Heavy quark diffusion in perturbative QCD at next-to-leading order

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We compute the momentum diffusion coefficient of a nonrelativistic heavy quark in a hot QCD plasma, to next-to-leading order in the weak coupling expansion. Corrections arise at $\mathcal{O}(g_4)$; physically they represent interference between overlapping scatterings, as well as soft, electric scale ($p \sim gT$) gauge field physics, which we treat using the hard thermal loop (HTL) effective theory. In 3-color, 3-flavor QCD, the momentum diffusion constant of a fundamental representation heavy quark at NLO is $\kappa = \frac{16g^2}{3} \alpha_s^2 T^3 (\ln \frac{1}{\alpha_s} + 0.07428 + 1.8869 g_s)$. The convergence of the weak coupling expansion is poor.

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The experimental program at RHIC and the future heavy ion program at the LHC are exploring the behavior of the QCD plasma at temperatures above the “deconfinement” temperature of $\sim 170$ MeV. So far the evidence is for a medium which interacts more strongly and thermalizes more quickly than expected. For instance, experimental results on elliptic flow are well explained by hydrodynamics [1] but only if the shear viscosity is much less than a naive extrapolation of weak coupling calculations [2, 3]. Similarly, heavy quarks display substantial elliptic flow and a degraded energy spectrum [4], implying stronger medium interactions than extrapolated weak-coupling calculations can easily accommodate [5].

This raises the general question: how well can we trust weak coupling calculations for dynamical quantities in hot QCD at couplings anywhere close to those probed in experiments? Naively the perturbative series converges (in possibly non-integer) powers of the strong coupling, $\alpha_s \equiv \frac{g^2}{4\pi} \sim 0.4$ for relevant temperatures. But perturbative series often show convergence which is much better or much worse than one would guess from the value of the coupling. In general determining how well a perturbative expansion converges requires evaluating a few terms in the expansion. Unfortunately, no dynamical transport quantity in QCD which involves large length or time scales (such as shear and bulk viscosity, electric conductivity, photon production, and heavy quark momentum diffusion and energy loss) is known beyond leading order. Most of the leading-order calculations are recent and quite involved.

Here we present a next-to-leading order calculation of the theoretically simplest of these quantities, the momentum diffusion coefficient of a nonrelativistic heavy quark. This coefficient (partially) characterizes how quickly heavy quarks are thermalized and swept up in the collective flow of the plasma.

A heavy quark, $M \gg T$, in or near equilibrium has a typical momentum $p \sim \sqrt{MT} \gg T$ large compared to the plasma scale and it therefore takes a parametrically long time for the momentum to change appreciably. This means that momentum changes accumulate from many uncorrelated “kicks,” so on long time scales $p$ will evolve via Langevin dynamics,

$$\frac{dp_i}{dt} = -\eta_D p_i + \xi_i(t), \quad \langle \xi_i(t)\xi_j(t') \rangle = \kappa \delta_{ij} \delta(t-t'). \quad (1)$$

The relaxation rate $\eta_D$ and the momentum diffusion constant $\kappa$ are related by a fluctuation-dissipation relation, $\eta_D = \frac{\kappa}{2MT}$, which follows on general thermodynamic grounds. Thus the dynamics of the nonrelativistic heavy quark is completely set by the single parameter $\kappa$. This parameter can be obtained by computing the mean squared momentum transfer per unit time in the underlying microscopic theory. In gauge theory, this mean squared momentum transfer equals the time integrated correlator of two electric field operators connected by fundamental Wilson lines [6]:

$$\kappa = \frac{g^2}{3d_H} \int_{-\infty}^{\infty} dT \text{Tr}_H (W(T;0)} \langle E^a_i(T)\delta^a_i W(T;0) E^b_j(0)\delta^b_j \rangle, \quad (2)$$

where $W(T;0)$ denotes a fundamental Wilson line running from $t = 0$ to $T$ along the static trajectory of the heavy quark and $d_H = 3$ is the dimension of the heavy quark's representation.

Intuitively, Eq. (2) is exactly the force-force correlator of Eq. (1), with the forces given by electric fields and the Wilson line representing the gauge rotation of the heavy quark due to propagation, which ensures gauge invariance. Because of operator ordering issues, the Wilson lines shown are not equivalent to connecting the $E$ fields with an adjoint Wilson line, and in fact such Wilson lines are even required in QED (diffusion of ions in a QED plasma depends on the ionic charge $Z$ in a more complicated way than $Z^2$ only because of these Wilson lines, which account for the reaction of the plasma to the presence of the charge).

We start by showing how this formula reproduces the well known [7] leading order momentum diffusion coefficient. At this order, (2) simplifies to a zero-frequency Wightman correlator of two $A^0$ fields (the $A^i$ fields do not contribute to the electric field operators at zero-frequency...
of Eq. (4) yields

\[ \frac{C_H g^2}{3} \int_0^{\infty} q^2 dq \int_0^{2q} \frac{p^3 dp}{(p^2 + m_q^2)^2} \]

where \( C_H = \frac{1}{2} \) is the Casimir of the heavy quark’s representation. This Wightman correlator can be evaluated in terms of the squared matrix elements of t-channel scattering processes involving the heavy quark, as illustrated in Fig. 1. These are the only processes which contribute in our case, Compton-like processes being suppressed in the low velocity limit. The result reduces to \[ \kappa_{LO} = \frac{g^4 C_H}{12 \pi^3} \int_0^{\infty} q^2 dq \int_0^{2q} \frac{p^3 dp}{(p^2 + m_q^2)^2} \]

\[ \left\{ N_f n_F(q)(1-n_F(q)) \left( 2 - \frac{m_q^2}{2q^2} \right) + N_c n_B(q)(1+n_B(q)) \left( 2 - \frac{m_q^2}{2q^2} + \frac{4\pi^2}{q^2} \right) \right\} \]

Here \( p \) is the transferred momentum and \( q \) is the energy of the light scattering target. Since the heavy quark is at rest, the initial and final light-particle energies are equal and \( p \) is purely spatial, which is why the medium modification of the exchanged gluon propagator is purely Debye screening with a Debye mass \( m_D^2 = g^2 T^2 (N_c + N_f/2) / 3 \). The inclusion of these HTL corrections is essential for obtaining the complete leading order result, otherwise \( \kappa \) would be infrared divergent in the region of soft momentum transfer \( p \). Formally taking \( m_D \ll T \), the integral is dominated by \( q \sim T \) and \( p \) in the parametric range \( m_D \lesssim p \lesssim T \). The strict leading-order evaluation of Eq. (4) yields

\[ \kappa \simeq \frac{C_n g^4 T^3}{18 \pi} \left[ N_c \left( \ln \frac{2T}{m_D + \xi} + \frac{N_f}{2} \right) \ln \frac{4T}{m_D + \xi} + \frac{N_c}{2} \right] \]

with \( \xi = \frac{1}{2} - \gamma_e + \frac{\zeta_2}{\zeta(2)} \simeq -0.64718 \).

When the exchange momentum \( p \) is hard, \( p \gg T \), then higher loop corrections to the propagators and vertices in Fig. 1 represent \( O(g^2) \) corrections. However, the expression (4) for \( \kappa \) receives an \( O(g) \) contribution from scatterings against soft gluons, \( q \approx m_D \). Both the dispersion relations and the interactions of such gluons are modified at the \( O(1) \) level; at leading order these modifications are described by hard thermal loops. Therefore there will be \( O(g) \) corrections to the above calculation. But this is not the only source of \( O(g) \) next-to-leading order (NLO) corrections.

Another source is associated with overlapping scattering events: the total scattering rate for a hard particle is \( \sim g^2 T \), and is dominated by t-Channel Coulombic scatterings involving soft momentum transfers. These soft scatterings have a duration of order \( \sim 1/m_D \sim 1/g^2T \) and therefore there is an \( O(g) \) probability that two such scattering events overlap with each other. This is relevant in QCD (though not in QED, see below) because each scattering color-rotates the participants.

We need a systematic way of evaluating these NLO effects. This is provided by a loopwise expansion for Eq. (2). The diagrams needed at NLO are shown in Fig. 2. The diagrammatic series is convergent in powers of \( g \) provided one incorporates HTL corrections in propagators and vertices wherever momenta are soft [9], unless a diagram is sensitive to the magnetic scale \( \sim g^2 T \), which would be signaled by an infrared divergence in the evaluation of a Feynman diagram. This does not occur in the current calculation; the diagrams shown in Fig. 2 are all IR and UV convergent, after the leading-order contribution is subtracted off from the transverse, pole-pole contribution of diagram \((A)\). Since the momenta are soft, the ordering issues for the Wilson lines are subdominant and we may replace the two Wilson lines in Eq. (2) with an adjoint Wilson line; all diagrams involve the group theoretic combination \( C_n C_a \) and we may represent the NLO correction as the coefficient \( C \) defined by

\[ \kappa = \frac{C_n g^4 T^3}{18 \pi} \left( \left[ N_c + \frac{N_f}{2} \right] \ln \frac{2T}{m_D + \xi} + \frac{N_f \ln 2}{2} + \frac{N_c m_D}{T} \right) \]

with \( O(g^2) \) corrections. There is no \( O(g) \) NLO correction in QED, where the (bare and HTL) vertices involved in diagrams \((A), (B), (C)\) do not exist and the Wilson line...
in $(D)$ is trivial. Since Eq. (2) involves unequal time correlators we have found it most convenient to evaluate it in the real-time (Schwinger-Keldysh) formalism. This required an extension of the HTL formalism to the closed time path in the Schwinger-Keldysh $(r, a)$ basis [10], which is convenient for treating soft physics because Bose-Einstein factors only arise in one propagator. We work in strict Coulomb gauge. The measurable, Eq. (2), is gauge invariant and only arise in one propagator. We work in strict Coulomb gauge. The measurable, Eq. (2), is gauge invariant and the HTL expansion should respect gauge invariance, so we expect the sum of diagrams systematically evaluated in powers of $g$ to produce gauge invariant results, though the results for individual diagrams probably are not.

The effect of diagram $(A)$ can be divided into the real and the imaginary part of the self-energy correction. The real part is the simplest to compute: it represents a correction to the Debye mass which can actually be evaluated within the 3-D dimensionally reduced theory [11]. 4D Coulomb gauge corresponds to 3D Landau gauge; in this gauge the self-energy receives a nonzero, momentum-dependent contribution when one propagator in the self-energy is transverse and the other is longitudinal $(A_0$ in the 3D theory). The correction is

\[
\frac{1}{(p^2 + m_0^2)^2} \rightarrow \frac{1}{(p^2 + m_0^2 + \delta m_0^2)^2} \quad \text{in Eq. (4),}
\]

\[
\delta m_0^2 = -4C_ag^2T \int \frac{d^3q}{(2\pi)^3} \frac{p^2 - (q \cdot P)^2/q^2}{(2\pi)^3 q^2((P - q)^2 + m_0^2)}.
\]

The contribution to $C$ is found by expanding $(p^2 + m_0^2 + \delta m_0^2)^{-2} - (p^2 + m_0^2)^{-2} \approx -2\delta m_0^2(p^2 + m_0^2)^{-3}$ and finding the shift to Eq. (4). Straightforward integration gives

\[
C_{re}(A) = \frac{3}{2\pi} \left(1 + \frac{e^2}{m_0^2}\right) \approx 0.77199.
\]

The next simplest contributions are from diagrams $(C)$ and $(D)$. Physically, $(C)$ accounts for real and virtual corrections in which the light scatterer undergoes an additional soft scattering or soft plasmon emission/absorption. Diagram $(D)$ is the same but for the heavy quark. In QED there is a cancellation between vertex orderings but in QCD one instead picks up a contribution from color operators. The contributions of these two diagrams are

\[
C_{(C)} = 6\pi^2 \int \frac{d^3p}{(2\pi)^3} \frac{p^2}{(1 + p^2)^2} \int \frac{d\Omega}{4\pi} \int \frac{d^4Q}{(2\pi)^4} G_{\mu\nu}(Q) v_{\mu} v_{\nu} \times \delta(v \cdot (P - Q)) + \delta(v \cdot (P + Q)) - 2\delta(v \cdot P),
\]

\[
C_{(D)} = \frac{3}{2\pi^4} \int_0^\infty p^2 dp \int_0^\infty q^2 dq \int_0^\infty d\omega \omega \times \frac{G_{\mu\nu}(\omega, p) - G_{\mu\nu}(0, p)}{\omega^2} G_{\mu\nu}(\omega, q).
\]

In writing these expressions we have scaled all momenta by $m_0$ and scaled out all powers of $T$. Here $v_{\mu} \equiv (1, v)$ and $G_{\mu\nu}$ is the ordering-averaged gauge field correlator, related to the retarded correlator via [15]

\[
G_{\mu\nu}(\omega, p) = (2\eta_{\mu\nu} + 1) \text{Re} G_{\mu\nu}(\omega, p) \approx \frac{2T}{\omega^2} \text{Re} G_{\mu\nu}(\omega, p).
\]

These expressions can be simplified somewhat but must be evaluated by numerical quadratures. We find [12]

\[
C_{(C)} = -0.132916(1) \quad \text{and} \quad C_{(D)} = 0.067526(1).
\]

The most involved calculation is for the imaginary contribution of the self-energy loop in diagram $(A)$. This bears some similarity to the calculation of the gluon damping rate by Braaten and Pisarski [13], but the “external” momentum $P$ is now spacelike. Therefore the integrals encountered are four rather than two dimensional (one must integrate over $p$ and $\theta_{pq}$), and the kinematics allow for processes involving two soft plasmons on their mass shells, as well as virtual corrections to the tree process of Fig. 1. The contribution to $(C)$ can be written

\[
C_{im}(A) = 6\pi \int \frac{d^3p}{(2\pi)^3} \frac{p^2}{(1 + p^2)^2} \int \frac{d^4Q}{(2\pi)^4} \left[-G_{\mu\nu}^{\mu\nu}(Q) G_{\mu\nu}^{\mu\nu}(R) M_{\mu\nu}(Q, R) M_{\mu\nu}(Q, R) + 2G_{\mu\nu}^{\mu\nu}(R) V_{\mu\nu} \left( G_{\mu\nu}^{\mu\nu}(Q) M_{\mu\nu}(Q, P) - G_{\mu\nu}^{\mu\nu}(Q) M_{\mu\nu}(Q, P) \right) + \frac{1}{2} V_{\mu\nu} V_{\mu'\nu'} G_{\mu\nu}^{\mu\nu}(Q) G_{\mu'\nu'}^{\mu'\nu'}(R) \right],
\]

where we have introduced

\[
M_{\mu\nu}(Q, R) = \int \frac{d\Omega}{4\pi} \frac{\mu^\mu \nu^\nu}{(v \cdot Q - i\epsilon)(v \cdot R - i\epsilon)},
\]

\[
V_{\mu\nu} = 2q^\mu \eta_{\mu\nu} + (R + P)_{\mu} \delta_{\nu}^\nu - (Q + P)_{\nu} \delta_{\mu}^\mu
\]

to denote objects that enter the HTL and tree vertices. The evaluation is lengthy [12], and rather remarkably, turns out to be separable into pole-pole, pole-cut and cut-cut contributions, in analogy to what was found by Braaten and Pisarski. Two subtractions are required.

First, as mentioned above, at large momenta the pole-pole contribution when both gauge bosons are transverse duplicates the tree process of Fig. 1; this must be subtracted. Further, evaluating the integrals in Eq. (3) for finite $m_0$ already incorporates an NLO correction besides what is in Eq. (5). We will take the leading contribution to be the result including this NLO correction (which corresponds to $C_{\text{Eq. (3)}} = 21/8\pi$). After these subtractions we obtain (numerically) $C_{im}(A) = 0.9097(1)$.

Diagram $(B)$ involves the correlator of three $A_0$ fields.
connected by an HTL 3-point function (the tree vertex vanishes), and accounts for interference between scattering events occurring on the light scatterer’s side and on the heavy quark’s side. One of the $A^i$ fields carries zero frequency, and the contributions can be organized according to whether the zero frequency propagator is cut or retarded,

\[ C_{\text{re}}(B) = 6\pi^2 \int \frac{d^3p}{(2\pi)^3} \frac{p}{(1+p^2)^2} \int \frac{d^3q}{(2\pi)^3} \frac{M^{00}(q, -r)}{1+(q^2+r^2)} \]  

\[ C_{\text{im}}(B) = 12\pi \int \frac{d^3p}{(2\pi)^3} \frac{p^2}{1+p^2} \int \frac{d^4Q}{(2\pi)^4} g^{r\tau}_r(R) G^{0\tau}_r(Q) M^{00}(Q, p) \]  

\[ \times \ln \left( \frac{2 p^2 + m^2}{\alpha} \right) \]  

\( \text{(13)} \)

The contributions $C_{\text{re}}(B)$ and $C_{\text{im}}(B)$ are closely analogous to the real and imaginary parts of diagram (A), respectively. We find \[ C_{\text{re}}(B) = -0.04829(1) \]  and $C_{\text{im}}(B) = -0.07338(1)$.

**Discussion**

The heavy quark diffusion coefficient can be computed beyond leading order in the weak coupling expansion. The first corrections arise at $O(g_s)$ and describe “soft” $p, \omega \sim g_s T$ physics including interference between scatterings and plasma corrections to interaction strengths. The calculation requires the HTL effective theory.

![Comparison of leading and NLO results for $N_f = 3$ QCD as a function of coupling.](attachment:image.png)

**FIG. 3:** Comparison of leading and NLO results for $N_f = 3$ QCD as a function of coupling.

The ratio of the NLO correction to the LO result is independent of the representation of the heavy quark and is proportional to the group’s adjoint Casimir $C_A$ ($C_A = N_c$ in SU($N_c$) gauge theory, 0 in QED). Numerically, we find (see Eq. (6)) $C = 1.4946 + C_{\text{Eq. (3)}}$, or, for 3 flavors,

\[ \kappa = \frac{16\pi}{3} \frac{\alpha_s}{\sqrt{s}} T^3 \left( \ln \frac{1}{g_s} + 0.07428 + 1.9026 g_s + O(g_s^2) \right) \]  

\( \text{(15)} \)

The correction is positive, meaning faster equilibration of heavy quarks. As shown in Fig. 3, for realistic values of the strong coupling the correction is large—a factor of 2 already at $\alpha_s = 0.03$.

Our result suggests that the convergence of the perturbative expansion for dynamical quantities is poor. Why? About $1/3$ of the NLO coefficient in Eq. (15) (the part we called $C_{\text{Eq. (3)}}$) is incorporated by integrating Eq. (4) numerically rather than expanding it into Eq. (5). Another third, $C_{\text{re}}(A)$, can be approximately included into Eq. (4) by giving the real part of the self-energy its full $p$ dependence rather than approximating it with its small $p$ limit, $m_2^2$. The remaining third represents complicated and nontrivial many-body physics.

It would be interesting to make similar calculations for other transport coefficients such as shear viscosity, and to extend the present calculation to $N_f=4$ SYM theory.

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[15] We use the $[-+++]$ metric and define the retarded Green function without a factor of $i$, so at the free level for a scalar field it is $-i/(Q^2 - i\epsilon\text{sgn}(Q^2))$. 