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A way to estimate the heavy quark thermalization rate from the lattice

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ABSTRACT: The thermalization rate of a heavy quark is related to its momentum diffusion coefficient. Starting from a Kubo relation and using the framework of the heavy quark effective theory, we argue that in the large-mass limit the momentum diffusion coefficient can be defined through a certain Euclidean correlation function, involving color-electric fields along a Polyakov loop. Furthermore, carrying out a perturbative computation, we demonstrate that the spectral function corresponding to this correlator is relatively flat at small frequencies. Therefore, unlike in the case of several other transport coefficients, for which the narrowness of the transport peak makes analytic continuation from Euclidean lattice data susceptible to severe systematic uncertainties, it appears that the determination of the heavy quark thermalization rate could be relatively well under control.

KEYWORDS: Thermal Field Theory, Lattice Gauge Field Theories, Heavy Quark Physics

Contents

1	Introduction	1
2	Reduction of the current-current correlator	2
2.1	Definitions	2
2.2	Heavy quark limit	5
2.3	Euclidean correlator	6
3	Perturbation theory	8
4	Correlator in lattice regularization	11
5	Conclusions and outlook	12
A	Examples of dynamics leading to a transport peak	13

1 Introduction

One of the very interesting discoveries of the RHIC program at Brookhaven National Laboratory has been that heavy quarks (particularly the charm quarks) appear to thermalize just about as effectively as the light quarks. This has been inferred from measuring the electron p_T -spectra produced by the decays of the heavy quarks, showing indications of the same type of hydrodynamic flow as experienced by the lighter quarks [1].

On the theoretical side, the historical starting point for a QCD-based understanding of the behavior of heavy quarks in a thermal environment was the determination of their energy loss rate to the leading order in the QCD coupling constant, α_s [2]. The energy loss is directly related to a number of other concepts, such as the diffusion and the thermalization rates of the heavy quarks [3, 4]. In particular, assuming that the effective value of α_s is relatively small leads to the thermalization rate $\Gamma \sim \alpha_s^2 T^2/M$, where T is the temperature and M is the heavy quark mass [4]. The comparable thermalization rate for a light quark or gluon is $\Gamma \sim \alpha_s^2 T$, or at very high energies $\Gamma \sim \alpha_s^2 T \sqrt{T/E}$ [5]. Hence heavy quarks with $M \gg T$ are expected to thermalize slowly, particularly at weak coupling.

As already mentioned, the empirical facts appear however to be in conflict with a slow thermalization rate [1]. This has led to a lot of new theoretical ideas, with the hope of bringing the theoretical determination of Γ beyond the leading order in α_s . In particular, possibilities for a lattice determination were explored [6]; computations in a strongly coupled theory with some similarities with QCD were carried out [7, 8]; phenomenological model treatments of bound states were considered [9]; and the first weak-coupling corrections to the leading order result were determined [10]. The studies [7]–[10] showed

that there could indeed be substantial corrections (of a positive sign) to the leading order result; at the same time, the study [6] showed that a direct lattice determination of the heavy quark related observables would be extremely hard, because the physics resides in a “transport peak” of a certain spectral function, of width $\Delta\omega \sim \Gamma \sim \alpha_s^2 T^2/M \ll T$, which regime is practically impossible to explore with Euclidean techniques.

The purpose of this paper is to reconsider the prospects for a lattice determination, making use of heavy quark effective theory [11] in order to systematically consider the behavior of the heavy quarks in the limit $M \gg T$. Essentially, this allows us to restrict the attention to the “numerator” of the thermalization rate, $\sim \alpha_s^2 T^2$, which remains finite in the heavy quark limit. In fact, our main goal will be to derive an observable measurable on the lattice which has its structure at “large” frequencies, $\omega \sim \alpha_s^{1/2} T \gg \Gamma$, and can be addressed much more easily than Γ itself.

We note that, in many respects, our study parallels that in ref. [8]. The main differences are that we use the imaginary-time formalism rather than the real-time one, in order to make contact with the Euclidean spacetime accessible to lattice techniques; and that we try to keep explicit track of $\mathcal{O}(\alpha_s)$ quantum corrections and renormalization issues.

The plan of this paper is the following. In section 2 we derive, by going through several intermediate steps, the observable alluded to above, consisting of color-electric fields along a Polyakov loop. In section 3 we analyze the corresponding spectral function perturbatively, demonstrating a relatively flat behavior at small $\omega \lesssim \alpha_s^{1/2} T$. In section 4 we suggest a lattice discretization for the object derived in section 2, while section 5 offers some conclusions and an outlook.

2 Reduction of the current-current correlator

In order to proceed with our derivation, we focus on one of the heavy quarks of physical QCD; either the charm or the bottom quark. We assume for the moment the use of dimensional regularization in order to regulate the theory (though we do not indicate this explicitly). Then there is only one large scale in the system, namely the (renormalized) heavy quark mass, M , and the task is to account for its effects analytically in the basic observable to be defined presently (eq.(2.1)). In section 4 we return to the complications emerging in lattice regularization.

2.1 Definitions

The diffusive motion of heavy quarks within a thermalized medium can be characterized by four different quantities, all of which are related to each other (at least in the weak-coupling limit). We start by defining the “diffusion coefficient”, D , proceeding then to the “relaxation rate” or “drag coefficient”, η_D , and the “momentum diffusion coefficient”, κ . The fourth quantity, the energy loss dE/dx , is historically the first one addressed within QCD [2]; yet it is not obvious how it could be related to the others on the non-perturbative level, so we omit it from the discussion below.

Among the three quantities, the one that can most directly be defined within quantum field theory is the diffusion coefficient D . Consider the spectral function related to the

current-current correlator,

$$\rho_V^{\mu\nu}(\omega) \equiv \int_{-\infty}^{\infty} dt e^{i\omega t} \int d^3\mathbf{x} \left\langle \frac{1}{2} [\hat{\mathcal{J}}^\mu(t, \mathbf{x}), \hat{\mathcal{J}}^\nu(0, \mathbf{0})] \right\rangle, \quad (2.1)$$

where $\hat{\mathcal{J}}^\mu \equiv \hat{\psi} \gamma^\mu \hat{\psi}$; $\hat{\psi}$ is the heavy quark field operator in the Heisenberg picture; $\langle \dots \rangle \equiv \mathcal{Z}^{-1} \text{Tr}[(\dots)e^{-\beta \hat{H}}]$ is the thermal expectation value; and $\beta \equiv 1/T$ is the inverse temperature. Diffusive motion leads to a pole in the spectral function at $\omega = -iD\mathbf{k}^2$, where \mathbf{k} is the momentum (already set to zero in eq.(2.1)). Solving for the pole position and making use of various symmetries leads to the Kubo relation (see, e.g., section 6 of ref. [12])

$$D = \frac{1}{3\chi^{00}} \lim_{\omega \rightarrow 0} \sum_{i=1}^3 \frac{\rho_V^{ii}(\omega)}{\omega}. \quad (2.2)$$

Here χ^{00} corresponds to a ‘‘susceptibility’’ related to the conserved charge $\int d^3\mathbf{x} \hat{\mathcal{J}}^0(t, \mathbf{x})$,

$$\chi^{00} \equiv \beta \int d^3\mathbf{x} \left\langle \hat{\mathcal{J}}^0(t, \mathbf{x}) \hat{\mathcal{J}}^0(t, \mathbf{0}) \right\rangle. \quad (2.3)$$

For a dilute system of heavy quarks, $T\chi^{00}$ defines their ‘‘number density’’.¹ Note that the conserved vector current $\hat{\mathcal{J}}^\mu$ does not require renormalization, so that the definitions in eqs.(2.2) and (2.3) are guaranteed to be ultraviolet finite at any order.

To define the other quantities, we need to assume that the spectral function around zero frequency possesses a narrow transport peak. Due to a heavy quark’s large inertia, this is certainly true for M sufficiently large, which we assume to be the case from now on. In this limit, the spectral function will on general grounds take the form of a Lorentzian,²

$$\sum_i \frac{\rho_V^{ii}(\omega)}{\omega} \stackrel{\omega \lesssim \omega_{UV}}{\approx} 3\chi^{00} D \frac{\eta_D^2}{\eta_D^2 + \omega^2}, \quad (2.4)$$

where ω_{UV} is a frequency scale at which the Lorentzian is overtaken by other types of physical processes.

The other two transport coefficients are then defined from the properties of the transport peak. We define the ‘‘drag coefficient’’ η_D to be the width of the Lorentzian, and the (a priori mass-dependent) ‘‘momentum diffusion coefficient’’ $\kappa^{(M)}$ to be M_{kin}^2 times the coefficient of the power-law falloff of its tails,

$$\kappa^{(M)} \equiv \frac{M_{\text{kin}}^2 \omega^2}{3T\chi^{00}} \sum_i \frac{2T\rho_V^{ii}(\omega)}{\omega} \Big|_{\eta_D \ll |\omega| \lesssim \omega_{UV}}. \quad (2.5)$$

Here M_{kin} refers to the heavy quark’s kinetic mass, to be defined presently (cf. eq.(2.7)). Later on we will define a transport coefficient κ from the $M \rightarrow \infty$ limit of $\kappa^{(M)}$.

¹In the non-relativistic limit and at zero chemical potential, $T\chi^{00} = 4N_c(MT/2\pi)^{3/2} \exp(-\beta M)$; however, our basic arguments hold also at a non-zero chemical potential for the heavy quarks, whereby the exponential suppression could be removed from $T\chi^{00}$.

²Two concrete examples for how such a dependence on ω can arise are reviewed in appendix A.

The physical motivation for the definition in eq.(2.5) is as follows. In the dilute limit the current $\hat{\mathcal{J}}^\mu$ couples individually to the heavy quarks; the spectral function $\rho_V^{\mu\nu}(\omega)$ is thus a product of their number density $T\chi^{00}$ times a contribution from one heavy quark. For a single quark, $\int d^3\mathbf{x} \hat{\mathcal{J}}^i \equiv \hat{v}^i$ represents a non-perturbative measurement of its velocity. Recalling Newton's law, $M_{\text{kin}} d\hat{\mathcal{J}}^i/dt$ is the force acting on the heavy quark; thus $\kappa^{(M)}$ is a correlator of that force with itself at different times, transformed into frequency space. The factor $2T/\omega$ relates the spectral function to a time-symmetric correlator, for which this classically motivated argumentation applies. Thus eq.(2.5) generalizes, in a non-perturbative way, the force-force correlator definition of κ given in ref. [8]. The condition on ω instructs us to integrate this force over a time scale, long compared with the medium's correlation time (set by $t \sim \omega_{\text{UV}}^{-1}$), but short compared with the dynamics of the heavy quark (set by $t \sim \eta_D^{-1}$).

The coefficients D , η_D and $\kappa^{(M)}$ thus defined are related by fluctuation-dissipation relations, which follow from the fact that the area under the transport peak defines the (coarse-grained) equal-time mean-squared velocity of a heavy quark,

$$\langle \mathbf{v}^2 \rangle \equiv \frac{1}{T\chi^{00}} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \sum_i \frac{2T\rho_V^{ii}(\omega)}{\omega} G_{\text{UV}}(\omega) . \tag{2.6}$$

Here we have introduced a cutoff function $G_{\text{UV}}(\omega)$ designed to isolate the transport peak from other types of physics, for instance $G_{\text{UV}}(\omega) = \theta(\omega_{\text{UV}} - |\omega|)$. In the time domain we are thus averaging over a time scale $t_{\text{UV}} \gtrsim \omega_{\text{UV}}^{-1}$. Such a time averaging is mandatory to make $\langle \mathbf{v}^2 \rangle$ finite and well-defined, since an instantaneous measurement of the heavy quark's velocity would induce it to radiate (or absorb) large amounts of energy, thereby changing its state. We emphasize that, were there no sharp zero-frequency peak in the spectral function, there would be no unambiguous notion of a heavy quark's (coarse-grained) mean squared velocity.

Motivated by the standard non-relativistic thermodynamic result, we can now define a kinetic mass via

$$\langle \mathbf{v}^2 \rangle \equiv 3 \frac{T}{M_{\text{kin}}} . \tag{2.7}$$

Eqs. (2.4)–(2.6) then yield the fluctuation-dissipation, or Einstein, relations:

$$D = \frac{2T^2}{\kappa^{(M)}} , \quad \eta_D = \frac{\kappa^{(M)}}{2M_{\text{kin}}T} , \tag{2.8}$$

both of which involve $\mathcal{O}(\eta_D/\omega_{\text{UV}})$ relative uncertainties. Note that $\eta_D \sim 1/M_{\text{kin}}$ in the large mass limit, assuming that $\kappa^{(M)}$ contains no (power-like) dependence on M_{kin} , justifying the narrow peak assumption.

Thermodynamic considerations relate the kinetic mass defined in eq.(2.7) to the standard notion. Namely, thanks to the slow dynamics of a heavy quark, one can (approximately) define a free energy $F(\mathbf{v})$ as a function of its velocity (time-averaged over a period $\sim t_{\text{UV}}$); expanding it as $F(\mathbf{v}) = M_{\text{rest}} + M_{\text{kin}}\mathbf{v}^2/2 + \mathcal{O}(\mathbf{v}^4)$ at small \mathbf{v} and taking a thermodynamic average should reproduce eq.(2.7).

The only approximations we have made so far concern the assumption of a narrow transport peak. Parametrically, in weakly coupled QCD [4], $\rho_V^{ii}(\omega)/(\chi^{00}\omega)$ has a peak value $D \sim 1/g^4 T$, where $g^2 \equiv 4\pi\alpha_s$; a width $\eta_D \sim g^4 T^2/M$; and a perturbative ultraviolet contribution which will start to depart from the $1/\omega^2$ Lorentzian tail at the scale $\omega_{UV} \sim gT$ (see section 3). Thus errors are of order $\eta_D/gT \sim g^3 T/M$. In strongly coupled multicolor ($N_c \rightarrow \infty$) $\mathcal{N} = 4$ Super-Yang-Mills theory [7], with a 't Hooft coupling $\lambda = g^2 N_c$, the width of the transport peak is $\eta_D \sim \sqrt{\lambda} T^2/M$, and the continuum takes over at $\omega_{UV} \sim T$; thus ambiguities are suppressed by $\sqrt{\lambda} T/M$.

Expecting the force-force correlator $\kappa^{(M)}$ to actually be mass-independent at large M_{kin} , as will be verified *a posteriori*, we are finally led to take the $M_{\text{kin}} \rightarrow \infty$ limit of eq.(2.5), inside of which it is essential to retain ω small but non-zero:

$$\kappa \equiv \frac{\beta}{3} \sum_{i=1}^3 \lim_{\omega \rightarrow 0} \omega^2 \left[\lim_{M \rightarrow \infty} \frac{M_{\text{kin}}^2}{\chi^{00}} \int_{-\infty}^{\infty} dt e^{i\omega t} \int d^3 \mathbf{x} \left\langle \frac{1}{2} \left\{ \hat{\mathcal{J}}^i(t, \mathbf{x}), \hat{\mathcal{J}}^i(0, \mathbf{0}) \right\} \right\rangle \right]. \quad (2.9)$$

The factor $2T/\omega$ has been accounted for by replacing the spectral function by a time-symmetric correlator. Eq. (2.9) will be the starting point for the further steps to be taken.

2.2 Heavy quark limit

Starting from the definition in eq.(2.9), our next goal is to carry out the limit $M \rightarrow \infty$. As a first step we note that, making use of time translational invariance and carrying out partial integrations, the definition in eq.(2.9) can be rephrased as

$$\kappa = \frac{\beta}{3} \sum_{i=1}^3 \lim_{\omega \rightarrow 0} \left[\lim_{M \rightarrow \infty} \frac{M_{\text{kin}}^2}{\chi^{00}} \int_{-\infty}^{\infty} dt e^{i\omega(t-t')} \int d^3 \mathbf{x} \left\langle \frac{1}{2} \left\{ \frac{d\hat{\mathcal{J}}^i(t, \mathbf{x})}{dt}, \frac{d\hat{\mathcal{J}}^i(t', \mathbf{0})}{dt'} \right\} \right\rangle \right]. \quad (2.10)$$

In order to evaluate the time derivatives here, let us rewrite the QCD Lagrangian, $\mathcal{L}_{\text{QCD}} = \bar{\psi}(i\gamma^\mu D_\mu - M)\psi + \mathcal{L}_{\text{light}}$, after a Foldy-Wouthuysen transformation [13]: expanding in $1/M$ and dropping total derivatives, this yields

$$\begin{aligned} \mathcal{L}_{\text{QCD}} = & \theta^\dagger \left(iD_0 - M + \frac{c_2 \mathbf{D}^2 + c_B \boldsymbol{\sigma} \cdot g\mathbf{B}}{2M} \right) \theta + \phi^\dagger \left(iD_0 + M - \frac{c_2 \mathbf{D}^2 + c_B \boldsymbol{\sigma} \cdot g\mathbf{B}}{2M} \right) \phi \\ & + \frac{i c_E}{2M} \left(\theta^\dagger \boldsymbol{\sigma} \cdot g\mathbf{E} \phi - \phi^\dagger \boldsymbol{\sigma} \cdot g\mathbf{E} \theta \right) + \mathcal{O} \left(\frac{1}{M^2} \right) + \mathcal{L}_{\text{light}}, \end{aligned} \quad (2.11)$$

where $D_i = \partial_i - igA_i$, $gB_i \equiv \frac{i}{2} \epsilon_{ijk} [D_j, D_k]$, $gE_i \equiv i[D_0, D_i]$, and θ, ϕ are two-component spinors. The mass M is the pole mass,³

$$M = m(\bar{\mu}) \left\{ 1 + \frac{3g^2 C_F}{(4\pi)^2} \left[\ln \frac{\bar{\mu}^2}{m^2(\bar{\mu})} + \frac{4}{3} \right] + \mathcal{O}(g^4) \right\}, \quad (2.12)$$

where $m(\bar{\mu})$ is the $\overline{\text{MS}}$ mass. In regularization schemes respecting Lorentz invariance, the coefficient c_2 must equal unity (because the combination needed for solving for the pole

³ This is true in schemes producing no additive mass renormalization, such as dimensional regularization. There is no multiplicative renormalization to M in eq.(2.11) either, because M could be shifted to zero by the field redefinitions $\theta \rightarrow e^{-iMt}\theta$, $\phi \rightarrow e^{iMt}\phi$ and would then remain zero quantum mechanically.

mass is $\sim p_0^2 - \mathbf{p}^2 - M^2$), and we assume this to be the case in the following. The matching coefficients c_B, c_E equal unity at leading order but have quantum corrections; these are not needed in the present study. Note that the linearly appearing “rest mass” M is normally shifted away (or rather replaced with 0^+); however, we prefer to keep it explicit for the moment, because the shifts needed are non-trivial at a non-zero temperature, where the Euclidean time extent is finite.

Setting $c_2 = 1$ in eq.(2.11), we can read off the conserved Noether current and the Hamiltonian in the heavy quark-mass limit:

$$\hat{\mathcal{J}}^0 = \hat{\theta}^\dagger \hat{\theta} + \hat{\phi}^\dagger \hat{\phi}, \quad (2.13)$$

$$\hat{\mathcal{J}}^j = \frac{i}{2M} \left[\hat{\theta}^\dagger (\overleftarrow{D}^j - \overrightarrow{D}^j) \hat{\theta} - \hat{\phi}^\dagger (\overleftarrow{D}^j - \overrightarrow{D}^j) \hat{\phi} \right] + \mathcal{O}\left(\frac{1}{M^2}\right), \quad (2.14)$$

$$\hat{H} = \int d^3\mathbf{x} \left[\hat{\theta}^\dagger (-gA_0 + M) \hat{\theta} - \hat{\phi}^\dagger (gA_0 + M) \hat{\phi} \right] + \mathcal{O}\left(\frac{1}{M}\right). \quad (2.15)$$

Here we treat the fermionic fields as operators but the gauge fields as c-numbers, anticipating a path integral treatment of the gauge fields. The time derivatives needed for eq.(2.10) can subsequently be taken according to the canonical equations of motion,

$$\frac{d\hat{\mathcal{J}}^i}{dt} = i[\hat{H}, \hat{\mathcal{J}}^i] + \frac{\partial \hat{\mathcal{J}}^i}{\partial t}, \quad (2.16)$$

where the partial derivative operates on the background gauge fields. The commutator is readily evaluated with the help of equal-time anticommutators, and we also note that since eq.(2.10) includes a spatial integral over the currents, partial integrations are allowed. Adding together the two parts in eq.(2.16) then yields

$$\frac{d\hat{\mathcal{J}}^i}{dt} = \frac{1}{M} \left\{ \hat{\phi}^\dagger gE^i \hat{\phi} - \hat{\theta}^\dagger gE^i \hat{\theta} \right\} + \mathcal{O}\left(\frac{1}{M^2}\right). \quad (2.17)$$

This can now be inserted into eq.(2.10), whereby the explicit factors of M duly cancel, since $M_{\text{kin}} = M$ up to $\mathcal{O}(T/M)$ thermal corrections which vanish in the heavy quark-mass limit:

$$\kappa = \frac{\beta}{3} \sum_{i=1}^3 \lim_{M \rightarrow \infty} \frac{1}{\chi^{00}} \int dt d^3\mathbf{x} \left\langle \frac{1}{2} \left\{ \left[\hat{\phi}^\dagger gE^i \hat{\phi} - \hat{\theta}^\dagger gE^i \hat{\theta} \right](t, \mathbf{x}), \left[\hat{\phi}^\dagger gE^i \hat{\phi} - \hat{\theta}^\dagger gE^i \hat{\theta} \right](0, \mathbf{0}) \right\} \right\rangle. \quad (2.18)$$

At this point the heavy quarks have become purely static; the ordering of the limits no longer matters, so we have set $\omega \rightarrow 0$ inside the Fourier transform.

Given that our derivation made no use of weak-coupling approximations, we believe that eq.(2.18) is free from (even finite) renormalization to all orders in perturbation theory, in the assumed regularization schemes with no additive mass renormalization and c_2 equal to unity. This shows, in particular, that κ is M -independent.

2.3 Euclidean correlator

Eq.(2.18) is a two-point function of gauge-invariant local operators; it therefore satisfies the standard KMS conditions which allow us to relate it to a Euclidean correlation function.

In particular, let us define the Euclidean correlator

$$G_E(\tau) \equiv -\frac{\beta}{3} \sum_{i=1}^3 \lim_{M \rightarrow \infty} \frac{1}{\chi^{00}} \int d^3\mathbf{x} \left\langle \left[\phi^\dagger g E_i \phi - \theta^\dagger g E_i \theta \right] (\tau, \mathbf{x}) \left[\phi^\dagger g E_i \phi - \theta^\dagger g E_i \theta \right] (0, \mathbf{0}) \right\rangle . \quad (2.19)$$

Hats have been left out because regular Euclidean path integral techniques apply for this object, and the minus sign accounts for the fact that a Euclidean electric field differs by a factor i from the Minkowskian one. The corresponding spectral function can be determined by inverting (for recent practical recipes see, e.g., refs. [14]⁴) the relation

$$G_E(\tau) = \int_0^\infty \frac{d\omega}{\pi} \rho(\omega) \frac{\cosh\left(\frac{\beta}{2} - \tau\right) \omega}{\sinh\frac{\beta\omega}{2}} , \quad (2.20)$$

or analytically from

$$\tilde{G}_E(\omega_n) \equiv \int_0^\beta d\tau e^{i\omega_n \tau} G_E(\tau) , \quad (2.21)$$

$$\rho(\omega) = \text{Im} \tilde{G}_E(\omega_n \rightarrow -i[\omega + i0^+]) . \quad (2.22)$$

The momentum diffusion coefficient then follows from

$$\kappa = \lim_{\omega \rightarrow 0} \frac{2T}{\omega} \rho(\omega) . \quad (2.23)$$

Note also that by making use of eq.(2.13), the susceptibility χ^{00} defined in eq.(2.3) can in the Euclidean theory be written as

$$\chi^{00} = \int_0^\beta d\tau \int d^3\mathbf{x} \left\langle \left[\phi^\dagger \phi + \theta^\dagger \theta \right] (\tau, \mathbf{x}) \left[\phi^\dagger \phi + \theta^\dagger \theta \right] (0, \mathbf{0}) \right\rangle . \quad (2.24)$$

In order to work out the contractions in eqs.(2.19), (2.24), we need the heavy quark propagators within the Euclidean theory

$$\mathcal{L}_E = \theta^\dagger (D_\tau + M) \theta + \phi^\dagger (D_\tau - M) \phi + \mathcal{O}\left(\frac{1}{M}\right) . \quad (2.25)$$

Making use of the equations of motion satisfied by the propagators, together with the proper boundary conditions, it can be shown that in the $M \rightarrow \infty$ limit and for $\tau > 0$,

$$\left\langle \theta_\alpha(\tau, \mathbf{x}) \theta_\beta^*(0, \mathbf{y}) \right\rangle = \delta^{(3)}(\mathbf{x} - \mathbf{y}) U_{\alpha\beta}(\tau, 0) e^{-\tau M} , \quad (2.26)$$

$$\left\langle \theta_\alpha(0, \mathbf{x}) \theta_\beta^*(\tau, \mathbf{y}) \right\rangle = -\delta^{(3)}(\mathbf{x} - \mathbf{y}) U_{\alpha\beta}(\beta, \tau) e^{(\tau-\beta)M} , \quad (2.27)$$

$$\left\langle \phi_\alpha(\tau, \mathbf{x}) \phi_\beta^*(0, \mathbf{y}) \right\rangle = \delta^{(3)}(\mathbf{x} - \mathbf{y}) U_{\alpha\beta}^\dagger(\beta, \tau) e^{(\tau-\beta)M} , \quad (2.28)$$

$$\left\langle \phi_\alpha(0, \mathbf{x}) \phi_\beta^*(\tau, \mathbf{y}) \right\rangle = -\delta^{(3)}(\mathbf{x} - \mathbf{y}) U_{\alpha\beta}^\dagger(\tau, 0) e^{-\tau M} , \quad (2.29)$$

⁴The inversion leads to well-known systematic uncertainties, and we have nothing concrete to add on how to treat those. However, as will be demonstrated below, our spectral function is smoother at small ω than the ones in refs. [14], which should somewhat ameliorate the problems in reconstructing the spectral function.

where U is now a straight fundamental Wilson line in the Euclidean time direction. With these propagators, we obtain

$$\begin{aligned} & \int d^3\mathbf{x} \left\langle \left[\phi^\dagger g E_i \phi - \theta^\dagger g E_i \theta \right] (\tau, \mathbf{x}) \left[\phi^\dagger g E_i \phi - \theta^\dagger g E_i \theta \right] (0, \mathbf{0}) \right\rangle \\ &= 4\delta^{(3)}(\mathbf{0}) e^{-\beta M} \left\langle \text{Re Tr} [U(\beta, \tau) g E_i(\tau, \mathbf{0}) U(\tau, 0) g E_i(0, \mathbf{0})] \right\rangle. \end{aligned} \quad (2.30)$$

Similarly, the susceptibility χ^{00} can be written as

$$\begin{aligned} \chi^{00} &= 4\delta^{(3)}(\mathbf{0}) e^{-\beta M} \int_0^\beta d\tau \left\langle \text{Re Tr} [U(\beta, \tau) U(\tau, 0)] \right\rangle \\ &= 4\delta^{(3)}(\mathbf{0}) e^{-\beta M} \beta \left\langle \text{Re Tr} [U(\beta, 0)] \right\rangle. \end{aligned} \quad (2.31)$$

In total, then,

$$G_E(\tau) = -\frac{1}{3} \sum_{i=1}^3 \frac{\left\langle \text{Re Tr} [U(\beta, \tau) g E_i(\tau, \mathbf{0}) U(\tau, 0) g E_i(0, \mathbf{0})] \right\rangle}{\left\langle \text{Re Tr} [U(\beta, 0)] \right\rangle}, \quad (2.32)$$

and κ can be obtained from the corresponding spectral function through eq.(2.23). Note that the correlation function $G_E(\tau)$ is *positive* (in a gauge with vanishing A_0 , one can think of it as $-\partial_\tau \partial_\sigma F(\tau - \sigma)|_{\sigma=0}$, where F is the correlation function of A_i). Eq. (2.32) is our main result. A related formula in Minkowski signature was given in ref. [8].

It is appropriate to remark that the meaning of eq.(2.32) is unclear in the confinement phase of pure $SU(N_c)$ gauge theory, where the expectation value of the Polyakov loop vanishes. In this situation, however, there would be a flux tube which drags the heavy quark in a way that is quite unlike diffusion, so it need not be surprising if the result for a diffusion coefficient were ill-defined.

3 Perturbation theory

The derivation of our main result, eq.(2.32), made no use of the weak-coupling expansion, and is meant to be applicable everywhere in the deconfined phase, particularly at the phenomenologically interesting temperatures of a few hundred MeV. Nevertheless, to gain some understanding on the general shape of the corresponding spectral function, we now go to very high temperatures, where the weak-coupling expansion is applicable. Our goal is to demonstrate explicitly that even in this regime, where spectral functions in general have more peaks and cusps than in a strongly-coupled regime, ours is relatively smooth.

The leading-order (free theory) behaviors of the correlation function in eq.(2.32) and of the spectral function in eq.(2.22) are easily found:

$$G_E(\tau) = g^2 C_F \pi^2 T^4 \left[\frac{\cos^2(\pi\tau T)}{\sin^4(\pi\tau T)} + \frac{1}{3 \sin^2(\pi\tau T)} \right] + \mathcal{O}(g^4), \quad (3.1)$$

$$\rho(\omega) = \frac{g^2 C_F}{6\pi} \omega^3 + \mathcal{O}(g^4), \quad (3.2)$$

where $C_F \equiv (N_c^2 - 1)/(2N_c)$. This shows that at the free level the spectral function has no zero-frequency peak, in contrast to the spectral functions relevant for transport coefficients and vector current correlators (which have δ -function peaks at this order). Given that $\rho(\omega)$ in eq.(3.2) vanishes faster than $\propto \omega$, the diffusion constant κ of eq.(2.23) is zero; we must work harder to find the leading non-trivial behavior at small frequency.

At next-to-leading order, $\mathcal{O}(g^4)$, the intercept κ becomes non-vanishing [4]:

$$\kappa = \frac{g^2 C_F T}{6\pi} m_D^2 \left(\ln \frac{2T}{m_D} + \frac{1}{2} - \gamma_E + \frac{\zeta'(2)}{\zeta(2)} + \frac{N_f \ln 2}{2N_c + N_f} \right) \left(1 + \mathcal{O}(g) \right), \quad (3.3)$$

where $m_D^2 = g^2 T^2 (N_c/3 + N_f/6)$. As indicated, corrections to this expression start already at $\mathcal{O}(g)$, and have in fact recently been determined [10].

In order to learn how “easy” it is to extract the intercept κ in practice, let us calculate more carefully the small- ω behavior of the spectral function in eq.(2.22). We restrict, in the following, to frequencies at most of the order of the plasmon (or Debye) scale, $\omega \lesssim gT$. Defining $\kappa(\omega)$ to be the product on the right-hand side of eq.(2.23), the difference $[\kappa(\omega) - \kappa]$ gets contributions only from soft momenta $k \sim m_D$, and can be calculated at tree-level using Hard Thermal Loop propagators. Moreover, the Wilson lines in eq.(2.32) can be set to unity. Inserting the gluon propagator

$$\langle A_\mu^a(x) A_\nu^b(y) \rangle = \delta^{ab} \int_K e^{iK \cdot (x-y)} \left[\frac{P_{\mu\nu}^T(K)}{K^2 + \Pi_T(K)} + \frac{P_{\mu\nu}^E(K)}{K^2 + \Pi_E(K)} + \xi \frac{K_\mu K_\nu}{(K^2)^2} \right], \quad (3.4)$$

where ξ is the gauge parameter, and carrying out the Fourier transform in eq.(2.21), we get

$$\tilde{G}_E(\omega_n) = -\frac{g^2 C_F}{3} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \left[\frac{2\omega_n^2}{\omega_n^2 + k^2 + \Pi_T(\omega_n, \mathbf{k})} + \frac{\omega_n^2 + k^2}{\omega_n^2 + k^2 + \Pi_E(\omega_n, \mathbf{k})} \right], \quad (3.5)$$

where $k \equiv |\mathbf{k}|$. After the analytic continuation in eq.(2.22), $\omega_n \rightarrow -i[\omega + i0^+]$, the self-energies become (see, e.g. ref. [12])

$$\Pi_T(-i(\omega + i0^+), \mathbf{k}) = \frac{m_D^2}{2} \left\{ \frac{\omega^2}{k^2} + \frac{\omega}{2k} \left[1 - \frac{\omega^2}{k^2} \right] \ln \frac{\omega + i0^+ + k}{\omega + i0^+ - k} \right\}, \quad (3.6)$$

$$\Pi_E(-i(\omega + i0^+), \mathbf{k}) = m_D^2 \left[1 - \frac{\omega^2}{k^2} \right] \left[1 - \frac{\omega}{2k} \ln \frac{\omega + i0^+ + k}{\omega + i0^+ - k} \right]. \quad (3.7)$$

This leads to Landau cut contributions at $k > \omega$, and plasmon pole contributions at $k < \omega$.

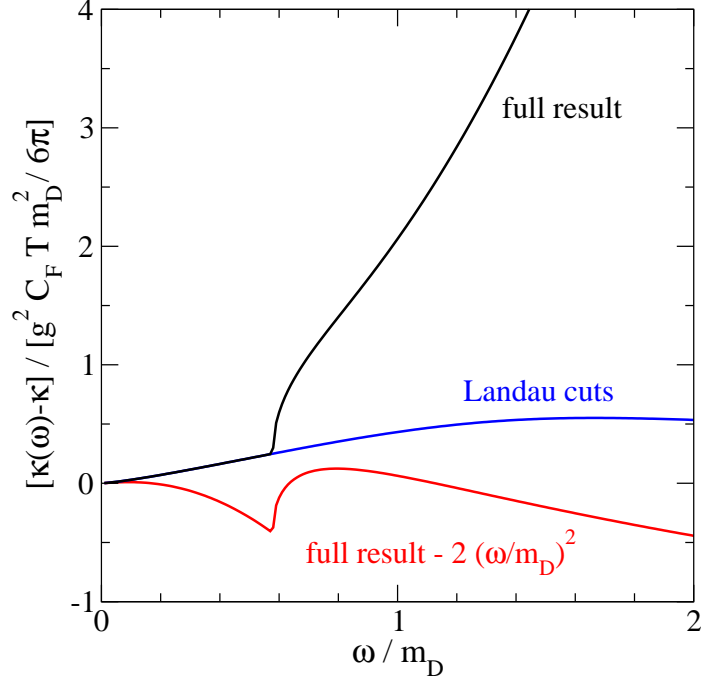


Figure 1. A numerical evaluation of eq.(3.8), in units of $g^2 C_F T m_D^2 / 6\pi$. The cusp is a feature of the weak-coupling expansion, as discussed in the text.

Concretely,

$$\begin{aligned}
 \kappa(\omega) - \kappa &= \frac{2g^2 C_F T}{3} \times \frac{4\pi}{(2\pi)^3} \times \pi m_D^2 \\
 &\times \left\{ \int_{\hat{\omega}}^{\infty} d\hat{k} \hat{k}^2 \frac{2\hat{\omega} \times \frac{\hat{\omega}}{4\hat{k}} \left(1 - \frac{\hat{\omega}^2}{\hat{k}^2}\right)}{\left(\hat{k}^2 - \hat{\omega}^2 + \frac{1}{2} \left[\frac{\hat{\omega}^2}{\hat{k}^2} + \frac{\hat{\omega}}{2\hat{k}} \left(1 - \frac{\hat{\omega}^2}{\hat{k}^2}\right) \ln \frac{\hat{k} + \hat{\omega}}{\hat{k} - \hat{\omega}} \right]\right)^2 + \left(\frac{\hat{\omega}\pi}{4\hat{k}}\right)^2 \left(1 - \frac{\hat{\omega}^2}{\hat{k}^2}\right)^2} \right. \\
 &+ \int_0^{\infty} d\hat{k} \hat{k}^4 \left[\frac{\theta(\hat{k} - \hat{\omega}) \times \frac{1}{\hat{\omega}} \times \frac{\hat{\omega}}{2\hat{k}}}{\left(\hat{k}^2 + 1 - \frac{\hat{\omega}}{2\hat{k}} \ln \frac{\hat{k} + \hat{\omega}}{\hat{k} - \hat{\omega}}\right)^2 + \left(\frac{\hat{\omega}\pi}{2\hat{k}}\right)^2} - \frac{1}{(\hat{k}^2 + 1)^2} \right] \\
 &+ 2\hat{\omega} \frac{\hat{k}_T^3 (\hat{\omega}^2 - \hat{k}_T^2)}{|3(\hat{k}_T^2 - \hat{\omega}^2)^2 - \hat{\omega}^2|} \Bigg|_{\hat{k}_T^2 - \hat{\omega}^2 + \frac{1}{2} \left[\frac{\hat{\omega}^2}{\hat{k}_T^2} + \frac{\hat{\omega}}{2\hat{k}_T} \left(1 - \frac{\hat{\omega}^2}{\hat{k}_T^2}\right) \ln \frac{\hat{\omega} + \hat{k}_T}{\hat{\omega} - \hat{k}_T} \right] = 0} \\
 &\left. + \frac{1}{\hat{\omega}} \frac{\hat{k}_E^3 (\hat{\omega}^2 - \hat{k}_E^2)}{|3(\hat{k}_E^2 - \hat{\omega}^2) + 1|} \Bigg|_{\hat{k}_E^2 + 1 - \frac{\hat{\omega}}{2\hat{k}_E} \ln \frac{\hat{\omega} + \hat{k}_E}{\hat{\omega} - \hat{k}_E} = 0} \right\}, \quad (3.8)
 \end{aligned}$$

where $\hat{\omega} \equiv \omega/m_D$ and $\hat{k} \equiv k/m_D$. The four terms correspond to the transverse cut, electric cut, transverse pole, and electric pole, respectively.

The outcome of a numerical evaluation of eq.(3.8) is plotted in figure 1, in units of the coefficient $g^2 C_F T m_D^2 / 6\pi$ multiplying the logarithm in eq.(3.3). For $\hat{\omega} < 1/\sqrt{3}$, the result comes exclusively from the Landau cuts; for $\hat{\omega} > 1/\sqrt{3}$, plasmon poles contribute as well.

For $\omega \gg m_D$, the result is dominated by the transverse pole, and extrapolates towards $\kappa(\hat{\omega} \gg 1) \rightarrow g^2 C_F T m_D^2 / 6\pi \times 2\hat{\omega}^2$, the free theory result.

The pattern in figure 1 illustrates an important point: even at weak coupling there is no transport peak around the origin; rather $\rho(\omega)/\omega$ displays a relatively flat behavior at $\omega \lesssim m_D/\sqrt{3}$, with a significant rise only above the Debye scale. The only singularity is associated with the onset of the plasmon contributions; however this should be smoothed out in the full dynamics. The amount of smoothing can be estimated from the (zero-momentum) plasmon damping rate calculated in ref. [15], $\Gamma_{\text{pl}} = 6.64g^2 N_c T / 24\pi$. Already for $\alpha_s = 0.05$ this gives (for $N_c = 3, N_f = 0 \dots 4$) a width $\Gamma_{\text{pl}}/m_D \gtrsim 0.2$ comparable to that of the cusp; therefore we expect the true behavior to be completely regular. A more detailed study of the shape, including the effects of interactions in the small- ω regime and ultraviolet features in the large- ω regime, is deferred to a future publication [16]. We also remark that the corresponding spectral functions computed for $\mathcal{N} = 4$ Super-Yang-Mills theory at infinite 't Hooft coupling show an analogous behavior, with the smooth infrared part ending in that case at $\omega \sim T$ [8, 17].

4 Correlator in lattice regularization

Let us finally move to lattice regularization. In principle correlators of the type in eq.(2.32) can be measured with standard techniques on the lattice, in fact even at low temperatures where the signal is very small [18]. There is the problem, however, that the lattice electric fields require in general multiplicative renormalization factors (see, e.g., ref. [19]); these depend on the details of the discretization chosen, and it is also not clear how they could be determined on the non-perturbative level.⁵

It appears, however, that the problem can at least be ameliorated if we choose a discretization of the electric fields inspired by lattice heavy quark effective theory (see, e.g., ref. [21]). The spatial components of the current (eq.(2.14)) could be thought of as

$$\hat{\mathcal{J}}^j = \frac{i}{2aM} \left[\hat{\theta}^\dagger(x + \hat{j}) U_j^\dagger(x) \hat{\theta}(x) - \hat{\theta}^\dagger(x) U_j(x) \hat{\theta}(x + \hat{j}) - (\hat{\theta} \longrightarrow \hat{\phi}) \right], \quad (4.1)$$

where a is the lattice spacing; \hat{j} is a unit vector in the j -direction; and U_j is a spatial link matrix. Discretizing also the time derivatives in eq.(2.10) and carrying out the contractions, we end up with a representation of eq.(2.32) which can best be represented graphically:

$$G_E(\tau) = \frac{\sum_{i=1}^3 \text{Re Tr} \langle \text{---} (\Gamma \text{---} \text{J}) \text{---} (\text{L---}\neg) \text{---} (\text{L---}\neg) \text{---} (\Gamma \text{---} \text{J}) \rangle}{-6a^4 \text{Re Tr} \langle \text{---} \text{---} \text{---} \rangle} \quad \begin{array}{c} x_i \\ \uparrow \\ x_0 \end{array} \quad (4.2)$$

Here the direct lines within parentheses are link matrices; reading from the right, the long horizontal Wilson lines in the numerator have lengths $\tau - a$ and $\beta - \tau - a$, if the sources are placed around $x_0 = a/2$ and $x_0 = \tau + a/2$, respectively; and the denominator stands for

⁵For recent progress with lattice magnetic fields, see ref. [20].

the trace of the Polyakov loop. It appears that eq.(4.2) should be less ultraviolet sensitive than the usual discretizations of the electric fields [18, 19].

Continuing with the framework of the lattice heavy quark effective theory, the renormalization of eq.(4.2) can also be discussed in concrete terms, and be related to two separate issues. First of all, the linearly appearing mass parameter M in eq.(2.11) is no longer the pole mass but requires additive renormalization; second, the coefficient c_2 can differ from unity due to the absence of (Euclidean) Lorentz invariance. It appears that both of these issues could be addressed perturbatively and, in fact, even non-perturbatively [21]. Since the explicit results depend on the particular lattice discretization chosen we do not, however, go into details here.

5 Conclusions and outlook

The main purpose of this paper has been to give a non-perturbative definition to the heavy quark momentum diffusion coefficient, κ , allowing in principle for its lattice measurement. The basic definition is given in terms of a certain limit of the vector current correlation function, eq.(2.9). Making use of heavy quark effective theory, we have furthermore shown that the definition can be reduced to a much simpler purely gluonic correlator, given in eq.(2.32), with κ then following from eq.(2.23).

An important consequence of these relations is that they show that κ does not contain any logarithms of the heavy quark mass M . Our formulae could in principle also serve as the starting point for a first computation of a finite-temperature real-time quantity to relative accuracy α_s , revealing in particular how the renormalization scale should be fixed.

Moving to the non-perturbative level, we have also suggested a particular discretization of eq.(2.32), given in eq.(4.2), which could be free of significant renormalization factors. It remains to be tested in practice, however, how noisy the correlator is, and how fast the continuum limit can be approached. In addition, current practical recipes [14] related to the inversion of eq.(2.20) suffer from uncontrolled systematic uncertainties which our method does not remove completely, although we hope that from the practical point of view they are less serious than in many other cases.

Assuming that a non-perturbative value can be obtained for κ , we can finally proceed to consider the thermalization rate of heavy quarks. A concrete and theoretically satisfactory meaning for a thermalization rate is provided by the heavy quark relaxation rate, or drag coefficient, denoted by η_D and defined around eq.(2.5) (the relation to thermalization follows from eq.(A.1)). Employing the fluctuation-dissipation relation in eq.(2.8), η_D can be estimated as $\eta_D \simeq \kappa/2MT$, where M is the heavy quark pole mass and T is the temperature. Although this relation does have ambiguities related to the definition of the quark mass (a pole mass has inherent non-perturbative ambiguities at the level of several hundreds of MeV [22]; a treatment free of this problem can only be given in terms of non-perturbatively renormalized heavy quark effective theory [21]), such ambiguities should be subdominant compared with the large corrections related to infrared sensitive thermal physics, at least for the bottom quarks. These large thermal corrections are prop-

erly captured by our definition of κ , so η_D should lie in the right ballpark as well. We are therefore very much looking forward to the first numerical estimates of κ .

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A Examples of dynamics leading to a transport peak

In this appendix, we review briefly two arguments through which the Lorentzian form of the transport peak in eq.(2.4) can be established explicitly.

Consider first non-relativistic quantum mechanics. Let us define $\hat{v}_i = \hat{p}_i/M_{\text{kin}}$, where \hat{p}_i is the momentum operator of the heavy quarks (i.e. the generator of translations in their Hilbert space). Suppose that we have, through some external source field, managed to prepare a non-equilibrium state where there is a heavy quark with a non-zero velocity. In thermal equilibrium, the average velocity must vanish, so we may expect the system to behave as

$$\frac{d}{dt}\langle\hat{v}_i(t)\rangle_{\text{non-eq}} = -\eta_D\langle\hat{v}_i(t)\rangle_{\text{non-eq}} + \mathcal{O}\left(\langle\hat{v}_i(t)\rangle_{\text{non-eq}}^2\right). \quad (\text{A.1})$$

Once t is so large that $\langle\hat{v}_i(t)\rangle_{\text{non-eq}} \sim [\langle\hat{v}_i^2\rangle_{\text{eq}}]^{1/2}$, Brownian motion sets in, and the system effectively equilibrates. In equilibrium we may define the correlator

$$\Delta_{ii}(t) \equiv \left\langle \frac{1}{2} \{\hat{v}_i(t), \hat{v}_i(0)\} \right\rangle_{\text{eq}}. \quad (\text{A.2})$$

This is an even function of t and must vanish for $t \rightarrow \infty$; in fact, at least on certain time scales, it can be argued that it vanishes with the *same* exponent as the non-equilibrium correlator in eq.(A.1) (see, e.g., section 118 of ref. [23]):

$$\Delta_{ii}(t) \stackrel{|t| \gg \beta}{\simeq} \bar{\Delta}_{ii} e^{-\eta_D |t|}, \quad (\text{A.3})$$

where $\bar{\Delta}_{ii}$ is a constant. Taking a Fourier transform yields

$$\tilde{\Delta}_{ii}(\omega) \equiv \int_{-\infty}^{\infty} dt e^{i\omega t} \Delta_{ii}(t) \stackrel{|\omega| \ll T}{\simeq} \bar{\Delta}_{ii} \frac{2\eta_D}{\omega^2 + \eta_D^2}, \quad (\text{A.4})$$

and making use of the general relation $\tilde{\Delta}_{ii}(\omega) = [1 + 2n_{\text{B}}(\omega)] \rho_{ii}(\omega)$ (see, e.g., ref. [12]), where $n_{\text{B}}(\omega) \equiv 1/[\exp(\beta\omega) - 1]$ and $\rho_{ii}(\omega)$ is the spectral function, we arrive at

$$\frac{\rho_{ii}(\omega)}{\omega} \stackrel{|\omega| \ll T}{\simeq} \frac{1}{2T} \tilde{\Delta}_{ii}(\omega) \stackrel{|\omega| \ll T}{\simeq} \bar{\Delta}_{ii} \frac{\beta\eta_D}{\omega^2 + \eta_D^2}. \quad (\text{A.5})$$

This indeed agrees with the functional form of eq.(2.4).

Another example is given by classical Langevin dynamics (see also ref. [6]). Essentially, we replace $\langle \hat{p}_i(t) \rangle_{\text{non-eq}} \rightarrow p_i(t)$, and assume the dynamics to be contained in

$$\dot{p}_i(t) = -\eta_D p_i(t) + \xi_i(t), \quad (\text{A.6})$$

$$\langle\langle \xi_i(t) \xi_j(t') \rangle\rangle = \kappa_{\text{cl}} \delta_{ij} \delta(t-t'), \quad \langle\langle \xi_i(t) \rangle\rangle = 0, \quad (\text{A.7})$$

with ξ a Gaussian stochastic noise field, and $\langle\langle \dots \rangle\rangle$ denoting an average over the noise. For a heavy particle the Gaussian nature follows from the central limit theorem and the slow time scale of its dynamics, while the auto-correlator $\kappa_{\text{cl}} = \int_{-\infty}^{\infty} dt \langle\langle \xi_i(t) \xi_i(0) \rangle\rangle$ can be chosen such as to match that of the underlying theory, eq.(2.5). It is easy to verify that within this dynamics, for a distribution with density $T\chi^{00}$ of heavy quarks, the equilibrium correlator is exactly eq.(2.4).

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