



Thermal contribution of unstable states

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Received: 18 February 2019 / Accepted: 2 April 2019

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Abstract Within the framework of the Lee model, we analyze in detail the difference between the energy derivative of the phase shift and the standard spectral function of the unstable state. The fact that the model is exactly solvable allows us to demonstrate the construction of these observables from various exact Green functions. The connection to a formula due to Krein, Friedal, and Lloyd is also examined. We also directly demonstrate how the derivative of the phase shift correctly identifies the relevant interaction contributions for consistently including an unstable state in describing the thermodynamics.

1 Introduction

Formal treatment of the interactions in a gas of particles at finite temperature is an important topic in thermal field theory [1–3]. In particular, a consistent description of the unstable states is imperative for understanding the hadron gas, see, e.g., Refs. [3–6]. Some questions of interest include: How are the bulk properties of the medium, such as pressure and energy density, affected by unstable particles? What are the effective ways to take these into consideration? What insights can be gained from comparing different approaches, e.g., the standard imaginary time formalism and those based on a virial expansion? [5, 7–13] In this work we tackle these issues using an effective Hamiltonian approach. Besides an intuitive modification driven by the spectral function of the unstable particle (the resonant contribution), we shall demonstrate how the very presence of an interaction modifies the 2-body states composed of the stable particles (the nonresonant contribution). The sum of these modifications recovers a well-known result [5, 14, 15], according to which the

derivative of the scattering phase shift can be identified as the density of state for computing the partition function.

Many thermal models have the widths of the resonances implemented but the nonresonant interactions are neglected. This can lead to misleading results when interpreting the contribution from an interaction channel [16, 17]. An illustrative example is the pion-pion scattering in the $I = 0$ channel, in which the famous $f_0(500)$ resonance, a.k.a. the σ -meson, is involved. The empirical phase shift, analyzed by the chiral perturbation theory [18], reveals that there are substantial (effective) repulsive corrections coming from the exchange interactions in the t- and u-channels. Additional cancellation also comes from the $I = 2$ channel. A model that corrects only for the width of the resonance is incapable of handling these effects. Some models try to remedy this by introducing extraneous repulsive forces, e.g., via an excluded volume. This, however, will generally lead to a model which contradicts the known phase shift [19].

In this study we consider a system of stable particles “ π ” (the pions) and unstable particle “ ρ ” (the ρ -mesons).¹ Each ρ can decay into two π 's via the interaction $\rho \rightarrow \pi\pi$. Chains of interactions, e.g., $\pi\pi \rightarrow \rho \rightarrow \pi\pi$, are also included. The fact that only two types of particles are considered drastically simplifies the discussion, but the main non-trivial features are kept.

We use a Lee-Model Hamiltonian (LH) [20, 21] to describe the interactions in the $\rho\pi$ system. Similar Hamiltonians have been used to explore various areas in physics, ranging from atomic physics and quantum optics [22–25] to baryon decays [26]. The Lee model offers a useful theoretical setup to study an interacting system [27–33] and in many aspects it resembles a quantum field theory [34]. In practice, the LH contains an unstable state $|\rho\rangle$, as well as a continuum of 2-body states $|\pi(\mathbf{q})\pi(-\mathbf{q})\rangle$ with all possible relative momenta \mathbf{q} of the pair. The decay $\rho \rightarrow \pi\pi$ is described by mixing terms of the form:

Electronic supplementary material The online version of this article (<https://doi.org/10.1140/epjc/s10052-019-6844-y>) contains supplementary material, which is available to authorized users.

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¹ These notions obviously mirror the case of a thermal hadron gas with pions and $\rho(770)$'s. However, our discussion generally applies to any thermal system with unstable states.

$\sim g (|\rho\rangle \langle \pi\pi| + |\pi\pi\rangle \langle \rho|)$. This gives the unstable particle ρ a width, i.e., a distribution in energies (or masses) dictated by the spectral function $A_\rho(E)$ [34–37], such that $A_\rho(E) \frac{dE}{2\pi}$ can be interpreted as the probability that the unstable ρ has energy between E and $E + dE$. The spectral function can be calculated from the imaginary part of the ρ -propagator. See Sect. 3 for details. For a narrow-width state this can be approximated by the Breit-Wigner (BW) formula [38,39],

$$A_\rho(E) \approx A_\rho^{BW}(E) = \frac{\Gamma_{\rho\pi\pi}}{(E - m_\rho)^2 + \frac{\Gamma_{\rho\pi\pi}^2}{4}}. \quad (1)$$

Note that the width $\Gamma_{\rho\pi\pi}$ is generally energy dependent, and the mass m_ρ can be modified by the real part of quantum loops. Thus, the decay probability is never exactly exponential. See, e.g., the theoretical treatment in Refs. [27,40] and the experimental results in Refs. [41–43]; and Ref. [44] for a discussion in a quantum field theory.

Based on the LH, the finite temperature properties of the system can be derived using the standard techniques of statistical mechanics. See Sect. 4 for details. Here we give a synopsis of our discussion. Consider the hypothetical limit where ρ and π 's are completely decoupled, i.e., $g = 0$ (or $\Gamma_{\rho\pi\pi} = 0$). The pressure of the system would be given by a sum of two contributions:

$$P_{\text{free}} = P_\pi^{(0)} + P_\rho^{(0)}, \quad (2)$$

where $P_a^{(0)} = P^{(0)}(E = m_a, T)$ denotes the pressure of an ideal gas of a species a , which depends on its mass (m_a) and degeneracy. The dependence on temperature T is understood. Even if the interaction is switched on, Eq. (2) can still be used as an estimate of the pressure for a narrow-width ρ . This is the fundamental premise of the hadron resonance gas (HRG) model [45,46]: contribution of resonances to the thermodynamics is approximated by an uncorrelated gas of zero-width particles.

As a next step in improving the approximation, we take into account the width of ρ via a weighed sum by $A_\rho(E)$:

$$P_\rho^{(0)} \rightarrow P_\rho = \int \frac{dE}{2\pi} A_\rho(E) \times P^{(0)}(E, T), \quad (3)$$

such that the total pressure is approximated as (Scheme-A):

$$P_{\text{Sch.A}} = P_\pi^{(0)} + P_\rho. \quad (4)$$

This scheme is employed in many versions of the HRG models, see e.g., Refs. [3,4,47–50]. See also the K-matrix-based approach [51,52]. However, Eq. (4) is not yet complete. According to the S-matrix formulation of statistical mechanics by Dashen et al. [5] (see also the discussion by Weinhold

et al. [15]), the correct result of the pressure at arbitrary g (or $\Gamma_{\rho\pi\pi}$) is given by (S-matrix scheme):

$$P_{\text{S-matrix}} = P_\pi^{(0)} + \int \frac{dE}{2\pi} B(E) \times P^{(0)}(E, T) \\ B(E) = 2 \frac{d}{dE} \mathcal{Q}_{\pi\pi}(E). \quad (5)$$

where $\mathcal{Q}_{\pi\pi}(E)$ is the phase shift for the scattering process $\pi\pi \rightarrow \pi\pi$. Here we summarize some key features of the S-matrix scheme:

- (i) Observe that there is no explicit ρ contribution in Eq. (5): The pressure is determined based on the scattering information of the asymptotic (stable) states alone. In fact, it is not compulsory to introduce the ρ state as an explicit degree of freedom. Its presence is encoded in the phase shift. This point will be made clear by direct model calculations.
- (ii) Equations (4) and (5) reduce to the free gas result (2) in the limit of $g \rightarrow 0$ (or $\Gamma_{\rho\pi\pi} \rightarrow 0$).² For the latter, we have

$$\delta_{\pi\pi}(E) \rightarrow \pi \theta(E - m_\rho) \\ B(E) \rightarrow 2\pi \delta(E - m_\rho). \quad (6)$$

- (iii) Generally, $B(E) \neq A_\rho(E)$, and Eqs. (4) and (5) are thus different. Systems which show substantial deviation are plenty: In addition to the case of $f_0(500)$ mentioned, nonresonant contribution is found to be important in the study of $\kappa(700)$ [16,17], the N^* and Δ resonances [53,54], the $S = -1$ hyperons [55], etc. It is also the case for the recently discovered X , Y , Z states [56–58]. As shown in a recent work [59], the state $X(3872)$ makes only a small contribution to the thermodynamics due to nonresonant effects. For what concerns other states, future studies based on Eq. (5) are needed.

In this work we verify Eq. (5), instead of Eq. (4), gives the correct description of the thermodynamics of an interacting system. This point had been raised in previous works, see e.g., Ref. [15], but the actual adoption of the scheme remains limited [54,60]. We hope that a more detailed account of the different spectral functions can raise the awareness of the issue in the community and further promote the use of the correct formula. We also establish their formal relations to the resolvent and the density of states. This gives an interesting perspective in describing the thermodynamics of an interacting system.

Using an LH, we derive the mismatch analytically, the result takes the form

² The $g = 0$ limits of $A_\rho(E)$ and $B(E)$ are not well-defined.

$$B(E) = A_\rho(E) + \sum_q \Delta A_{2\pi}(E; q), \tag{7}$$

where the second term in the R.H.S. describes the the modification of the spectral function of the 2-body $|\pi\pi\rangle$ state. Such a term is present even in the absence of the resonance, e.g., taking the large m_ρ limit (see Sect. 3). The correct expression of the pressure can be decomposed as:

$$P_{S\text{-matrix}} = P_\pi^{(0)} + P_\rho + \Delta P_{2\pi}, \tag{8}$$

where

$$\Delta P_{2\pi} = \int \frac{dE}{2\pi} \sum_q \Delta A_{2\pi}(E; q) \times P^{(0)}(E, T). \tag{9}$$

As we shall see, the last term is in general not negligible and can even be dominant at low temperatures.

The paper is organized as follows: In Sect. 2 the details of the Lee model are presented. Then, in Sect. 3, the spectral functions for both ρ and $\pi\pi$, and the phase shift are introduced. Here the important Eq. (7) is derived. In Sect. 4 the thermodynamic properties of the system are determined analytically, with special focus on the pressure with its various contributions. A numerical example shows that $\Delta P_{2\pi}$ can be sizable and in general should not be neglected. Finally, discussions and conclusions are given in Sect. 5.

2 The Lee model

The Lee model [20] describing the $\rho \leftrightarrow \pi\pi$ system can be formulated as follows.³ Introducing the basis states in the center-of-mass (CM) frame:

$$|\rho\rangle, \{|q\rangle\}, \tag{10}$$

where q is the momentum label for the two-pion state

$$|\pi(\mathbf{q})\pi(-\mathbf{q})\rangle. \tag{11}$$

The Hamiltonian of the system can be represented as an $(1 + N_q) \times (1 + N_q)$ -matrix. The non-interacting Hamiltonian H_0 is a diagonal matrix with

$$\begin{aligned} H_0|\rho\rangle &= \Delta_0|\rho\rangle, \\ H_0|q\rangle &= \epsilon(q)|q\rangle. \end{aligned} \tag{12}$$

³ In the following we measure energy with respect to $2m_\pi$, and the nonrelativistic dispersion relation $\epsilon(q) = q^2/m_\pi$ is used. We also choose to present our model in a discretized form. This prepares for the later numerical treatment of solving the system on a momentum grid. [61]. It is easy to go to the continuum by taking $\sum_q C(q)^2 (\dots) \rightarrow \int \frac{d^3q}{(2\pi)^3} (\dots)$.

The interaction V describes the coupling of ρ with the $|q\rangle$ states

$$V = \sum_q g_{\text{eff}} C(q) (|\rho\rangle\langle q| + |q\rangle\langle \rho|), \tag{13}$$

such that

$$\begin{aligned} V|\rho\rangle &= \sum_{q'} g_{\text{eff}} C(q')|q'\rangle \\ V|q\rangle &= g_{\text{eff}} C(q)|\rho\rangle. \end{aligned} \tag{14}$$

We use

$$C(q)^2 = \frac{4\pi q^2}{(2\pi)^3} \delta q \tag{15}$$

to implement the spherical degeneracy. Note that $\delta q = \frac{2\pi}{L}$ in the finite volume formulation, L being the size of the box. The coupling g_{eff} is generally q -dependent. The full Hamiltonian then reads

$$H = H_0 + V. \tag{16}$$

With the Hamiltonian defined, we can construct the resolvent operators

$$\begin{aligned} G_0(E) &= \frac{1}{E - H_0 + i\epsilon} \\ G(E) &= \frac{1}{E - H + i\epsilon}, \end{aligned} \tag{17}$$

which can be understood again as $(1 + N_q) \times (1 + N_q)$ matrices. In the remainder of this paper we will suppress the E dependence unless there is a chance for confusion.

The well-known relations from the Lippmann-Schwinger equation can also be directly realized:

$$\begin{aligned} G &= G_0 + G_0VG \\ &= G_0 + G_0TG_0, \end{aligned} \tag{18}$$

and

$$\begin{aligned} T &= V + VG_0T \\ &= V + VGV \\ &= VGG_0^{-1}. \end{aligned} \tag{19}$$

In this paper, we investigate the inclusion of an unstable state in the description of thermodynamics using the S-matrix formulation. The key operators of interest in this scheme is the scattering operator [13,62]

$$\begin{aligned} \hat{S} &= G_0^* G^{*-1} G G_0^{-1} \\ &= I + (G_0 - G_0^*) \times V G G_0^{-1} \\ &= I - 2\pi i \delta(E - H_0) \times T. \end{aligned} \tag{20}$$

Since ρ is not an asymptotic state, the actual scattering matrix S is extracted from the (lower-right) $N_q \times N_q$ block of \hat{S} . In addition, we introduce an operator \mathcal{K} , due to Krein, Friedal and Lloyd (KFL) [63,64], defined as the difference of the spectral functions

$$\begin{aligned} \mathcal{K} &= -\text{Im} [(G - G^*) - (G_0 - G_0^*)] \\ &= A - A_0 \\ &= \Delta A, \end{aligned} \tag{21}$$

where we have identified the spectral function operator

$$\begin{aligned} A(E) &= -2 \text{Im} G = -\text{Im} (G - G^*) \\ A_0(E) &= -2 \text{Im} G_0 = -\text{Im} (G_0 - G_0^*). \end{aligned} \tag{22}$$

These operators are deeply connected with the scattering phase shift \mathcal{Q} and the effective spectral function B . The latter is defined as

$$B(E) = 2 \frac{\partial}{\partial E} \mathcal{Q}(E). \tag{23}$$

There are multiple ways to extract the phase shift \mathcal{Q} from the resolvents (or Green functions). (See Eqs. (36), (48)). These and the explicit relations among the various observables will be demonstrated in the context of the Lee model in Sect. 3.

3 Phase shift and effective spectral function

In the Lee model various theoretical quantities, e.g. the propagator and the self-energy of ρ , can be analytically computed. It is a useful exercise to revisit these formulas as it helps to build an understanding the physical content of the KFL operator \mathcal{K} and the derivative of the phase shift.

3.1 The ρ -propagator

The ρ -propagator G_ρ can be computed from $\langle \rho | G(E) | \rho \rangle$, i.e. the first diagonal entry of the matrix $G(E)$, as

$$\begin{aligned} G_\rho &\equiv \langle \rho | G | \rho \rangle \\ &= \langle \rho | G_0 | \rho \rangle + \langle \rho | G_0 V G_0 | \rho \rangle \\ &\quad + \langle \rho | G_0 V G_0 V G_0 | \rho \rangle + \dots, \end{aligned} \tag{24}$$

where each term can be directly worked out:

$$\begin{aligned} \langle \rho | G_0 | \rho \rangle &= G_\rho^0 = \frac{1}{E - \Delta_0 + i\varepsilon} \\ \langle \rho | G_0 V G_0 | \rho \rangle &= 0, \end{aligned} \tag{25}$$

and

$$\langle \rho | G_0 V G_0 V G_0 | \rho \rangle = G_\rho^0 \left(\sum_q C(q)^2 g_{\text{eff}}^2 G_{2\pi}^0(E; q) \right) G_\rho^0. \tag{26}$$

It is clear that the propagator G_ρ can be re-summed to all orders via

$$\begin{aligned} G_\rho &= G_\rho^0 + G_\rho^0 \Sigma_\rho G_\rho^0 + G_\rho^0 \Sigma_\rho G_\rho^0 \Sigma_\rho G_\rho^0 + \dots \\ &= \frac{1}{(G_\rho^0)^{-1} - \Sigma_\rho}, \end{aligned} \tag{27}$$

where the self-energy of ρ can be explicitly computed by

$$\begin{aligned} \Sigma_\rho &\equiv \langle \rho | V G_0 V | \rho \rangle \\ &= \sum_q C(q)^2 g_{\text{eff}}^2 G_{2\pi}^0(E; q). \end{aligned} \tag{28}$$

A relation that will prove useful later is the energy-derivative of Σ_ρ :

$$\frac{\partial}{\partial E} \Sigma_\rho = -1 \times \sum_q C(q)^2 g_{\text{eff}}^2 G_{2\pi}^0(E; q) G_{2\pi}^0(E; q). \tag{29}$$

which is easily seen by noting

$$\begin{aligned} G_{2\pi}^0(E; q) &= \frac{1}{E - \varepsilon(q) + i\varepsilon} \implies \frac{\partial}{\partial E} G_{2\pi}^0(E; q) \\ &= -G_{2\pi}^0(E; q) \times G_{2\pi}^0(E; q) \end{aligned} \tag{30}$$

3.2 The 2-pion propagator

Now we turn to the 2-pion states. The propagator $G_{2\pi}(E; q)$ can be explicitly worked out from the corresponding diagonal entries of $G(E)$:

$$\begin{aligned} G_{2\pi}(E; q) &= \langle q | G | q \rangle \\ &= G_{2\pi}^0(E; q) + \langle q | G_0 T G_0 | q \rangle \\ &= G_{2\pi}^0(E; q) + G_{2\pi}^0(E; q) \times \langle q | T | q \rangle \\ &\quad \times G_{2\pi}^0(E; q). \end{aligned} \tag{31}$$

We now show that the diagonal T-matrix is directly related to the full propagator G_ρ . This is an important relation, as it dictates how the properties of the unstable state can be

inferred from the scattering of the stable particles. To see that we employ the following expression of the T-matrix:

$$\langle q|T|q\rangle = \langle q|V|q\rangle + \langle q|VGV|q\rangle. \tag{32}$$

The first term is 0 since V is off-diagonal. The second term gives

$$\langle q|VGV|q\rangle = g_{\text{eff}}^2 C(q)^2 \times G_\rho \tag{33}$$

and hence

$$\langle q|T|q\rangle = g_{\text{eff}}^2 C(q)^2 \times G_\rho. \tag{34}$$

This relates the amplitude of $\pi\pi$ scatterings to the ρ -propagator. Indeed, in the simple setting of the Lee model, all the physical information concerning the unstable state ρ can be extracted from the diagonal T-matrix $\langle q|T|q\rangle$.

Finally, the full propagator $G_{2\pi}(E; q)$ can be obtained in closed form as

$$G_{2\pi}(E; q) = G_{2\pi}^0(E; q) + G_{2\pi}^0(E; q) \times \left(C(q)^2 g_{\text{eff}}^2 G_\rho \right) G_{2\pi}^0(E; q). \tag{35}$$

3.3 Effective spectral function

We are now ready to examine the expressions of the phase shift \mathcal{Q} , the effective spectral function B and the operator \mathcal{K} in the context of the Lee model.

The phase shift can most simply be extracted from G_ρ via⁴

$$\begin{aligned} \mathcal{Q}(E) &= \text{Im} \ln G_\rho \\ &= \tan^{-1} \frac{\text{Im} \Sigma_\rho}{E - \Delta_0 - \text{Re} \Sigma_\rho}. \end{aligned} \tag{36}$$

The effective spectral function B is known to be related to the interacting part of the density of state. In the Lee model, it is

$$\begin{aligned} B(E) &= 2 \frac{\partial}{\partial E} \mathcal{Q}(E) \\ &= 2 \frac{\partial}{\partial E} \text{Im} \ln G_\rho \\ &= -2 \text{Im} \left(G_\rho \frac{\partial}{\partial E} G_\rho^{-1} \right) \\ &= -2 \text{Im} \left[G_\rho \frac{\partial}{\partial E} (E - \Delta_0 - \Sigma_\rho) \right] \\ &= -2 \text{Im} G_\rho + 2 \text{Im} \left(G_\rho \times \frac{\partial}{\partial E} \Sigma_\rho \right), \end{aligned} \tag{37}$$

⁴ One can obtain the phase shift directly from the S-matrix. See Eq. (48).

using the relation previously obtained

$$\frac{\partial}{\partial E} \Sigma_\rho = -1 \times \sum_q C(q)^2 g_{\text{eff}}^2 G_{2\pi}^0(E; q) G_{2\pi}^0(E; q), \tag{38}$$

we get

$$\begin{aligned} B &= -2 \text{Im} G_\rho + 2 \text{Im} \left(G_\rho \times \frac{\partial}{\partial E} \Sigma_\rho \right) \\ &= -2 \text{Im} G_\rho - 2 \text{Im} \left[G_\rho \sum_q C(q)^2 g_{\text{eff}}^2 G_{2\pi}^0(E; q) G_{2\pi}^0(E; q) \right] \\ &= -2 \text{Im} G_\rho - 2 \text{Im} \sum_q (G_{2\pi}(E; q) - G_{2\pi}^0(E; q)). \end{aligned} \tag{39}$$

Comparing with the expression of the KFL operator \mathcal{K} in Eq. (21), we obtain

$$\begin{aligned} B(E) &= A_\rho(E) + \sum_q \Delta A_{2\pi}(E; q) \\ &= A_\rho^0(E) + \text{tr} \mathcal{K} \\ &= A_\rho^0(E) + \left(\Delta A_\rho(E) + \sum_q \Delta A_{2\pi}(E; q) \right). \end{aligned} \tag{40}$$

Relation (40) constitutes the main result of this work. It demonstrates how the operator B extracts the physical content, including the contribution from the unstable state ρ , of the system. From the first line of Eq. (40), we see that B includes the contribution from the full spectral function A_ρ and the 2-pion nonresonant interaction $\sum_q \Delta A_{2\pi}(E; q)$. The second line offers an alternative, but equivalent interpretation: B includes the contribution from the bare- ρ , together with the interaction contribution contained in $\text{tr} \mathcal{K}$. The latter includes contributions from the change in the energy spectra of both the ρ and the 2-pion states.

To understand relation (40) better, we consider the interesting limit of vanishing coupling $g_{\text{eff}} \rightarrow 0$. At this limit, the KFL operator \mathcal{K} vanishes by definition. However the phase shift derivative operator B would give

$$B \rightarrow A_\rho^0, \tag{41}$$

that is, it becomes a Dirac-delta function for the bare ρ state. It follows that the phase shift \mathcal{Q} would become a step function $\mathcal{Q} \rightarrow \pi \times \theta(E - \Delta_0)$. This is an intuitive limit for describing a ρ that decouples from the pions: ρ becomes a stable state, its width ceases to exist and the state should be included as particles in the asymptotic state. These are automatically implemented when the effective spectral function B is used.

Another interesting limit is that of large bare resonant mass $\Delta_0 \gg E$. In this case, the resonant structure is suppressed, and the nonresonant term dominates. One can show that as $E \rightarrow 0$

$$\begin{aligned}
 B &\approx 2 (\text{Re } G_\rho) \times \frac{\partial}{\partial E} \text{Im}(\Sigma_\rho) \\
 &\approx 2 a_l \times \frac{\partial}{\partial E} q^{2l+1}.
 \end{aligned}
 \tag{42}$$

where a_l is the scattering length of the channel and l is the relative orbital angular momentum between the pions. Note that terms that are proportional to $\text{Im}(\Sigma_\rho)$ are subleading relative to $\frac{\partial}{\partial E} \text{Im}(\Sigma_\rho)$, as the latter is of $\mathcal{O}(q^{2l-1})$. This should be distinguished from the residual effect of the resonance width at threshold, which is of $\mathcal{O}(q^{2l+1})$. Thus, even an energy dependent Breit-Wigner model can not capture the effect of this term. In addition, the scattering lengths are well constrained by the chiral perturbation theory, and indeed the stated form of B was derived [65].

3.4 Numerical results

As a numerical exercise, we solve the Lee Model on a momentum grid following the method of Ref. [61]. The Hamiltonians are constructed directly as an $(1 + N_q) \times (1 + N_q)$ matrix. The various Green functions are computed by matrix inversions. The method is very robust, and the procedure is as follows:

- (i) Construct the matrices H and H_0 .
- (ii) For each E , construct the matrices

$$\begin{aligned}
 M_1(E) &= E I - H_0 + i\varepsilon I \\
 M_2(E) &= E I - H + i\varepsilon I;
 \end{aligned}
 \tag{43}$$

and invert

$$\begin{aligned}
 \hat{G}_0(E) &= \{M_1(E)\}^{-1} \\
 \hat{G}(E) &= \{M_2(E)\}^{-1}.
 \end{aligned}
 \tag{44}$$

- (iii) Extract the quantities of interest. For example, the propagators are obtained from

$$\begin{aligned}
 G_\rho &= \hat{G}(1, 1) \\
 G_\rho^0 &= \hat{G}_0(1, 1) \\
 G_{2\pi}(q_i) &= \hat{G}(i, i) \\
 G_{2\pi}^0(q_i) &= \hat{G}_0(i, i).
 \end{aligned}
 \tag{45}$$

where q_i is the discrete momentum of the i -th grid.

- (iv) The spectral functions A 's can be obtained from the propagators by simply taking the imaginary part. To calculate the B function, one possible method is

$$\begin{aligned}
 B(E) &= -2 \text{Im tr } (G(E) - G_0(E)) \\
 &\quad + 2 \text{Im } \hat{G}_0(1, 1).
 \end{aligned}
 \tag{46}$$

In this exercise, we have chosen an appropriate P-wave coupling to describe the physical ρ -meson:

$$g_{\text{eff}} = g \times q \times e^{-\frac{q^2}{2\Lambda^2}},
 \tag{47}$$

with parameters $g = 23.5 \text{ GeV}^{-3/2}$, $\Delta_0 = 0.64 \text{ GeV}$, and $\Lambda = 0.4 \text{ GeV}$. The form factor renders the real part of the self-energy finite.⁵ It can be motivated in a quantum field theory with non-local interactions or dressing of vertex [66–69]. For what concerns us here it parametrizes the finite-size effects of the hadrons. See Ref. [70] for a rigorous treatment within the QFT framework.

The numerical results for \mathcal{Q} and various spectral functions are shown in Fig. 1. We have computed the phase shift on the momentum grid, ($1 + N_q = 800$; $L \approx 800 \text{ fm}$; $\varepsilon = 0.01 \text{ GeV}$), in two ways: one uses G_ρ via Eq. (36) (grey squares), the other uses the scattering matrix S via Eq. (48) (black circles). Both results agree quite well with the continuum limit, although they appear to have different convergence property.⁶

A key feature to note is the apparent shift of the strength of B , compared to A_ρ , towards lower energies. This effect originates from the nonresonant scattering term $\sum_q \Delta A_{2\pi}(E; q)$, and is needed, in addition to A_ρ , for a complete description of the interacting system.

3.5 Phase shift from S-matrix

In Eq. (36) we extracted the phase shift \mathcal{Q} from the ρ -propagator. The same information is also available from the 2-pion sector via the S-matrix. In Ref. [13], the following recipe has been proposed to extract the phase shift from an $N_q \times N_q$ S-matrix

$$\begin{aligned}
 \mathcal{Q} &= \frac{1}{2} \times \text{Im tr } \ln S \\
 &= \frac{1}{2} \times \text{Im } \ln \det S \\
 &\approx \frac{1}{2} \times \text{Im } \ln(1 + i \times \text{tr } \hat{t}).
 \end{aligned}
 \tag{48}$$

where we have introduced the \hat{t} operator, defined as

$$\hat{t} = -2\pi \delta(E - H_0) \times T.
 \tag{49}$$

⁵ The imaginary part is finite even without a regulator. We checked that its value is only slightly modified by the form factor.

⁶ Within this model one can also study how the phase shift and the spectral functions depend on the lattice size. This may help in understanding phase shift extraction in LQCD [61, 71].

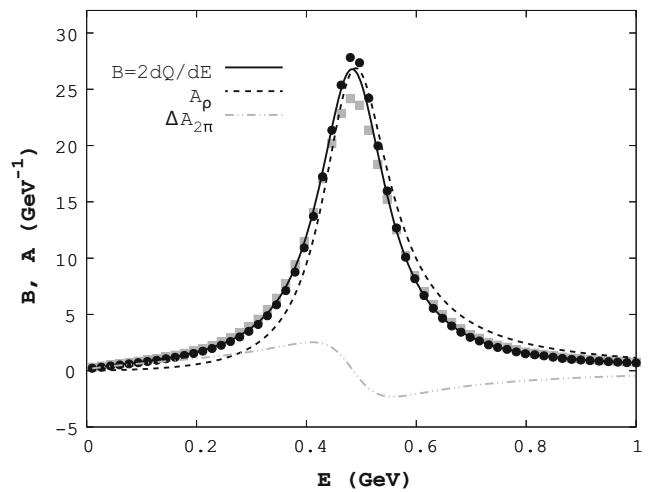
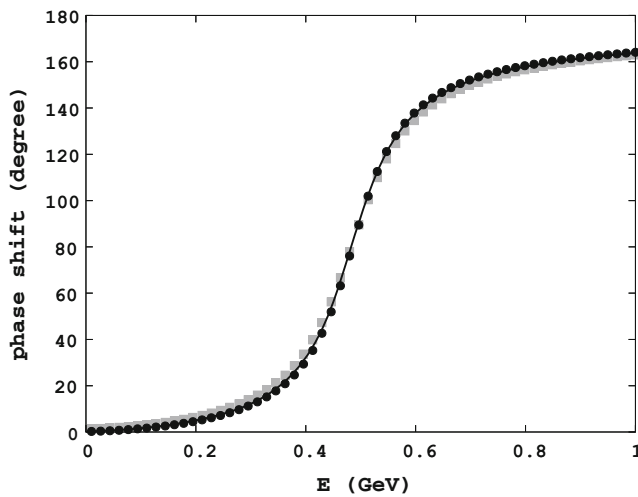


Fig. 1 Phase shift computed from the Lee model (Eq. (36)) and the corresponding effective spectral functions (Eqs. (22), (23)) for the ρ -meson. E is the energy of the relative motion. Note that $B = A_\rho +$

$\Delta A_{2\pi}$. The points are the numerical results obtained from the momentum grid method: Grey squares indicate results based on Eq. (36), while black circles indicate results based on Eq. (48). See text

From Eqs. (28) and (34) we see

$$\begin{aligned} \text{tr } \hat{t} &= -2 \sum_q \left(\pi \delta(E - \varepsilon(q)) \times g_{\text{eff}}^2 C(q)^2 \right) \times G_\rho \\ &= 2 \text{Im } \Sigma_\rho \times G_\rho, \end{aligned} \tag{50}$$

and indeed it is straightforward to verify the same result of the phase shift as in Eq. (36):

$$\begin{aligned} &\frac{1}{2} \times \text{Im } \ln(1 + i \times \text{tr } \hat{t}) \\ &= \frac{1}{2} \times \text{Im } \ln \left(G_\rho^{-1*} / G_\rho^{-1} \right) \\ &= \tan^{-1} \frac{\text{Im } \Sigma_\rho}{E - \Delta_0 - \text{Re } \Sigma_\rho}. \end{aligned} \tag{51}$$

The approximation in the last line of Eq. (48) was shown to be valid for some simple cases such as s-channel-only interaction or structureless scattering. We shall now show that the approximation is exact in the Lee model.

Consider the expansion of the logarithm of the S-matrix via the Mercator series

$$\begin{aligned} \text{tr } \ln S &= \text{tr } \ln(I + i \times \hat{t}) \\ &= \sum_{m=1}^{\infty} \frac{(-1)^{m+1} i^m}{m} \text{tr } (\hat{t}^m). \end{aligned} \tag{52}$$

The approximation in Eq. (48) becomes exact if \hat{t} satisfies the following property

$$\text{tr } (\hat{t}^m) \rightarrow (\text{tr } \hat{t})^m, \tag{53}$$

giving

$$\begin{aligned} \sum_{m=1}^{\infty} \frac{(-1)^{m+1} i^m}{m} \text{tr } (\hat{t}^m) &\rightarrow \sum_{m=1}^{\infty} \frac{(-1)^{m+1} i^m}{m} (\text{tr } \hat{t})^m \\ &= \ln(1 + i \times \text{tr } \hat{t}). \end{aligned} \tag{54}$$

Note the effective replacement of I with 1 in the above.

Inspecting the interaction term of the Lee Model in Eq. (13), we see that the matrix element of \hat{t} takes the product form

$$\hat{t}_{q_1 q_2} = u_{q_1} v_{q_2}. \tag{55}$$

It follows that

$$\begin{aligned} (\hat{t}^2)_{q_1 q_2} &= \sum_{q_3} u_{q_1} v_{q_3} u_{q_3} v_{q_2} \\ &= u_{q_1} v_{q_2} \text{tr } \hat{t}, \end{aligned} \tag{56}$$

and hence $\text{tr } (\hat{t}^2) = (\text{tr } \hat{t})^2$ and so on for higher power. This demonstrates that criteria (53) is satisfied by a class of \hat{t} which involves separable potentials, i.e. the ones that are from a Kronecker (direct) product.

Furthermore, we add that from Cayley Hamilton theorem, the determinant of \hat{t} essentially vanishes. In fact, all eigenvalues of \hat{t} are zero, except one, which is $\text{tr } \hat{t}$. This is another way to understand why the approximation made in Eq. (48) is justified. The full implication of this result is not yet completely clear, and will be explored in a future work.

4 Thermodynamics

The change in the density of state due to interactions, as revealed by the KFL \mathcal{H} operator or the B function, is the key input for the S-matrix formulation of statistical mechanics [5,6]. The approach is based on the method of cluster expansions, and for the second virial coefficient the result is exact. We retrace a few basic steps in relating the scattering phase shift to the thermal partition function.

Our starting point is the cluster expansion of the grand partition function

$$Z(T, V, \xi) = \text{tr} e^{-\beta(H-\mu N)} = \sum_N Z_N \xi^N, \tag{57}$$

where ξ is the fugacity, related to the particle chemical potential via $\xi = e^{\mu/T}$. Z_N is the N-body partition function. The corresponding expansion for the logarithm of Z reads

$$W(T, V, \xi) = \ln Z = \sum_N W_N \xi^N, \tag{58}$$

and one can work out

$$\begin{aligned} W_1 &= Z_1 \\ W_2 &= Z_2 - \frac{1}{2} Z_1^2 \\ W_3 &= Z_3 - Z_1 Z_2 - \frac{1}{3} Z_1^3 \dots \end{aligned} \tag{59}$$

The interacting part of the partition function satisfies⁷

$$W_2 - W_2^{(0)} = Z_2 - Z_2^{(0)}, \tag{60}$$

The latter can be re-expressed via

$$\begin{aligned} Z_2 - Z_2^{(0)} &= \text{Tr} \left(e^{-\beta H_2} - e^{-\beta H_2^{(0)}} \right) \\ &= V \int \frac{d^3 P}{(2\pi)^3} \frac{dE}{2\pi} e^{-\beta E_{\text{sys}}(\mathbf{P}, q)} D(E) \\ &= \beta V \times (T \lambda_T^3) e^{-\beta m_{\text{tot}}} \times \int \frac{dE}{2\pi} e^{-\beta E} D(E). \end{aligned} \tag{61}$$

where we have integrated out the CM motion in the total energy of the 2-body system

$$E_{\text{sys}}(\mathbf{P}, q) = m_{\text{tot}} + \frac{\mathbf{P}^2}{2m_{\text{tot}}} + E, \tag{62}$$

⁷ For simplicity we neglect corrections due to quantum statistics and focus on the $\mu = 0$ case.

with m_{tot} being the total mass. E is the energy of the relative motion

$$E = \frac{q^2}{2m_{\text{red}}}, \tag{63}$$

where m_{red} is the reduced mass. We have made use of the form of the nonrelativistic dispersion (see e.g., Ref. [13] for a relativistic formulation) to integrate out the CM momentum \mathbf{P} and obtain the thermal wavelength λ_T

$$\lambda_T^3 \equiv \int \frac{d^3 P}{(2\pi)^3} e^{-\beta \frac{\mathbf{P}^2}{2m_{\text{tot}}}}. \tag{64}$$

Note that the bare ρ state is not counted in the trace of $Z_2^{(0)}$. The remaining integral in Eq. (61) requires the input of $D(E)$, which is the change in the density of state due to interactions.

Now we are ready to examine the thermal contribution of an unstable state ρ based on the input from the Lee model. The first thing to notice is that the L.H.S. of Eq. (61) can be directly computed from the eigenvalues (λ_n) of the Hamiltonian:⁸

$$\begin{aligned} \text{Tr} e^{-\beta H} &= \sum_{\lambda_n} e^{-\beta \lambda_n} \\ &= -2 \text{Im} \int \frac{dz}{2\pi} e^{-\beta z} \text{Tr} G(z). \end{aligned} \tag{65}$$

The result is shown as points in Fig. 2. This in turns indicates what is the correct $D(E)$ to use. The S-matrix formulation of statistical mechanics by Dashen *et al.* [5] dictates the choice of $D(E) \rightarrow B(E) = 2 \frac{\partial}{\partial E} \mathcal{Q}(E)$. This means that we compute the thermodynamic pressure via

$$P_{\text{S-matrix}} \approx P_{\pi}^{(0)} + \Delta P_B. \tag{66}$$

ΔP_B includes the contribution of the unstable state $|\rho\rangle$ and nonresonant $\pi\pi$ interaction:

$$\Delta P_B = P_{\rho} + \Delta P_{2\pi}. \tag{67}$$

From Eq. (40) and the discussion it is clear that one can incorporate the same physical content of the thermal medium with a different choice of $D(E)$, though with a different interpretation. For example, one can choose instead $D(E) \rightarrow \text{tr} \mathcal{H}$, and in this case the contribution of A_{ρ}^0 needs to be added separately as

⁸ In fact, computations involving the difference between the fully interacting system and the free case, e.g., $G(z) - G_0(z)$, are numerically more stable [72]. This also opens up the possibility of solving the system with other numerical techniques, such as the use of a harmonic oscillator basis in the expansion [73].

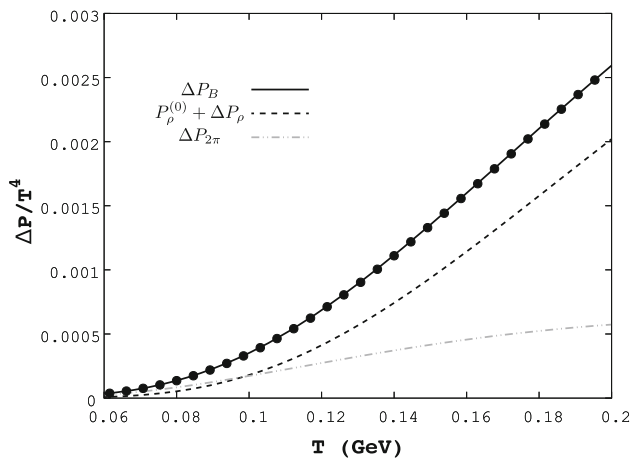


Fig. 2 Interacting contributions to the thermodynamics pressure (normalized to T^4) from different effective spectral functions. The top line (B) is equal to the sum of the contributions from the lower two (see Eq. (69)). The points are the results obtained by directly constructing the partition function from the eigenvalues of the Hamiltonian. See text

$$\begin{aligned}
 P_{\text{KFL}} &\approx P_{\pi}^{(0)} + P_{\rho}^{(0)} + \Delta P_{\mathcal{K}} \\
 &= P_{\pi}^{(0)} + P_{\rho}^{(0)} + \Delta P_{\rho} + \Delta P_{2\pi}.
 \end{aligned}
 \tag{68}$$

Here $\Delta P_{\mathcal{K}}$ contains the contribution from ΔA_{ρ} and $\Delta A_{2\pi}$. Note that as $g \rightarrow 0$, $\Delta P_{\mathcal{K}} \rightarrow 0$; while $\Delta P_B \rightarrow P_{\rho}^{(0)}$. The two results in Eqs. (66) and (68) are equivalent, i.e.

$$\begin{aligned}
 \Delta P_B &= P_{\rho}^{(0)} + \Delta P_{\mathcal{K}} \\
 &= P_{\rho}^{(0)} + \Delta P_{\rho} + \Delta P_{2\pi}.
 \end{aligned}
 \tag{69}$$

which is just restating the relation (40).

The various partial pressures are shown in Fig. 2. Due to the contribution from the nonresonant $\pi\pi$ state, the pressure based on B is substantially larger than the one based on A_{ρ} alone. We stress that only the former one gives a consistent description of the thermodynamics, as can be verified by the direct construction of the partition function from the eigenvalues of the Hamiltonian (black circles). Therefore Eq. (5) should be used instead of Eq. (4).

These observations are in accord with the previous analysis based on a Φ -derivable approach [15]. The B -function-based description requires only the input from the scattering of asymptotic states. This underlines an important concept in the formulation: In computing the density of states it is not mandatory to introduce the unstable state as an explicit degree of freedom. For approaches that use only stable states as degrees of freedom, such as an effective field theory where resonances are dynamically generated [74], the same density of states would be obtained as long as the phase shifts agree. And when an empirical phase shift $\mathcal{Q}(E)$ is used, the function $B(E)$ becomes model independent, while the splitting

into $A_{\rho}(E)$ and $\sum_q \Delta A_{2\pi}(E; q)$ is model dependent. The Lee model studied here provides a clear picture of such a splitting, and demonstrates how an unstable state should be included in the description of the thermodynamics.

5 Conclusion

In the context of the Lee model we have clarified the relation between the energy derivative of the phase shift and the spectral functions of the degrees of freedom composing the system. We have also illustrated how these quantities enter the thermal description of the system via the S-matrix formulation of the statistical mechanics. This consolidates our understanding of the connection between this and the standard approach based on thermal Green functions. In particular, we have shown that the thermodynamic trace requires the inclusion of the nonresonant contribution ($\Delta A_{2\pi}$), in addition to, and independent of, the effect coming from the width of the unstable state ΔA_{ρ} .

Besides acting as an effective density of state, an alternative interpretation of the energy derivative of the phase shift is the concept of time delay [75, 76]: particles spend longer or shorter in the interaction region due to the attractive or repulsive nature of the interaction. In the contexts of transport models and resonance identification, it was argued [77, 79–82] that such a time delay, instead of the inverse width $1/\Gamma(E)$, should be used to measure the life-time of a resonance. A related problem is the study of the survival probability of an unstable state. According to Fonda et al. [40], the standard exponential decay law is valid only in the limited case of an energy-independent Breit-Wigner distribution. Rescattering effect, apparently related to $\Delta A_{2\pi}$, would lead to non-exponential behavior [83]. A clearer theoretical understanding of B and A_{ρ} could provide further insights into these topics.

So far we have restricted our discussion to Fock space up to two body. It will be extremely interesting to extend the scheme to include multi-channel and multi-body scatterings [13, 21, 55, 84, 85], and understand how these interactions would influence thermodynamic quantities. This can be a useful framework to analyze the observables in Heavy Ion Collision experiments, such as hadron yields and the momentum distributions of light hadrons [60, 86–88]. We defer this more challenging problem to future research.

Acknowledgements PML thanks Eric Swanson for stimulating discussions. He also acknowledges fruitful discussions with Hans Feldmeier, Bengt Friman, and Piotr Bozek. The authors are also grateful for the constructive conversations with Wojciech Broniowski, Wojciech Florkowski, and Stanislaw Mrowczynski. PML was partly supported by the Polish National Science Center (NCN), under Maestro Grant No. DEC-2013/10/A/ST2/00106 and by the Short Term Scientific Mission (STSM) program under COST Action CA15213 (refer-

ence number: 41977). FG acknowledges financial support from the Polish National Science Centre (NCN) through the OPUS project no. 2015/17/B/ST2/01625.

Data Availability Statement This manuscript has associated data in a data repository. [Authors' comment: The phase shift data analyzed are extracted from Refs. [89,90]. Results of our model calculation are available in the supplementary datafile.]

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