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Volume dependence of spectral weight functions

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It has been suggested that the volume dependence of the spectral weight could be utilized as a probe to distinguish single and multiparticle states in Monte Carlo simulations. In a recent study using a solvable model, the Lee model, we found that this criteria is not applicable for broad resonances. In this paper, the same question is addressed within the finite-size formalism outlined by Lüscher. A similar conclusion has been reached. This is first studied using a quantum-mechanical scattering model. Then, following analogous arguments as in the original Lüscher's formalism, the result is generalized to massive quantum field theories under the same conditions as the conventional Lüscher's formulas. A possibility of extracting resonance parameters using the spectral weight function is also pointed out.

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I. INTRODUCTION

Low-energy hadron-hadron scattering plays an important role in the understanding of nonperturbative physics of strong interaction. Because of its genuine nonperturbative nature, such problems can only be studied from first principles using nonperturbative methods like lattice QCD. Lüscher has outlined a finite-size formalism which enables one to calculate the elastic scattering phase shifts using lattice simulations [1–5]. Over the years, extensive numerical simulations have been carried out to the study on hadron-hadron scattering using Lüscher's formalism, both within the quenched approximations and using gauge field configurations with dynamical quarks [6–16].

In typical lattice studies on hadron spectroscopy and hadron-hadron scattering, the most important physical quantity is the energy of the system which is obtained via the measurements of various correlation functions. However, since a quantum field theory does not conserve particle numbers in general, the distinction between single-particle and multiparticle states becomes an important and delicate issue in lattice calculations. In the infinite volume, the difference is obvious since they have different kinematic behaviors: single-particle states have discrete energy eigenvalues when viewed in their rest frame while multiparticle states usually have continuous spectra starting from the corresponding threshold. However, when performing a lattice simulation in a finite volume, all energy eigenvalues in the finite box become discrete. Therefore, other means have to be applied in order to identify the particle nature of a corresponding state.

In principle, differences between single-particle and multiparticle states still persist in a finite volume. For example, although both have discrete spectra, the level spacing between neighboring multiparticle scattering states becomes infinitesimally small while the level spacing between the neighboring single-particle states remains finite as the volume goes to infinity. However, it is difficult to utilize this difference as a practical criteria since this requires the computation of excited energy eigenvalues in Monte Carlo simulations which is usually quite challenging. Another method suggested by various authors is to use the so-called spectral weight function as the identifier. This is the quantity which can be measured directly (and relatively easily) from Monte Carlo simulations, together with the corresponding energy eigenvalue. In a finite volume, the volume dependence of the spectral weight for a eigenstate is expected to show different behavior for single-particle and multiparticle states. For example, one expects the following empirical rule to hold: the spectral weight for a single-particle state (if properly normalized) should exhibit little volume dependence, while for a two-particle state, it is expected to show a $1/L^3$ dependence with L being the size of the cubic box. This expected difference in volume dependence can be measured in lattice simulations by performing the same calculation in two distinct volumes. As an example, this strategy has been used in Ref. [17] to study the possible penta-quark state. Using this technique, the authors concluded that the expected penta-quark (single-particle) states measured in their lattice calculations are in fact kaon-nucleon two-particle scattering states. However, this conclusion is not so settled even in the first-principle lattice QCD calculations [18–20]. Therefore, the volume dependence of the spectral weight indeed can provide us useful information on the particle nature of the corresponding state.

In a previous model study, we have shown that the above mentioned empirical rule to distinguish single-particle and multiparticle states are in fact only valid for stable particles and narrow resonances. Using a solvable model, the Lee model, we showed that this rule is violated for broad resonances [21]. A general formula for the spectral weight was obtained which can show either single- or two-particle volume behavior depending whether the width of the resonance is narrow or broad.

In this paper, we attempt to generalize this conclusion that we obtained in the Lee model, to the case of general massive quantum field theory. For this purpose, the general Lüscher's formalism is adopted. In previous studies, people have been focusing mainly on the energy eigenvalue (which directly enters the famous Lüscher's formula) of the system within Lüscher's formalism. However, since the spectral weight function $W(E, L)$ of a given state with energy E in a cubic box of size L is intimately related to the overlap of the exact energy eigenfunction with the free scattering states, we have to study the wave function of a energy eigenstate in a finite volume. In this paper, our study focuses on the wave function in the A_1^+ sector and a formula for the spectral weight is thus obtained within the nonrelativistic quantum mechanics model. By studying the volume dependence of the spectral weight in the large volume limit, we arrive at basically the same conclusion as we drew from the previous Lee model study. Then, following Lüscher's arguments, this result is generalized to massive quantum field theory. Our results also opens up a possibility of extracting the resonance parameters from the spectral weight function on various volumes.

This paper is organized as follows. In Sec. II, we briefly review the quantum-mechanical model in the infinite volume. In Sec. III, the quantum-mechanical model is studied on a three-dimensional torus of size L. In this section, we derive the relevant formulas for the spectral weight function and study its volume dependence. It is found that similar conclusion is reached as in our previous study using the Lee model. We then argue that, under the same restrictions as in Lüscher's formula, our results found in the quantum-mechanical model can be generalized to massive quantum field theory. The possibility of extracting resonance parameters from spectral weight is also discussed. In Sec. IV, we will conclude with some general remarks. Details on the evaluation of a function $F(k^2)$ are listed in the Appendix.

II. THE MODEL IN THE INFINITE VOLUME

Consider a quantum-mechanical model whose Hamiltonian is given by

$$H = -\frac{1}{2m}\nabla^2 + V(r), \tag{1}$$

where the potential $V(r)$ is zero for $r > a$ with some $a > 0$. We now discuss the energy eigenstates satisfying $H\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$. One can expand the eigenfunction in terms of spherical harmonics:

$$\Psi(\mathbf{r}) = \psi_{lm}(r)Y_{lm}(\mathbf{n}), \tag{2}$$

where $\mathbf{r} = r\mathbf{n}$ and $\psi_{lm}(r)$ is the radial wave function satisfying the radial Schrödinger equation,

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2 - 2mV(r)\right)\psi_{lm}(r) = 0, \tag{3}$$

and where $E = k^2/(2m)$ is the energy eigenvalue of the state. It is well known that, there exists only one solution to the radial Schrödinger equation that is bounded near the origin. This solution will be denoted as $u_l(r; k)$. To fix the normalization, we impose the condition

$$\lim_{r\to 0} r^{-l}u_l(r; k) = 1; \tag{4}$$

the solution to the radial Schrödinger equation then has the form

$$\psi_{lm}(r) = b_{lm}u_l(r; k), \tag{5}$$

with some constant b_{lm} to be fixed by other conditions (normalization, boundary conditions, etc.).

In the region $r > a$ where the interaction vanishes, the solution $u_l(r; k)$ is expanded in terms of spherical Bessel functions[1]:

$$u_l(r; k) = \alpha_l(k)j_l(kr) + \beta_l(k)n_l(kr). \tag{6}$$

The coefficients $\alpha_l(k)$ and $\beta_l(k)$ have a simple relation with the scattering phase shift:

$$e^{2i\delta_l(k)} = \frac{\alpha_l(k) + i\beta_l(k)}{\alpha_l(k) - i\beta_l(k)}, \qquad \tan\delta_l(k) = \frac{\beta_l(k)}{\alpha_l(k)}. \tag{7}$$

In the low-energy limit, $k \to 0$, one normally defines

$$\alpha_l^0 = \lim_{k\to 0} k^l\alpha_l(k), \qquad \beta_l^0 = \lim_{k\to 0} k^{-l-1}\beta_l(k), \tag{8}$$

and the threshold parameters[2]

$$a_l \equiv \frac{\beta_l^0}{\alpha_l^0}. \tag{9}$$

In particular, a_0 for $l = 0$ is referred to as the s-wave scattering length. Other a_l's for $l > 0$ are sometimes also called scattering lengths in the corresponding channel, although they do not have the dimension of a length.[3] The threshold parameters a_l are important because they characterize the behaviors in low-energy scattering processes. For example, we have

$$\delta_l(k) \simeq a_l k^{2l+1} + O(k^{2l+3}), \qquad (\mathrm{mod}\ \pi). \tag{10}$$

III. THE MODEL ON A TORUS

We now enclose the system we discussed in the previous section in a large cubic box and impose the periodic boundary condition in all three spatial directions. The potential itself is also modified to $V_L(\mathbf{r})$ by periodically extending over the whole space $V_L(\mathbf{r}) = \sum_{\mathbf{n}\in\mathbb{Z}^3} V(|\mathbf{r} + \mathbf{n}L|)$. For later convenience, we define the so-called "outer

[1] In this paper, we have adopted the same convention for spherical Bessel functions as in Ref. [4] which agrees with Messiah's book [22].

[2] Assuming $\alpha_l^0 \neq 0$ which is usually the case.

[3] From normalization condition (4), it is easy to verify that the spectral parameters a_l have the length dimension of $2l + 1$.

region'' as

$$\Omega = \{\mathbf{r}:|\mathbf{r} + \mathbf{n}L| > a, \quad \text{for all } \mathbf{n} \in \mathbb{Z}^3\}. \tag{11}$$

This is the region where the potential vanishes identically. We assume the size of the box is L which is much larger than any of the physical scales in the system. In particular, we need to have $L \gg 2a$ so that the outer region admits free spherical wave solutions (asymptotic states). We now would like to study the change in the energy eigenvalues, the corresponding wave functions, and their possible connections with the scattering phase shifts in the infinite volume. Our discussion here will focus on the case of a cubic box whose relevant symmetry group being the cubic group $O(\mathbb{Z})$. Generalization to an arbitrary rectangular box can be performed easily by changing the symmetry group to the corresponding ones (D_4 or D_2, etc.).

Since the boundary condition breaks rotational symmetry explicitly, we anticipate that energy eigenstates of the system will not have a definite angular momentum in general. To be specific, the original eigenstate in the s-wave will acquire mixtures from higher angular momentum modes (mainly $l = 4$ for a cubic box). However, since the original radial wave function $u_l(r; k)$ and the spherical harmonics forms a complete set in the functional space, we may still expand the true eigenfunction in the box in terms of them:

$$\Psi(\mathbf{r}; k) = \sum_{lm} b_{lm} u_l(r; k) Y_{lm}(\mathbf{n}), \tag{12}$$

where the coefficients are to be determined by boundary conditions and normalization.

In the outer region Ω, the solutions are those singular, periodic solutions for the Helmholtz equation. Thus we may write

$$\Psi(\mathbf{r}; k)|_{\mathbf{r}\in\Omega} = \sum_{lm} v_{lm} G_{lm}(\mathbf{r}; k^2). \tag{13}$$

In the meantime, the outer solution can also be expanded in terms of spherical harmonics and the spherical Bessel functions $j_l(kr)$ and $n_l(kr)$:

$$G_{lm}(\mathbf{r}; k^2) = \frac{(-)^l k^{l+1}}{4\pi}\Big[Y_{lm}(\Omega_{\mathbf{r}}) n_l(kr) + \sum_{l'm'} \mathcal{M}_{lm;l'm'} Y_{l'm'}(\Omega_{\mathbf{r}}) j_{l'}(kr)\Big]. \tag{14}$$

The explicit expression for $\mathcal{M}_{l'm';lm}(k_i^2)$ is given in Ref. [4] which we quote here:

$$\mathcal{M}_{lm;js}(k^2) = \sum_{l'm'} \frac{(-)^s i^{j-l} \mathcal{Z}_{l'm'}(1, q^2)}{\pi^{3/2} q^{l'+1}} \times \sqrt{(2l+1)(2l'+1)(2j+1)} \begin{pmatrix} l & l' & j \\ 0 & 0 & 0 \end{pmatrix} \times \begin{pmatrix} l & l' & j \\ m & m' & -s \end{pmatrix}. \tag{15}$$

Here we have used the Wigner's $3j$ symbols and $q = kL/(2\pi)$. The zeta function $\mathcal{Z}_{lm}(s, q^2)$ is defined as

$$\mathcal{Z}_{lm}(s, q^2) = \sum_{\mathbf{n}} \frac{\mathcal{Y}_{lm}(\mathbf{n})}{(\mathbf{n}^2 - q^2)^s}. \tag{16}$$

From the analytically continued formula, it is obvious from the symmetry of $O(\mathbb{Z})$ that, for $l \le 4$, the only nonvanishing zeta functions at $s = 1$ are $\mathcal{Z}_{00}$ and $\mathcal{Z}_{40}$. This is in accordance with the fact that s-wave and g-wave mix with each other in a cubic box. In what follows, we will focus on the s-wave eigenfunction.

A. Lüscher's formula in the A_1^+ sector revisited

In the remaining part of this paper, we will be only concerned with the energy eigenfunctions in the A_1^+ sector, which is the analogue of s-wave in a cubic box.

A good approximation for the s-wave dominated eigenfunction can be written as a superposition of $l = 0$ and $l = 4$ spherical harmonics with the s-wave component much larger than that of g-wave. To explicitly construct this type of wave functions, we notice that the eigenfunction in A_1^+ sector has to be invariant under cubic symmetries. It is easy to verify that; there are only two homogeneous harmonic polynomials which are invariant under cubic symmetry up to $l \le 4$. They can be conveniently expressed as

$$\mathcal{Y}_{00} = \frac{1}{\sqrt{4\pi}}, \qquad \mathcal{Y}_{40} + \frac{\sqrt{70}}{14}(\mathcal{Y}_{4,4} + \mathcal{Y}_{4,-4}) = \frac{15}{4\sqrt{\pi}}\Big(x^4 + y^4 + z^4 - \frac{3}{5} r^4\Big). \tag{17}$$

So, we may write the eigenfunction in A_1^+ sector as

$$\Psi^{(A_1^+)}(\mathbf{r}; k) = b_{00} u_0(r; k) Y_{00} + b_{40} u_4(r; k) \times \Big(Y_{40} + \frac{\sqrt{70}}{14}(Y_{4,4} + Y_{4,-4})\Big) + \cdots, \tag{18}$$

with $|b_{40}| \ll b_{00}$ in the large volume limit. In other words, to ensure cubic symmetry, the general coefficients b_{lm} at $l = 4$ with different m values must have definite ratios. In the outer region, using relation (6), we have

$$\Psi^{(A_1^+)}(\mathbf{r};k)|_{\mathbf{r}\in\Omega} = b_{00}[\alpha_0 j_0(kr) + \beta_0 n_0(kr)]Y_{00}(\Omega_{\mathbf{r}}) + b_{40}[\alpha_4 j_4(kr) + \beta_4 n_4(kr)] \times \left(Y_{40} + \frac{\sqrt{70}}{14}(Y_{4,4} + Y_{4,-4})\right) + \cdots. \tag{19}$$

On the other hand, we know that, in the outer region Ω, the eigenfunction can also be expanded into singular periodic solutions of Helmholtz equation. Since $G_{lm} \equiv \mathcal{Y}_{lm}(\nabla)G(\mathbf{r};k^2)$ with $G(\mathbf{r};k^2)$ being rotationally invariant, we see that in order to keep the eigenfunction invariant under cubic symmetry, we must have the combination $G_{40} + \sqrt{70}/14(G_{4,4} + G_{4,-4})$ in the expansion. Thus we may write[4]

$$\Psi^{(A_1^+)}(\mathbf{r};k)|_{r\in\Omega} = \left(\frac{4\pi}{k}\right)v_{00}\left[G_{00} + \frac{v_{40}}{k^4}\left(G_{40} + \frac{\sqrt{70}}{14} \times [G_{4,4} + G_{4,-4}]\right) + \cdots\right]. \tag{20}$$

The fact that such a combination respects cubic symmetry can also be checked explicitly. Using the expressions (14) and (15), we may write the expansion for G_{00} as

$$G_{00} = \frac{k}{4\pi}\left[(n_0 + m_{00}j_0)Y_{00} + \sqrt{\frac{7}{12}}m_{04}j_4 \times \left(Y_{40} + \frac{\sqrt{70}}{14}[Y_{44} + Y_{4,-4}]\right)\right], \tag{21}$$

where we have introduced $m_{00} = \mathcal{M}_{00;00}$ and $m_{04} = 2\sqrt{3/7}\mathcal{M}_{40;00}$ for later convenience (see Ref. [4] for the notation). Similarly, for the higher angular momentum functions, we have

$$\begin{aligned} G_{40} &= \frac{k^5}{4\pi}[n_4 Y_{40} + \mathcal{M}_{40;00}j_0 Y_{00} + \mathcal{M}_{40;20}j_2 Y_{20} + \mathcal{M}_{40;40}j_4 Y_{40} + \mathcal{M}_{40;44}j_4(Y_{44} + Y_{4,-4})], \\ G_{4,4} + G_{4,-4} &= \frac{k^5}{4\pi}[n_4(Y_{4,4} + Y_{4,-4}) + 2\mathcal{M}_{44;00}j_0 Y_{00} + 2\mathcal{M}_{44;20}j_2 Y_{20} + 2\mathcal{M}_{44;40}j_4 Y_{40} + (\mathcal{M}_{44;4,-4} + \mathcal{M}_{44;44})j_4(Y_{44} + Y_{4,-4})]. \end{aligned} \tag{22}$$

In the above expansions, we have also utilized the following properties of the matrix elements $\mathcal{M}_{lm;l'm'}$:

$$\mathcal{M}_{lm;l'm'} = \mathcal{M}_{l'm';lm} = \mathcal{M}_{l,-m;l',-m'}. \tag{23}$$

[4]For simplicity of the following equations, we have scaled out an overall factor $(4\pi/k)$ and an extra factor of $(1/k^4)$ for the coefficient of G_{40}.

Note that in the expansion of G_{40} and $G_{44} + G_{4,-4}$ in Eq. (22), there are terms with $l = 2$, $m = 0$ spherical harmonics. However, when we construct the combination $G_{40} + (\sqrt{70}/14)(G_{44} + G_{4,-4})$, the terms with $l = 2$ cancel out explicitly since $\mathcal{M}_{40;20} + (\sqrt{70}/7)\mathcal{M}_{44;20} = 0$ which can be checked by looking into Table E.1 in Ref. [4]. Therefore we finally have

$$G_{40} + \frac{\sqrt{70}}{14}(G_{44} + G_{4,-4}) = \frac{k^5}{4\pi}\left[\sqrt{\frac{12}{7}}m_{04}j_0 Y_{00} + (n_4 + m_{44}j_4) \times \left(Y_{40} + \frac{\sqrt{70}}{14}[Y_{44} + Y_{4,-4}]\right)\right], \tag{24}$$

where $m_{44} = \mathcal{M}_{40;40} + \cdots$. At this stage, it is worthwhile to point out that m_{00}, m_{04}, and m_{44} that we introduced here are exactly those reduced matrix elements of $\mathcal{M}$ in the A_1^+ sector. Please refer to Ref. [4] for further detailed explanations (especially Table E.1 and Table E.2 in the reference).

Collecting relevant information from the expansions obtained thus far, i.e. Eq. (20), (21), and (24), we have

$$\Psi^{(A_1^+)}(\mathbf{r};k)|_{r\in\Omega} = v_{00}\left[\left(n_0 + m_{00}j_0 + v_{40}\sqrt{\frac{12}{7}}m_{04}j_0\right)Y_{00} + \left(\left[\sqrt{\frac{7}{12}}m_{04} + v_{40}m_{44}\right]j_4 + v_{40}n_4\right) \times \left(Y_{40} + \frac{\sqrt{70}}{14}(Y_{4,4} + Y_{4,-4})\right)\right] + \cdots. \tag{25}$$

We should now match the two solutions given by Eq. (19) and (25) in the outer region Ω. This yields the following set of linear equations:

$$v_{00} = b_{00}\beta_0, \qquad v_{00}\left(m_{00} + \sqrt{\frac{12}{7}}v_{40}m_{04}\right) = b_{00}\alpha_0, \tag{26}$$

$$v_{00}v_{40} = b_{40}\beta_4, \qquad v_{00}\left(\sqrt{\frac{7}{12}}m_{04} + v_{40}m_{44}\right) = b_{40}\alpha_4. \tag{27}$$

These four equations can be viewed as a set of homogeneous linear equations for the four coefficients: v_{00}, b_{00}, $v_{00}v_{40}$, and b_{40}. Demanding a nontrivial solution to exist requires the corresponding determinant of the 4×4 matrix to vanish. Another simple way to proceed is to divide the second equation by the first and similarly divide the fourth one by the third. This will eliminate all coefficients except for v_{40}. We then arrive at

$$\cot\delta^{(0)} = m_{00} + \sqrt{\frac{12}{7}} v_{40} m_{04},$$
$$\cot\delta^{(4)} = m_{44} + \sqrt{\frac{7}{12}} m_{04}/v_{40}. \tag{28}$$

Eliminating v_{40} from the above two equations then yields

$$(\cot\delta^{(0)} - m_{00})(\cot\delta^{(4)} - m_{44}) = m_{04} m_{04}. \tag{29}$$

This is exactly the equation obtained by general Lüscher's method when we only consider the mixing between $l = 0$ and $l = 4$ waves [4]. Therefore, using more explicit construction, not only have we recovered Lüscher's formula, we also obtained an explicit approximate expression for the energy eigenfunction in the A_1^+ channel which is given by Eq. (18) in general and given by Eq. (20) in the outer region.

B. The spectral weight function and its normalization

Now we would like to derive a formula for the spectral weight function which can be measured in a Monte Carlo simulation. Instead of working with general states, we will focus on the single- and two-particle states. These states naturally arise in the lattice study of hadron-hadron scattering and hadron spectrum. In such simulations, one constructs an operator (also known as the interpolating field operator), or operators if more than one is needed, within a specific symmetry sector of the theory. The correlation matrix among these operators are then computed by ensemble averaging over different gauge field configurations that is generated in a Monte Carlo simulation.

For this purpose, we pass over to the second-quantized version of our quantum-mechanical scattering model. In this model, two distinguishable particles scatter via a potential $V(r)$ where r being the distance between them. The center-of-mass coordinate of the two-particle system is separated out and the mass parameter m in the Hamiltonian (1) refers to the reduced mass of the two-particle system. For each type of particle, a local scalar field operator $\pi_i(\mathbf{x}, t)$, with $i = 1, 2$ designating different types of particles, is introduced together with its momentum-space counterpart[5]:

$$\pi_i(\mathbf{x}, t) = \frac{1}{\sqrt{L^3}} \sum_{\mathbf{p}} \tilde{\pi}_i(\mathbf{p}, t) e^{i\mathbf{p}\cdot\mathbf{x}},$$
$$\tilde{\pi}_i(\mathbf{p}, t) = \frac{1}{\sqrt{L^3}} \int d^3\mathbf{x}\, \pi_i(\mathbf{x}, t) e^{-i\mathbf{p}\cdot\mathbf{x}}. \tag{30}$$

They satisfy the usual equal-time commutation relations: $[\pi_i(\mathbf{p}, t), \pi_j^\dagger(\mathbf{k}, t)] = \delta_{\mathbf{pk}}\delta_{ij}$. Using free states made up of two particles, one from each type, one can form a state:

$$|\Phi\rangle = \mathcal{O}^\dagger(0)|0\rangle = \frac{1}{L^{3/2}} \sum_{\mathbf{P}} \tilde{\Phi}(\mathbf{P}) \tilde{\pi}_1^\dagger(\mathbf{P}, 0) \tilde{\pi}_2^\dagger(-\mathbf{P}, 0)|0\rangle, \tag{31}$$

with the interpolating operator $\mathcal{O}(t)$ defined by

$$\mathcal{O}(t) = \frac{1}{\sqrt{L^3}} \sum_{\mathbf{P}} \tilde{\Phi}^*(\mathbf{P}) \tilde{\pi}_1(\mathbf{P}, t) \tilde{\pi}_2(-\mathbf{P}, t). \tag{32}$$

Requiring such a state to be normalized as $\langle\Phi|\Phi\rangle = 1$ yields the condition

$$\frac{1}{L^3} \sum_{\mathbf{P}} |\tilde{\Phi}(\mathbf{P})|^2 = 1. \tag{33}$$

If such a state were a bound state of two particles, $\tilde{\Phi}(\mathbf{P})$ would be the corresponding momentum-space wave function normalized according to the above equation.

We can now define the corresponding correlation function:

$$\mathcal{C}(t) = \langle 0|\mathcal{O}(t)\mathcal{O}^\dagger(0)|0\rangle = \sum_E |\langle E|\mathcal{O}^\dagger(0)|0\rangle|^2 e^{-Et}, \tag{34}$$

where E and $|E\rangle$ represents the eigenvalue and eigenstate of the full Hamiltonian, respectively. By fitting the time dependence of the correlation function obtained from Monte Carlo simulations, the exact eigenvalue E, and the corresponding spectral weight function $W(E)$, which is the coefficient in front of the exponential, is obtained. If we denote the overlap of two wave functions,

$$O(E) = \langle E|\mathcal{O}^\dagger(0)|0\rangle = \int d^3\mathbf{r}_1 d^3\mathbf{r}_2 \langle E|\mathbf{r}_1, \mathbf{r}_2\rangle\langle\mathbf{r}_1, \mathbf{r}_2|\mathcal{O}^\dagger(0)|0\rangle, \tag{35}$$

the spectral weight function is simply given by

$$W(E) = |\langle E|\mathcal{O}^\dagger(0)|0\rangle|^2 = |O(E)|^2. \tag{36}$$

At this point, it is worthwhile to point out that the spectral weight function $W(E)$ defined above depends explicitly on the normalization of $\mathcal{O}$.

Because of translational symmetry, the exact wave function $\langle\mathbf{r}_1, \mathbf{r}_2|E\rangle$ will only depend on the relative coordinate $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$. It is independent of the center-of-mass coordinate $\mathbf{r}_c$. This means that, if the eigenstate $|E\rangle$ is normalized according to $\langle E|E\rangle = 1$ as it should, the wave function $\langle\mathbf{r}_1, \mathbf{r}_2|E\rangle \equiv \langle\mathbf{r}|E\rangle$ should be normalized according to

$$\int_{\mathcal{T}_3} d^3\mathbf{r} |\langle\mathbf{r}|E\rangle|^2 = \int_{\mathcal{T}_3} d^3\mathbf{r} |\Psi^{(A_1^+)}(\mathbf{r}; k)|^2 = \frac{1}{L^3}. \tag{37}$$

Therefore, in order to compute the volume dependence of the spectral weight function, we first have to fix the normalization of $\Psi^{(A_1^+)}(\mathbf{r}; k)$ according to this convention.

C. Normalization of the energy eigenstates in A_1^+ sector

As discussed in the previous subsection, the wave function in the A_1^+ sector in Eq. (18) must be normalized

[5]For simplicity, we assume that the two particles are distinguishable.

properly on the torus $\mathcal{T}_3$ according to Eq. (37). The integral of the eigenfunction on the torus runs over two regions: the inner region, where the explicit form of the wave function is not known, and the outer region Ω, where an approximate form of the function is given by Eq. (20). Although we do not know the exact form of the eigenfunction in the inner region, we do know that the eigenfunction is bounded in this region. Since it is assumed that the interaction region is of size a with $a \ll L$, therefore the integral in the normalization condition (37) is dominated by the integral of the function in the outer region Ω. Therefore, we may modify the normalization condition to

$$\int_\Omega d^3\mathbf{r}|\Psi^{(A_1^+)}(\mathbf{r};k)|^2 \simeq \frac{1}{L^3}. \tag{38}$$

Since in the large volume limit, the eigenfunction is dominated by the s-wave contribution, we may use the first term in Eq. (20) and write

$$\left(\frac{4\pi}{k}\right)^2|v_{00}|^2\left(\int_{\mathcal{T}_3} d^3\mathbf{r}|G_{00}(\mathbf{r};k)|^2 - \int_B d^3\mathbf{r}|G_{00}(\mathbf{r};k)|^2\right) \simeq \frac{1}{L^3}, \tag{39}$$

where the second integral is over the interaction ball region, $B = \{\mathbf{r}: r \le a, \mathrm{mod}\, L\}$. We now use the definition for G_{00}:

$$G_{00}(\mathbf{r};k) = \frac{1}{\sqrt{4\pi}L^3}\sum_{\mathbf{p}}\frac{e^{i\mathbf{p}\cdot\mathbf{r}}}{\mathbf{p}^2 - k^2}, \tag{40}$$

where the summation of $\mathbf{p} = (2\pi/L)\mathbf{n}$ is for all three-dimensional integers $\mathbf{n} \in \mathbb{Z}^3$. Substituting this expression into the first term and Eq. (25) into the second integral in Eq. (39) we get

$$\frac{k^2}{16\pi^2|v_{00}|^2L^3} \simeq \frac{1}{4\pi L^3}\sum_{\mathbf{p}}\frac{1}{(\mathbf{p}^2 - k^2)^2} - \frac{k^2}{16\pi^2} \times \int_0^a r^2 dr(n_0(kr) + m_{00}j_0(kr))^2. \tag{41}$$

The integral in the second term maybe evaluated directly within $r < a$. We thus obtain

$$\frac{1}{|v_{00}|^2L^3} \simeq \frac{4\pi}{k^2L^3}\sum_{\mathbf{p}}\frac{1}{(\mathbf{p}^2 - k^2)^2} - \frac{a}{2k^2\sin^2\Delta} \times \left[1 - \left(\frac{\sin ka}{ka}\right)\cos(ka + 2\Delta)\right], \tag{42}$$

where we have utilized the definition $m_{00} = \cot\Delta$. In the large volume limit, the first term on the right-hand side of the above equation is much larger than the second (see the Appendix for the explanation of this assertion). If we drop the second term, we then arrive at

$$\left(\frac{4\pi}{k}\right)^2|v_{00}|^2L^3 \simeq 4\pi\left(\frac{1}{L^3}\sum_{\mathbf{p}}\frac{1}{(\mathbf{p}^2 - k^2)^2}\right)^{-1} \equiv \frac{4\pi}{F'(k^2)}, \tag{43}$$

where we have defined the function

$$F(k^2) = \frac{1}{L^3}\sum_{\mathbf{p}}\frac{f(\mathbf{p}^2)}{\mathbf{p}^2 - k^2}, \tag{44}$$

where we have introduced a cutoff function $f(\mathbf{p}^2)$ to regulate possible ultraviolet divergences. The property of this function in the large volume limit is addressed in the Appendix. The relevant formula for us is given by Eq. (A10).

D. Spectral weight in A_1^+ sector

We now evaluate the spectral weight using Eq. (36) with the exact energy eigenfunction given approximately by $\Psi^{(A_1^+)}(\mathbf{r};k) \simeq (4\pi/k)v_{00}G_{00}(\mathbf{r};k)$. The overlap of the two wave function is approximately given by

$$O = \left(\frac{4\pi}{k}\right)v_{00}^*\frac{1}{\sqrt{4\pi L^3}}\sum_{\mathbf{P}}\frac{\tilde{\Phi}(\mathbf{P})}{\mathbf{P}^2 - k^2}. \tag{45}$$

Using the expression (43) and the expression in Eq. (A10), we finally obtain $W(E) = |O|^2$ as

$$W(E) = \frac{8\pi k|\varphi_L(k^2)|^2}{\cot\delta_0(k) + \frac{2\pi k^2}{\Delta\mathbf{p}^2}\csc^2\delta_0(k)} = \frac{8\pi k|\varphi_L(k^2)|^2}{\cot\delta_0(k) + \frac{2\pi E}{\Delta E}\csc^2\delta_0(k)}, \tag{46}$$

where the function $\varphi_L(k^2)$ is defined as

$$\varphi_L(k^2) = \frac{1}{L^3}\sum_{\mathbf{P}}\frac{\tilde{\Phi}(\mathbf{P})}{\mathbf{P}^2 - k^2}. \tag{47}$$

In the large volume limit, following similar derivation as in our discussion of function $F(k^2)$, this function goes over to

$$\varphi_\infty(k^2) = \mathcal{P}\int\frac{d^3\mathbf{p}}{(2\pi)^3}\frac{\tilde{\Phi}(\mathbf{p})}{\mathbf{p}^2 - k^2} + \frac{k\tilde{\Phi}(k^2)}{4\pi}\cot\delta_0(k). \tag{48}$$

Thus the function $\varphi_L(k^2)$ has little volume dependence in the large volume limit. Therefore, the explicit volume dependence of the spectral weight function $W(E)$ comes mainly from the denominator in Eq. (46). Normally, if $\cot\delta_0(k)$ is not changing rapidly, the second term in the denominator of Eq. (46), which is proportional to L^3, dominates the result and one finds that the spectral weight is proportional to $1/L^3$. This is the typical two-particle spectral weight function.

In particular, if there exists a resonance at energy $E = E_\star$, then close to this resonance energy region, one has approximately

$$\cot\delta(E) \simeq \frac{E_\star - E}{\Gamma/2}, \tag{49}$$

where Γ is the physical width of the resonance. In this case, we obtain

$$W(E) \simeq \frac{8\pi k_\star |\varphi_\infty(k_\star^2)|^2}{(\frac{E_\star - E}{\Gamma/2}) + (\frac{2\pi E}{\Delta E})[1 + (\frac{E_\star - E}{\Gamma/2})^2]}. \tag{50}$$

Note that the numerator of the above expression does not depend on the volume of the box. The first term in the denominator also does not depend on the volume explicitly.[6] Therefore, only the second term in the denominator depends on the volume of the box in an explicit manner via the quantity ΔE. For large enough volume, as long as Γ remains finite, we have $\Gamma \gg \Delta E$ and the quantity in the denominator is dominated by the second term and the spectral weight itself is roughly proportional to $1/L^3$ which is typical for a two-particle scattering state.

The case for an extremely narrow resonance needs to be considered differently. The reason for this is that, in the derivations so far that lead to Eq. (50), we have implicitly assumed that *all functions*, e.g, $\tilde{\Phi}(\mathbf{P})$ etc., are smooth functions on the scale of ΔE. This allows us to approximate the summations by a principle integral part and an analytically computable series (see the derivations in the Appendix). However, for an extremely narrow resonance for which $\Gamma \ll \Delta E$, this assumption becomes invalid. For example, the two-particle operators that overlap with the narrow resonance substantially will have a wave function $\tilde{\Phi}(\mathbf{P})$ that changes rapidly around the resonance energy $E_\star$. In fact, if we take a simple Breit-Wigner form, the wave function will change substantially within the energy range $[E_\star - \Gamma/2, E_\star + \Gamma/2]$. Since in this case $\Gamma \ll \Delta E$, this wave function does not satisfy our assumption that it is smooth over a range of ΔE and thus the derivation given above cannot apply to such a case. In real lattice calculations, such a scenario basically indicates that the volume is not large enough and the narrow resonance simply cannot decay and it behaves more like a single stable particle. For example, for simulations in which $2m_\pi < m_\rho$ but the energy for the pion pair with nonvanishing momenta are larger than mass of the ρ due to the smallness of the volume, the ρ meson in this case effectively cannot decay into pion pairs and a single-particle description of it remains a good approximation. However, as we pointed out already, as long as the volume is large enough (and the mass parameters are such that the decay can occur in infinite volume), any resonance with a finite width will mix with multiparticle final states (the decay products) and its spectral weight function will eventually show a multiparticle behavior.

[6]The exact energy eigenvalue E depends on the volume slightly which is usually called the finite volume correction for that state in lattice simulations.

E. Generalization to massive quantum field theory

Our results on the volume dependence of the spectral weight is obtained within a quantum-mechanical model. In this subsection, we would like to generalize these results to massive quantum field theory, following the line of arguments in Lüscher's formalism [5]. Using an effective Schrödinger equation (derived from the Bethe-Salpeter equation) [2], Lüscher has argued that, if the size of the box is large enough such that all quantum field theory effects are suppressed exponentially, the results obtained within the quantum-mechanical model can be carried over to the case of massive quantum field theory literally [2,5]. Here, we will assume that the same conditions are satisfied and thus our results obtained within the quantum-mechanical model are expected to be valid for massive quantum field theory.

F. Possibility of extracting the resonance parameters from the spectral weight

The relation established in Eq. (50) opens up a possibility for extracting the width of a resonance if the spectral weight can be measured in the simulation. Assuming that there exists a single resonance in the energy region that we are interested in, and the contribution from this single resonance dominates the scattering. Thus, by fitting the function $W(E, L)$[7] for different E and L (hence different ΔE as well), it is possible to extract the width parameter Γ together with the resonance position $E_\star$ of the resonance. Note that in previous lattice calculations, focus has been mainly put on the energy levels, i.e. the values of E, only. No attention is paid to the associated spectral weight function $W(E, L)$ which in fact can be obtained from the fitting procedure of the corresponding correlation functions *with almost no extra costs*. The study in this paper indicates that, the spectral weight function at various volumes also contains valuable information about the scattering and might also be utilized in some way. In fact, it can be used as an cross-check for the scattering phase obtained from the energy levels. Of course, this is only a possibility at this stage. The feasibility of this method has to be check in realistic simulations.

IV. CONCLUSIONS

In this paper, we have studied the volume dependence of the spectral weight function which is accessible in Monte Carlo lattice simulations. Motivated by our previous study in the Lee model, Lüscher's formalism is adopted. It is first studied in a quantum-mechanical model and then generalized to massive quantum field theories, assuming that the polarization effects are exponentially suppressed

[7]To emphasize its dependence on the box size L, we have used $W(E, L)$ to denote the spectral weight function $W(E)$ given in Eq. (50).

following Lüscher's arguments. It is shown that, for a resonance of definite width, the spectral weight function will exhibit typical two-particle volume dependence, i.e. a $1/L^3$ dependence, as long as the volume is large enough. In particular, we expect this scenario to be true also for QCD which governs the scattering of hadrons and therefore our result is relevant for lattice QCD simulations. Possibilities of using the spectral weight function to extract the resonance parameters is also discussed.

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APPENDIX: THE FUNCTION $F(k^2)$

To study the normalization of the wave function $\Psi^{(A_1^+)}(\mathbf{r}; k)$ in the large volume limit, we define the function:

$$F(k^2) = \frac{1}{L^3}\sum_{\mathbf{p}} \frac{f(\mathbf{p}^2)}{\mathbf{p}^2 - k^2}, \tag{A1}$$

where we have introduced a cutoff function $f(\mathbf{p}^2)$. The relevant function appearing in the normalization condition (43) is given by the derivative of $F(k^2)$ with respect to k^2:

$$F'(k^2) = \frac{1}{L^3}\sum_{\mathbf{p}} \frac{f(\mathbf{p}^2)}{(\mathbf{p}^2 - k^2)^2}. \tag{A2}$$

We now follow the argument in Ref. [21] to estimate the value of $F(k^2)$ for arbitrary value of k^2 in the large L limit. We separate the summation into two parts with $|\mathbf{p}^2 - k^2| \geq \epsilon$ and $|\mathbf{p}^2 - k^2| < \epsilon$. The first part goes smoothly to the principle-valued integral $\phi(k^2)$ while the second summation may be written as

$$\begin{aligned}\frac{1}{L^3}\sum_{\mathbf{p},|\mathbf{p}^2-k^2|<\epsilon} \frac{1}{\mathbf{p}^2 - k^2} &= \frac{1}{L^3}\sum_{n=-\infty}^{\infty} \frac{1}{\mathbf{p}_\star^2 + n\Delta\mathbf{p}^2 - k^2} \\ &= -\frac{\pi}{L^3\Delta\mathbf{p}^2}\cot\left[\pi\left(\frac{k^2 - \mathbf{p}_\star^2}{\Delta\mathbf{p}^2}\right)\right],\end{aligned} \tag{A3}$$

where $\mathbf{p}_\star^2$ is the value of $\mathbf{p}^2$ that is closest to k^2; $\Delta\mathbf{p}^2$ is the typical level spacing between neighboring $\mathbf{p}^2$ values which can be estimated by

$$\frac{L^3}{(2\pi)^3} 2\pi\sqrt{\mathbf{p}^2}\Delta\mathbf{p}^2 = 1 \mapsto L^3\Delta\mathbf{p}^2 = \frac{(2\pi)^2}{\sqrt{\mathbf{p}^2}}. \tag{A4}$$

Therefore we obtain

$$F(k^2) = \phi(k^2) - \frac{k}{4\pi}\cot\left[\pi\left(\frac{k^2 - \mathbf{p}_\star^2}{\Delta\mathbf{p}^2}\right)\right]. \tag{A5}$$

However, since it is easy to verify that

$$F(k^2) = \frac{\mathcal{Z}_{00}(1; q^2)}{2\pi^{3/2}L} \simeq \frac{k}{4\pi}\cot\delta_0(k), \tag{A6}$$

where we have utilized the approximate relation (Lüscher's formula)

$$\cot\delta_0(k) = \frac{\mathcal{Z}_{00}(1; q^2)}{\pi^{3/2}q}. \tag{A7}$$

We therefore seem to have $\phi(k^2) = 0$ in which case we recover the DeWitt's formula

$$\delta_0(k) = -\pi\left(\frac{k^2 - \mathbf{p}_\star^2}{\Delta\mathbf{p}^2}\right). \tag{A8}$$

If one evaluates $\phi(k^2)$ explicitly, one gets

$$\phi(k^2) = \mathcal{P}\int \frac{d^3\mathbf{p}}{(2\pi)^3}\frac{1}{\mathbf{p}^2 - k^2} = 4\pi\Lambda + 2\pi k\ln\left|\frac{\Lambda - k}{\Lambda + k}\right|, \tag{A9}$$

with a sharp momentum cutoff Λ. This expression indeed goes to zero if we drop the constant term and taking $\Lambda \to \infty$. Consequently we have for the function $F'(k^2)$,

$$\begin{aligned}F'(k^2) &= -\frac{1}{8\pi k}\cot\left[\pi\left(\frac{k^2 - \mathbf{p}_\star^2}{\Delta\mathbf{p}^2}\right)\right] \\ &\quad + \frac{k}{4\Delta\mathbf{p}^2}\csc^2\left[\pi\left(\frac{k^2 - \mathbf{p}_\star^2}{\Delta\mathbf{p}^2}\right)\right] \\ &= \frac{1}{8\pi k}\cot\delta_0(k) + \frac{k}{4\Delta\mathbf{p}^2}\csc^2\delta_0(k),\end{aligned} \tag{A10}$$

where in the second line we have used DeWitt's formula. Since $\Delta\mathbf{p}^2 \propto L^{-3}$, we find that $F'(k^2) \propto L^3$ in the large volume limit. This justifies the assertion made after Eq. (42) in the main text.

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