chemical equilibration rate as a transport coefficient

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Abstract: Motivated by indications that heavy (charm and bottom) quarks interact strongly at temperatures generated in heavy ion collision experiments, we suggest a non-perturbative definition of a heavy quark chemical equilibration rate as a transport coefficient. Within leading-order perturbation theory (corresponding to 3-loop level), the definition is argued to reduce to an expression obtained from the Boltzmann equation. Around $T \sim 400\,\mathrm{MeV}$, an order-of-magnitude estimate for charm yields a rate $\Gamma_{\rm chem}^{-1} \gtrsim 60\,\mathrm{fm/c}$ which remains too slow to play a practical role in current experiments. However, the rate increases rapidly with T and, due to non-linear effects, also if the initial state contains an overabundance of heavy quarks.

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Contents

1 Introduction

In a fully thermalized medium, the momenta of bosons and fermions are distributed according to the Bose and Fermi distributions, respectively, parametrized by a single temperature, T, and chemical potentials associated with conserved global charges. In contrast, the most important cosmological relics, such as Light Element Abundances, Dark Matter, or Baryon Asymmetry, rely on deviations from thermal equilibrium. In a canonical Dark Matter scenario, for instance, the overall abundance of the Dark Matter particles is determined through a "freeze-out" period, which takes place when their annihilation rate becomes too slow to track the total number density determined by the Fermi distribution, which decreases exponentially when $\pi T \ll M$, where M denotes the particle mass. Since the number densities of particles and antiparticles remain equal, this deviation cannot in relativistic field theory be represented through a chemical potential, and we speak of chemical non-equilibrium. (Typically, elastic scatterings with the plasma particles still continue after this period, so that kinetic equilibrium is maintained down to lower temperatures, cf. e.g. ref. [1].) A freeze-out process leading to chemical non-equilibrium is also responsible for the $\sim 20\%$ primordial helium abundance observed in the Universe today, cf. e.g. ref. [2].

Analogous processes are assumed to play a role in heavy ion collisions. In particular, for $\pi T \ll M$, the kinetic equilibration rate of heavy quarks scales as $\Gamma_{\rm kin} \sim \alpha_s^2 \ln(\alpha_s) T^2/M$ [3]–[6], whereas the chemical equilibration rate scales as $\Gamma_{\rm chem} \sim \alpha_s^2 T^{\frac{3}{2}} \exp(-M/T)/M^{\frac{1}{2}}$ [8, 9]. Experimental data from RHIC and LHC suggest that charm quarks do have time to kinetically equilibrate, thereby participating in hydrodynamic flow (cf. e.g. refs. [10, 11]), and

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theoretical efforts to understand this up to the non-perturbative level are under way [12]–[14]. Building on earlier studies of strange quarks [15] it is believed, in contrast, that chemical equilibration does *not* take place; the number density of charm quarks and antiquarks is essentially assumed to remain as determined by an initial hard process [16], implying that there are *more* heavy quarks present than would be due for chemical equilibrium (cf. e.g. ref. [17]).

The purpose of this study is to suggest a definition of a chemical equilibration rate of heavy quarks near equilibrium, similarly to what was achieved for their kinetic equilibration rate earlier on [18, 19]. A definition should be possible in the heavy-quark limit $M \gg \pi T$, in which the rate itself is much slower than typical "fast" plasma rates, $\Gamma_{\rm fast} \sim \alpha_s^n T$, $n \geq 1$. (If no scale separation is present between M and πT, then pair creations and annihilations take place as fast as elastic processes, and the massive degrees of freedom are to a good approximation in full thermal equilibrium with the strongly interacting heat bath.)

The plan of this paper is the following. After some general considerations in section 2, we recall the derivation of the chemical equilibration rate to leading order in α_s, making use of the Boltzmann equation, in section 3. This is followed by a reminder that loop corrections are likely to be substantial at any realistic temperature, in section 4. A non-perturbative formulation is put forward in section 5. Subsequently we argue, in section 6, that in the weak-coupling limit the expression of section 5 reduces to the result of section 3. A brief discussion of implications as well as prospects for non-perturbative studies concludes this writeup in section 7.

2 General considerations

Assume that the system possess an approximately conserved particle number. Let us denote the corresponding number density[1] by $n(t)$. In thermal equilibrium the value of n fluctuates around its equilibrium value. To treat the non-equilibrium problem we follow the general method described in ref. [7]. Let $\delta n(t) \equiv n(t) - n_{\rm eq}$ at some time t be large compared to the mean fluctuation. It will then evolve towards its equilibrium value. Let us assume that the characteristic time scale τ for this evolution is much larger than the other relaxation times of the system. We only want to resolve time scales of order τ. Then the non-equilibrium state is completely characterized by the instantaneous value of δn. Therefore the time derivative of δn can only depend on the value of δn and on thermodynamic quantities of the system such as temperature and chemical potentials. When δn is sufficiently small, one can expand $\delta\dot{n}$ in powers of δn and keep only the linear term,

$$\delta\dot{n}(t) = -\Gamma_{\rm chem}\delta n(t) \,. \tag{2.1}$$

The coefficient $\Gamma_{\rm chem}$ only depends on thermodynamic quantities.

[1] It is important to consider the number density rather than the differential phase space distribution, because otherwise it would be difficult to distinguish between processes changing the kinetic and the chemical decomposition of the system.

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Let us now be specific and choose n to be the sum of quark and antiquark number densities,

$$n \equiv n_{_Q} + n_{_{\overline{Q}}} \,. \tag{2.2}$$

We consider the heavy quark baryon number density $n_{_Q} - n_{_{\overline{Q}}}$ to vanish (i.e. the baryon chemical potential to be zero). We are interested in the limit that $\pi T \ll M$. For heavy particles, $\{\delta\dot{n}(t)\}_{\rm loss} \sim e^{-2M/T}$, because a heavy quark-antiquark pair gets annihilated, and $\delta n(t) \sim n_{\rm eq} \sim e^{-M/T}$. Therefore Γ itself scales as $\sim e^{-M/T}$, implying that this rate is much slower than most other processes in the system. In particular, this rate is slower than the kinetic equilibration rate. Therefore the heavy quarks can be considered to be in kinetic equilibrium, which means that they move very slowly. These almost static quarks experience rare number changing reactions, and a non-perturbative description of the resulting dynamics, incorporating both the non-equilibrium evolution of eq. (2.1) as well as equilibrium fluctuations, is presented in eqs. (5.11)–(5.20) below.

3 Boltzmann equation

If the system is weakly coupled, one can usually compute the coefficient $\Gamma_{_{\rm chem}}$ in eq. (2.1), at least to leading order, from the Boltzmann equation. If we take into account $2 \to 2$ scattering processes and consider the limit $\pi T \ll M$, it takes the form (cf. e.g. ref. [20])

$$\dot{n} = -c\left(n^2 - n_{\rm eq}^2\right) \equiv \dot{n}_{\rm loss} + \dot{n}_{\rm gain} \,, \tag{3.1}$$

where $\dot{n}_{\rm loss} \equiv -c\, n^2$. In equilibrium, with $n(t) \equiv n_{\rm eq}$, gain and loss terms must cancel each other, and the number density is constant. Now linearize (3.1) as described in section 2, which gives $\delta\dot{n} = -2c\, n \delta n$. Thus we can obtain $\Gamma_{_{\rm chem}}$ from the loss term in eq. (3.1) via

$$\Gamma_{_{\rm chem}} = -2\,\frac{\dot{n}_{\rm loss}}{n_{\rm eq}} \,. \tag{3.2}$$

An analogous discussion, implemented by introducing separate "chemical potentials" for the quarks and antiquarks, can be found in ref. [15].

Now we compute $\Gamma_{_{\rm chem}}$ using eq. (3.2) with tree-level matrix elements. The relevant loss processes are shown in figure 1. Inserting the number of degrees of freedom of the initial state, $2N_{\rm c}$, the decay rate according to eq. (3.2) can be written as

$$\begin{aligned}
\Gamma_{_{\rm chem}} = {} & \frac{2}{2N_{\rm c}\int_{\mathbf{k}} f_{\rm F}(E_k)} \int \prod_{a=1}^{2} \frac{{\rm d}^3\mathbf{k}_a}{(2\pi)^3 2E_{k_a}} \prod_{i=1}^{2} \frac{{\rm d}^3\mathbf{p}_i}{(2\pi)^3 2\epsilon_{p_i}} \, (2\pi)^4 \delta^{(4)}(\mathcal{P}_1 + \mathcal{P}_2 - \mathcal{K}_1 - \mathcal{K}_2) \\
& \times f_{\rm F}(E_{k_1}) f_{\rm F}(E_{k_2}) \biggl\{ \frac{1}{2} \sum |\mathcal{M}_1|^2 \left[1 + f_{\rm B}(\epsilon_{p_1})\right] \left[1 + f_{\rm B}(\epsilon_{p_2})\right] \\
& \qquad + N_{\rm f} \sum |\mathcal{M}_2|^2 \left[1 - f_{\rm F}(\epsilon_{p_1})\right] \left[1 - f_{\rm F}(\epsilon_{p_2})\right] \biggr\} \,.
\end{aligned} \tag{3.3}$$

Here $\int_{\mathbf{k}} \equiv \int \frac{{\rm d}^3\mathbf{k}}{(2\pi)^3}$; $\mathbf{k}_a$ are momenta in the initial state and $\mathbf{p}_i$ those in the final state; $E_{k_a} \equiv \sqrt{k_a^2 + M^2}$ is the energy of a massive particle and $\epsilon_{p_i} \equiv |\mathbf{p}_i|$ is that of a massless

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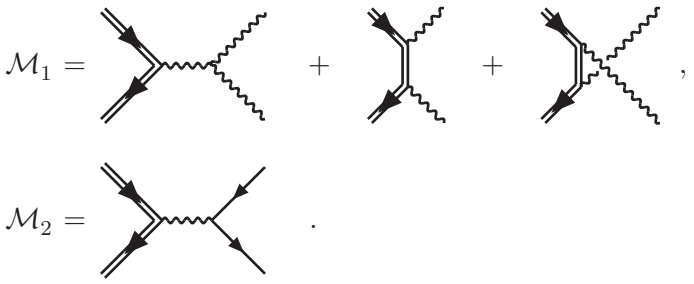

Figure 1. Scatterings through which an overabundance of heavy quarks can disappear, assuming that there is an exponentially small thermal distribution of antiquarks present (or vica versa). A double line indicates heavy quarks, a single line light quarks, and a wiggly line gluons.

one; and $f_{\rm F}, f_{\rm B}$ are the Fermi and Bose distributions, respectively. The sums are taken over the quantum numbers of all on-shell degrees of freedom, i.e. $2N_{\rm c}$ for quarks and antiquarks, and $2d_A$ for gluons, with $d_A \equiv N_{\rm c}^2 - 1$. By $N_{\rm f}$ we denote the number of light quark flavours, and later on $C_F \equiv d_A/(2N_{\rm c})$ will also appear. The factor $\frac{1}{2}$ in front of the gluonic amplitude accounts for the two final state particles being identical [15].

Taking the amplitude $\mathcal{M}_2$ of figure 1 as an example, a text-book calculation yields (cf. e.g. refs. [21, 22])

$$\sum |\mathcal{M}_2|^2 = \frac{4g^4 C_F N_{\rm c}}{s^2}\Big[(M^2-t)^2 + (M^2-u)^2 + 2M^2 s\Big] \,, \tag{3.4}$$

where s, t, u are the standard kinematic invariants: $s \equiv (\mathcal{P}_1 + \mathcal{P}_2)^2 = (\mathcal{K}_1 + \mathcal{K}_2)^2$; $t \equiv (\mathcal{P}_1 - \mathcal{K}_1)^2 = (\mathcal{P}_2 - \mathcal{K}_2)^2$; and $u \equiv (\mathcal{P}_1 - \mathcal{K}_2)^2 = (\mathcal{P}_2 - \mathcal{K}_1)^2$.

The result simplifies further in the heavy-quark limit. Because of Boltzmann suppression of $f_{\rm F}(E_{k_a})$ at $M \gg \pi T$, we can consider the decaying heavy quark and antiquark to be almost at rest with respect to the thermal medium:

$$\mathcal{K}_1 \approx \left(M + \frac{k_1^2}{2M}, \mathbf{k}_1\right) \,, \quad \mathcal{K}_2 \approx \left(M + \frac{k_2^2}{2M}, \mathbf{k}_2\right) \,, \tag{3.5}$$

with $k_a \sim \sqrt{\pi T M} \ll M$. In contrast p_1 and p_2 are large because they have to carry away the energy liberated in the pair annihilation. So $\mathbf{k}_1 + \mathbf{k}_2$ can be approximated as zero in the phase space constraints, and the Fermi distributions $f_{\rm F}(\epsilon_{p_i})$ can be omitted:

$$\begin{aligned} \Gamma_{\rm chem}^{(q\bar{q})} \approx{}& \frac{e^{-M/T}}{4N_{\rm c}M^2} \int \frac{{\rm d}^3\mathbf{k}_2}{(2\pi)^3}\, e^{-\frac{k_2^2}{2MT}} \\ &\times \frac{1}{(2\pi)^2} \int \frac{{\rm d}^3\mathbf{p}_1}{2\epsilon_{p_1}} \int \frac{{\rm d}^3\mathbf{p}_2}{2\epsilon_{p_2}}\, \delta^{(3)}(\mathbf{p}_1 + \mathbf{p}_2)\delta(\epsilon_{p_1} + \epsilon_{p_2} - 2M)\, N_{\rm f} \sum |\mathcal{M}_2|^2 \,. \end{aligned} \tag{3.6}$$

Here we cancelled a factorized integral against the one in the denominator. Noting also that

$$s \approx 4M^2 \,, \quad t \approx -M^2 \,, \quad u \approx -M^2 \,, \tag{3.7}$$

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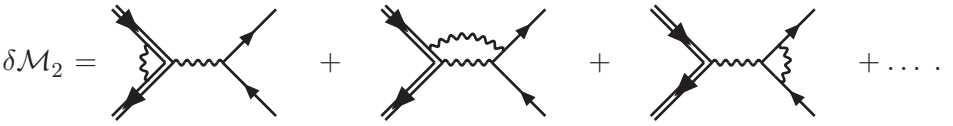

Figure 2. Examples of 1-loop corrections to the scattering amplitude $\mathcal{M}_2$ of figure 1.

we get $\sum|\mathcal{M}_2|^2 \approx 4g^4 C_F N_c$. The remaining integrals are trivially carried out, and we obtain

$$\Gamma_{\text{chem}}^{(q\bar{q})} \approx \frac{g^4 C_F N_f}{8\pi M^2}\left(\frac{TM}{2\pi}\right)^{\frac{3}{2}} e^{-M/T} \,. \tag{3.8}$$

A similar computation can be carried out with gluons, represented by the amplitude $\mathcal{M}_1$ of figure 1. Again the result is well-known (cf. e.g. refs. [21, 22]), and reads

$$\begin{aligned}\sum|\mathcal{M}_1|^2 \;=\; 4g^4 C_F N_c\Bigg\{ & 4N_c\,\frac{(M^2-t)(M^2-u)}{s^2} \;+\; (2C_F - N_c)\frac{2M^2(s-4M^2)}{(M^2-t)(M^2-u)} \\ & +2C_F\left[\frac{(M^2-t)(M^2-u)-2M^2(M^2+t)}{(M^2-t)^2} \;+(t\leftrightarrow u)\right] \\ & -2N_c\left[\frac{(M^2-t)(M^2-u)+M^2(u-t)}{s(M^2-t)} \;+(t\leftrightarrow u)\right]\Bigg\} \,. \end{aligned} \tag{3.9}$$

In the heavy-quark limit, eq. (3.7), this simplifies to $\sum|\mathcal{M}_1|^2 \approx 4g^4 C_F N_c(4C_F - N_c)$. The phase space integration goes through as before, and recalling the $\frac{1}{2}$ in eq. (3.3), eq. (3.8) gets completed into

$$\Gamma_{\text{chem}} \approx \frac{g^4 C_F}{8\pi M^2}\left(N_f + 2C_F - \frac{N_c}{2}\right)\left(\frac{TM}{2\pi}\right)^{\frac{3}{2}} e^{-M/T} \,. \tag{3.10}$$

Numerically $2C_F - N_c/2 = \frac{7}{6}$ for $N_c = 3$; for $N_f = 0$ this agrees with eq. (10) of ref. [9]. (We note, however, that for three light flavours, i.e. $N_f = 3$, fermionic final states are significantly more important than purely gluonic ones.)

4 Towards loop corrections

The result of eq. (3.10) could well suffer from large radiative corrections. A few representative examples of next-to-leading order (NLO) amplitudes are shown in figure 2. In particular, the first amplitude, iterated by further rungs connecting the heavy quark and antiquark to each other, is responsible for binding the particles to a quarkonium-like resonance. In the context of Dark Matter co-annihilation, such a threshold enhancement is assumed to play a potentially important role, cf. e.g. refs. [23, 24]. However, this is not the only class of processes in our case: as illustrated in figure 2, all participating particles carry a colour charge, so that there may also be final-state interactions, as well as "non-factorizable" terms connecting the initial and final states.

For future reference, we remark that there is one Euclidean observable in which rungs between the heavy particles can also appear but which is nevertheless very well understood.

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This is the heavy quark-number susceptibility, formally defined as

$$\chi_f \equiv \int_{\mathbf{x}} \Big\langle (\bar{\psi}\gamma_0\psi)(\tau,\mathbf{x})(\bar{\psi}\gamma_0\psi)(0,\mathbf{0}) \Big\rangle_T \,, \quad 0 \leq \tau \leq \beta \,, \quad \beta \equiv \frac{1}{T} \,. \tag{4.1}$$

Because of charge conservation the argument τ can be chosen at will. With vanishing chemical potentials, the susceptibility measures the mean number of heavy particles created by thermal fluctuations, and is therefore closely related to the distribution function $f_{\rm F}(E_{k_2})$ on which the heavy quarks scatter in eq. (3.3).

We recall that in the free limit the susceptibility evaluates to

$$\chi_f = 4N_{\rm c} \int \frac{{\rm d}^3\mathbf{k}}{(2\pi)^3} \, f_{\rm F}(E_k) \left[1 - f_{\rm F}(E_k)\right] \,. \tag{4.2}$$

For massless quarks the integral can be carried out in a closed form, yielding $\chi_f = N_{\rm c}T^3/3$, to which loop corrections are known up to a high order [25], generically decreasing the susceptibility from the free value. To us more relevant is the non-relativistic limit,

$$\chi_f \approx 4N_{\rm c} \int \frac{{\rm d}^3\mathbf{k}}{(2\pi)^3} e^{-E_k/T} \approx 4N_{\rm c} \left(\frac{MT}{2\pi}\right)^{\frac{3}{2}} e^{-M/T} \,. \tag{4.3}$$

Here the temperature dependence is precisely the same as that in eq. (3.8). Lattice data indicate that the susceptibility grows rapidly with the temperature and, in the charm case, overcomes the exponential suppression already at temperatures of a few hundred MeV [26]–[28], in line with the general expectation [29]. We will keep these observations in mind when estimating the numerical importance of the exponential suppression in section 7.

5 Non-perturbative formulation

Motivated by the remarks in section 4, the goal now is to suggest a non-perturbative *definition* of the heavy quark chemical equilibration rate. This could allow for a systematic computation of higher order corrections, or in principle be subjected e.g. to a lattice investigation.

In relativistic theories there is no obvious definition for a particle number operator. Here we are interested in heavy quarks and antiquarks with very small velocities. In this case the energy of quarks and antiquarks is roughly given by the sum of their rest energies or, in other words, by their number density times the heavy quark mass M. Therefore the energy density of heavy quarks and antiquarks is a good measure for their number density. We propose to define the relaxation time of the number density $n = n_Q + n_{\overline{Q}}$ through the real time correlation function of the heavy quark Hamilton operator.

We start by introducing an operator describing heavy quark energy loss, both through elastic and through inelastic processes (section 5.1); define then a "transport coefficient" related to this operator, capturing the desired rate (section 5.2); and finally simplify one of the correlators appearing by considering the heavy-quark limit (section 5.3).

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5.1 Operator for heavy quark energy loss

A form of the fermionic energy-momentum tensor which is symmetric, gauge-invariant, and leads to a correct finite trace anomaly, reads [30, 31]

$$T_{\rm f}^{\mu\nu} \;\equiv\; \frac{i}{4}\bar{\psi}\Big(\gamma^\mu \overleftrightarrow{D}^\nu + \gamma^\nu \overleftrightarrow{D}^\mu\Big)\psi - \eta^{\mu\nu}\,\mathcal{L}_{\rm f}\,. \tag{5.1}$$

Here $\eta^{\mu\nu} \equiv {\rm diag}(+---)$ and

$$\bar{\psi}\gamma^\mu \overleftrightarrow{D}^\nu\psi \;\equiv\; \bar{\psi}\gamma^\mu \overrightarrow{D}^\nu\psi - \bar{\psi}\gamma^\mu \overleftarrow{D}^{\nu\dagger}\psi\,, \tag{5.2}$$

with $\overrightarrow{D}^\nu\psi \equiv (\partial^\nu - igA^\nu)\psi$, $\bar{\psi}\,\overleftarrow{D}^{\nu\dagger} \equiv \bar{\psi}(\overleftarrow{\partial}^\nu + igA^\nu)$, and g denoting the bare gauge coupling. The Lagrangian can be written with a similar notation as

$$\mathcal{L}_{\rm f} = \bar{\psi}\left(\frac{i}{2}\overleftrightarrow{\not{D}} - M\right)\psi\,. \tag{5.3}$$

The heavy quark Hamilton operator is now defined by taking a spatial integral over $T_{\rm f}^{00}$, with the fields promoted to operators:

$$\hat{H} \equiv \int_{\mathbf{x}} \hat{T}_{\rm f}^{00} \;=\; \int_{\mathbf{x}} \hat{\bar{\psi}}\left(-\frac{i}{2}\gamma^j \overleftrightarrow{D}_j + M\right)\hat{\psi}\,. \tag{5.4}$$

Summation over repeated spatial indices is understood. Obviously, $\hat{H}$ could be written in other forms by use of the Dirac equation, but for us it appears to be beneficial to employ a version with spatial derivatives only, because then partial integrations are formally allowed.

In order to derive the operator for energy loss, let us also write down the Dirac equation in an explicit form, by placing time derivatives on the left-hand side:

$$\partial_t\hat{\psi} = \Big[-i(M\gamma^0 - gA_0) - \gamma^0\gamma^j\overrightarrow{D}_j\Big]\hat{\psi}\,, \tag{5.5}$$

$$\partial_t\hat{\bar{\psi}} = \hat{\bar{\psi}}\Big[i(M\gamma^0 - gA_0) - \overleftarrow{D}_j^\dagger\gamma^j\gamma^0\Big]\,. \tag{5.6}$$

In all of what follows, equations of motion are used for fermions only; derivatives acting on gauge fields are left "as is", formally assuming that gauge fields form a differentiable off-shell background over which a path integral is to be carried out at a later stage.

The task now is to construct $\partial_t\hat{H}$. The derivative can act on any of the three possible locations in eq. (5.4):

$$\partial_t\hat{H} = \int_{\mathbf{x}}\left\{\Big(\partial_t\hat{\bar{\psi}}\Big)\Big(-i\gamma^j\overrightarrow{D}_j + M\Big)\hat{\psi} + \hat{\bar{\psi}}\Big(-g\gamma^j\partial_0 A_j\Big)\hat{\psi} + \hat{\bar{\psi}}\Big(i\gamma^j\overleftarrow{D}_j^\dagger + M\Big)\Big(\partial_t\hat{\psi}\Big)\right\}\,. \tag{5.7}$$

Inserting eqs. (5.5), (5.6) and carrying out one partial integration, numerous cancellations take place, and we are finally left with

$$\partial_t\hat{H} \;=\; -g\int_{\mathbf{x}}\hat{\bar{\psi}}\gamma^j\Big(\partial_0 A_j - \partial_j A_0 - igA_0A_j + igA_jA_0\Big)\hat{\psi} \;=\; -g\int_{\mathbf{x}}\hat{\bar{\psi}}\,\gamma^j F_{0j}\hat{\psi}\,. \tag{5.8}$$

So, in the presence of interactions ($g \neq 0$), the energy carried by heavy quarks is not conserved.

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It appears that eq. (5.8) has a classical interpretation. If a charged particle feels a Lorentz force,

$$\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = q\Big(\mathbf{E} + \mathbf{v}\times\mathbf{B}\Big)\,, \tag{5.9}$$

then its energy changes as

$$\frac{\mathrm{d}E}{\mathrm{d}t} = \nabla_{\mathbf{p}}E\cdot\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = \mathbf{v}\cdot\frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = q\mathbf{v}\cdot\mathbf{E}\,. \tag{5.10}$$

Recalling that $\hat{\bar{\psi}}\gamma^j\hat{\psi}$ are the spatial components of a current this is seen to agree in form with eq. (5.8). However, being a Fock space operator, $\partial_t\hat{H}$ of eq. (5.8) describes also number-changing reactions; in particular, if the initial state has more quarks and antiquarks than would be due for chemical equilibrium, a net pair annihilation should take place, and in the large-time limit the corresponding matrix elements dominate the statistical average of $\partial_t\hat{H}$.

5.2 Defining a transport coefficient

To describe the depletion of an overabundance of heavy quarks through a single coefficient, we follow a general method which has also been used for determining their *kinetic equilibration rate* [18, 19]. The goal is to relate the non-equilibrium rate of interest, eq. (2.1), to an equilibrium correlator, eq. (5.14) (see ref. [7] for a general argument concerning such relations). In order to achieve this goal, the logic is to use an "effective" classical picture to describe the long time physics of chemical equilibration. The parameters of this description are subsequently matched to reproduce quantum-mechanical correlators. As we will see, the consistency of the description will be tested at the matching stage.

As discussed in section 2, large deviations from an equilibrium value tend to decrease, with a rate that we want to determine (cf. eq. (2.1)); however, small deviations can also be generated by the occasional inverse reactions.[2] This is formally the same physics as in Brownian motion, described by a Langevin equation,

$$\delta\dot{n}(t) \,=\, -\Gamma_{\mathrm{chem}}\,\delta n(t) + \xi(t)\,, \tag{5.11}$$

$$\big\langle\!\big\langle\, \xi(t)\,\xi(t')\,\big\rangle\!\big\rangle \,=\, \Omega_{\mathrm{chem}}\,\delta(t-t')\,, \qquad \big\langle\!\big\langle \xi(t)\big\rangle\!\big\rangle = 0\,, \tag{5.12}$$

where δn is the non-equilibrium excess; ξ is a stochastic noise, whose autocorrelation function is parametrized by Ω_{chem}; and $\langle\!\langle\ldots\rangle\!\rangle$ denotes an average over the noise. The noise is uncorrelated because the time scale considered is much larger than any others in the system.[3]

[2] In a heavy ion collision there may not be enough time for inverse reactions to take place *in practice*; but that does not change the *theoretical role* that they play in relating the non-equilibrium problem to a corresponding equilibrium one. In other words, within the linear response regime the value of the coefficient Γ_{chem} is independent of initial conditions and of for how long we observe the dynamics.

[3] At very short time scales, the noise is no longer white but has a structure. By definition, the structure can be resolved by inspecting the spectral function corresponding to the "force-force" correlator. As demonstrated in section 6, the spectral function has support down to small frequencies, with an overall magnitude $\Omega_{\mathrm{chem}} \sim e^{-2M/T}$. Noise becomes coloured at a frequency scale ω_{UV} above which the shape of the spectral function changes from its small-frequency asymptotics. This is related to the physics of colour-electric fields, so we may expect $\omega_{\mathrm{UV}} \gtrsim \alpha_s^2 T$. This is much larger than the frequency scales that we are concerned with, and plays no role in the following.

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Now, eq. (5.11) can be solved explicitly, given an initial value $\delta n(t_0)$:

$$\delta n(t) = \delta n(t_0)\, e^{-\Gamma_{\rm chem}(t-t_0)} + \int_{t_0}^{t} {\rm d}t'\, e^{\Gamma_{\rm chem}(t'-t)} \xi(t') \,. \tag{5.13}$$

Making use of this solution and taking an average over the noise, we can determine the 2-point correlation function of unequal time fluctuations of δn:

$$\begin{aligned} \Delta_{\rm cl}(t,t') & \equiv \lim_{t_0\to-\infty} \langle\!\langle\, \delta n(t)\, \delta n(t') \,\rangle\!\rangle \\ & = \lim_{t_0\to-\infty} \int_{t_0}^{t} {\rm d}t_1\, e^{\Gamma_{\rm chem}(t_1-t)} \int_{t_0}^{t'} {\rm d}t_2\, e^{\Gamma_{\rm chem}(t_2-t')} \langle\!\langle\, \xi(t_1)\, \xi(t_2) \,\rangle\!\rangle \\ & = \Omega_{\rm chem} \lim_{t_0\to-\infty} \int_{t_0}^{t} {\rm d}t_1\, e^{\Gamma_{\rm chem}(t_1-t)} \int_{t_0}^{t'} {\rm d}t_2\, e^{\Gamma_{\rm chem}(t_2-t')} \delta(t_1-t_2) \\ & = \frac{\Omega_{\rm chem}}{2\Gamma_{\rm chem}}\, e^{-\Gamma_{\rm chem}|t-t'|} \,. \end{aligned} \tag{5.14}$$

The limit $t_0 \to -\infty$ here guarantees that any initial transients have died out; therefore, $\Delta_{\rm cl}$ is an *equilibrium* correlation function. Subsequently, making use of $\partial_t \partial_{t'} |t-t'| = -2\delta(t-t')$, we obtain

$$\partial_t \partial_{t'} \Delta_{\rm cl}(t,t') = -\frac{\Omega_{\rm chem}\Gamma_{\rm chem}}{2}\, e^{-\Gamma_{\rm chem}|t-t'|} + \Omega_{\rm chem}\, \delta(t-t') \,. \tag{5.15}$$

Fourier transforming eqs. (5.14) and (5.15) leads to

$$\tilde{\Delta}_{\rm cl}(\omega) \equiv \int_{-\infty}^{\infty} {\rm d}t\, e^{i\omega(t-t')} \Delta_{\rm cl}(t,t') \;=\; \frac{\Omega_{\rm chem}}{\omega^2 + \Gamma_{\rm chem}^2} \,, \tag{5.16}$$

$$\omega^2 \tilde{\Delta}_{\rm cl}(\omega) = \int_{-\infty}^{\infty} {\rm d}t\, e^{i\omega(t-t')} \partial_t \partial_{t'} \Delta_{\rm cl}(t,t') \;=\; \frac{\omega^2\, \Omega_{\rm chem}}{\omega^2 + \Gamma_{\rm chem}^2} \,. \tag{5.17}$$

It is also useful to note that, setting the time arguments equal, we can define a "susceptibility" as

$$\langle (\delta n)^2 \rangle_{\rm cl} \equiv \lim_{t_0\to-\infty} \langle\!\langle\, \delta n(t)\, \delta n(t) \,\rangle\!\rangle = \frac{\Omega_{\rm chem}}{2\Gamma_{\rm chem}} \,, \tag{5.18}$$

where we made use of eq. (5.14).

Combining eqs. (5.16)–(5.18), various strategies can be envisaged for determining the quantity that we are interested in, namely the non-equilibrium rate $\Gamma_{\rm chem}$. A particularly fruitful approach is to take eqs. (5.17), (5.18) as starting points, obtaining

$$\Omega_{\rm chem} = \lim_{\Gamma_{\rm chem} \ll \omega \ll \omega_{\rm UV}} \omega^2 \tilde{\Delta}_{\rm cl}(\omega) \,, \tag{5.19}$$

$$\Gamma_{\rm chem} = \frac{\Omega_{\rm chem}}{2\langle (\delta n)^2 \rangle_{\rm cl}} \,. \tag{5.20}$$

Here $\omega_{\rm UV}$ is a frequency scale at which some microscopic physics which is not described by the effective classical picture sets in, typically $\omega_{\rm UV} \sim \alpha_s^2 T$, and it has been assumed (cf. section 2) that $\Gamma_{\rm chem}$ *is parametrically small compared with* $\omega_{\rm UV}$. In our case this is so because $\Gamma_{\rm chem}$ is exponentially suppressed as $\sim e^{-M/T}$. With this input, all real-time information is in the numerator of the equilibrium correlator $\omega^2 \tilde{\Delta}_{\rm cl}(\omega)$.

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After these preparatory steps, we can promote the determination of $\Gamma_{\rm chem}$ to the quantum level. It just remains to note that since in the classical limit observables commute, a suitable quantum version of the equilibrium correlator is

$$\Delta_{\rm qm}(t,t') \equiv \left\langle \frac{1}{2}\left\{\delta\hat{n}(t),\delta\hat{n}(t')\right\}\right\rangle . \tag{5.21}$$

So, eqs. (5.19), (5.20) can be rephrased as

$$\Omega_{\rm chem} = \lim_{\Gamma_{\rm chem}\ll\omega\ll\omega_{\rm UV}} \omega^2 \int_{-\infty}^{\infty} {\rm d}t\, e^{i\omega(t-t')} \left\langle \frac{1}{2}\left\{\delta\hat{n}(t),\delta\hat{n}(t')\right\}\right\rangle , \tag{5.22}$$

or

$$\Omega_{\rm chem} = \lim_{\Gamma_{\rm chem}\ll\omega\ll\omega_{\rm UV}} \int_{-\infty}^{\infty} {\rm d}t\, e^{i\omega(t-t')} \left\langle \frac{1}{2}\left\{\frac{{\rm d}\hat{n}(t)}{{\rm d}t},\frac{{\rm d}\hat{n}(t')}{{\rm d}t'}\right\}\right\rangle , \tag{5.23}$$

together with

$$\Gamma_{\rm chem} = \frac{\Omega_{\rm chem}}{2\langle(\delta\hat{n})^2\rangle} . \tag{5.24}$$

The denominator of eq. (5.24) is nothing but the variance, $\langle(\delta\hat{n})^2\rangle = \langle\hat{n}^2\rangle - \langle\hat{n}\rangle^2$. The consistency of the matching is tested at least to some extent by whether the variance is UV-finite (for most composite operators this is not the case).

The formulae introduced can be applied on a non-perturbative level by re-expressing them through the imaginary-time formalism. This means that we first define a Euclidean correlator, $\Omega(\tau)$; Fourier-transform it, $\tilde{\Omega}(\omega_n) = \int_0^\beta {\rm d}\tau\, e^{i\omega_n\tau}\Omega(\tau)$, where $\omega_n = 2\pi nT$, $n\in\mathbb{Z}$ (this requires the presence of an UV regulator, or the subtraction of short-distance divergences); and obtain the spectral function from its imaginary part, $\rho_\Omega(\omega) = {\rm Im}\,\tilde{\Omega}(\omega_n\to -i[\omega+i0^+])$. The symmetric combination needed in eq. (5.23) is given by $\Omega_{\rm chem} = \lim_{\Gamma_{\rm chem}\ll\omega\ll\omega_{\rm UV}} 2T\rho_\Omega(\omega)/\omega$.

The argumentation above can directly be transported to the case at hand, with $\hat{n}$ replaced by $\hat{H}$ from eq. (5.4). Denoting by E_j the *Euclidean* electric field, which contains an additional i from a Wick rotation, the imaginary-time correlator referred to above reads (we divide by volume in order to define intensive quantities)

$$\begin{aligned}\Omega(\tau) &\equiv \frac{1}{V}\left\langle \partial_t\hat{H}(\tau)\,\partial_t\hat{H}(0)\right\rangle_{\rm qc} \\ &= -g^2\int_{\mathbf{x}}\left\langle \left[\bar{\psi}\gamma^j E_j\psi\right](\tau,\mathbf{x})\left[\bar{\psi}\gamma^k E_k\psi\right](0,\mathbf{0})\right\rangle_{\rm qc} ,\end{aligned} \tag{5.25}$$

where $gE_k \equiv i[D_\tau, D_k]$, and $\langle\ldots\rangle_{\rm qc}$ refers to connected quark contractions (the reason for this choice is discussed in figure 3). Hats have been left out in the second row because this correlator can be evaluated with regular path integral techniques. Similarly, the correlator related to energy fluctuations becomes

$$\begin{aligned}\Delta(\tau) &\equiv \frac{1}{V}\left\langle \hat{H}(\tau)\,\hat{H}(0)\right\rangle_{\rm c} \\ &= \int_{\mathbf{x}}\left\langle \left[\bar{\psi}\left(-\frac{i}{2}\gamma^j\overleftrightarrow{D}_j + M\right)\psi\right](\tau,\mathbf{x})\left[\bar{\psi}\left(-\frac{i}{2}\gamma^k\overleftrightarrow{D}_k + M\right)\psi\right](0,\mathbf{0})\right\rangle_{\rm c} ,\end{aligned} \tag{5.26}$$

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where $\langle\ldots\rangle_{\rm c}$ refers to the connected part, i.e. $\langle\hat{H}(\tau)\hat{H}(0)\rangle_{\rm c}\equiv\langle\hat{H}(\tau)\hat{H}(0)\rangle-\langle\hat{H}(0)\rangle^2$. We can interpret $\Delta(\tau)$ as the susceptibility needed in eq. (5.24) to the extent that it is τ-independent and therefore finite at $\tau\to 0$ (cf. eq. (4.1)); this turns out to be the case in the limit $\pi T\ll M$, where it corresponds to a quasi-conserved quantity: $\Delta(\tau)\approx\frac{1}{V}\langle(\delta\hat{H})^2\rangle$ (cf. eq. (5.31)).

5.3 Heavy quark limit

The correlators in eqs. (5.25), (5.26) can be understood physically, and also written in somewhat simpler forms, if two-component spinors corresponding to non-relativistic degrees of freedom are employed. We choose a representation for the Dirac matrices with

$$\gamma^0\equiv\begin{pmatrix}\mathbb{1} & 0\\ 0 & -\mathbb{1}\end{pmatrix}\,,\quad \gamma^k\equiv\begin{pmatrix}0 & \sigma_k\\ -\sigma_k & 0\end{pmatrix}\,,\quad k=1,2,3\,, \tag{5.27}$$

where σ_k are the Pauli matrices. The Dirac spinors are written as

$$\psi\equiv\begin{pmatrix}\theta\\ \chi\end{pmatrix}\,,\quad \bar{\psi}\equiv(\theta^\dagger\,,\,-\chi^\dagger)\,. \tag{5.28}$$

Clearly θ corresponds to $\mathbb{P}_+\psi$ and χ to $\mathbb{P}_-\psi$, with the projection operators defined as $\mathbb{P}_\pm\equiv\frac{1}{2}\left(\mathbb{1}\pm\gamma^0\right)$. With this notation the operator entering eq. (5.25) can be expressed as

$$\partial_t H=-ig\int_{\mathbf{x}}\left[\theta^\dagger\sigma\cdot\mathbf{E}\,\chi+\chi^\dagger\sigma\cdot\mathbf{E}\,\theta\right]\,. \tag{5.29}$$

Note that this operator is *different* from that relevant for heavy quark *kinetic* equilibration: electric fields appear in both cases but here they come together with $\theta^\dagger\chi$, $\chi^\dagger\theta$, whereas in ref. [19] the combinations $\theta^\dagger\theta$, $\chi^\dagger\chi$ appeared. Eq. (5.26) can also be expressed in the new notation, with the Hamiltonian becoming

$$H=\int_{\mathbf{x}}\left[M\big(\theta^\dagger\theta-\chi^\dagger\chi\big)-\frac{i}{2}\left(\theta^\dagger\sigma\cdot\overleftrightarrow{\mathbf{D}}\chi+\chi^\dagger\sigma\cdot\overleftrightarrow{\mathbf{D}}\theta\right)\right]\,. \tag{5.30}$$

For a proper physical interpretation, it is useful to change the ordering of χ^*_α, χ_β. It then becomes clear that χ^* represents an antiparticle to θ; a most direct way to see this is from the number density operator: $\bar{\psi}\gamma^0\psi=\bar{\psi}(P_+-P_-)\psi=\theta^\dagger\theta+\chi^\dagger\chi=\theta^\dagger\theta-\chi^{*\dagger}\chi^*$. What this implies is that operators of the types $\theta^\dagger\chi$, $\chi^\dagger\theta$, appearing in eq. (5.29), create or annihilate quark-antiquark pairs; and that the leading term of the Hamilton operator in eq. (5.30) counts particles *plus* antiparticles, assigning each energies given by their rest mass.

After these remarks we can simplify the correlator $\Delta(\tau)$ of eq. (5.26). In the heavy-quark limit the leading term comes from $M(\theta^\dagger\theta-\chi^\dagger\chi)$ in eq. (5.30). But since in the same limit the cross term gives no contribution, the (disconnect part of) the 2-point correlator is the same as that for $\bar{\psi}\gamma^0\psi=\theta^\dagger\theta+\chi^\dagger\chi$. So,

$$\Delta(\tau)\;\approx\;M^2\chi_f\;=\;M^2\int_{\mathbf{x}}\Big\langle(\bar{\psi}\gamma_0\psi)(\tau,\mathbf{x})(\bar{\psi}\gamma_0\psi)(0,\mathbf{0})\Big\rangle_T\,, \tag{5.31}$$

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where χ_f is from eq. (4.1). As required, eq. (5.31) is independent of τ. Unfortunately, for $\Omega(\tau)$ of eq. (5.25), it is not clear to us whether any similar simplification is possible; the reasons for this are discussed at the beginning of section 6.

To summarize, from the Euclidean correlator, $\Omega(\tau)$ in eq. (5.25), we can in principle construct the Matsubara representation, $\tilde{\Omega}(\omega_n) \equiv \int_0^\beta \mathrm{d}\tau\, e^{i\omega_n\tau}\Omega(\tau)$, if an ultraviolet regulator or subtraction is present. After analytic continuation, $\rho_\Omega(\omega) = \mathrm{Im}\,\Omega(\omega_n \to -i[\omega+i0^+])$, the decay rate of eq. (5.24) follows from

$$\Gamma_{\mathrm{chem}} \equiv \frac{\lim_{\omega\to 0^+}\frac{2T\rho_\Omega(\omega)}{\omega}}{2\chi_f M^2} = \lim_{\omega\to 0^+}\left\{\frac{T\rho_\Omega(\omega)}{\omega\chi_f M^2}\right\}. \tag{5.32}$$

We remark that since eq. (5.25) involves composite operators for non-conserved quantities, the issue of renormalization is non-trivial. Unfortunately a satisfactory discussion goes beyond the scope of the present work.

6 Perturbative evaluation

So far we have made no approximation based on the weak-coupling expansion. At high T, however, the renormalized gauge coupling can be assumed small; we would like to make use of this limit in order to compare the general formulae with those in section 3.

It is now important to be more precise about the nature of the heavy-quark limit. Even though we made use of the "non-relativistic" spinors θ and χ in section 5.3 in order to obtain a physical interpretation for the operators appearing, the function $\Omega(\tau)$ *cannot* actually be evaluated with non-relativistic kinematics. A trivial reason is that with non-relativistic dispersion relations, a heavy quark and antiquark can annihilate into a single gluon; this non-sensical reaction would spoil the physics. In addition, in the t and u-channel processes of figure 1 the heavy quarks are deeply virtual, cf. eq. (3.7). That said, some parts of the analysis can still be simplified, but *a priori* the quark propagators need to be fully relativistic.

The relevant graphs are shown in figure 3. It is easy to see that the leading-order graph, (a), does not contribute: after analytic continuation and taking the cut we are faced with the decay of a heavy quark and a heavy antiquark into a gluon, which is forbidden by relativistic kinematics. At NLO, in contrast, there are non-vanishing contributions; let us show this explicitly by evaluating the fermionic graph in figure 4.

To get started, we note that in its original form the amplitude squared of eq. (3.4) reads

$$\begin{aligned} N_{\mathrm{f}}\sum|\mathcal{M}_2|^2 &= g^4 N_{\mathrm{f}}\mathrm{Tr}\,[T^aT^b]\mathrm{Tr}\,[T^aT^b] \\ &\quad\times\frac{\mathrm{Tr}\,[\gamma^\mu\mathcal{P}\!\!\!/_1\,\gamma^\nu\mathcal{P}\!\!\!/_2\,]\mathrm{Tr}\,[\gamma_\mu(\mathcal{K}\!\!\!/_1+M)\gamma_\nu(\mathcal{K}\!\!\!/_2-M)]}{(\mathcal{P}_1+\mathcal{P}_2)^4}\,, \end{aligned} \tag{6.1}$$

where T^a are the Hermitean generators of $\mathrm{SU}(N_{\mathrm{c}})$, normalized as $\mathrm{Tr}\,[T^aT^b] = \frac{\delta^{ab}}{2}$; whereas

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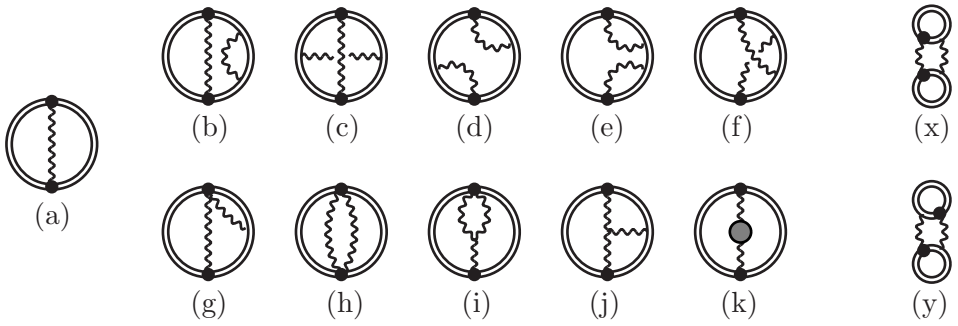

Figure 3. The graphs contributing to the correlator $\Omega(\tau)$ defined in eq. (5.25), up to $\mathcal{O}(g^4)$ (time runs vertically). The double lines denote heavy quarks; the small dots the composite operators; and the grey blob the 1-loop gauge field self-energy. Graphs (a)-(k) look similar to those relevant for computing the correlator yielding the heavy quark kinetic equilibration rate [32], but the kinematic regime is different. The additional graphs (x) and (y) amount to a renormalization of the gluonic part of the energy-momentum tensor by virtual heavy quarks, and have been excluded from the definition in eq. (5.25) by restricting to connected quark contractions.

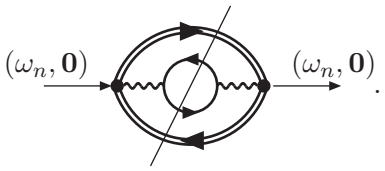

Figure 4. The part of diagram (k) of figure 3 sensitive to light quarks, after a Fourier transformation to Euclidean frequency ω_n and a rotation by 90 degrees. The diagonal line indicates a cut.

the imaginary time diagram of figure 4 can be written as

$$\begin{aligned}\tilde{\Omega}^{(q\bar{q})}(\omega_n) \,=\, & -g^4 N_{\rm f} \mathrm{Tr}\,[T^a T^b]\,\mathrm{Tr}\,[T^a T^b] \\ & \times \oint\!\!\!\!\!\!\sum_{\{P_1 P_2 K_1 K_2\}} \frac{\delta(\omega_n + P_1 + P_2 - K_1 - K_2)\,\varepsilon_{\mu;\alpha}(P_1+P_2)\varepsilon_{\nu;\beta}(P_1+P_2)}{P_1^2 P_2^2 (K_1^2+M^2)(K_2^2+M^2)} \\ & \times \frac{\mathrm{Tr}\,[\gamma_\alpha(i\not{P}_1)\gamma_\beta(i\not{P}_2)]\mathrm{Tr}\,[\gamma_\mu(i\not{K}_1+M)\gamma_\nu(i\not{K}_2-M)]}{(P_1+P_2)^4}\,. \end{aligned} \tag{6.2}$$

Here four-momenta and Dirac-matrices are Euclidean; ω_n within the δ is a short-hand for $(\omega_n, \mathbf{0})$; δ is normalized so that $\oint\!\!\!\!\!\!\sum_P \delta(P) = 1$; sum-integrals are standard, with $\oint\!\!\!\!\!\!\sum_{\{\ldots\}}$ denoting fermionic Matsubara frequencies; and

$$\varepsilon_{\mu;\alpha}(P) \equiv P_0\,\delta_{\mu\alpha} - P_\mu\,\delta_{0\alpha} \tag{6.3}$$

originates from the electric fields. A close kinship between eqs. (6.1), (6.2) is immediately observed, but to see that they really lead to the same physics requires a careful analysis.

We note, first of all, that the index μ appearing in eq. (6.3) can only be spatial. Therefore, in the heavy-quark part

$$\mathrm{Tr}\,[\gamma_\mu(i\not{K}_1+M)\gamma_\nu(i\not{K}_2-M)] = 4\big[\delta_{\mu\nu}(K_1\cdot K_2 - M^2) - K_{1\mu}K_{2\nu} - K_{1\nu}K_{2\mu}\big]\,, \tag{6.4}$$

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we can drop the terms $-K_{1\mu}K_{2\nu} - K_{1\nu}K_{2\mu}$ and the spatial part of $K_1 \cdot K_2$, because the heavy quarks will be non-relativistic, cf. eq. (3.5). The part containing final-state momenta,

$$\begin{aligned}
&\delta_{i\mu}\delta_{i\nu}\varepsilon_{\mu;\alpha}(P_1+P_2)\varepsilon_{\nu;\beta}(P_1+P_2)\mathrm{Tr}\,[\gamma_\alpha(i\not{P}_1)\gamma_\beta(i\not{P}_2)] \\
&\qquad = 4\,\varepsilon_{i;\alpha}(P_1+P_2)\varepsilon_{i;\beta}(P_1+P_2)\big[\delta_{\alpha\beta}P_1\cdot P_2 - P_{1\alpha}P_{2\beta} - P_{1\beta}P_{2\alpha}\big]\,, \qquad (6.5)
\end{aligned}$$

can in turn be re-expressed as ($P_i \equiv (p_{ni}, \mathbf{p}_i)$)

$$\varepsilon_{i;\alpha}\,\varepsilon_{i;\beta}\,\delta_{\alpha\beta} = 3(P_1+P_2)^2 - 2(\mathbf{p}_1+\mathbf{p}_2)^2\,, \qquad (6.6)$$

$$\varepsilon_{i;\alpha}\,\varepsilon_{i;\beta}\,P_{1\alpha}P_{2\beta} = (P_1+P_2)^2 p_{n1}p_{n2} - P_1^2(p_{n1}+p_{n2})p_{n2} - P_2^2(p_{n1}+p_{n2})p_{n1}\,. \qquad (6.7)$$

The latter two terms of eq. (6.7) do not contribute due to the antisymmetry in one of the summation variables (for instance, in the middle term, after first carrying out $T\sum_{p_{n1}}$ the expression is antisymmetric in p_{n2}), so we get

$$\begin{aligned}
\tilde{\Omega}^{(q\bar{q})}(\omega_n) \approx -8g^4 C_F N_c N_f \sum\!\!\!\!\!\!\int_{\{P_1P_2K_1K_2\}} \delta(\omega_n + P_1 + P_2 - K_1 - K_2)\frac{k_{n1}k_{n2} - M^2}{(K_1^2+M^2)(K_2^2+M^2)} \\
\times\frac{1}{P_1^2}\bigg\{\frac{3}{2P_2^2} - \frac{3}{(P_1+P_2)^2} + \frac{2(\mathbf{p}_1+\mathbf{p}_2)^2}{(P_1+P_2)^4} - \frac{(\mathbf{p}_1+\mathbf{p}_2)^2}{P_2^2(P_1+P_2)^2} - \frac{2p_{n1}p_{n2}}{P_2^2(P_1+P_2)^2}\bigg\}\,. \qquad (6.8)
\end{aligned}$$

To carry out the Matsubara sums, we write

$$\delta(\omega_n + p_{n1} + p_{n2} - k_{n1} - k_{n2}) = \int_0^\beta \mathrm{d}\tau\, e^{i(\omega_n + p_{n1} + p_{n2} - k_{n1} - k_{n2})\tau}\,. \qquad (6.9)$$

Then,

$$T^2\sum_{\{k_{n1}k_{n2}\}} \frac{(k_{n1}k_{n2} - M^2)e^{-i(k_{n1}+k_{n2})\tau}}{(k_{n1}^2+E_{k_1}^2)(k_{n2}^2+E_{k_2}^2)} \approx -\frac{1}{2}\frac{e^{(\beta-\tau)(E_{k_1}+E_{k_2})} + e^{\tau(E_{k_1}+E_{k_2})}}{(e^{\beta E_{k_1}}+1)(e^{\beta E_{k_2}}+1)}\,, \qquad (6.10)$$

where we again approximated $E_{k_a} \approx M$ in the spin part (but not in the exponential functions), whereby the "crossed terms" cancelled in the sum. As far as the second row of eq. (6.8) is concerned, we note that in the 2nd and 3rd terms a shift $p_{n2} \to p_{n2} - p_{n1}$ factorizes the p_{n1}-dependence from the τ-dependence. These terms lead to a vanishing contribution to the transport coefficient defined in eq. (5.32); the reason is that since neither ϵ_{p_1} nor ϵ_{p_2} appears in the time dependence, we are left with the phase space constraints $\delta(E_{k_1} + E_{qk_1} - q)$ or $\delta(E_{k_1} + E_{qk_1} + q)$, where $E_{qk_1} \equiv \sqrt{(\mathbf{q}-\mathbf{k_1})^2 + M^2}$ and $\mathbf{q} \equiv \mathbf{p}_1 + \mathbf{p}_2$. These constraints cannot get realized and so the factorized terms can be omitted.[4]

[4] In the case with the "double pole", i.e. the 3rd term of eq. (6.8), one can replace $(P_1+P_2)^2 \to (P_1+P_2)^2 + m_0^2$; consider first a single pole; and take subsequently a derivative with respect to m_0^2. The relevant phase space constraint becomes $\delta(E_{k_1} + E_{qk_1} - \epsilon_q)$, with $\epsilon_q \equiv \sqrt{q^2+m_0^2}$. This does not get realized if $m_0 < 2M$, so the function vanishes exactly in this regime, and thereby the derivative vanishes as well.

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Non-trivial contributions arise from the remaining three terms of eq. (6.8). Defining

$$\tilde{\mathcal{I}}_1(\omega_n) \equiv \int_0^\beta \mathrm{d}\tau\, e^{i\omega_n\tau}\, \frac{e^{(\beta-\tau)(E_{k_1}+E_{k_2})}+e^{\tau(E_{k_1}+E_{k_2})}}{(e^{\beta E_{k_1}}+1)(e^{\beta E_{k_2}}+1)}\, T^2 \sum_{\{p_{n1}p_{n2}\}} \frac{e^{i(p_{n1}+p_{n2})\tau}}{P_1^2 P_2^2}\,, \tag{6.11}$$

$$\tilde{\mathcal{I}}_2(\omega_n) \equiv \int_0^\beta \mathrm{d}\tau\, e^{i\omega_n\tau}\, \frac{e^{(\beta-\tau)(E_{k_1}+E_{k_2})}+e^{\tau(E_{k_1}+E_{k_2})}}{(e^{\beta E_{k_1}}+1)(e^{\beta E_{k_2}}+1)}\, T^2 \sum_{\{p_{n1}p_{n2}\}} \frac{e^{i(p_{n1}+p_{n2})\tau}(\mathbf{p}_1+\mathbf{p}_2)^2}{P_1^2 P_2^2 (P_1+P_2)^2}\,, \tag{6.12}$$

$$\tilde{\mathcal{I}}_3(\omega_n) \equiv \int_0^\beta \mathrm{d}\tau\, e^{i\omega_n\tau}\, \frac{e^{(\beta-\tau)(E_{k_1}+E_{k_2})}+e^{\tau(E_{k_1}+E_{k_2})}}{(e^{\beta E_{k_1}}+1)(e^{\beta E_{k_2}}+1)}\, T^2 \sum_{\{p_{n1}p_{n2}\}} \frac{e^{i(p_{n1}+p_{n2})\tau}p_{n1}p_{n2}}{P_1^2 P_2^2 (P_1+P_2)^2}\,; \tag{6.13}$$

analytically continuing $\rho_i(\omega) = \mathrm{Im}\,\tilde{\mathcal{I}}_i(\omega_n \to -i[\omega + i0^+])$; taking the limit $\omega \to 0$; and keeping only the terms that give a non-vanishing contribution, some work leads to

$$\lim_{\omega\to 0^+} \frac{T\rho_1(\omega)}{\omega} = \frac{f_{\mathrm{F}}(\epsilon_{p_1}) f_{\mathrm{F}}(\epsilon_{p_2})[1-f_{\mathrm{F}}(E_{k_1})][1-f_{\mathrm{F}}(E_{k_2})]}{4\epsilon_{p_1}\epsilon_{p_2}}\, 2\pi\delta(\epsilon_{p_1}+\epsilon_{p_2}-E_{k_1}-E_{k_2})\,, \tag{6.14}$$

$$\lim_{\omega\to 0^+} \frac{T\rho_2(\omega)}{\omega} = \lim_{\omega\to 0^+} \frac{T\rho_1(\omega)}{\omega} \times \frac{(\mathbf{p}_1+\mathbf{p}_2)^2}{(\mathbf{p}_1+\mathbf{p}_2)^2-(\epsilon_{p_1}+\epsilon_{p_2})^2}\,, \tag{6.15}$$

$$\lim_{\omega\to 0^+} \frac{T\rho_3(\omega)}{\omega} = \lim_{\omega\to 0^+} \frac{T\rho_1(\omega)}{\omega} \times \frac{-\epsilon_{p_1}\epsilon_{p_2}}{(\mathbf{p}_1+\mathbf{p}_2)^2-(\epsilon_{p_1}+\epsilon_{p_2})^2}\,. \tag{6.16}$$

In the non-relativistic limit, $M \gg \pi T$, the subsequent spatial integrals can also be carried out. Indeed detailed balance,

$$\begin{aligned} &f_{\mathrm{F}}(\epsilon_{p_1}) f_{\mathrm{F}}(\epsilon_{p_2})[1-f_{\mathrm{F}}(E_{k_1})][1-f_{\mathrm{F}}(E_{k_2})]\delta(\epsilon_{p_1}+\epsilon_{p_2}-E_{k_1}-E_{k_2}) \\ &\quad = f_{\mathrm{F}}(E_{k_1}) f_{\mathrm{F}}(E_{k_2})[1-f_{\mathrm{F}}(\epsilon_{p_1})][1-f_{\mathrm{F}}(\epsilon_{p_2})]\delta(\epsilon_{p_1}+\epsilon_{p_2}-E_{k_1}-E_{k_2})\,, \end{aligned} \tag{6.17}$$

guarantees that the momenta k_1, k_2 are non-relativistic, like in eq. (3.5). Momentum conservation requires that $\mathbf{p_1}+\mathbf{p_2}$ is also non-relativistic, and that $f_{\mathrm{F}}(\epsilon_{p_i})$ are exponentially small. So, from eqs. (6.8)–(6.17),

$$\begin{aligned} \lim_{\omega\to 0^+} \frac{T\rho_\Omega^{(q\bar{q})}(\omega)}{\omega} &\approx 4g^4 C_F N_{\mathrm{c}} N_{\mathrm{f}} \int_{\mathbf{p_1 p_2 k_1 k_2}} \frac{f_{\mathrm{F}}(E_{k_1}) f_{\mathrm{F}}(E_{k_2})}{4\epsilon_{p_1}\epsilon_{p_2}} \\ &\quad \times (2\pi)^4 \delta^{(4)}(\mathcal{P}_1+\mathcal{P}_2-\mathcal{K}_1-\mathcal{K}_2)\left\{\frac{3}{2} - \frac{2\epsilon_{p_1}\epsilon_{p_2}}{(\epsilon_{p_1}+\epsilon_{p_2})^2}\right\} \\ &\approx \frac{g^4 C_F N_{\mathrm{c}} N_{\mathrm{f}}}{M^2} \int_{\mathbf{p_1 p_2 k_1 k_2}} f_{\mathrm{F}}(E_{k_1}) f_{\mathrm{F}}(E_{k_2})\, (2\pi)^4 \delta^{(3)}(\mathbf{p_1}+\mathbf{p_2})\delta(2p_1-2M) \\ &= \frac{g^4 C_F N_{\mathrm{c}} N_{\mathrm{f}}}{2\pi} \int_{\mathbf{k_1}} f_{\mathrm{F}}(E_{k_1}) \int_{\mathbf{k_2}} f_{\mathrm{F}}(E_{k_2})\,. \end{aligned} \tag{6.18}$$

Dividing by χ_f from eq. (4.3), eq. (5.32) finally yields

$$\Gamma_{\mathrm{chem}}^{(q\bar{q})} \approx \frac{g^4 C_F N_{\mathrm{f}}}{8\pi M^2} \left(\frac{MT}{2\pi}\right)^{\frac{3}{2}} e^{-M/T}\,. \tag{6.19}$$

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This agrees with eq. (3.8).

As far as the gluonic contributions are concerned, the situation is complicated by the many diagrams appearing in figure 3; indeed we have checked that all diagram classes, with two, three and four heavy quark propagators, need to be summed together in order to obtain gauge-independent results. Nevertheless, without getting lost in excruciating detail, we can draw on eqs. (6.1), (6.2) to present a short but "suggestive" argument that things work out as before. For the s-channel process, the vacuum amplitude squared reads

$$\begin{aligned}\sum |\mathcal{M}_1|^2_{ss} \,=\, & g^4 \mathrm{Tr}\,[T^a T^b] f^{acd} f^{bcd} \;\; \mathbb{P}_T^{\sigma\tilde{\sigma}}(\mathcal{P}_1)\, \mathbb{P}_T^{\rho\tilde{\rho}}(\mathcal{P}_2) \\ & \times \frac{\mathrm{Tr}\,[\gamma^\mu(\not{K}_1 + M)\gamma^\nu(\not{K}_2 - M)]}{(\mathcal{P}_1+\mathcal{P}_2)^4} \\ & \times \big[\eta_{\sigma\rho}(\mathcal{P}_2-\mathcal{P}_1)_\mu - \eta_{\rho\mu}(\mathcal{P}_1+2\mathcal{P}_2)_\sigma + \eta_{\mu\sigma}(2\mathcal{P}_1+\mathcal{P}_2)_\rho\big] \\ & \times \big[\eta_{\tilde{\sigma}\tilde{\rho}}(\mathcal{P}_2-\mathcal{P}_1)_\nu - \eta_{\tilde{\rho}\nu}(\mathcal{P}_1+2\mathcal{P}_2)_{\tilde{\sigma}} + \eta_{\nu\tilde{\sigma}}(2\mathcal{P}_1+\mathcal{P}_2)_{\tilde{\rho}}\big] \,. \end{aligned} \tag{6.20}$$

Here $\mathbb{P}_T$ denotes the projector from a sum over the on-shell gluon polarizations, and Feynman gauge was used for the inner gluon line. On the other hand, the gluonic equivalent of the process in figure 4 can be written in Feynman gauge as

$$\begin{aligned}\delta\tilde{\Omega}^{(gg)}(\omega_n) \,=\, & -\frac{1}{2}\, g^4 \mathrm{Tr}\,[T^a T^b]\, f^{acd} f^{bcd} \\ & \times \oint\!\!\!\!\!\!\sum_{P_1 P_2 \{K_1 K_2\}} \frac{\delta(\omega_n + P_1 + P_2 - K_1 - K_2)\, \varepsilon_{\mu;\alpha}(P_1+P_2)\varepsilon_{\nu;\beta}(P_1+P_2)}{P_1^2 P_2^2 (K_1^2+M^2)(K_2^2+M^2)} \\ & \times \frac{\mathrm{Tr}\,[\gamma_\mu(i\not{K}_1 + M)\gamma_\nu(i\not{K}_2 - M)]}{(P_1+P_2)^4} \\ & \times \big[\delta_{\sigma\rho}(iP_2-iP_1)_\alpha - \delta_{\rho\alpha}(iP_1+2iP_2)_\sigma + \delta_{\alpha\sigma}(2iP_1+iP_2)_\rho\big] \\ & \times \big[\delta_{\sigma\rho}(iP_2-iP_1)_\beta - \delta_{\rho\beta}(iP_1+2iP_2)_\sigma + \delta_{\beta\sigma}(2iP_1+iP_2)_\rho\big] \,. \end{aligned} \tag{6.21}$$

Establishing a precise equivalence between all indices requires adding other gluonic contributions on both sides, but a comparison with eqs. (6.1), (6.2), for which we carried out a detailed analysis, allows us to anticipate that things work out here as well, including the important factor $\frac{1}{2}$ in front of the gluonic channels in eq. (3.3), clearly visible in eq. (6.21).

7 Discussion

The question of whether or not heavy quarks chemically equilibrate in heavy ion collisions is sometimes addressed by comparing the observed total yield with that predicted by a thermal distribution at the *final* (pionic) freeze-out temperature. In this paper, we have have asked whether chemical equilibrium could be reached earlier on, at a *higher* temperature. Since there are many heavy quarks in the initial state, one simply needs to get rid of some of them, to arrive at a thermal ensemble. The rate for this is suppressed by $e^{-M/T}$,

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which is the density of antiquarks seen by any given heavy quark. If this suppression can be overcome then, for a while, heavy quarks could be part of the thermal medium, before re-decoupling again above the final pionic freeze-out, explaining why more heavy quarks and antiquarks are observed than is due for chemical equilibrium.

Taking the expression from eq. (3.10); factorizing from it the susceptibility of eq. (4.3); normalizing the susceptibility to its value in the massless limit, to be denoted by $\chi_0 \equiv N_{\rm c}T^3/3$; and setting $N_{\rm c} = 3$, the result for the chemical equilibration rate reads

$$\Gamma_{\rm chem} \;\simeq\; \frac{2\pi\alpha_s^2 T^3}{9M^2}\left(\frac{7}{6} + N_{\rm f}\right)\frac{\chi_{\rm f}}{\chi_0}\,. \tag{7.1}$$

Setting furthermore $N_{\rm f} = 3$, $\alpha_s \sim 0.3$, $M \sim 1.5\,\mathrm{GeV}$, and estimating χ_f/χ_0 from refs. [27, 28], we obtain $\Gamma^{-1}_{\rm chem} \sim 10\,\mathrm{fm/c}$ at $T \sim 600\,\mathrm{MeV}$, and $\Gamma^{-1}_{\rm chem} \gtrsim 60\,\mathrm{fm/c}$ at $T \sim 400\,\mathrm{MeV}$. If true, these time scales indicate that chemical equilibrium is unlikely to be reached in current heavy ion collision experiments, where the highest temperatures are around $T \sim 400\,\mathrm{MeV}$ and the time scale is around $10\,\mathrm{fm/c}$.

The estimate presented in eq. (7.1) is a rough one. In principle, a non-perturbative value could be obtained from eq. (5.32) through numerical lattice Monte Carlo simulations and a subsequent analytic continuation. For the latter step, short-distance singularities need to be subtracted, as has recently been elaborated upon in connection with other transport coefficients [33, 34]. This task is undoubtedly a hard one: as an analysis of graph (a) of figure 3 shows, for $\omega \gg M$ the spectral function behaves as

$$\rho_\Omega(\omega) \stackrel{\omega\gg M}{=} \frac{g^2 C_F N_{\rm c}}{120(4\pi)^3}\left[\omega^6 + \mathcal{O}(\omega^2 M^4)\right]\,, \tag{7.2}$$

implying that the Euclidean correlator diverges as $\Omega(\tau) \sim 1/\tau^7$ for $\tau \ll M^{-1}$. To subtract this dominant and any subdominant divergences perturbatively, and still retain a statistically significant signal containing the thermal physics, would require a very precise analysis. (Alternatively one could start with the correlator $\Delta(\tau)$ of eq. (5.26), although this is dominated by a constant mode, which poses problems for some methods of analytic continuation.)

Nevertheless, our non-perturbative formulation may have other uses; for instance, it may be amenable to an order-of-magnitude estimate in the confined phase through chiral effective theories, similarly to what has previously been achieved in the case of the heavy flavour kinetic equilibration rate [35]–[38]. Possibly it could also be combined with non-relativistic QCD (NRQCD) where the hard ($p \sim M$) momentum fields have been integrated out perturbatively. Indeed it is possible to include the effects of $Q\overline{Q}$ annihilation in NRQCD, through a 4-fermion interaction in the effective Lagrangian, where the effective coupling has an imaginary part [39]. In this case one cannot consider $\Omega(\tau)$ of eq. (5.25) because the chromo-electric field is hard and should have been integrated out; but one could compute $\Delta(\tau)$ of eq. (5.26) instead.

We end by remarking that whereas our non-perturbative formulation is only valid near equilibrium, the Boltzmann description can also be applied beyond it. Since $\Gamma_{\rm chem}$ is proportional to the density of the antiquarks, cf. eqs. (3.1)–(3.3), we may expect a correspondingly faster rate in the real world where the heavy antiquarks appear in overabundance.

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