An in-Medium Heavy-Quark Potential from the $Q\bar{Q}$ Free Energy

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Abstract

We investigate the problem of extracting a static potential between a quark and its antiquark in a quark-gluon plasma (QGP) from lattice-QCD computations of the singlet free energy, $F_{Q\bar{Q}}(r)$. We utilize the thermodynamic $T$-matrix formalism to calculate the free energy from an underlying potential ansatz resummed in ladder approximation. Imaginary parts of both $Q\bar{Q}$ potential-type and single-quark selfenergies are included as estimated from earlier results of the $T$-matrix approach. We find that the imaginary parts, and in particular their (low-) energy dependence, induce marked deviations of the (real part of the) potential from the calculated free energy. When fitting lattice results of the latter, the extracted potential is characterized by significant long-range contributions from remnants of the confining force. We briefly discuss consequences of this feature for the heavy-quark transport coefficient in the QGP.

Keywords: Heavy-quark potential, Bethe-Salpeter Equation, Quark-Gluon Plasma

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1. Introduction

Heavy-flavor (HF) particles, containing charm or bottom quarks, play a central role in the analysis of strongly interacting matter as produced in ultrarelativistic heavy-ion collisions (URHICs) [1]. The nuclear modification factor and elliptic flow of $D$ and $B$ mesons (as well as their semileptonic decay leptons) are key measures to establish and quantify the strong-coupling nature of the QCD medium [2–4], while the production patterns of charmonia and bottomonia [5–8] are believed to encode information on its deconfinement properties. For both observables, a good understanding of the in-medium interactions of the heavy quarks and quarkonia is mandatory.

Lattice-QCD (lQCD) computations allow to study the properties of heavy-quark (HQ) systems in the quark-gluon plasma (QGP) from first principle. In particular, euclidean correlation functions of quarkonia, HQ susceptibilities and static $Q\bar{Q}$ free energies have been computed with good precision [9, 10]. A non-perturbative $T$-matrix approach (“Brueckner theory”) for quarkonia and heavy quarks in the QGP has been developed to interpret the QCD results [11, 12], and the calculated spectral functions and transport coefficients have been applied to both hidden [13] and open HF observables [14] in URHICs. The main theoretical uncertainty in this and other approaches based on the Schrödinger equation [15, 16] remains the definition of the driving kernel or potential. Thus far, it has been bracketed by using either the temperature dependent free or internal energies (or combinations thereof), which, roughly speaking, led to a rather weakly or strongly coupled systems, respectively.

In the present paper we address this uncertainty by utilizing the thermodynamic $T$-matrix to derive an expression for the singlet HQ free energy, $F_{Q\bar{Q}}(r)$. Previous work to extract the HQ potential has been done both nonperturbatively from lQCD using an effective Schrödinger equation and potential for the Wilson loop [20–23], and within weak-coupling schemes [18, 24, 25]. Here, we take a diagramatic approach by defining the potential within a field-theoretic scattering equation, which leads to a slightly different Schrödinger (or Dyson) equation than in previous work. Starting from the finite-temperature Bethe-Salpeter equation (BSE) for a static quark and antiquark in a mixed coordinate-frequency representation, we resum the ladders into a closed form expression which naturally serves as the definition of the in-medium driving kernel.

The pertinent spectral function can then be straightforwardly related to the HQ free energy. A key element in evaluating the resulting expression is the energy dependence of the spectral function, in particular of imaginary parts induced by both one- and two-body correla-
tions, i.e., single-quark self-energies and Q\Bar{Q} potential-type contributions. The former have been calculated before within the selfconsistent T-matrix formalism [26], while for the latter we take guidance from perturbative calculations [18, 24, 25]. The real part of the potential will be taken from a field-theoretic ansatz for a screened Cornell potential [27], where four parameters characterize its strength and screening properties. This set-up will then be deployed to conduct a fit to lQCD data for the static color-singlet free energy.

2. Static Q\Bar{Q} Free Energy in Ladder Approximation

Our objective in this section is to relate the static correlation function of (infinitessively massive) quark and antiquark to the HQ free energy, \( F_{Q\Bar{Q}}(r) \) [18, 28, 30], and evaluate it in ladder approximation (BSE or T-matrix scheme). Toward this end we first formally carry out the ladder-diagram resumation of the BSE in the imaginary-time (Matsubara) formalism, and then reduce the BSE to the T-matrix (potential approximation).

The one-particle propagator in the infinite-mass limit is given by [18]

\[
G^{(1)}(v_n, r') = \frac{1}{\beta M - \Sigma_{1}^{(1)}(v_n)} \int \frac{d^3 p'}{(2\pi)^3} e^{iv_n \cdot p'} G^{(1)}(v_n, p') ,
\]

where the \( \delta \)-function implies that the particle never moves; \( \Sigma_{1}^{(1)} \) denotes the single-particle selfenergy and \( M \) is its (heavy) mass; \( v_n = (2n + 1)\pi/\beta \) is a discrete fermionic Matsubara frequency (\( n \) integer, \( T = 1/\beta \); temperature), adopting the conventions of Ref. [31] with \( \hbar = 1 \). The two-particle Green function inherits the \( \delta \)-function structure [18]:

\[
G^{(2)}(-ir, r_1, r_2| r_1', r_2') \equiv \delta (r_1 - r_1') \delta (r_2 - r_2') G^{(1)}(v_n, r) ,
\]

where \( r = |r_1 - r_2| \). Here and in the following the “tilde” notation is used to denote the reduced Green function without the spatial \( \delta \)-functions. The static Q\Bar{Q} free energy, \( F_{Q\Bar{Q}} \), can be defined in terms of the Q\Bar{Q} Green function as [18]

\[
F_{Q\Bar{Q}}(r) = -\frac{1}{\beta} \ln \left( G^{(2)}(-i\beta, r) \right) .
\]

The task in the following is to calculate \( \tilde{G}^{(2)}(-ir, r) \) in Eq. (2) within a BSE (or potential model) in the Matsubara formalism. In a “mixed” frequency-coordinate representation it is given by

\[
\tilde{T}(z_{\lambda}, v_n, v_m|r) = K(v_n - v_m, r) - \frac{1}{\beta} \sum_k K(v_n - v_k, r) \times G^{(2)}_{0}(z_{\lambda} - v_k, v_k) \tilde{T}(z_{\lambda}, v_k, v_m|r) \]

where \( K(v_n - v_m, r) \) is the interaction kernel and

\[
G^{(2)}_{0}(z_{\lambda} - v_m, v_m|r) \equiv \tilde{G}^{(1)}(z_{\lambda} - v_m) \tilde{G}^{(1)}(v_m) \]

the uncorrelated two-particle propagator. The external frequency \( z_{\lambda} \) is conserved because of imaginary-time translation invariance. The full two-particle Green function takes the form [32, 33]

\[
\tilde{G}(z_{\lambda}, r) = G^{(2)}_{0}(z_{\lambda}) + \frac{1}{\beta^2} \sum_{\lambda,\lambda'} \tilde{G}^{(2)}_{0}(z_{\lambda} - v_k, v_k) \tilde{T}(z_{\lambda}, v_k, v_m|r) \tilde{G}^{(2)}_{0}(z_{\lambda} - v_k, v_k) ,
\]

where we defined \( G^{(2)}_{0}(z_{\lambda}) \) \( \equiv -\frac{1}{\beta} \sum_{\lambda} \tilde{G}^{(2)}_{0}(z_{\lambda} - v_k, v_k) \), and likewise for \( \tilde{G}(z_{\lambda}, r) \). The discrete energy dependencies and summations render Eq. (4) of matrix type, \( T_{mn} = K_{nm} + \sum_{\lambda} [K G^{(2)}_{0}\lambda] K_{km} \), which is amenable to a formal solution via matrix inversion, \( T_{mn} = \sum_{\lambda} [1 - K G^{(2)}_{0}\lambda]^{-1} K_{km} \), which, however, is not very practical.

To proceed, we adopt a potential approximation, i.e., neglecting energy transfers in the interaction kernel so that \( K(v_n - v_m, r) \rightarrow V(z_{\lambda}, r) \); we keep a possible dependence on the external energy parameter \( z_{\lambda} \), in analogy to what has been done, e.g., in the description of electromagnetic plasmas [34] where a “dynamical screening” can induce such a dependence. With this approximation, the Matsubara summations in Eq. (4) decouple and one can resum the geometric series to find

\[
\tilde{T}(z_{\lambda}, v_n, v_m|r) =
V(z_{\lambda}, r) \frac{1}{1 - V(z_{\lambda}, r) G^{(2)}_{0}(z_{\lambda})} \equiv \tilde{T}(z_{\lambda}, r)
\]

The corresponding full two-particle Green function can also be written in compact form as

\[
\tilde{G}(z_{\lambda}, r) = \frac{1}{[G^{(2)}_{0}(z_{\lambda})]^{-1} - V(z_{\lambda}, r)} .
\]

The above expression is a key formula of our derivation, as it can serve as the definition of the interaction kernel.
in the $T$-matrix formalism. It slightly differs from what has been adopted in previous approaches \cite{26,27,28}, as can be seen from inspecting the resulting Dyson equation for the meson spectral function.

Next we use the analyticity of the Green function to obtain the correlation function in imaginary-time via a spectral representation,

$$\tilde{G}^{\tau}(−i\tau,r)=\int_{−\infty}^{\infty}dE^{′}\sigma_{V}(E^{′},r)e^{E^{′}(β−\tau)}\varepsilon^{\beta E}−1,$$  \hspace{1cm} (9)

with the spectral function corresponding to Eq. (6),

$$\sigma_{V}(E,r)=−\frac{1}{\pi}\tilde{G}_{I}(E+i\epsilon|r).$$  \hspace{1cm} (10)

We use the subscript “$V$” to indicate that the spectral function is calculated in potential approximation. Here and in the following, the subscripts ”$R$” and ”$I$” are short-hand notations for the real and imaginary part of a given quantity. Since we work in the static limit ($M → \infty$), we redefine the spectral function relative to the $Q\bar{Q}$ threshold by a shift $E = E′ − 2M$, i.e.,

$\tilde{\sigma}_{V}(E,r) \equiv \sigma_{V}(E + 2M,r)$, which further simplifies Eq. (9) to

$$\tilde{G}^{\tau}(−i\tau,r) \equiv \tilde{G}^{\tau}(−i\tau,r)\varepsilon^{−i2Mr} = \int_{−\infty}^{\infty}dE^{′}\tilde{\sigma}_{V}(E^{′},r)e^{−iE^{′}}\varepsilon^{−βE}$$  \hspace{1cm} (11)

Combining Eqs. (9), (10) and (11), we arrive at the final expression for $F_{Q\bar{Q}}(r)$ within the $T$-matrix approach,

$$F_{Q\bar{Q}} = −\frac{1}{\beta}\ln\left[\int_{−\infty}^{\infty}dE\tilde{\sigma}_{V}(E,r)e^{−βE}\right].$$  \hspace{1cm} (12)

In the following section, in the spirit of a variational approach, we will fit a physically motivated ansatz for the potential to IQCD data of the in-medium free energy.

3. Potential Extraction from the Free Energy

The two-particle Green function in medium receives contributions from the (medium-modified) interaction kernel, $V$, and from the single-particle selfenergies, $\Sigma^{(1)}$, arising from individual interactions of each particle with the heat bath which figure into $G^{(0)}_{I}$. Both are, in principle, complex quantities and are contained in our $T$-matrix expression for the full two-particle Green function, Eq. (8); we write the pertinent spectral function as

$$\tilde{\sigma}_{V}(E,r) = \frac{1}{\pi}\tilde{G}_{I}(E + 2M + i\epsilon|r) \approx \frac{1}{\pi} \left[ V_{I}(E,r) + \Sigma_{I}^{(2)}(E) \right] \frac{1}{E - V_{I}(E,r) - \Sigma_{I}^{(2)}(E)^{2} + \Sigma_{I}^{(2)}(E)} ,$$  \hspace{1cm} (13)

where we use $\Sigma^{(2)}$ to denote the two-particle selfenergy that arises from the uncorrelated single-particle selfenergies \cite{26,27}. We now make concrete ansätze for the potential and selfenergies in terms of a field-theoretic model for the in-medium Cornell potential \cite{27} and previous results from the $T$-matrix formalism \cite{28}. The former leads to the following real parts of potential and uncorrelated selfenergy,

$$V_{R}(E,r) = \frac{4}{3} \alpha_{s} e^{-m_{r}/r} - \sigma \frac{e^{-m_{r}/r}}{m_{r}}$$  \hspace{1cm} (14)

$$\Sigma_{R}^{(2)}(E) = -\frac{4}{3} \sigma_{s} m_{D} + \frac{1}{m_{s}} ,$$  \hspace{1cm} (15)

corresponding to the $r$-dependent and $r$-independent terms of the screened Cornell potential, respectively (additional contributions from the uncorrelated 2-particle propagator are small \cite{26} and therefore neglected in the present exploratory calculation). Their strengths are characterized by the strong coupling, $\alpha_{s} = g^{2}/(4\pi)$, and string tension $\sigma$, along with corresponding screening masses $m_{D}$ and $m_{s}$, respectively. As in our previous work \cite{13,14}, we utilize the latter as independent fit parameters, where, for simplicity, we choose a linear ansatz, $m_{D,s} = c_{D,s} g T$ with two constant coefficients, $c_{D,s}$ (which turn out to be close of order one).

The imaginary part of the uncorrelated 2-particle selfenergy, $\Sigma_{I}^{(2)}$, follows from the folding integral of the single-particle propagators which contain the respective in-medium selfenergies. In principle, this quantity follows automatically from a selfconsistent calculation, once the potential is specified, as was carried out in Ref. \cite{26}. For our exploratory study in the present work, we do not enforce selfconsistency but instead employ the energy dependence of $\Sigma_{I}^{(1)}$ as found in Ref. \cite{26} (see Fig. 3 in there) to compute $\Sigma_{I}^{(2)}$. It turns out that the latter can be well represented by Gaussian form,

$$\Sigma_{I}^{(2)}(E) = D \exp \left[ -\frac{(E - \Sigma_{I}^{(1)})^{2}}{2(CT)^{2}} \right] \frac{4}{3} \sigma_{I} T .$$  \hspace{1cm} (16)

With $C \approx 1.6$ we can reproduce the energy dependence of the single-particle width of Ref. \cite{26}, being very similar for both internal and free energies as underlying potential. The strength parameter $D$, however, which we
define relative to the perturbative value, \( \frac{1}{4} \alpha_s T \), markedly depends on the underlying potential, varying by a factor of 2-3 between free and internal energies; as mentioned above, we here use it as a fit parameter.

Finally, we have to specify the imaginary part of the potential; its magnitude and \( r \) dependence has been determined previously in the weak coupling limit as \( V^\text{ext}_I = \frac{1}{4} \alpha_s T \Phi(m_{Qr}) \) \cite{24, 25}, where \( \Phi(x) \) is a smoothly varying function which vanishes for \( x=0 \) and approaches 1 for large \( x \). However, in our definition of the potential, we have identified the non-zero part at infinite distance with the uncorrelated selfenergy. Upon subtracting this part and again allowing for a nonperturbative enhancement with the same strength parameter \( D \) and energy dependence as in Eq. (16) we arrive at the form

\[
V_I(E, r) = D \exp \left( -\frac{(E - \frac{V_f^2}{2})^2}{2(C T)^2} \right) \frac{4}{3} \alpha_s T \left[ \Phi(B m_{Qr}) - 1 \right].
\]

(17)

To accommodate the possibility that the imaginary part of the string interaction can have a different \( r \) dependence than given by \( \Phi \) (albeit with the same asymptotic limits), we rescaled its argument by a constant \( B \) (which turns out to be close to one). We note that nontrivial energy dependencies in both imaginary parts, \( V_I \) and \( \Sigma^2 \), are crucial to ensure convergence of the integration in Eq. (12). In this sense, the potential is required to go beyond the static approximation.

As an example of our method we perform a fit to a set of free energies computed in lattice QCD with \( N_f = 2 + 1 \) dynamical flavors \cite{35}, for temperatures \( T=1.2, 1.7, 2.2 T_c \), with \( T_c=196 \text{ MeV} \) \cite{35}. The following parameter values were used: The Coulomb Debye mass is \( m_D = 1.22 g T \), close to the expected HTL value, while the string interaction is screened less with \( m_r = 0.8 g T \); for the string tension itself a constant value of \( \sigma = 1.58 \text{ GeV/fm} \) turns out to be sufficient, which is larger than in vacuum but significantly smaller than in previous fits to the in-medium free energy \cite{12, 27}.

For the strong coupling we utilize a weak temperature running, \( \alpha_s = 0.288 - 0.05 \left( \frac{T}{1.2 T_c} - 1 \right) \), decreasing from 0.288 at 1.2\( T_c \) to 0.238 at 2.4\( T_c \). For the dimensionless coefficients we have \( B = 0.73 \), which delays the approach of \( \Phi \) to its asymptotic value of one, and \( C=2.07 \) in Eq. (10), which produces slightly longer tails in the energy dependence of the HQ selfenergies than in the microscopic calculations of Ref. \cite{26}.

The resulting fit to the IQCD free energies is displayed in Fig. 1, showing good agreement. Reproducing the temperature dependence essentially ensures that the internal energies, \( U = F + TS \) with \( S = -dF/dT \), also agree with the lattice data. The underlying two-body potential turns out to lie significantly above \( F_{Q0} \) but below \( U_{Q0} \) at intermediate and long distances. However, the potential differs from both free and internal energy in that its derivative, characterizing the interquark force, is larger than for both \( F_{Q0} \) and \( U_{Q0} \), in a region around \( r \approx 1 \text{ fm} \). This is a remnant of the confining string term in the hot medium, caused by the relatively small screening mass, \( m_r \). Even though this force is not so large, it has a rather long range, encompassing a relatively large volume. In the heavy-light quark sector, this enables heavy quarks to effectively couple to more particles in the heat bath, relative to a short-range force. Our preliminary calculations of the HQ diffusion coefficient indeed indicate that the latter is comparable to earlier calculations using the internal energy \cite{12}, which has a stronger force but over a shorter range. In this sense, the potential obtained in the present study may still imply a strongly coupled QGP.

The above example of a fit is not unique, mostly due to uncertainties in the imaginary parts, which in the future will have to be calculated in a selfconsistent scheme as laid out in Ref. \cite{26}. However, several qualitative, model-independent observations can be made. First, if the imaginary parts, \( (V + \Sigma^2)(E) \), are taken to zero, the spectral function \( \sigma^V \) becomes a \( \delta \) function in energy and the potential in the denominator is forced to become the free energy, thus recovering the weak-coupling analysis of Ref. \cite{12}. This underlines the key role of the imaginary parts of both potential and single-quark selfenergy in raising the potential above the free energy, i.e., rendering a stronger force. The \( E \)-dependence of \( (V + \Sigma^2)(E) \) (the “width of the width”), encoded in the width parameter \( C \), also plays an important role, which reiterates the need for microscopic calculations, such as the \( T \)-matrix approach. The dependence on the real part is more robust and “model independent” in the sense that it can be largely determined by the small distance behavior of free energy where \( \Phi(x) \) forces the imaginary part to become small. Let us also comment on the magnitude of the string tension exceeding its vacuum value by about 60\%. This appears to be a rather generic feature within the screened Cornell potential ansatz. In previous works utilizing this ansatz \cite{12, 27}, where the strength of the string term was additionally allowed to develop a temperature dependence, fits to the free energy preferred string tensions of up to a factor 3-4 times.

\footnote{The imaginary parts implicit in our fit are comparable to what was found before with the internal energy as potential, which indicates that they are in the expected ballpark of the selfconsistent solution.}
the vacuum, albeit with a much stronger screening than
in our present potential fit. As a result, the in-medium free energy never exceeds the vacuum potential (as in
our present work). Similar features are also found in applications of the Dyson-Schwinger approach to quarko-
nia at finite $T$ [36]. A possible microscopic mechanism
for an enhanced string tension could be the release of magnetic monopole in the near-$T_c$ region, as suggested,
e.g., in Ref. [37].

4. Conclusions and Outlook

Utilizing a thermodynamic $T$-matrix approach, we
have derived an expression for the static heavy-quark free energy that directly relates to the underlying in-
teraction kernel, resummed in ladder approximation.
The such defined kernel serves as our definition of an
in-medium potential, $V_{QQ}(r)$, in the context of a dia-
grammatic many-body approach. Key elements of this
framework are a non-trivial energy dependence of the pertinent $Q\bar{Q}$ spectral function, induced by the imagi-
nary parts of both one- and two-body type, i.e., in the
single-quark selfenergies and the potential. We have
applied this set-up to fit lattice-QCD "data" for the
color-singlet free energy in the spirit of a variational
scheme for the underlying potential. To facilitate this,
we made an ansatz for the real part of the potential in
terms of a screened Cornell potential, augmented with
an imaginary part motivated by perturbative studies but
with variable magnitude. We additionally accounted for
complex heavy-quark self-energies with an energy de-
pendence motivated by earlier selfconsistent implemen-
tations of the many-body theory. The resummations
of the interaction kernel, with a nonperturbative string
term, and of the selfenergies are required in a regime of
strong coupling, as expected for the QGP at tempera-
tures not too far above $T_c$. Indeed, our resulting potential
significantly deviates from the weak coupling limit
(in which case it would be close to the free energy), and
exhibits a rather long-range remnant of the confining
force surviving well above $T_c$. The associated imagi-
nary parts are large, not inconsistent with what was ob-
tained earlier using the internal energy as a potential ap-
proximation. First estimates indicate that the pertinent
HQ diffusion coefficient is around $D_s(2\pi T) \approx 3 \sim 5$, suggestive for a strong coupling regime.

Several further investigations are in order to scruti-
nize our initial estimates within the $T$-matrix approach.
First, the calculation needs to be carried out selfconsis-
tently, by computing the heavy-quark selfenergies from
the underlying $T$-matrices and reinserting the former in
the latter [26]. Second, the free energies should be up-
dated with the most recent lattice-QCD results. Third,
quarkonium correlators, HQ susceptibilities and trans-
port coefficients should be computed and systematically
compared to lattice data. The role of possible three-
body correlations may need to be addressed. If the the-
eoretical framework passes these tests, applications to
heavy-quark and quarkonium phenomenology are war-
anted.

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