

In-medium heavy quark-antiquark T matrix without partial-wave expansion

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The T matrix of the heavy quark-antiquark ($Q\bar{Q}$) pair interacting through a screened Cornell potential in the quark-gluon plasma is computed without employing the partial-wave expansion. This is compared with the results obtained using the conventional method of partial-wave expansion. Through a comprehensive survey over a range of screening mass and center-of-mass (c.m.) energy, which, when combined, determine the orbital angular momentum involved in the scattering, it is demonstrated that a substantial number of partial-wave terms are necessary to precisely match the full scattering amplitude directly obtained from the method without partial-wave expansion. For moderate screening masses (corresponding to one to two times the crossover transition temperature) and c.m. energy, the number of partial waves required for satisfactory matching turns out as large as 10–20, substantially larger than what one would expect based on simply measuring the magnitudes of the first few partial-wave amplitudes. This highlights the efficacy and advantage of the new method in directly obtaining the full scattering amplitude needed for further computation of physical observables, which is illustrated by comparing the calculations of heavy quark-antiquark scattering cross section and heavy quark drag coefficient between the two methods. We also employ the new method to calculate the T matrix at c.m. energies below the $Q\bar{Q}$ mass threshold, and demonstrate the presence of bound states of different orbital quantum numbers simultaneously in a single energy scan.

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I. INTRODUCTION

Ultrarelativistic high-energy collision experiments aim to create and study the quark-gluon plasma (QGP), a novel phase of nuclear matter. Quarkonia—bound states of heavy quark-antiquark pairs ($Q\bar{Q}$, where Q is a charm or bottom quark)—serve as key probes for understanding color-force modifications in QGP [1–3]. As different heavy quarkonia are characterized by different sizes in vacuum, they are expected to be influenced progressively in the inverse order of their binding energies when immersed in the medium. The earliest prediction of a sequential quarkonia suppression [4], primarily due to color-charge screening of $Q\bar{Q}$ potential in QGP, has been observed experimentally in the bottomonia sector [5]. However, a static screening scenario alone is insufficient; in-medium dynamical effects, such as inelastic collisions [6,7], reflecting the imaginary part of the potential [8], generate state-dependent dissociation widths. At LHC energies, the enhanced production of charm quarks enables charmonium regeneration from uncorrelated $c\bar{c}$ pairs [9–11], while bottomonium regeneration occurs via in-medium transitions to different bound states of a single correlated pair [12,13]. The

regeneration rate, through the fluctuation-dissipation theorem, is related to the dissociation rate [14] and consequently to the imaginary potential. Theoretically, the strength of screening (mass shift), the in-medium binding energies and the reaction rates are all encoded in the quarkonia spectral functions [15].

The in-medium quarkonia spectral properties can be computed through the first-principles lattice QCD approach, which provides information on both the real and imaginary parts of the $Q\bar{Q}$ potential [16–18]. Due to the heavy quark mass $M_Q \gg T$, the energy k_0 of the exchanged gluons between the $Q\bar{Q}$ pair is parametrically smaller than their momentum $|\vec{k}| \approx T$, implying that a static picture remains valid in the QGP medium. Therefore, it is anticipated that the predominant interactions between the $Q\bar{Q}$ pair are of potential nature, which can then be resummed by the scattering T -matrix equation. The thermodynamical T -matrix framework has been employed in the computation of spectral functions of quarkonia, heavy-light mesons, and diffusion coefficient for heavy quarks in the QGP [19–23]. Its advantages lie in providing a unified framework to analyze both the bound and the continuum states of $Q\bar{Q}$ pair in medium [20]. It is based on a three-dimensional (3D) reduction of the relativistically covariant four-dimensional Bethe-Salpeter equation. The two most common methods for the 3D reduction in literature are those of Blankenbecler-Sugar [24] and Thompson [25]. The 3D reduction enables one to solve the two-body Bethe-Salpeter scattering amplitude using an instantaneous (thus nonrelativistic) potential as input, while retaining the relativistic unitarity [24,25]. Higher-order relativistic corrections can also be appropriately included in this approach [20,22]. Lattice QCD data of quarkonia correlators and heavy quark

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susceptibilities, when applied to this approach, may provide first-principles constraints for the extraction of in-medium $Q\bar{Q}$ potential as well as spectral functions [22,23]. On the other hand, direct application of the phenomenologically motivated potential in this approach, e.g., the Cornell-type potential parameterized with color screening has also turned out useful in the T -matrix calculations of in medium-heavy quark systems [26,27].

The conventional T -matrix calculations of $Q\bar{Q}$ system have employed the partial-wave expansion method (termed PWE in this work) [19–23,28], to simplify the numerical solution of the 3D reduced T -matrix equation. It is advantageous when the $Q\bar{Q}$ potential exhibits rotational symmetry. The T -matrix equation in PWE method assumes the form of a one-dimensional integral equation, which can be formulated as a matrix inversion problem [28]. In problems with small angular momentum, the scattering rates can be computed with first few partial-wave amplitudes. Similarly, the PWE method is suitable for computing spectral functions or bound states for a specific channel with definite orbital angular momentum (e.g., s-wave or p-wave). However, there are situations where these advantages break down. First, when the $Q\bar{Q}$ potential is not rotationally symmetric, e.g., in cases where one aims to address the anisotropy of the QGP medium or if the c.m. momentum of $Q\bar{Q}$ pair cannot be neglected. Second, the full T matrix is related to the its PWE components as (see Sec. II A for details)

$$T(\vec{q}', \vec{q}) = 4\pi \sum_{l=0}^{\infty} (2l+1) T_l(q', q) P_l(\hat{q}' \cdot \hat{q}). \quad (1)$$

The convergence of the sum in the above equation is marred by the presence of the degeneracy factor $(2l+1)$ and Legendre polynomials of order l [denoted by $P_l(x)$]. First, the factor $(2l+1)$ can counter the decrease of the partial-wave amplitudes T_l as l increases and thus significantly slow down the convergence of the PWE series. Furthermore, the oscillatory nature of Legendre polynomials may necessitate the inclusion of a substantial number of PWE terms to achieve precise matching with the full amplitude on the left-hand side, which is usually a smooth function of the involved variables and is needed for precision calculations of phenomenological observables, e.g., heavy quark elliptic flow coefficient [26]. The magnitude of the angular momentum involved in a problem depends upon the impact parameter and the momentum of the projectile, implying that a large number of PWE terms will be required to reproduce the full amplitude in case one of them is large. Consequently, it is worthwhile to explore the solution of T -matrix equations without employing the partial wave expansion (termed no-PWE in this work). Indeed, the no-PWE method has been pursued for the nonrelativistic Lippmann-Schwinger equation addressing the nucleon-nucleon scattering in vacuum [29–31].

In this work, we apply the no-PWE method [31] to compute the $Q\bar{Q}$ scattering mediated by a temperature dependent potential [32] in the QGP. We calculate the pertinent T matrix utilizing both PWE and no-PWE methods and compare them against each other for a wide range of Debye screening masses m_D and c.m. energies E_{CM} . Working with the Thompson form

of 3D-reduced T -matrix equation [19], we demonstrate for the scattering problem (i.e., E_{CM} above the $Q\bar{Q}$ mass threshold) that the number of PWE terms required to match the full amplitude obtained directly from the no-PWE method is substantially larger than one would expect from simply measuring the magnitudes of first few partial-wave amplitudes, especially at small screening mass or large E_{CM} . This is further illustrated and corroborated by calculating two kinds of physical quantities, namely the heavy quark-antiquark scattering differential cross section and the heavy quark drag coefficient, both involving the pertinent full on-shell T matrices that are computed using PWE versus no-PWE methods. Applying the no-PWE method to the bound state problem where E_{CM} is below the mass threshold, we demonstrate that the no-PWE T matrix can accommodate all bound states of different orbital angular momentum simultaneously, for the first time in literature to our knowledge. For the purpose of simply demonstrating the power of the no-PWE method for computing the T matrix, we refrain from coupling the two-body $Q\bar{Q}$ scattering equation to the one-body Q self-energy equation in the present work, which would require a self-consistent iteration of the integral system and will be pursued in the future.

The article is organized as follows. In Sec. II the basics of 3D-reduced T -matrix equation is outlined. Following the brief account of the PWE method and its numerical implementation in Sec. II A, the formalism of the no-PWE method and details of its numerical implementation are discussed in Secs. II B and II C. Then in Sec. III we move on to present in detail the numerical computations and results of our work. First we discuss in Sec. III A the behavior of first few partial-wave amplitudes for a range of screening masses. Next, in Sec. III B we discuss the comparison between the PWE and no-PWE methods for the scattering problem, by varying the screening mass m_D and E_{CM} over a wide range. In Sec. III C the half-off-shell T -matrix amplitudes are compared between the PWE and no-PWE approaches. In Sec. IV the $Q\bar{Q}$ scattering cross section and heavy quark drag coefficient are calculated and compared between the PWE and no-PWE methods. In the last Sec. V, we discuss the computation of below mass threshold T matrix (pertaining to bound state problem) in the no-PWE approach, from the perspectives of both numerical demonstration and analytical understanding. In Sec. VI we conclude our work and present a short summary, with potential applications in future work.

II. T -MATRIX FORMALISM

The starting point of our analysis is 3D-reduced [24,25] form of the four-dimensional Bethe-Salpeter equation, which has been conventionally used in $Q\bar{Q}$ T -matrix calculations. We work in the c.m. (CM) frame setting $\vec{P}_{\text{CM}} = 0$. The 3D-reduced equation is given as

$$T(E_{\text{CM}}, \vec{q}', \vec{q}) = V(\vec{q}', \vec{q}) + \int \frac{d^3k}{(2\pi)^3} V(\vec{q}', \vec{k}) \times G_{Q\bar{Q}}(E_{\text{CM}}, k) T(E_{\text{CM}}, \vec{k}, \vec{q}). \quad (2)$$

The 3D-reduction in essence puts the propagator of virtual heavy quark(antiquark) on its positive (negative) mass shell.

The 3D-reduced two-body propagator is constructed in such way that the unitarity properties of the four-dimensional Bethe-Salpeter equation are preserved. The complete two-body kernel is approximated by the potential term $V(\vec{q}', \vec{q})$, which does not depend upon E_{CM} . Replacing the two-body interaction kernel with the potential term amounts to approximating the full scattering series with the ladder approximation. We also ignore any relativistic corrections to the potential term, as implemented in Refs. [20,22], or the spin structure of the T and V matrices and the resulting complications that arise thereafter.

The propagation of heavy quark-antiquark pairs is governed by $G_{Q\bar{Q}}(E_{\text{CM}}, k)$. We employ the Thompson propagator [19,25], for its simple form and similarity to the nonrelativistic case:

$$G_{Q\bar{Q}}(E_{\text{CM}}, k) = \frac{1}{E_{\text{CM}} - 2\omega_k - 2i\Sigma_I(\omega_k, k)} [1 - 2n_F(\omega_k, T)]. \quad (3)$$

Here, $\omega_k = \sqrt{k^2 + M^2} + \Sigma_R(\omega_k, k)$ and $\Sigma_R(\omega_k, k)$, $\Sigma_I(\omega_k, k)$ represent the real and imaginary parts of the heavy quark (antiquark) self-energy in the medium, respectively. $n_F(\omega_k, T)$ denotes the Fermi-Dirac thermal distribution function for heavy quarks (antiquarks):

$$n_F(\omega_k, T) = \frac{1}{e^{\omega_k/T} + 1}. \quad (4)$$

The factor of $[1 - 2n_F(\omega_k, T)]$ accounts for the thermal modification of the two-body propagator $G_{Q\bar{Q}}(E, k)$. The complete many-body treatment of this problem requires solving a coupled self-energy equation for the heavy quark (antiquark), which is inserted back into Eq. (2). The self-energy stems from interactions between heavy quarks (antiquarks) with thermal light quarks/antiquarks and gluons present in the medium. In this work, we disregard this additional modification of single heavy quark (antiquark) properties and set the real part to zero, $\Sigma_R(\omega_k, k) = 0$. We employ a constant, albeit small, imaginary part $\Sigma_I \approx -10$ MeV in the propagator to mitigate the delta-function-like poles of the propagator. Given that our primary focus in this work is solely on the formal comparison of PWE and no-PWE methods, we defer further details regarding these additional considerations to a future work.

A. PWE method

The two-body interaction kernel is approximated by the potential interactions $V(\vec{q}', \vec{q})$. Assuming the potential in position space to be given by a local, scalar term, but independent of the spin of the $Q, \bar{Q}$ particles, the T and V matrices in the momentum space are expanded in terms of their partial-wave components

$$V(\vec{q}', \vec{q}) = 4\pi \sum_{l=0}^{\infty} (2l+1) V_l(q', q) P_l(\hat{q}' \cdot \hat{q}),$$

$$T(\vec{q}', \vec{q}) = 4\pi \sum_{l=0}^{\infty} (2l+1) T_l(q', q) P_l(\hat{q}' \cdot \hat{q}), \quad (5)$$

with the $V(\vec{q}', \vec{q})$ obtained from the Fourier transform of the position space potential

$$V(\vec{q}', \vec{q}) = \int d^3r V(\vec{r}) e^{i(\vec{q}-\vec{q}') \cdot \vec{r}}. \quad (6)$$

Here $\hat{q} = \vec{q}/|\vec{q}|$ is the unit vector, and $P_l(x)$ is the Legendre polynomial of order l . Integrating out the angle associated with $\vec{k}$ in Eq. (2) using the orthogonality relation for the Legendre polynomials and matching the component of $P_l(x)$ on both sides, one obtains the T -matrix equation for its l th component

$$T_l(E, q', q) = V_l(q', q) + \frac{2}{\pi} \int_0^\infty dk k^2 V_l(q', k) \times G(E, k) T_l(E, k, q), \quad (7)$$

where

$$V_l(q', q) = \int dr r^2 j_l(q'r) j_l(qr) V(r), \quad (8)$$

and $j_l(r)$ is the spherical Bessel function of order l . After the partial-wave expansion, the resulting T -matrix equation is solved using the algorithm of Haftel-Tabakin [28]. After the discretizations of momentum variables using the Gauss-Legendre quadratures, denoted as q_j , Eq. (7) can be written in the matrix form as

$$[T_l(E)]_{ij} = [V_l]_{ij} + \frac{2}{\pi} \sum_k w_k q_k^2 [V_l]_{ik} [G(E)]_{kk} [T_l(E)]_{kj},$$

$$[T_l(E)] = (1 - [V_l][G(E)])^{-1} [V_l], \quad (9)$$

and can be solved using standard matrix inversion routines. Throughout this work we use the notation [...] to represent the matrix form of T or V matrices.

B. no-PWE method

In Ref. [31] the nonrelativistic Lippmann-Schwinger equation for a nucleon-nucleon system in vacuum was solved without employing the partial-wave expansion. After the 3D reduction has been performed, the Thompson T -matrix equation is formally similar to the Lippmann-Schwinger equation, with main difference occurring in the two-body propagator and the thermal corrections to it, both of which in the case of $\vec{P}_{\text{CM}} = 0$ can be made independent of angular coordinates. As such, the no-PWE method of Ref. [31] can be extended to the Thompson equation. We first write the 3D-reduced T -matrix equation [Eq. (2)] as

$$T(q', q, x') = V(q', q, x') + \int_0^\infty \frac{dk k^2}{(2\pi)^3} \int_{-1}^1 dx'' \int_0^{2\pi} d\phi'' V(q', k, y) \times G_{Q\bar{Q}}(E, k) T(k, q, x''), \quad (10)$$

where $x' = \hat{q}' \cdot \hat{q}$, $y = \hat{q}' \cdot \hat{k}$, $x'' = \hat{k} \cdot \hat{q}$, and we have suppressed the E dependence of $T(E, \vec{q}', \vec{q})$ for brevity. Setting $\hat{q} = \hat{z}$ and using the angular coordinates for the unit vectors $\hat{q}' = \hat{q}'(\theta', \phi')$, $\hat{q}'' = \hat{q}''(\theta'', \phi'')$, we can express y as a

function of x', x'' as

$$y = x'x'' + \sqrt{1-x'^2}\sqrt{1-x''^2}\cos(\phi'' - \phi'). \quad (11)$$

Since no term depends upon ϕ' we conveniently set it to zero. Substituting this back in Eq. (10), we get

$$T(q', q, x') = \frac{1}{2\pi} v(q', q, x', 1) + \int_0^\infty \frac{dk}{(2\pi)^3} \int_{-1}^1 \times dx'' v(q', k, x', x'') G_{Q\bar{Q}}(E, k) T(k, q, x''), \quad (12)$$

where we have introduced

$$v(q', q, x', x'') = \int_0^{2\pi} d\phi'' V(q', q, x'x'' + \sqrt{1-x'^2}\sqrt{1-x''^2}\cos\phi''). \quad (13)$$

In the next section we discuss how to numerically solve the no-PWE T -matrix equation.

C. Numerical method for no-PWE

After the discretizations of momentum and the angular variables, the resulting quantities in Eq. (12) are arrays of dimension 3 or higher, and cannot be solved with the method of matrix inversion used in the PWE case and a different numerical method has to be implemented to solve the no-PWE T -matrix equation, which we discuss in this section. Noting that in Eq. (12) (remember that the CM energy dependence has been suppressed), the only variables present in the equation are q' and x' , which through the kernel term $v(q', q, x', x'')$ couple the T matrix on the right-hand side (RHS) and LHS. We can utilize this by solving the equation for each q independently. To understand the numerical method, first we convert Eq. (12) into its discrete version by using the Gauss-Legendre quadratures to convert the integration over the momentum and angular variables, k and x , respectively, into a discrete sum. The array $T(E, q', q, x')$ for a given E and q can be rearranged into a vector of length $N_q \times N_x$ as $[T]_i$, where N_q and N_x are number of grid points for the Gauss-Legendre quadratures for the momentum and the angular variables. Using the same method, the term $v(q', q, x', 1)$ can also be converted into a vector of the same length, corresponding to a fixed q . The integration kernel can be expressed as

$$[K(E)]_{ij} = \frac{k_j^2}{(2\pi)^3} [w(k)]_{g(j)} [w(x)]_{f(j)} [v]_{ij} [G(E)]_j, \quad (14)$$

where $[v]_{ij} = v(q'_i, k_j, x'_i, x''_j)$ is a two-dimensional matrix of size $(N_q \times N_x) \times (N_q \times N_x)$, and $[w(k)]$, $[w(x)]$ are Gauss-Legendre weights corresponding to the momentum and angular integration variables k and x'' . The function $f(i)$, $g(i)$ are remainder and modulo functions, respectively,¹ to assign

¹Since i, j run over the entire range $i, j \in [1, N_q \times N_x]$, we pick the corresponding values of $[w(q)]$ and $[w(x)]$ using i/N_x (modulo operator) and $i \% N_x$ (remainder operator), respectively.

$[w(k)]$ and $[w(x)]$ to their corresponding q_i and x_j , as all variables have to be casted into a vector of length $N_q \times N_x$. After vectorization of all the terms in the stated manner, for a particular q_k one obtains the following matrix equation:

$$[T(E)]_i^k = \frac{1}{2\pi} [v]_i^k + [K(E)]_{ij} [T(E)]_j^k, \\ [T(E)]^k = (1 - [K(E)])^{-1} \frac{1}{2\pi} [v]^k. \quad (15)$$

This is similar in form to the PWE matrix equation, which is expected since both of them are linear equations, and can be solved using the method of matrix inversion. Then by looping over the entire range of q_k and joining the solution $T^{k'}$ s for each case, one obtains the full solution $T(q', q, x)$. The E_{CM} dependence of $T(E, q', q, x)$ enters the T -matrix equation through the dependence of two-body propagator $G_{Q\bar{Q}}(E, k)$ on E_{CM} , and can be addressed independently of other variables present in Eq. (12). Before moving to the next section, we note that we scale the Gauss-Legendre quadratures u 's, obtained in the range $(0, 1)$, for the momentum integration range $(0, \infty)$ using the transformation

$$q = b \tan\left(\frac{u\pi}{2}\right), \quad (16)$$

where the constant $b \approx 1$ GeV is a scaling parameter.

Before embarking on real calculations, we make a comment on the numerical cost of the two methods. The most numerically intensive part of calculating the T matrix resides in the inversion of the kernel matrix $\{1 - [V_l][G(E)]\}$ [Eq. (9)], for the PWE method, and $[1 - K(E)]$ [Eq. (15)] for the no-PWE method. The numerical cost for calculating the PWE T matrix can be estimated as $C_{\text{PWE}} \approx L_{\text{Max}} \times N_q^3$, where L_{Max} is the number of partial-wave terms needed for convergence, while the numerical cost for the no-PWE case scales as $C_{\text{no-PWE}} \approx (N_q \times N_x)^3$. Therefore, even in cases where many partial-wave terms, say $L_{\text{Max}} \approx 20$ –40, are needed for convergence, the PWE method is order of magnitude numerically cheaper ($C_{\text{PWE}}/C_{\text{no-PWE}} \approx L_{\text{Max}}/N_x^3$, with typical $N_x \approx 16$ –24) than the no-PWE method, modulo the cost in the numerical evaluation of the $V_l(q', q)$ [Eq. (8)] matrices required in the PWE method [whereas the $V(q', q, x', x)$ needed in the no-PWE method can be analytically evaluated]. Although the no-PWE method is not superior to the PWE method in terms of the computational cost, the advantage of the no-PWE method lies in its efficacy to directly compute the full amplitude once for all, allowing one to avoid computing each partial-wave amplitude for all l , especially when many T_l 's are needed for evaluating physical quantities, as to be demonstrated below.

III. SCATTERING STATE PROBLEM: $E_{\text{CM}} > 2M_c$

We first discuss the $Q\bar{Q}$ scattering problem, characterized by $E_{\text{CM}} > 2M_c$, where M_c is the mass of open charm quark in the QGP medium. The magnitude of angular momentum in a scattering problem depends upon two factors, the impact parameter and the incoming momentum of the projectile. The impact parameter in the $Q\bar{Q}$ scattering problem is determined

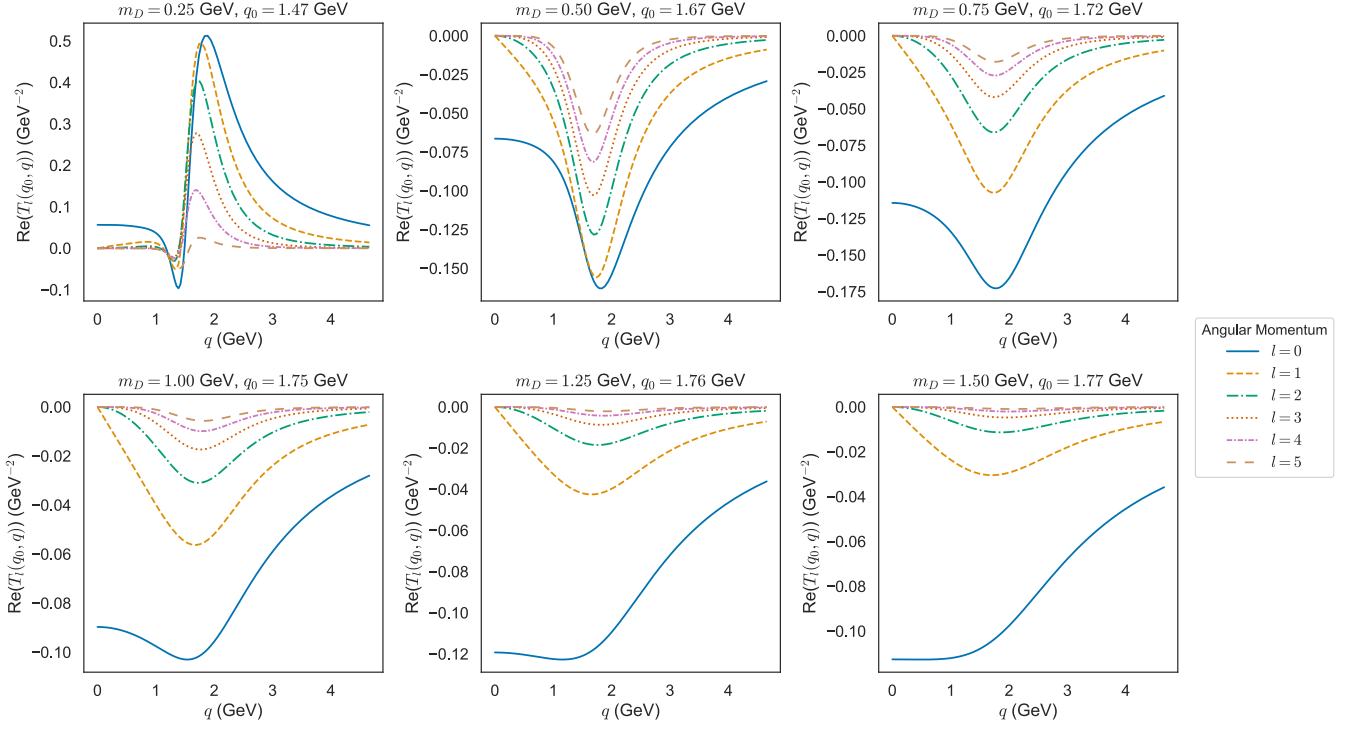


FIG. 1. The first five $\text{Re}[T_l(q_0, q)]$ [$\text{Re}(T)$ denotes real part of the T matrix in here and rest of the plots] as a function of q are shown for six different values of screening mass we consider. The value of on-shell momentum q_0 and the corresponding screening mass m_D are given in the title of the plot.

by the effective range of the $Q\bar{Q}$ potential $V(r, T)$, whereas the incoming momentum in the problem depends upon the CM energy E_{CM} . Several works [16,33] have addressed the determination of $V(r, T)$ on lattice, and have found that the potential exhibit screening, which increases with increasing medium temperature. To model the function $V(r, T)$, we employ a Cornell-type potential

$$V(r, T) = \frac{-\alpha}{r} e^{-m_D(T)r} + \frac{\sigma}{m_D(T)} (1 - e^{-m_D(T)r}), \quad (17)$$

which is characterized by a screening mass $m_D(T)$, and rest of the parameters are same as those used in Ref. [32], $\alpha = 0.471$, $\sigma = 0.192 \text{ GeV}^2$. The temperature dependence of $V(r, T)$ is solely contained in the screening mass $m_D(T)$, and we can vary the effective interaction range or the impact parameter in the scattering problem by varying $m_D(T)$.

The bare mass of charm quark is set to $M_c^0 = 1.32 \text{ GeV}$. The function $V(r, T)$ employed in Eq. (17) tends to a finite value $\sigma/m_D(T)$ as $r \rightarrow \infty$. Its Fourier transform $V(\vec{q}', \vec{q})$ exists only if $V(r, T)$ goes to zero as $r \rightarrow \infty$, therefore we subtract the $V(r = \infty, T) = \sigma/m_D(T)$ part from the potential function and add this to the heavy quark bare mass (following the line of work in Refs. [20,22]), as a temperature-dependent contribution to $M_Q(T)$ arising due to its interaction with the thermal medium, $M_c = M_c^0 + \sigma/2m_D$. This also affects the threshold value $E_{\text{th}} = 2M_c(T)$ below which bound states are formed, as $2M_c(T)$ decreases with increasing temperature or $m_D(T)$.

A. Partial-wave amplitudes T_l

In this section we first discuss partial-wave amplitudes T_l and their convergence, for a range of screening masses, which are later employed in the comparison between the PWE and no-PWE methods. As the QGP medium expands and cools down, the $Q\bar{Q}$ pair undergoes scattering at different temperatures, and $m_D(T)$ changes throughout the medium evolution. To model this we consider six different screening masses $m_D = \{0.25, 0.5, 0.75, 1, 1.25, 1.5\} \text{ (GeV)}$, which is wide enough to cover a moderate range of temperature $T_c - 3 T_c$, where $T_c \approx 160 \text{ MeV}$ is the pseudocritical temperature denoting the crossover temperature for the QCD. The c.m. energy is fixed to $E_{\text{CM}} = 4.5 \text{ GeV}$ for the results presented in this section.

In a physical problem only the on-shell amplitude $T_l(q_0, q_0)$ is needed, where q_0 is the on-shell momentum in the scattering problem given by the on-shell condition $q_0 = \sqrt{E_{\text{CM}}^2/4 - M_c^2}$. To obtain the on-shell amplitude the T -matrix Eq. (7) needs to be solved at least for the half-off-shell case, $T_l(q_0, q)$, therefore we work with half-off-shell partial-wave amplitudes in this section. The comparison of first six half-off-shell $T_l(q_0, q)$ as a function of q is presented in Fig. 1 for the real part, and in Fig. 2 for the imaginary part. In the figure, though $E_{\text{CM}} = 4.5 \text{ GeV}$ is fixed, the on-shell momentum changes slightly as the charm quark mass depends upon m_D through the relation $M_c = M_c^0 + \frac{\sigma}{2m_D}$.

The overall observation is that both the real and imaginary part of the partial-wave amplitudes reduce as l increases. For the real part of T_l , except for the two lowest screening masses,

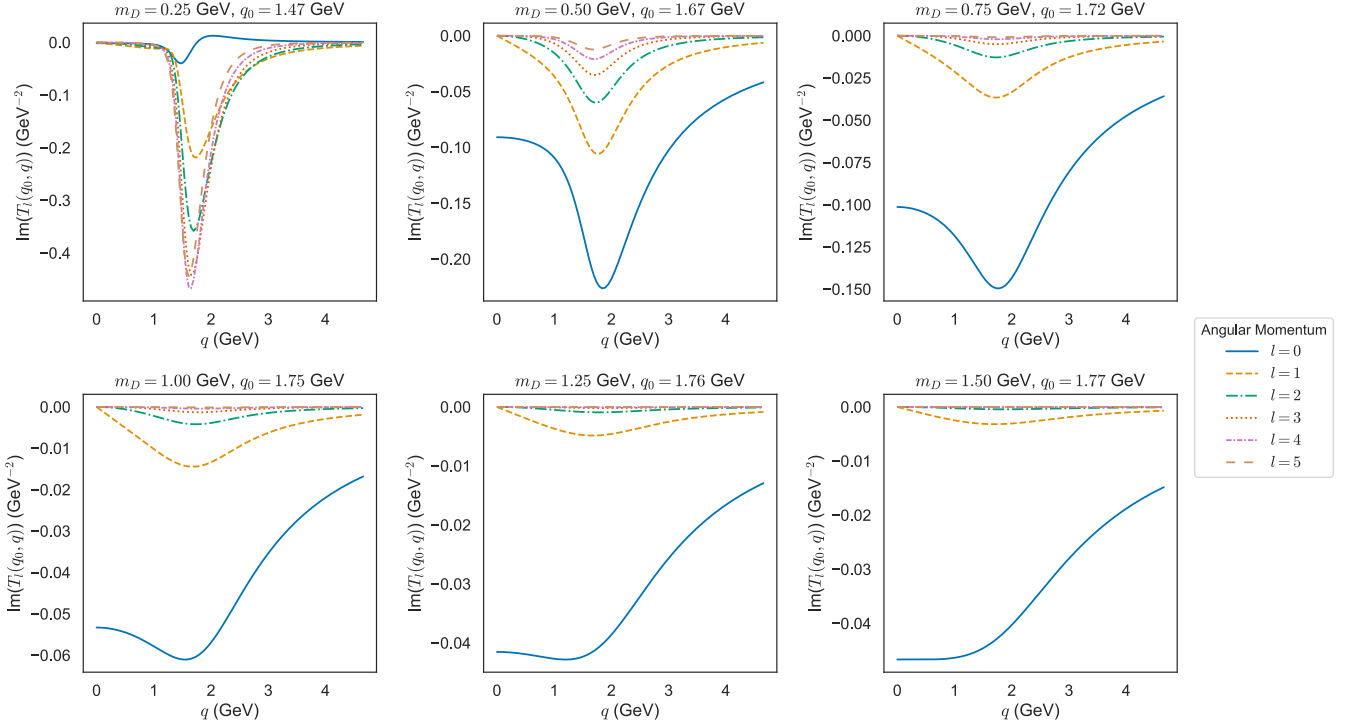


FIG. 2. The first five $\text{Im}[T_l(q_0, q)]$ [$\text{Im}(T)$ denotes imaginary part of the T matrix in here and rest of the plots] as a function of q are shown for six different values of screening mass we consider. Rest same as Fig. 1.

corresponding to $m_D = 0.25$ and 0.5 GeV, at which the half-off-shell $\text{Re}T_l(q_0, q)$ decreases rather slowly with increasing l , for the rest of the screening mass $m_D = 0.75$ – 1.5 GeV the real part of $T_l(q_0, q)$ all shows an order of magnitude decrease from $l = 0$ to $l = 5$. It is interesting to note that resummation of the strong attractive potential at the lowest screening mass $m_D = 0.25$ GeV results in a significant positive $\text{Re}T_l$ for $q > q_0$, which disappears for weaker potentials at higher screening masses. The shape of $\text{Re}T_l(q_0, q)$ and $\text{Im}T_l(q_0, q)$ in Figs. 1 and 2 depends upon their corresponding potential kernel $V_l(q', q)$ in Eq. (8). For $q' \approx q$ or $q' \ll q$, the Bessel functions are out of phase, and due to large oscillations, which increase as q increases, the integral becomes comparatively smaller. This is seen in Figs. 1 and 2, where the half-off-shell amplitudes $\text{Re}T_l(q_0, q)$ and $\text{Im}T_l(q_0, q)$ have their peaks occurring near $q \approx q_0$ region.

For a fixed l , the magnitude of $\text{Re}T_l$ generally becomes smaller as m_D increases. This can be understood from the fact that, when the screening mass increases, the effective range of interaction potential and thus the orbital angular momentum involved in the scattering decreases, and consequently higher partial-wave amplitudes corresponding to larger l values must become smaller. The imaginary part of the half-off-shell $T_l(q_0, q)$ at $m_D = 0.25$ GeV, first increases with l up to $l = 4$, and then starts decreasing as one goes to higher l 's (in the figure only up to $l = 5$ terms are plotted but higher terms become smaller as l keeps increasing). For the rest of the

screening masses $m_D = 0.5$ – 1.5 GeV the imaginary part all diminishes even faster than the real part with increasing l , and the $l \geq 3$ terms are already barely visible for $m_D \geq 0.5$ GeV.

Based on the above observation of the diminishing behavior of these first few partial-wave amplitudes with increasing angular momentum, one would expect that the first three to five partial-wave amplitudes should be enough to be summed over to arrive at the full amplitude needed for further precision calculation of physical quantities. However we will see in the next section that substantially larger number of PWE terms are necessary for reproducing the full T -matrix amplitudes, even at large screening masses $m_D = 0.75, 1$ GeV.

B. PWE vs no-PWE: On-shell amplitudes

The partial-wave T -matrix amplitudes are related to the full T matrix (or the no-PWE T matrix) as

$$T(q', q, x) = 4\pi \sum_{l=0}^{L_{\text{Max}}} (2l+1) P_l(x) T_l(q', q), \quad (18)$$

where L_{Max} is the minimum number of partial-wave terms required to reproduce the no-PWE full T matrix. In Eq. (18), the degeneracy of the l th channel is given by the factor of $(2l+1)$, which increases with increasing l and acts to counter the decrease in the partial-wave amplitudes T_l 's, therefore slowing down the convergence of the partial wave expansion in Eq. (18). Further, Legendre polynomials put another angle-dependent weight for each T_l , which oscillate for all values of x except $x = 1$ [$P_l(x = 1) = 1$]. Therefore the sum of different partial-wave amplitudes does not monotonically

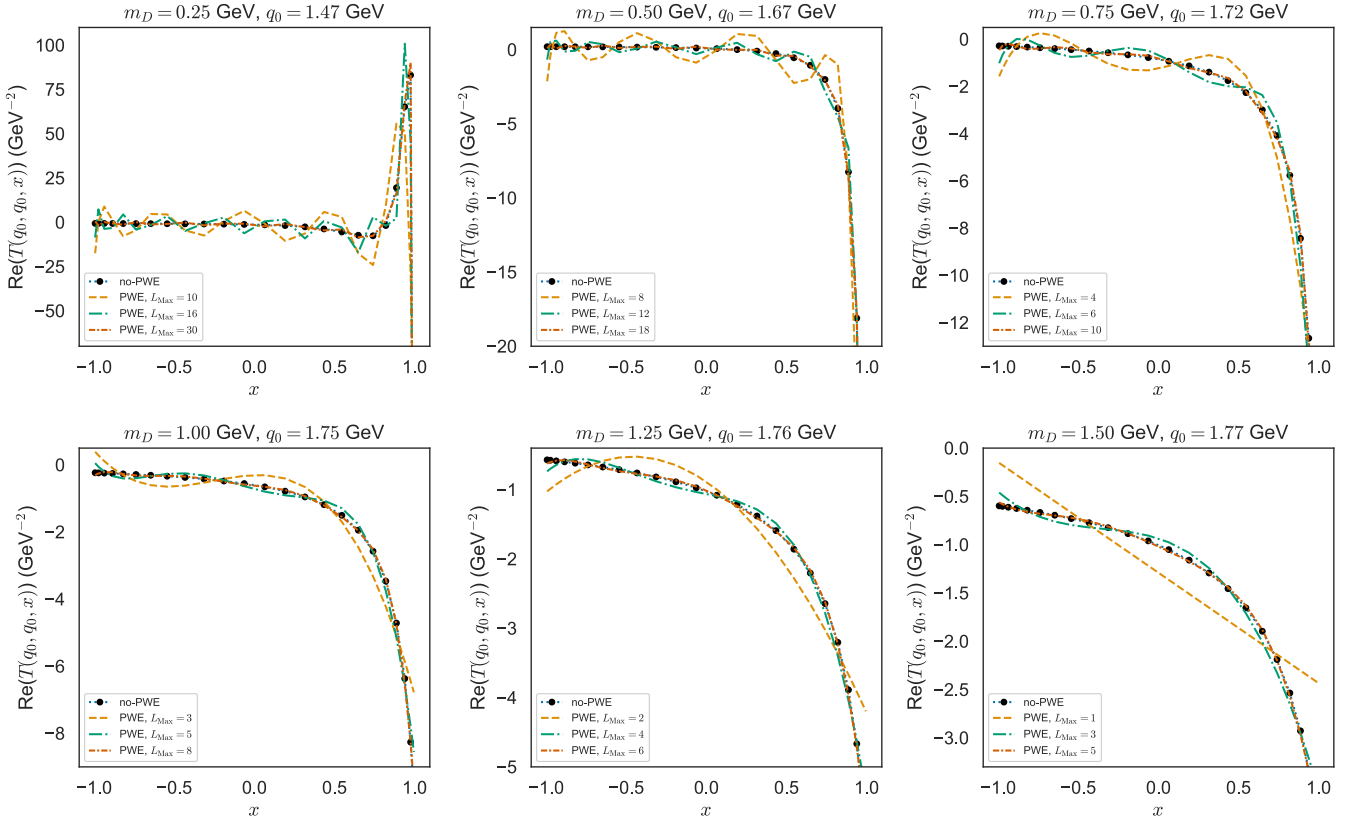


FIG. 3. $\text{Re}[T(E, q_0, q_0, x)]$ as a function of x is compared between the PWE and no-PWE methods, for six different values of screening mass. The labels on PWE curves denote the number of partial-wave terms summed. The value of on-shell momentum q_0 and the corresponding screening mass m_D are given in the title of the plot.

converges to the no-PWE (full) T matrix but rather approaches it in an oscillatory manner. These two factors combined render the overall convergence of the sum in Eq. (18) substantially slower than what the fast decay of the magnitude of the first few partial-wave amplitudes (cf. Figs. 1 and 2) would suggest otherwise.

To demonstrate this, in this section we compare the T matrix computed in the PWE and no-PWE methods, and determine the value of L_{Max} in Eq. (18) for a wide range of screening masses and c.m. energies. We demonstrate that the number of PWE terms required in Eq. (18) for the on-shell amplitude can get as large as $l \approx 10$ – 20 for our considered range of screening masses and CM energies.

In the first case we fix the CM energy to $E_{\text{CM}} = 4.5$ GeV, and vary the screening mass in $Q\bar{Q}$ potential over the same range $m_D = 0.25$ – 1.5 GeV as done in Figs. 1 and 2, thus probing the effect of varying the impact parameter (thus orbital angular momentum) in the scattering problem. The value of on-shell momenta considered in our work vary around $q_0 \approx 1.5$ GeV, which is the typical value of near-thermalized charm quark momentum, as simulated in the phenomenological transport models [26]. The comparison of the diagonal component of the on-shell T -matrix amplitudes, $T(q_0, q_0, x)$, as a function of x for PWE and no-PWE methods for six different values of m_D , are presented in Figs. 3 and 4 for the real and the imaginary part, respectively. At any screening mass m_D , the convergence is substantially slower for the PWE

T -matrix sum in Eq. (18) than suggested by the apparent magnitudes of the first few partial-wave terms T_l 's (cf. Figs. 1 and 2). For a precise agreement between the two methods, up to $l = 30$ PWE terms are necessary for the lowest value of $m_D = 0.25$ GeV. For $m_D = 0.5$ GeV and $m_D = 0.75$ GeV that correspond to most phenomenologically relevant QGP temperature range of $T \approx 200$ – 400 MeV, at least $l = 18$ and $l = 10$ PWE terms are needed, respectively, for a precise matching of the real part. This number drops to $l = 5$ for the largest $m_D = 1.5$ GeV we consider.

Conversely, we find that the number of partial-wave terms needed to match the imaginary part of T matrix between PWE and no-PWE methods is substantially less than that for the real part, in general. For $m_D = 0.25$ GeV, only $l = 18$ terms are needed, for $m_D = 0.5$ GeV only $l = 10$ and for $m_D = 0.75$ GeV only $l = 6$, PWE terms are required for a precise matching with the no-PWE results, as compared to $l = 30$, $l = 18$, and $l = 10$ terms for the real part, respectively. To understand this, we resort to the phase shift analysis in the scattering theory, where the partial-wave amplitudes can be computed as a function of phase shift δ_l for the l th channel. The real part of the T matrix is proportional to $\cos(\delta_l) \sin(\delta_l)$ while the imaginary part is proportional to $\sin^2(\delta_l)$ [31]. The phase shift δ_l becomes small as one goes to higher l , so that the real part becomes approximately proportional to δ_l while the imaginary part to δ_l^2 appearing at a higher order. Due to this, the imaginary part in general requires less

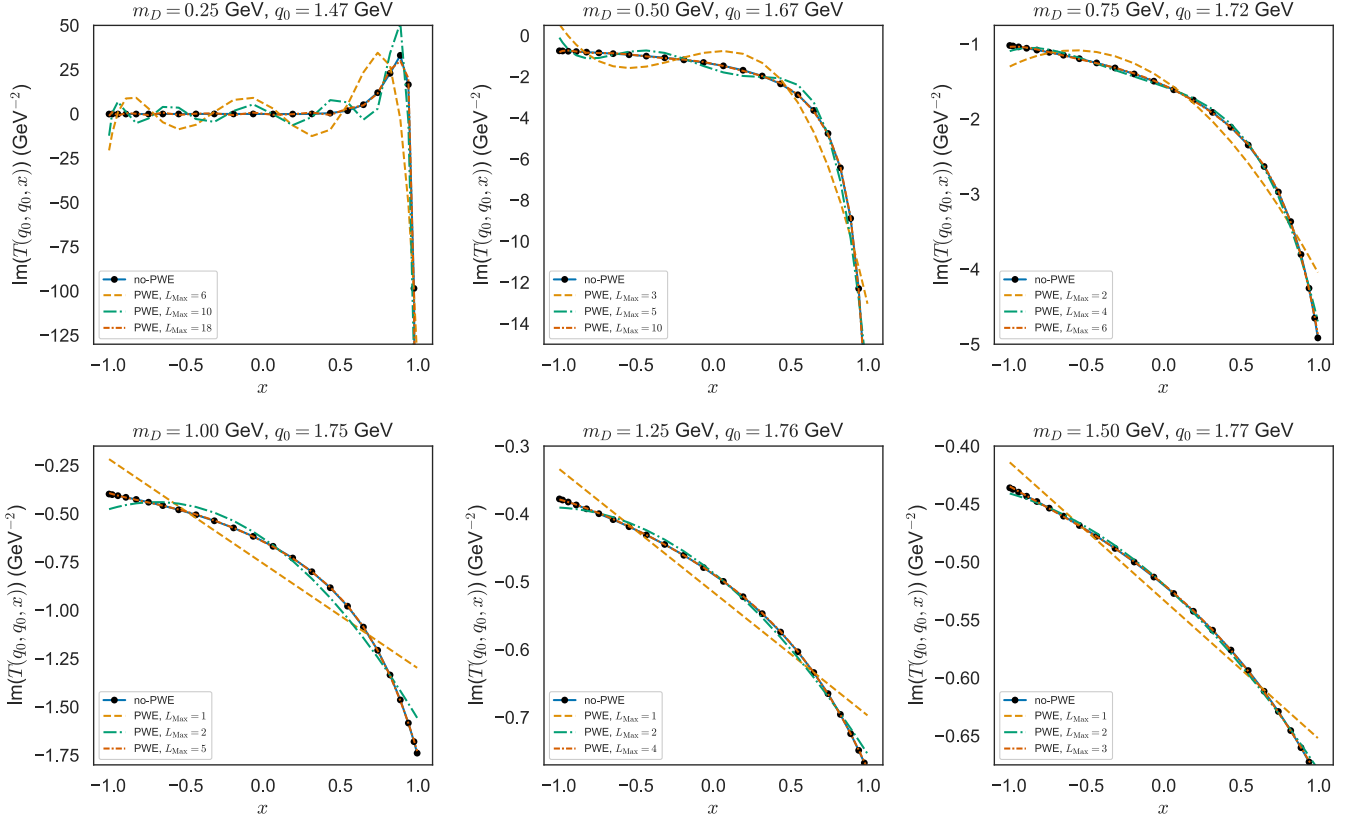


FIG. 4. $\text{Im}[T(E, q_0, q_0, x)]$ as a function of x is shown for six different values of screening mass we consider. Rest of the details are same as the Fig. 3.

partial-wave terms to match a no-PWE calculation than the real part of T matrix.

In the second case, we change the on-shell momentum in our problem, given by $q_0 = \sqrt{E_{\text{CM}}^2/4 - M_c^2}$, which corresponds to changing the orbital angular momentum involved in the scattering by changing the incoming momentum of the projectile, while keeping the impact parameter fixed by employing a fixed screening mass $m_D = 0.75$ GeV. We work with four different values of $E_{\text{CM}} = 4, 4.5, 5, 5.5$ GeV. For our calculation this covers a range of 1.4–2.3 GeV for the on-shell momentum q_0 . The comparison of real and imaginary parts of the T matrix computed in the PWE and no-PWE methods, for four different values of E_{CM} , are presented in Fig. 5. We observe that at $E_{\text{CM}} = 4$ GeV only $l = 8$ terms are required for a precise matching of the real parts between the two methods, which increases to $l = 10$ for $E_{\text{CM}} = 4.5$ GeV, $l = 12$ for $E_{\text{CM}} = 5$ GeV and finally to $l = 16$ for $E_{\text{CM}} = 5.5$ GeV, the largest E_{CM} we consider. In contrast, for a precise matching of the imaginary part of T matrix in the two approaches, $l = 4$ terms are sufficient for $E_{\text{CM}} = 4$ GeV, increasing to $l = 5$ for $E_{\text{CM}} = 4.5$ GeV, $l = 6$ for $E_{\text{CM}} = 5$ GeV, and finally $l = 8$ for $E_{\text{CM}} = 5.5$ GeV, all significantly less than those numbers for the real part. These calculations demonstrate that, for a moderate increase in the c.m. energy from $E_{\text{CM}} = 4$ GeV to 5.5 GeV, the number of PWE terms required for a precise matching to the full amplitude doubles for both the real and the imaginary part, reiterating the

conclusion drawn from the first case study that the convergence of the PWE series is not as fast as one would expect based on simply looking at the magnitudes of first few terms.

C. PWE vs no-PWE: Half-off-shell amplitudes

One needs to solve for at least the half-off-shell T matrix for obtaining the physical on-shell amplitudes, therefore in this section we discuss the convergence of half-off-shell partial-wave amplitudes against the no-PWE full amplitude. In Figs. 6 and 7 the real and imaginary parts of the half-off-shell T -matrix amplitudes $T(q_0, q, x)$ as a function of off-shell momentum q are compared between the PWE and no-PWE methods, for three different values of x and two different screening masses $m_D = 0.5$ GeV and $m_D = 1$ GeV. The c.m. energy is fixed at $E_{\text{CM}} = 4.5$ GeV. The value of corresponding on-shell momenta are given in the title of the plots.

One observes that for both the real and imaginary parts of these half-off-shell amplitudes, when the off-shell momentum q is far away from the on-shell momentum q_0 , the required numbers of PWE terms for a precise matching to the no-PWE results are substantially less than in the on-shell region, characterized by $q \approx q_0$, with a spread of ≈ 1 –2 GeV in the off-shell momentum. This can be understood by observing the behavior of the half-off-shell partial-wave amplitudes plotted in Figs. 1 and 2. Near the on-shell region $q \approx q_0$, the partial-wave amplitudes $\text{Re}T_l(q_0, q)$ and $\text{Im}T_l(q_0, q)$ achieve their maximum strengths. Furthermore, the decrease of these

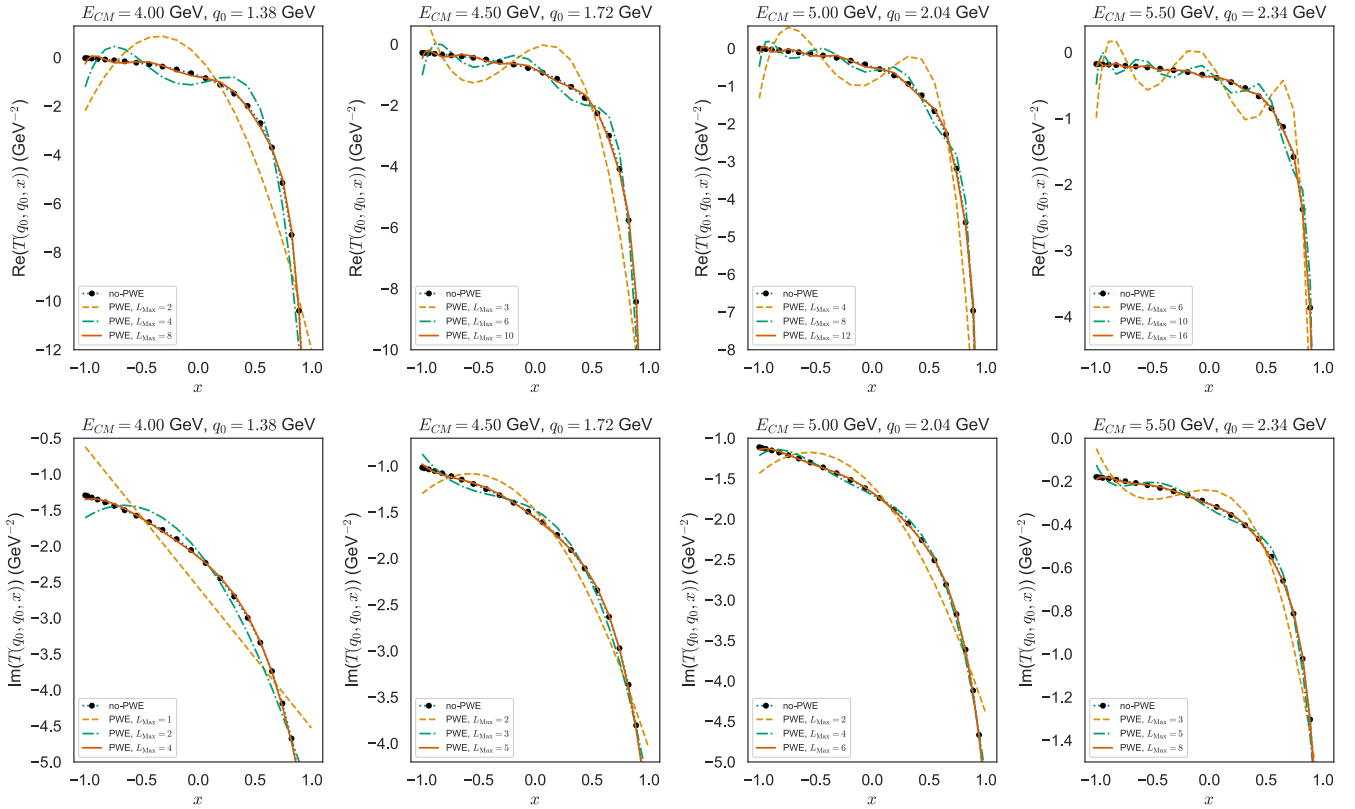


FIG. 5. The $\text{Re}[T(E, q_0, q_0, x)]$ (top row) and the $\text{Im}[T(E, q_0, q_0, x)]$ (bottom row) as a function of x , is shown for four different values of E_{CM} . Values of E_{CM} and the corresponding on-shell momentum q_0 are given in the title.

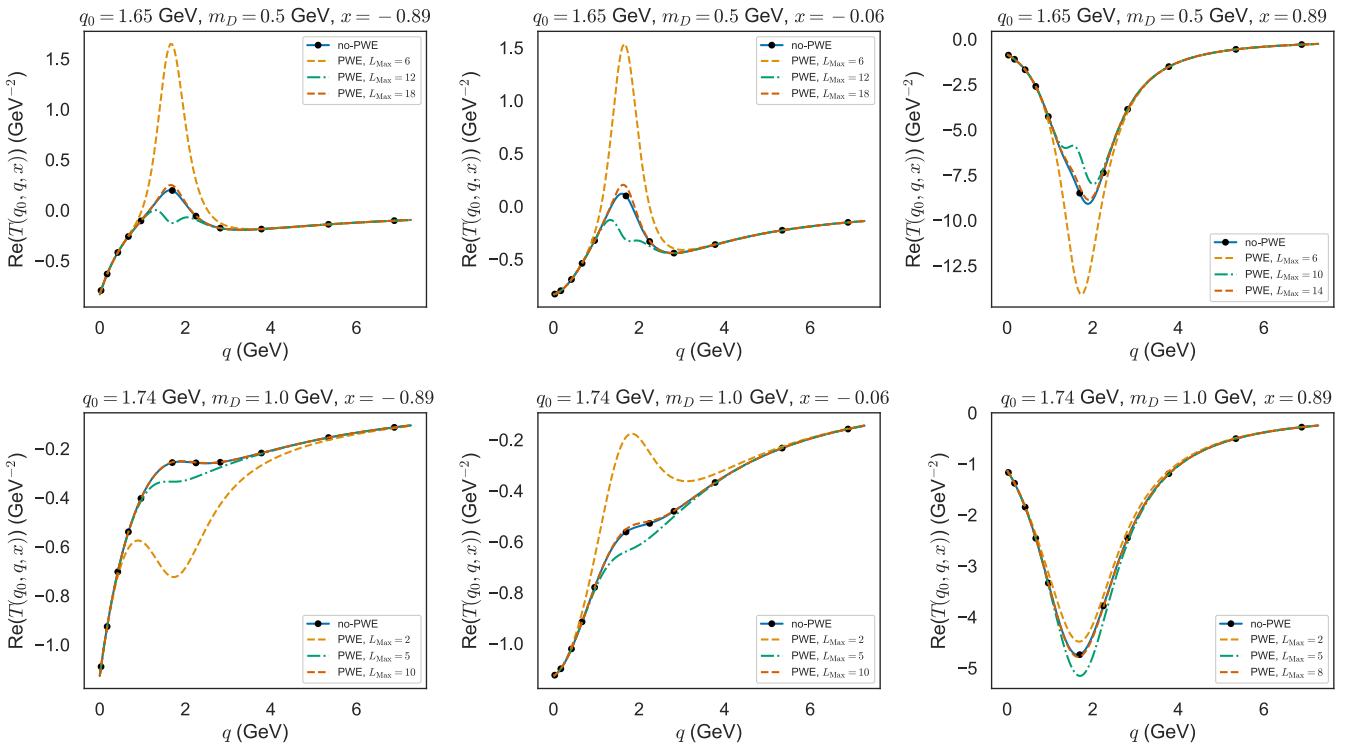


FIG. 6. The real part of the half-off-shell $\text{Re}[T(E, q_0, q, x)]$ as a function of q , is compared between the PWE and no-PWE approach, for three different values of x , corresponding to the screening mass $m_D = 0.5$ GeV (top row) and $m_D = 1.0$ GeV (bottom row). The c.m. energy is fixed at $E_{\text{CM}} = 4.5$ GeV, and the values of on-shell momentum q_0 and x are given in the title of the plots.

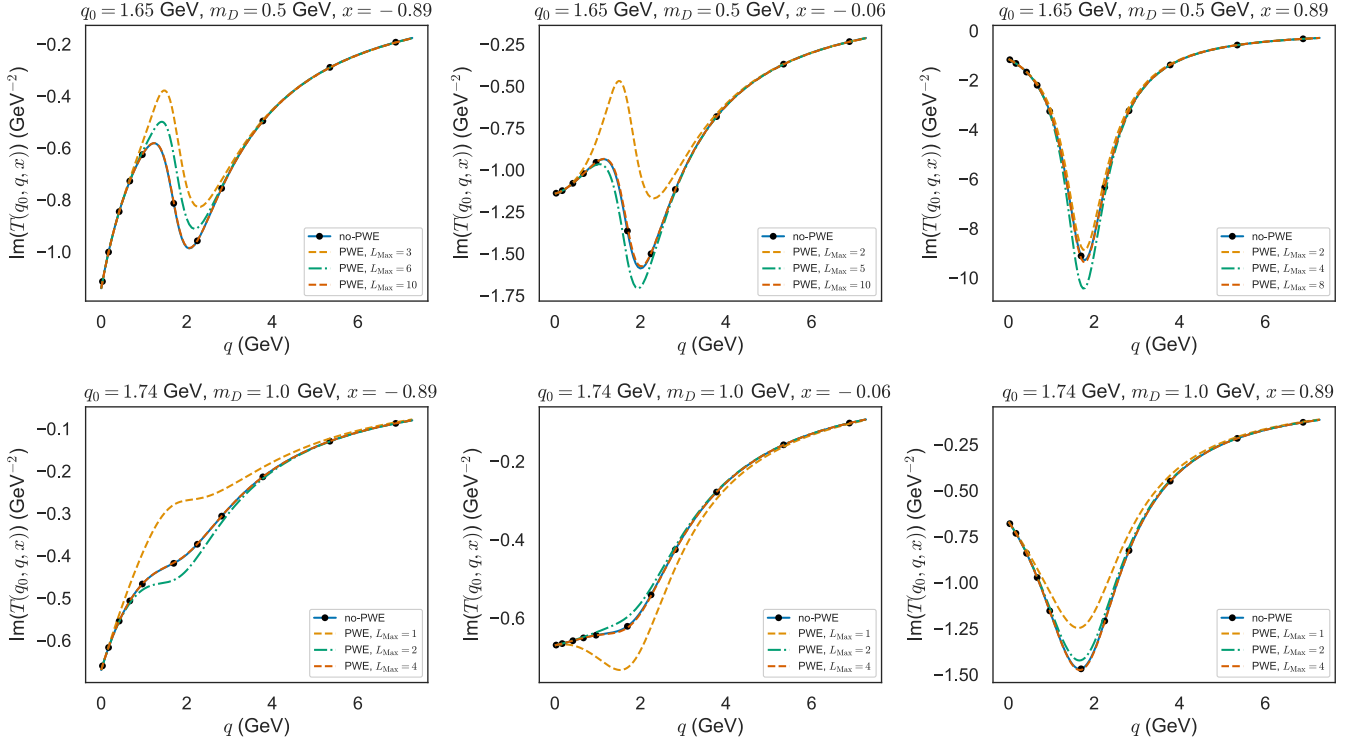


FIG. 7. The imaginary part of the half-off-shell $\text{Im}[T(E, q_0, q, x)]$ as a function of q , is compared between the PWE and no-PWE approach for three different values of x , corresponding to the screening mass $m_D = 0.5$ GeV (top row) and $m_D = 1.0$ GeV (bottom row). Rest of the parameters are same as described in the figure above.

half-off-shell partial-wave amplitudes with increasing l is much slower in the on-shell region, when compared to the off-shell region $q \gg q_0$ or $q \ll q_0$ where the lowest few $\text{Re}T_l(q_0, q)$ and $\text{Im}T_l(q_0, q)$ for $l \approx 0-2$ possess much larger strengths than higher partial waves and thus dominate the PWE sum in Eq. (18). Near the on-shell region, the slowly decreasing (when l increases) partial-wave amplitudes are further augmented by the factor $2l + 1$, and the Legendre polynomials $P_l(x)$, which introduce oscillations, making the convergence of the PWE sum even slower.

When increasing m_D from 0.5 GeV to 1 GeV, the number (L_{Max}) of these half-off-shell PWE terms required for a good matching to the no-PWE amplitude also becomes significantly smaller, same as found for the on-shell amplitudes in Figs. 3–5. But what is more interesting here is the x dependence of the L_{max} for these half-off-shell amplitudes. For a given m_D , at $x = 0.89$, which is close to the forward direction ($\theta_{\vec{q}\vec{q}'} \approx 0$ and thus $x \approx 1$), the magnitude of both the real and imaginary part of the full no-PWE amplitude is much larger than at other $x = -0.89$ or -0.06 (as already seen from the x dependence of the on-shell amplitudes in Figs. 3–5). This is because at the forward angle with $P_l(x \approx 1) \approx 1$ for any l , different partial-wave amplitudes add up constructively through Eq. (18), in contrast to the destructive sum at other angles due to oscillations arising from the Legendre polynomials. For the same reason, at $x = 0.89$ the width of the near-on-shell region over which a substantial number of PWE terms through Eq. (18) are needed for a precise matching to the no-PWE results appears to be narrower and the corresponding L_{Max} turns out smaller, compared to the cases at the other two angles.

IV. PHYSICAL QUANTITIES: PWE VS NO-PWE

To further demonstrate the efficacy of the no-PWE method, in this section we discuss the calculation of two physical quantities, namely the $Q\bar{Q}$ differential scattering cross section and the heavy quark drag coefficient, both of which involve the computation of the full on-shell scattering amplitudes.

A. $Q\bar{Q}$ differential scattering cross section

The differential cross section for the scattering of a charm quark and charm antiquark pair ($Q\bar{Q}$) interacting via a color singlet potential is given in the c.m. frame by

$$\frac{d\sigma}{d\Omega} = \frac{1}{64\pi^2 E_{\text{CM}}^2} |\overline{\mathcal{M}}|^2, \quad (19)$$

where $\mathcal{M}$ is the $Q\bar{Q}$ scattering amplitude (the bar denoting the sum over the final state color and spin degeneracies and the average over the initial state degeneracies), related to the on-shell T matrix through

$$\mathcal{M} = \sqrt{16E_{\vec{Q}}(-\vec{q}')E_{\vec{Q}}(\vec{q}')E_{\vec{Q}}(-\vec{q})E_{\vec{Q}}(\vec{q})} T(E_{\text{CM}}, \vec{q}', \vec{q}), \quad (20)$$

where the factors $\sqrt{2E_{\vec{Q}/\vec{Q}'}}$ convert the T -matrix element defined with nonrelativistically normalized single particle momentum eigenstates into the relativistically normalized and thus Lorentz invariant amplitude $\mathcal{M}$, and $\vec{q}, \vec{q}'$ denote the incoming and outgoing relative momentum.

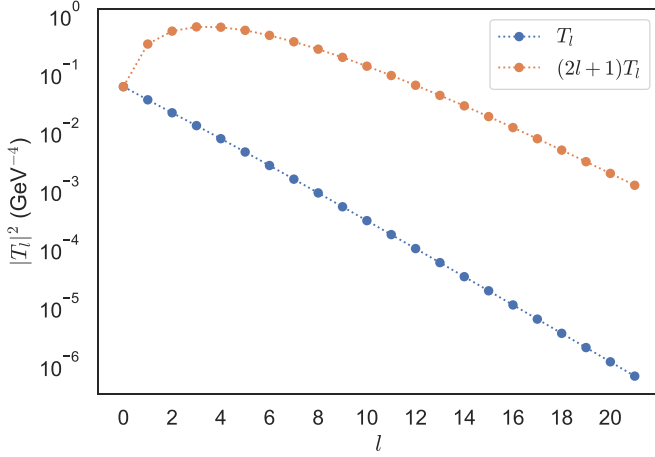


FIG. 8. The magnitudes of the $Q\bar{Q}$ on-shell partial-wave amplitudes $|T_l|^2$ are compared with and without the accompanying factor of $(2l+1)$ for different l , at $E_{\text{CM}} = 4.5$ GeV and $m_D = 0.5$ GeV.

In Fig. 8 the magnitudes of the on-shell partial-wave amplitudes for the $Q/\bar{Q}$ scattering are compared with and without the accompanying factor of $2l+1$, highlighting its importance in enhancing the contributions of higher l terms in the sum of Eq. (18) to obtain the full amplitude. One observes that though $|T_l|^2$ decreases monotonically as l increases, $|(2l+1)T_l|^2$ first keeps increasing till $l=4$ and then decreases from thereon for larger l . This decrease however is slowed down by almost a factor of 1000 compared to the case without this factor, thus significantly reducing the convergence speed of the sum in Eq. (18). In Fig. 9, the $Q\bar{Q}$ differential scattering cross section, for $E_{\text{CM}} = 4.5$ GeV and $m_D = 0.5$ GeV, is shown for three different representative x values ($x = \hat{q} \cdot \hat{q}'$) as a function of L_{Max} , which is the number of partial-wave terms summed over in obtaining the full PWE T matrix and compared with the results from no-PWE calculation. One sees that, at all three x values, the differential cross sections from summing over partial-wave amplitudes are far from a monotonic function of L_{Max} . Instead, they whether exhibit peaks at moderate $L_{\text{Max}} \approx 6-10$ (for $x = -0.89$ and 0.97) or suffer from severe fluctuations (for $x = 0.19$, primarily due to the oscillating behavior of the pertinent Legendre polynomials),

before starting to approach the full results from the no-PWE method at $L_{\text{Max}} \approx 20$. This thus alludes to the advantage of the no-PWE method of being able to obtain the full amplitude and thus the cross section once for all without concern about the convergence of the sum over partial-wave amplitudes in the PWE method. One also notes, incidentally, that the differential cross section in the near-forward direction ($x = 0.97$) is comparatively much larger.

B. Heavy quark drag coefficient

In this section we calculate the charm quark drag coefficient, which is a key input for evaluating the heavy quark thermalization and flow in heavy-ion collisions [26,34]. For a heavy quark interacting with the light QGP particles, the exchanged energy $k_0 \approx \vec{k}^2/M_Q$ is parametrically much smaller than the exchanged momentum $|\vec{k}| \approx T$ as the QGP temperature $T \ll M_Q$, implying that one can approximate the heavy-light interactions as mediated by a static potential and apply the T -matrix approach to compute their scattering rates [26,34]. Here we focus on heavy-light antiquark ($Q\bar{q}$) scattering in the color singlet channel with the potential taken to be the same as the $Q\bar{Q}$ potential [Eq. (17)] and compare the PWE and the no-PWE methods.

The drag coefficient $A(p)$, defined as [35]

$$A(p) = \gamma_{\bar{q}} \frac{1}{2E_p} \int \frac{d^3q}{(2\pi)^3 E_q} \int \frac{d^3q'}{(2\pi)^3 E_{q'}} \int \frac{d^3p'}{(2\pi)^3 E_{p'}} \times (2\pi)^4 \delta^4(p' + q' - p - q) |\overline{\mathcal{M}}|^2 \times (1 - n_F(E_{q'})) n_F(E_q) \left(1 - \frac{\vec{p} \cdot \vec{p}'}{|\vec{p}|^2} \right), \quad (21)$$

measures the momentum relaxation (thermalization) rate of a heavy quark due to its elastic collisions with light particles from the QGP medium, with $\gamma_{\bar{q}}$ being the light antiquark degeneracy. Here p, p', q, q' denote the four-momentum of the incoming and outgoing heavy quark and light antiquark, respectively. The thermal mass of light quarks, which is typically of the order of the temperature of the medium, is set to $m_q = 0.4$ GeV, and we use a slightly larger single-particle

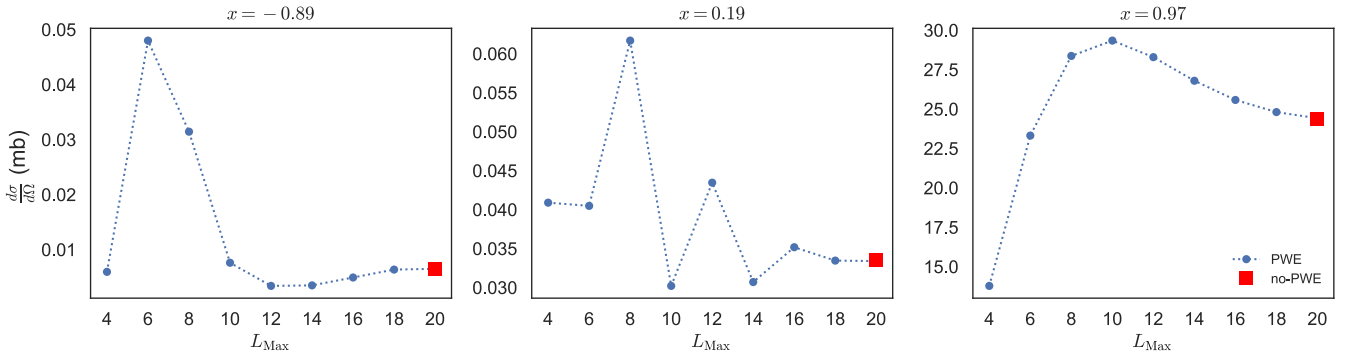


FIG. 9. The $Q\bar{Q}$ differential scattering cross section is compared as a function of L_{Max} , between the PWE and no-PWE methods, at three different scattering angle $x = \hat{q} \cdot \hat{q}'$ (given in the title of the plots), for $E_{\text{CM}} = 4.5$ GeV and $m_D = 0.5$ GeV. Clearly the remnant of the partial-wave series relative to the no-PWE full results can be positive or negative depending on the L_{Max} of the series.

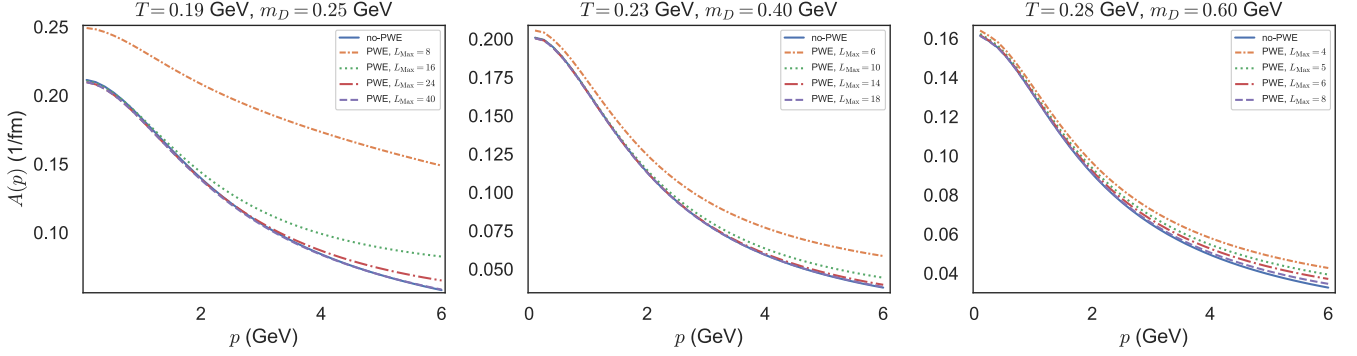


FIG. 10. The charm quark drag coefficient, calculated for the singlet interaction channel, is shown for three different temperatures (given in the title of the plots).

width $\Sigma_{Q/q} = -50$ MeV (compared to the default small value of -10 MeV otherwise used throughout the work) for the sake of numerical stability in evaluating the multidimensional integration over the scattering amplitude squared in Eq. (21) (quantitatively, this choice does not alter the results in any significant manner). We also assume that the scattering amplitude does not depend strongly upon the CM momentum so that using the T matrix computed in the $Q\bar{q}$ CM frame is a good approximation.

In Fig. 10, the heavy quark drag coefficient is compared between the PWE and no-PWE methods at three different screening masses $m_D = 0.25, 0.40, 0.60$ GeV, corresponding to temperatures $T = 0.19, 0.23, 0.28$ GeV as converted using the pertinent relation from lattice QCD studies [36]. Here an overall observation is that for phenomenologically relevant temperatures $T \approx 0.2\text{--}0.3$ GeV (middle and right plots), as many as 8–18 partial-wave terms are needed to make a perfect match of the PWE results with the no-PWE results in the whole explored momentum range. While the number of partial-wave terms $L_{\text{Max}} \approx 5\text{--}10$ required for the match is generally moderate for low momenta $p < 3$ GeV, it goes up rapidly at higher heavy quark momenta, simply because the CM energy $E_{\text{CM}} = \sqrt{(E_p + E_q)^2 - (\vec{p} + \vec{q})^2}$ and thus the involved angular momentum increases. At lower temperatures $T < 0.2$ GeV (left plot), this number gets significantly larger, requiring $L_{\text{Max}} \approx 24\text{--}40$ to make the match up to $p \approx 3\text{--}6$ GeV. In contrast, a substantially smaller $L_{\text{Max}} = 8$ [34] was previously explored in the same context (yet using a weaker potential [34]), implying an overestimate of the drag coefficient at low temperatures. A quantitative assessment of the impact of neglecting higher partial waves within the PWE approach (as compared the no-PWE T matrix) on charm quark phenomenological observables (e.g., elliptic flow) would require performing realistic simulations for heavy quark diffusion with the drag coefficients computed in these two approaches.

In summary, this thus further confirms the efficacy and advantage of the no-PWE method in obtaining the physical quantities in a single computation, bypassing the hurdle of determining the value of L_{Max} for a good convergence, especially in scenarios where a range of CM energies or screening masses are involved.

V. BOUND STATE PROBLEM: $E_{\text{CM}} < 2M_c$

When the c.m. energy E_{CM} falls below the mass threshold $2M_c$, the solution of Thomson equation Eqs. (2) and (3) is anticipated to exhibit bound state poles when E_{CM} approaches E_{nl} , where $E_{nl} < 2M_c$ represents the bound state energy of the $Q\bar{Q}$ eigenstate characterized by its principal and orbital quantum numbers, n and l , respectively. In the conventional PWE approach, each PWE component T_l has to be solved in a separate integral equation [Eq. (7)], therefore one needs to scan the energy range separately for each distinct orbital quantum number l . For $E_{\text{CM}} < 2M_c$ the on-shell momentum becomes imaginary, while the T -matrix equation is defined and solved in terms of real momenta. Several works in literature [19,20] have suggested an analytical continuation of the T matrix from the imaginary momentum axis to $q' = 0$, $q = 0$ and have employed the zero-zero component $T(E_{\text{CM}}, 0, 0)$ to demonstrate the bound state poles, manifesting as peaks in the real and the imaginary parts. Though this method works for demonstrating the S-wave pole, for bound states of higher orbital quantum numbers, $l > 0$, one faces problem as the seed potential term $V_l(q', q) \xrightarrow{q', q \rightarrow 0} 0$ [see Eq. (8)], therefore

suppressing the peak structure in the T matrix. To overcome this hurdle, the authors in Ref. [20] plotted the determinant of the transition matrix $\{1 - [V_l][G(E)]\}$, which is zero at the pole location, to demonstrate the P-wave bound states, though this method also relies on a separate scan of the energy range for bound states of distinct orbital quantum numbers.

The no-PWE T matrix, in principle, contains contributions from all the bound states of different orbital quantum numbers, which implies that a single energy scan is sufficient to demonstrate their presence or absence. In spirit of the on-shell plots in Figs. 3–5, we plot the real and imaginary parts of the diagonal term $T(E, q, q, x)$ as a function of CM energy E in Fig. 11, for a small screening mass $m_D = 0.18$ GeV in the potential for which $V(r, T)$ resemble the vacuum potential, demonstrating peak structures corresponding to multiple bound states of distinct principal and orbital quantum numbers in a single energy scan, for the first time in literature, to our knowledge. In Fig. 11, results from solving the nonrelativistic Schrödinger equation for the $Q\bar{Q}$ pair are also shown, to ascertain the quantum numbers of the bound state poles obtained

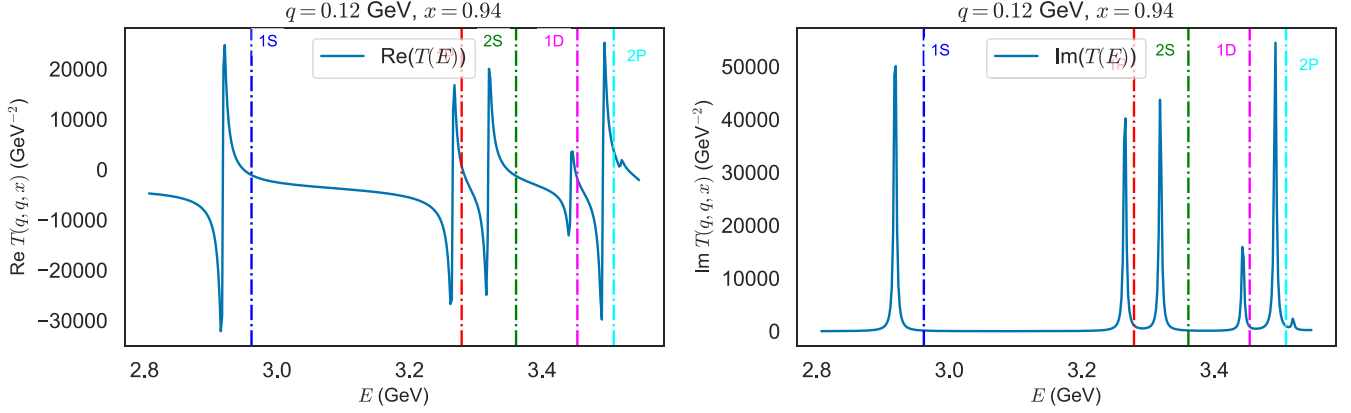


FIG. 11. The $\text{Re}[T(E, q, x)]$ (left) and $\text{Im}[T(E, q, x)]$ (right) part of $Q\bar{Q}$ T matrix obtained from solving the Thompson equation with a small screening mass $m_D = 0.18$ GeV, are plotted as a function of E_{CM} . The values of q and x given in the title of the plot are determined such that the residue strength of the bound states of distinct orbital and principal quantum numbers, is large enough to render them visible, simultaneously. The bound state masses obtained from solving the Schrödinger equation are plotted as vertical lines and labeled with their quantum numbers, serving as a reference for the pole masses obtained from the Thompson equation.

in the Thompson equation. The T -matrix poles exhibit a small but noticeable shift downward compared to the eigenvalues obtained from the Schrödinger equation. The real and imaginary parts of the T matrix around pole energies exhibit peak structures even in the off-shell momentum of the T matrix, and P or D wave states can be demonstrated in a similar manner to the S-wave state, something which is not possible with the $T_l(E_{\text{CM}}, 0, 0)$ component [19].

To understand why this is possible in principle, we scrutinize the nonrelativistic Lippmann-Schwinger equation, which is formally similar to the 3D reduced Thompson equation, the main difference lying in the two-body propagators (Green's function), which in the Lippmann-Schwinger case contain the full nonrelativistic Hamiltonian operator H , facilitating derivation of analytical results without the complications present in the relativistic Thompson equation. Thus by analyzing the former, one can gain insights into the behavior of residue at the pole locations for the latter. The Lippmann-Schwinger equation can be written in the form

$$T = V + V G_{\text{NR}} V, \quad (22)$$

where $G_{\text{NR}}(E, \vec{k}) = (E - H + i\Sigma_I)^{-1}$, V is the nonrelativistic potential operator and $H = 2M_c + k^2/M + V$ is the nonrelativistic Hamiltonian operator of the $Q\bar{Q}$ system, excluding the c.m. kinetic energy term. Inserting complete set of states of H ,

$$\mathbb{I} = \sum_{nl} |\psi_{nl}\rangle \langle \psi_{nl}| + \int_{\alpha} |\psi_{\alpha}\rangle \langle \psi_{\alpha}|,$$

where $|\psi_{nl}\rangle$ and $|\psi_{\alpha}\rangle$ represent the bound and scattering states of H , respectively, and considering the T matrix in the momentum eigenstate basis $|\vec{q}\rangle$, $|\vec{q}'\rangle$, we obtain

$$T(E, \vec{q}', \vec{q}) = \langle \vec{q}' | V | \vec{q} \rangle + \sum_{nl} \frac{\langle \vec{q}' | V | \psi_{nl} \rangle \langle \psi_{nl} | V | \vec{q} \rangle}{E - E_{nl} + i\Sigma_I} + \int_{\alpha} \frac{\langle \vec{q}' | V | \psi_{\alpha} \rangle \langle \psi_{\alpha} | V | \vec{q} \rangle}{E - E_{\alpha} + i\Sigma_I}. \quad (23)$$

For scattering states we have $E_{\alpha} > 2M_c$ while $E_{nl} < 2M_c$ for the bound states, therefore when the CM energy E is below mass threshold in Eq. (23), one can make a distinction between the pole terms containing the factor $(E - E_{nl} + i\Sigma_I)^{-1}$ from other terms, which do not contain any singularity, and Eq. (23) can be separated into two parts as

$$T(E, \vec{q}', \vec{q}) = \sum_{nl} \frac{\langle \vec{q}' | V | \psi_{nl} \rangle \langle \psi_{nl} | V | \vec{q} \rangle}{E - E_{nl} + i\Sigma_I} + (\text{regular terms}). \quad (24)$$

We can express the scalar product containing the potential operator as

$$\begin{aligned} \langle \vec{q}' | V | \psi_{nl} \rangle &= \int d^3 q_1 \int d^3 r \langle \vec{q}' | \vec{r} \rangle \langle \vec{r} | V | \vec{q}_1 \rangle \langle \vec{q}_1 | \psi_{nl} \rangle \\ &= \int d^3 q_1 \int d^3 r \frac{e^{i(\vec{q}' \cdot \vec{r} - \vec{q}_1 \cdot \vec{r})}}{(2\pi)^3} V(r) \psi_{nl}(q_1) Y_{lm}(\hat{q}_1), \end{aligned} \quad (25)$$

which after expanding the exponential factors in terms of spherical harmonics

$$e^{i\vec{q} \cdot \vec{r}} = 4\pi \sum_{lm} i^l j_l(qr) Y_{lm}(\hat{q}) Y_{lm}^*(\hat{r}) \quad (26)$$

and doing the angular integrations, yields

$$\begin{aligned} \langle \vec{q}' | V | \psi_{nl} \rangle &= \int d q_1 q_1^2 V_l(q, q_1) \psi_{nl}(q_1) Y_{lm}(\hat{q}) \\ &= g_l(q) Y_{lm}(\hat{q}), \end{aligned} \quad (27)$$

where $g_l(q)$ is defined as

$$g_l(q) = \int d q' q'^2 \frac{2}{\pi} V_l(q, q') \psi_{nl}(q'), \quad (28)$$

and $V_l(q', q)$ was defined in Eq. (8). Finally, using the identity

$$P_l(\hat{q}' \cdot \hat{q}) = \frac{4\pi}{2l+1} \sum_m Y_{lm}(\hat{q}') Y_{lm}^*(\hat{q}) \quad (29)$$

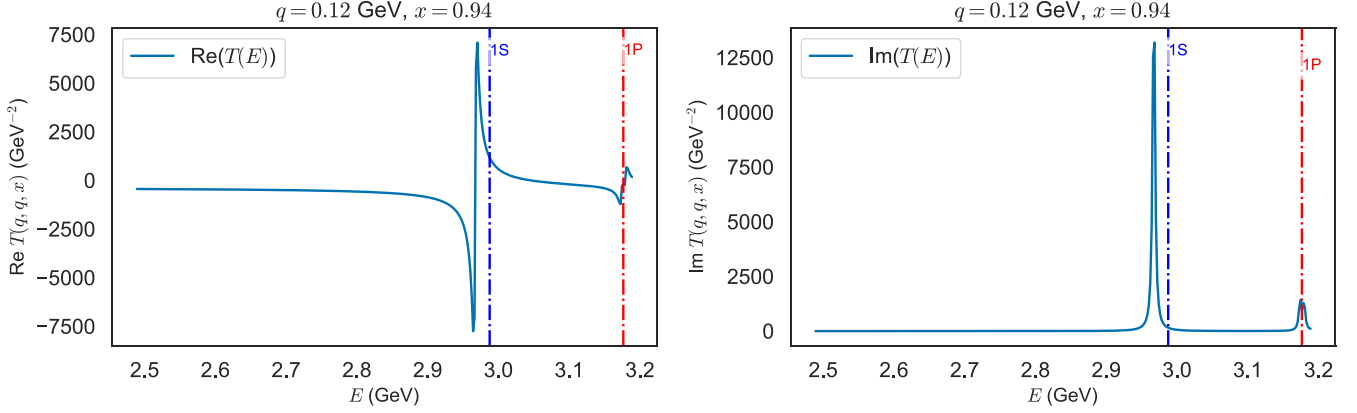


FIG. 12. The results from solving the Thompson equation for $\text{Re}[T(E, q, q, x)]$ (left) and $\text{Im}[T(E, q, q, x)]$ (right) are plotted as a function of E_{CM} for the screening mass $m_D = 0.35$ GeV. The values of q and x given in the title are same as those used in Fig. 11. With the increase in screening mass is, higher excited states melt away, leaving only the 1S and 1P states. The vertical lines are bound state masses obtained from solving the Schrödinger equation.

and Eq. (27), Eq. (24) can be written as

$$T(E, \vec{q}', \vec{q}) = \sum_{nl} \frac{R_l(q', q, x)}{E - E_{nl} + i\Sigma_l} + (\text{regular terms}), \quad (30)$$

where $x = \hat{q}' \cdot \hat{q}$ and

$$R_l(q', q, x) = \frac{2l+1}{4\pi} g_l(q') g_l(q) P_l(x). \quad (31)$$

Using Eq. (30) we see that when E is close to a pole energy E_{nl} , the regular terms are negligible and T matrix is dominated by the pole term containing the residue $R_l(q', q, x)$, which for the real $\text{Re}(T)$ and imaginary part $\text{Im}(T)$ of the T matrix (ignoring the regular terms) are given by

$$\begin{aligned} \text{Re}(T) &= \sum_{nl} \frac{(E - E_{nl}) R_l(q', q, x)}{(E - E_{nl})^2 + \Sigma_l^2}, \\ \text{Im}(T) &= \sum_{nl} \frac{\Sigma_l R_l(q', q, x)}{(E - E_{nl})^2 + \Sigma_l^2}. \end{aligned} \quad (32)$$

Equation (32) demonstrate that at the pole positions both real and imaginary parts of the T matrix have a peak for even off-shell values of q and q' and the pole locations are independent of the momenta q' , q and the angular variable x , as only the residue strength depends upon these variables. For a fixed q' , q , and x , the real part changes its sign around the pole position, while the imaginary part exhibit a peak, which vanishes at the nonpole energies. Since the residue term $R_l(q', q, x)$ depends upon the product of functions $g_l(q)$, $g_l(q')$ and $P_l(x)$, for the angular variable x we find that using $x \approx 1$ is best suited for demonstrating the presence of peak structures in different l states, as $P_l(x \rightarrow 1) \rightarrow 1$ for all l whereas for other values of x , $P_l(x)$ oscillates between positive and negative values affecting the residue term, and makes the peak structure less visible for some states. The suitable value of q is determined as such for which the function $g_l(q)$ is not small for any quantum numbers nl under consideration. Therefore an optimal combination of the variables q and x can be selected to ensure that the residue strength at all pole locations is significant enough, for rendering the peak

structures visible for all bound states simultaneously. This provides explanation for our results in Figs. 11, 12, and for the values of q and x used in there.

The binding energy of the $Q\bar{Q}$ bound states decreases with an increase in the QGP temperature, or equivalently the screening mass m_D , which is the basis of the melting picture originally formulated in Ref. [4]. In Fig. 12 we have plotted the real and imaginary parts of the T matrix for a larger screening mass $m_D = 0.35$ GeV. As the screening mass increases, the excited states 2S, 1D, and 2P have melted and only 1S and 1P, two lowest-lying bound states survive. The binding energies of the $Q\bar{Q}$ bound states are related to their pole mass as $E_\psi(T) = 2M_Q(T) - M_\psi(T)$, where $M_\psi(T)$ is the pole mass of the state labeled as ψ at temperature T . The binding energies decrease significantly from $E_{1S} = 0.794$ GeV, $E_{1P} = 0.442$ GeV for the screening mass $m_D = 0.18$ GeV, to $E_{1S} = 0.223$ GeV, $E_{1P} = 0.0126$ GeV when the screening mass is increased to 0.35 GeV, due to the weakening of $Q\bar{Q}$ potential at larger screening mass.

VI. SUMMARY

A comprehensive comparison between the conventional partial-wave expansion method and a new method without partial-wave expansion is conducted for solving the $Q\bar{Q}$ scattering T -matrix equation in the QGP. By comparing the new method against the PWE method for a wide range of screening masses and c.m. energies, which, when combined, determine the orbital angular momentum in the scattering problem, it was demonstrated that the number of partial-wave amplitudes needed for a precise matching with the full no-PWE amplitude is substantially larger than what one would expect from measuring the magnitude of the first few partial-wave amplitudes. The presence of the degeneracy factor $2l+1$ and Legendre polynomial $P_l(x)$ corresponding to the l th angular momentum channel in the partial wave sum, significantly slows down the convergence of PWE amplitudes to the full no-PWE amplitude.

We first discussed the leading half-off-shell partial-wave amplitudes, and found both the real and imaginary parts

exhibit a monotonic decrease with increasing l , except for the two lowest screening masses for which the decrease is rather slow or not monotonic. By comparing the on-shell scattering amplitudes calculated in the PWE and the no-PWE methods, we demonstrated that the minimum number $L_{\max}$ of partial-wave amplitudes required for a precise matching between the two methods, decreases monotonically as the screening of $Q\bar{Q}$ potential becomes stronger, or the c.m. energy is lowered. For phenomenologically relevant values of screening masses and c.m. energies, $L_{\max}$ can reach as high as $l \approx 10\text{--}20$. The comparison of half-off-shell amplitudes calculated in the two methods, demonstrates that the near-on-shell region requires larger number of the PWE terms for a precise matching, while in the far-off-shell region significantly lower number of PWE terms are sufficient. The calculation of physical quantities, namely the $Q\bar{Q}$ differential scattering cross section and the charm quark drag coefficient, further demonstrates that at moderate temperatures, the required number of partial-wave terms for a precise matching with the no-PWE results can be unexpectedly large. These calculations suggest that for a precision calculation of $Q\bar{Q}$ observables, which requires calculating the full in-medium scattering amplitude (i.e., T matrix), the no-PWE method may be of desired efficacy and advantage in obtaining the full amplitudes in a once-for-all manner, although at increased numerical cost compared to the conventional PWE method. In particular, the oscillations introduced by the Legendre polynomials throughout the intermediate values of x when summing over PWE amplitudes of different l s to approximate the full T matrix can lead to persistent fluctuations around the genuine value and thus cause significant uncertainties.

In calculations of below mass threshold T matrix pertaining to the $Q\bar{Q}$ bound states, first working with a small screening mass $m_D = 0.18$ GeV, which resembles a vacuum potential, we demonstrated that the no-PWE method can be employed for determination of all bound states of distinct orbital quantum numbers in a single energy scan, which is impossible in the partial wave T -matrix equation. Using the nonrelativistic Lippmann-Schwinger equation as a proxy that allows for convenient analytical derivations, we showed that the bound states peak structures in the real and imaginary parts of T matrix are present in the whole off-shell domain, given the momentum and angular coordinate are selected in a manner that the residue strength at pole locations are sufficiently large for all bound states simultaneously. The bound state peaks of all but the $1S$ and $1P$ states, melt away when the screening mass is increased to $m_D = 0.35$ GeV and the

binding energies of the two remaining bound states also reduce significantly.

There are several directions along which our present work can be further developed. First, calculations of heavy quarkonium spectral functions whether on the lattice or from the T -matrix approach have been thus far restricted to vanishing c.m. momentum. The conventional PWE method of the T -matrix approach may be further complicated by the presence of another momentum vector in this connection. On the contrary, the no-PWE method is expected to be more suited for this purpose, since in the collinear frame with total (c.m.) momentum $P = (P^0, 0, 0, P^3)$, the two-particle propagator $G_{Q\bar{Q}}$ can still be made independent of the intermediate azimuthal angle ϕ'' [37]. It is the latter fact that renders the T -matrix equation tractable without partial-wave expansion [cf. Eqs. (10), (11) in Sec. II B]. In particular, in order to perform a complete calculation, we need to solve the coupled integral system of both two-body scattering T -matrix equation and the one-body single- Q self-energy equation, which has been neglected in the present work but ensures a self-consistent many-body treatment. Second, the T -matrix equation can be extended to the case of heavy quark-light quark/antiquark/gluon scattering, based on the realization that energy transfer between the heavy quark and light QGP constituent is still parametrically small compared to the three-momentum transfer and thus the interaction remains of potential type [22]. For this, the application of the no-PWE method may allow for a more direct and precise computation of the full scattering amplitude, which can then be used to evaluate the heavy quark transport coefficient. We defer these considerations for future works.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available upon publication because it is not technically feasible and/or the cost of preparing, depositing, and hosting the data would be prohibitive within the terms of this research project. The data are available from the authors upon reasonable request.

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