A general study on the volume dependence of spectral weights in lattice field theory

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Abstract

It has been suggested that the volume dependence of the spectral weight could be utilized to distinguish single and multi-particle states in Monte Carlo simulations. In a recent study using a solvable model, the Lee model, we found that this criteria is applicable only for stable particles and narrow resonances, not for the broad resonances. In this paper, the same question is addressed within the finite size formalism outlined by Lüscher. Using a quantum mechanical scattering model, the conclusion that was found in previous Lee model study is recovered. Then, following similar arguments as in Lüscher’s, it is argued that the result is valid for a general massive quantum field theory under the same conditions as the Lüscher’s formulae. Using the spectral weight function, a possibility of extracting resonance parameters is also pointed out.

Key words: Spectral weight, finite-size technique, lattice QCD.
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1 Introduction

Low-energy hadron-hadron scattering plays an important role in the understanding of non-perturbative physics of strong interaction. Due to its genuine non-perturbative nature, such problems can only be studied from first principles using non-perturbative methods like lattice QCD. Lüscher has outlined a finite-size formalism which enables us to calculate the elastic scattering phase

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shifts using lattice simulations \cite{12,345}. 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 \cite{6,7,8,9,10,11,12,13,14,15,16}.

In lattice study 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- and multi-particle 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 multi-particle states usually have continuous spectrum 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- and multi-particle states still persist in a finite volume. For example, although both have discrete spectra, the level spacing between neighboring multi-particle 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 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- and multi-particle states. For example, one expects the following empirical rule: the spectral weight to show little volume dependence for a single particle state (if properly normalized), while for a two-particle state, it is expected to show a $1/L^3$ dependence where $L$ 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. \cite{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 \cite{18,19,20}. Therefore, the volume dependence of the spectral weight indeed can provide us useful information about the particle nature of the corresponding state.
In a previous model study, we have shown that the above mentioned empirical rule to distinguish single- and multi-particle 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 \cite{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 $W(E, L)$ of a given state is intimately related to the overlap of the exact energy eigenfunction with the free scattering states, we have to study the wavefunction of a energy eigenstate in a finite volume. In this paper, our study focuses on the wavefunction in the $A_1^+$ sector and a formula for the spectral weight is thus obtained within the non-relativistic quantum mechanics model. By studying the volume dependence of the spectral weight in the large volume limit, we arrive at 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 show a possibility of extracting the resonance parameters from the spectral weight function on various volumes.

This paper is organized as follows. In Sec. 2 we briefly review the quantum-mechanical model in the infinite volume. In Sec. 3 the quantum-mechanical model is studied on a three-dimensional torus of size $L$. In this section, we derive the relevant formulae 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. 4 we will conclude with some general remarks. Details on the evaluation of a function $F(k^2)$ are listed in the appendix.

2 The Model in the Infinite Volume

Consider a quantum mechanical model whose Hamiltonian is given by:

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

(1)
where the potential $V(r)$ is zero for $r > a$ with some $a > 0$. We now discuss the energy eigenstates satisfying: $H\Psi(r) = E\Psi(r)$. One can expand the eigenfunction in terms spherical harmonics:

$$\Psi(r) = \psi_{lm}(r)Y_{lm}(\mathbf{n}) .$$  \hfill (2)

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

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

where $E = k^2/(2m)$ being the energy eigenvalue of the state. It is well-known that, there exist 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:

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

and the solution to the radial Schrödinger equation then has the form:

$$\psi_{lm}(r) = b_{lm}u_l(r; k) ,$$  \hfill (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 $u_l(r; k)$ are expanded in terms of spherical Bessel functions:

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

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

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

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

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

\footnote{In this paper, we have adopted the same convention as in Ref. \cite{4}, which agrees with Messiah’s book \cite{22}.}
and the threshold parameters:

\[ a_l \equiv \frac{\beta_l^0}{\alpha_l^0}. \]  

(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. The threshold parameters \( a_l \) are important because they characterize the behaviors in low-energy scattering processes. For example, we have:

\[ \delta_l(k) \simeq a_l k^{2l+1} + O(k^{2l+3}) , \quad (\text{mod } \pi) . \]  

(10)

3 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 \( V_L(r) \) by periodically extending over the whole space: \( V_L(r) = \sum_{n \in \mathbb{Z}^3} V(|r + nL|) \). For later convenience, we define the so-called “outer region” as:

\[ \Omega = \{ r : |r + nL| > a , \text{ for all } n \in \mathbb{Z}^3 \} . \]  

(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 scale 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

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3 Assuming \( \alpha_l^0 \neq 0 \) which is usually the case.

4 From normalization condition \( [\alpha_l^0] \); it is easy to verify that the spectral parameters \( a_l \) has the length dimension of \( 2l + 1 \).
spherical harmonics forms a complete set in the functional space, we may still expand the true eigenfunction in the box in terms of them:

$$\Psi(r; k) = \sum_{lm} b_{lm} u_l(r; k) Y_{lm}(n).$$  \hfill (12)

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

In the outer region $\Omega$, the solution are those singular, periodic solutions for the Helmholtz equation. Thus we may write:

$$\Psi(r; k)|_{r \in \Omega} = \sum_{lm} v_{lm} G_{lm}(r; k^2).$$ \hfill (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 $n_l(kr)$:

$$G_{lm}(r; k^2) = \frac{(-)^{l} k^{l+1}}{4\pi} \left[ Y_{lm}(\Omega r)n_l(kr) + \sum_{l'm'} M_{lm;l'm'} Y_{l'm'}(\Omega r)j_{l'}(kr) \right],$$ \hfill (14)

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

$$M_{lm;l'm'}(k^2) = \sum_{l''m''} \frac{(-)^{s} q^{s-l+l'} Z_{l'm'}(1, q^2)}{\pi^{3/2} q^{l'+1}} \sqrt{(2l + 1)(2l' + 1)(2j + 1)} \times \left( \begin{array}{ccc} l & l' & j \\ 0 & 0 & 0 \\ m & m' & -s \end{array} \right).$$ \hfill (15)

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

$$Z_{lm}(s, q^2) = \sum_{n} \frac{Y_{lm}(n)}{(n^2 - q^2)^s}. \hfill (16)$$

From the analytically continued formula, it is obvious from the symmetry of $O(\mathbb{Z})$ that, for $l \leq 4$, the only non-vanishing zeta functions at $s = 1$ are: $Z_{00}$, and $Z_{40}$. This is in accordance with the fact that $s$-wave and $g$-wave mixes with each other in a cubic box. In what follows, we will focus on the $s$-wave eigenfunction.
3.1 Lüscher’s formula in the $A_1^+$ sector revisited

In the remaining part of this paper, we will be only concerned with the energy eigen-functions 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 eigen-function 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 $l \leq 4$. They can be conveniently expressed as:

$$Y_{00} = \frac{1}{\sqrt{4\pi}}, \quad Y_{40} + \frac{\sqrt{70}}{14} (Y_{4,4} + Y_{4,-4}) = \frac{15}{4\sqrt{\pi}} \left( x^4 + y^4 + z^4 - \frac{3}{5} r^4 \right).$$

(17)

So, we may write the eigen-function in $A_1^+$ sector as:

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

(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:

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

(19)

On the other hand, we know that, in the outer region $\Omega$, the eigen-function can also be expanded into singular periodic solutions of Helmholtz equation. Since $G_{lm} = \nabla_l G(r; k^2)$ with $G(r; k^2)$ being rotationally invariant, we see that in order to keep the eigen-function 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:

$$\Psi^{(A_1^+)}(r; k)|_{r \in \Omega} = \left( \frac{4\pi}{k} \right)^5 v_{00} \left[ G_{00} + \frac{v_{40}}{k^4} \left( G_{40} + \frac{\sqrt{70}}{14} (G_{4,4} + G_{4,-4}) \right) + \cdots \right].$$

(20)

\footnote{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 $G_{40}$.}
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:

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

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

$$G_{40} = \frac{k^5}{4\pi} \left[ n_4 Y_{40} + M_{40;00} j_0 Y_{00} + M_{40;20} j_2 Y_{20} + M_{40;44} j_4 (Y_{44} + Y_{4,-4}) \right],$$

$$G_{4,4} + G_{4,-4} = \frac{k^5}{4\pi} \left[ n_4 (Y_{4,4} + Y_{4,-4}) + 2M_{44;00} j_0 Y_{00} + 2M_{44;20} j_2 Y_{20} + 2M_{44;44} j_4 + (M_{44;44} + M_{44;44}) j_4 (Y_{44} + Y_{4,-4}) \right], \quad (22)$$

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

$$M_{lm;l'm'} = M_{l'm';lm} = M_{l,-m;l',-m'}. \quad (23)$$

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

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

where $m_{44} = M_{40;44} + \cdots$. 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), Eq. (21) and Eq. (24), we have:
\[ \Psi^{(A^+_1)}(r; k)|_{r \in \Omega} = v_{00} \left( n_0 + m_{00} j_0 + v_{40} \sqrt{\frac{12}{7}} m_{04} j_0 \right) Y_{00} 
\]
\[ + \left( \left[ \sqrt{\frac{7}{12}} m_{04} + v_{40} m_{44} \right] j_4 + v_{40} n_4 \right) \left( Y_{40} + \frac{\sqrt{70}}{14} (Y_{4,4} + Y_{4,-4}) \right) \] + \]  

(25)

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

\[ v_{00} = b_{00} \beta_0 , \quad v_{00} \left( m_{00} + \sqrt{\frac{12}{7}} v_{40} m_{04} \right) = b_{00} \alpha_0 , \]  
\[ (26) \]

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

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 non-trivial solution to exist requires the corresponding determinant of the \( 4 \times 4 \) 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:

\[ \cot \delta^{(0)} = m_{00} + \sqrt{\frac{12}{7}} v_{40} m_{04} , \quad \cot \delta^{(4)} = m_{44} + \frac{\sqrt{70}}{14} m_{04}/v_{40} . \]  
\[ (28) \]

Eliminating \( v_{40} \) from the above two equations then yields:

\[ \left( \cot \delta^{(0)} - m_{00} \right) \left( \cot \delta^{(4)} - m_{44} \right) = m_{04} m_{04} . \]  
\[ (29) \]

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 eigen-function in the \( A^+_1 \) channel which is given by Eq. (18) in general and given by Eq. (20) in the outer region.

### 3.2 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 \( \pi_i(x,t) \), with \( i = 1, 2 \) designating different types of particles, is introduced together with its momentum space counterpart:

\[
\pi_i(x,t) = \frac{1}{\sqrt{L^3}} \sum_p \tilde{\pi}_i(p,t)e^{ip\cdot x}, \quad \tilde{\pi}_i(p,t) = \frac{1}{\sqrt{L^3}} \int d^3x \pi_i(x,t)e^{-ip\cdot x} \quad (30)
\]

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

\[
|\Phi\rangle = \mathcal{O}^\dagger(0)|0\rangle = \frac{1}{L^{3/2}} \sum_P \tilde{\Phi}(P)\tilde{\pi}_1^\dagger(P,0)\tilde{\pi}_2^\dagger(-P,0)|0\rangle, \quad (31)
\]

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

\[
\mathcal{O}(t) = \frac{1}{\sqrt{L^3}} \sum_P \tilde{\Phi}^* (P)\tilde{\pi}_1(P,t)\tilde{\pi}_2(-P,t). \quad (32)
\]

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

\[
\frac{1}{L^3} \sum_P |\tilde{\Phi}(P)|^2 = 1. \quad (33)
\]

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

We can now define the corresponding correlation function:

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

\footnote{For simplicity, we assume that the two particles are distinguishable.}
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 wavefunctions:

$$O(E) = \langle E|\mathcal{O}^\dagger(0)|0\rangle = \int d^3r_1 d^3r_2 \langle E|r_1, r_2\rangle \langle r_1, r_2|\mathcal{O}^\dagger(0)|0\rangle,$$

the spectral weight function is simply given by:

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

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

Due to translational symmetry, the exact wave-function $\langle r_1, r_2|E\rangle$ will only depend on the relative coordinate $r = r_2 - r_1$. It is independent of the center-of-mass coordinate $r_c$. This means that, if the eigenstate $|E\rangle$ is normalized according to $\langle E|E\rangle = 1$ as it should, the wave-function $\langle r_1, r_2|E\rangle \equiv \langle r|E\rangle$ should be normalized according to:

$$\int_{T^3} d^3r \langle r|E\rangle|^2 = \int_{T^3} d^3r |\Psi^{(A^+_1)}(r; k)|^2 = \frac{1}{L^3}.$$  

Therefore, in order to compute the volume dependence of the spectral weight function, we first have to fix the normalization of $\Psi^{(A^+_1)}(r; k)$ according to this convention.

### 3.3 Normalization of the energy eigenstates in $A^+_1$ sector

As discussed in the previous subsection, the wavefunction in the $A^+_1$ sector in Eq. \ref{eq:wavefunction} must be normalized properly on the torus $T_3$ according to Eq. \ref{eq:37}. The integral of the eigen-function on the torus runs over two regions: the inner region where the explicit form of the wavefunction is not known and the outer region $\Omega$ where an approximate form of the function is given by Eq. \ref{eq:20}. Although we do not know the exact form of the eigen-function 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 \ref{eq:37} is dominated by the integral of the function in the outer region $\Omega$. Therefore, we may modify the normalization
condition to:

\[ \int_\Omega d^3 r |\Psi(\hat{A}^1_r)(r; k)|^2 \simeq \frac{1}{L^3}. \] (38)

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

\[ \left( \frac{4\pi}{k} \right)^2 |v_{00}|^2 \left( \int \int d^3 r |G_{00}(r; k)|^2 - \int_{B} d^3 r |G_{00}(r; k)|^2 \right) \simeq \frac{1}{L^3}, \] (39)

where the second integral is over the interaction ball region: \( B = \{ r : r \leq a, \text{mod} L \} \). We now use the definition for \( G_{00} \):

\[ G_{00}(r; k) = \frac{1}{\sqrt{4\pi L^3}} \sum_p \frac{e^{ip \cdot r}}{p^2 - k^2}, \] (40)

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

\[ \frac{k^2}{16\pi^2 |v_{00}|^2 L^3} \simeq \frac{1}{4\pi L^3} \sum_p \frac{1}{(p^2 - k^2)^2} - \frac{k^2}{16\pi^2} \int_0^a r^2 dr \left( n_0(kr) + m_{00}j_0(kr) \right)^2, \] (41)

The integral in the second term maybe evaluated directly within \( r < a \). We thus obtain:

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

where we have utilized the definition: \( m_{00} = \cot \Delta \). In the large volume limit, the first term on the r.h.s. of the above equation is much larger than the second (see appendix [A] for the explanation of this assertion). If we drop the second term, we then arrive at:

\[ \left( \frac{4\pi}{k} \right)^2 |v_{00}|^2 L^3 \simeq 4\pi \left( \frac{1}{L^3} \sum_p \frac{1}{(p^2 - k^2)^2} \right)^{-1} \equiv \frac{4\pi}{F'(k^2)}, \] (43)

where we have defined the function:

\[ F(k^2) = \frac{1}{L^3} \sum_p \frac{f(p^2)}{p^2 - k^2}, \] (44)
where we have introduced a cutoff function $f(p^2)$ to regulate possible ultraviolet divergences. The property of this function in the large volume limit is addressed in appendix A. The relevant formula for us is given by Eq. (A.10).

3.4 Spectral weight in $A_1^+$ sector

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

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

Using the expression (43) and the expression in Eq. (A.10), we finally obtain $W(E) = |O|^2$ as:

$$W(E) = \frac{8\pi k|\varphi_L(k^2)|^2}{\cot \delta_0(k) + \frac{2\pi k^2}{\Delta E} \csc^2 \delta_0(k)} = \frac{8\pi k|\varphi_L(k^2)|^2}{\cot \delta_0(k) + \frac{2\pi E}{\Delta E} \csc^2 \delta_0(k)},$$  \hspace{1cm} (46)

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

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

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

$$\varphi_{\infty}(k^2) = \mathcal{P} \int \frac{d^3p}{(2\pi)^3} \frac{\tilde{\Phi}(p)}{p^2 - k^2} + \frac{k\tilde{\Phi}(k^2)}{4\pi} \cot \delta_0(k).$$  \hspace{1cm} (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. However, if there exists a rather narrow resonance at energy $E = E_\star$, then close to this resonance energy, one has approximately:

$$\cot \delta(E) \simeq \frac{E_\star - E}{\Gamma/2},$$  \hspace{1cm} (49)
where \( \Gamma \) is the physical width of the resonance. In this case, we obtain:

\[
W(E) \simeq \frac{4\pi k_s \Gamma|\varphi(k^2_s)|^2}{(E^* - E) + \pi E^* \frac{E^*}{\Delta E}}.
\] (50)

If \( \Gamma/\Delta E \ll 1 \), then the quantity in the denominator is dominated by the first term and the spectral weight shows a typical single-particle behavior. This means that an extremely narrow resonance behaves like a stable particle. If on the other hand \( \Gamma/\Delta E \gg 1 \), which is always true for an extremely large volume (assuming the width of the resonance remains finite), 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. We therefore arrive at the conclusion that the volume dependence of the spectral weight near a resonance is controlled by the ratio \( \Gamma/\Delta E \).

### 3.5 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 [3]. Using an effective Schrödinger equation (derived from the Bethe-Salpeper 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.

### 3.6 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, we simply rewrite Eq. (50) as:

\[
\frac{1}{W(E, L)} \simeq \frac{1}{4\pi k_s |\varphi(k^2_s)|^2} \left( \frac{E^* - E}{\Gamma} + \frac{\pi E^*}{\Delta E} \right).
\] (51)
Therefore, by fitting the function $1/W(E, L)$ for different $E$ and $L$ (hence different $\Delta E$ as well), it is possible to extract the width parameter $\Gamma$ together with the resonance position $E_*$ 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.

4 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, it is expected that the spectral weight function shows little volume dependence for a stable or narrow resonance while for a broad resonance, it exhibits a typical $1/L^3$ dependence, the same as a two-particle scattering state. To verify this scenario, Lüscher’s formalism is adopted. It is first shown in a quantum mechanical model and then generalized to any massive quantum field theory, assuming that the polarization effects are exponentially suppressed following Lüscher’s arguments. 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. Our final result for the spectral weight is summarized in Eq. (46) which exhibits either single- or two-particle volume dependence depending on the value of $\Gamma/\Delta E$ where $\Gamma$ is the physical width of the resonance and $\Delta E$ is the typical level spacing near the resonance in the finite volume. Possibilities of using the formula to extract the width of a resonance is also discussed.

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A  The function $F(k^2)$

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

$$F(k^2) = \frac{1}{L^3} \sum_p \frac{f(p^2)}{p^2 - k^2}, \quad (A.1)$$

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

$$F'(k^2) = \frac{1}{L^3} \sum_p \frac{f(p^2)}{(p^2 - k^2)^2}. \quad (A.2)$$

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: $|p^2 - k^2| \geq \epsilon$ and $|p^2 - k^2| < \epsilon$. The first part goes smoothly to the principle-valued integral $\phi(k^2)$ while the second summation may be written as:

$$\frac{1}{L^3} \sum_{p, |p^2 - k^2| < \epsilon \Delta p^2} \frac{1}{p^2 - k^2} = \frac{1}{L^3} \sum_{n=-\infty}^{\infty} \frac{1}{p^2 + n\Delta p^2 - k^2} = -\frac{\pi}{L^3 \Delta p^2} \cot \left[ \pi \left( \frac{k^2 - p^2}{\Delta p^2} \right) \right], \quad (A.3)$$

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

$$\frac{L^3}{(2\pi)^3} 2\pi \sqrt{p^2 \Delta p^2} = 1 \quad \Rightarrow \quad L^3 \Delta p^2 = \frac{(2\pi)^2}{\sqrt{p^2}} \quad (A.4)$$

Therefore we obtain:

$$F(k^2) = \phi(k^2) - \frac{k}{4\pi} \cot \left[ \pi \left( \frac{k^2 - p^2_*}{\Delta p^2} \right) \right]. \quad (A.5)$$

However, since it is easy to verify that:

$$F(k^2) = \frac{Z_{00}(1; q^2)}{2\pi^{3/2} L} \simeq \frac{k}{4\pi} \cot \delta_0(k), \quad (A.6)$$
where we have utilized the approximate relation (Lüscher’s formula):

\[
\cot \delta_0(k) = \frac{Z_{00}(1; q^2)}{\pi^{3/2} q}.
\]  

(A.7)

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

\[
\delta_0(k) = -\pi \left( \frac{k^2 - p^2}{\Delta p^2} \right). 
\]  

(A.8)

If one evaluate \( \phi(k^2) \) explicitly, one gets:

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

(A.9)

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

\[
F'(k^2) = -\frac{1}{8\pi k} \cot \left[ \pi \left( \frac{k^2 - p^2}{\Delta p^2} \right) \right] + \frac{k}{4\Delta p^2} \csc^2 \left[ \pi \left( \frac{k^2 - p^2}{\Delta p^2} \right) \right]
\]  

\[= \frac{1}{8\pi k} \cot \delta_0(k) + \frac{k}{4\Delta p^2} \csc^2 \delta_0(k),
\]  

(A.10)

where in the second line we have used DeWitt’s formula. Since \( \Delta p^2 \propto L^{-3} \), 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.

References

[1] M. Lüscher. Volume dependence of the energy spectrum in massive quantum field theories. 1. stable particle states. Commun. Math. Phys., 104:177, 1986.

[2] M. Lüscher. Volume dependence of the energy spectrum in massive quantum field theories. 2. scattering states. Commun. Math. Phys., 105:153, 1986.

[3] M. Lüscher and U. Wolff. How to calculate the elastic scattering matrix in two-dimensional quantum field theories by numerical simulation. Nucl. Phys. B, 339:222, 1990.

[4] M. Lüscher. Two particle states on a torus and their relation to the scattering matrix. Nucl. Phys. B, 354:531, 1991.
[5] M. Lüscher. Signatures of unstable particles in finite volume. *Nucl. Phys. B*, 364:237, 1991.

[6] R. Gupta, A. Patel, and S. Sharpe. I=2 pion scattering amplitude with wilson fermions. *Phys. Rev. D*, 48:388, 1993.

[7] M. Fukugita, Y. Kuramashi, H. Mino, M. Okawa, and A. Ukawa. Hadron scattering lengths in lattice qcd. *Phys. Rev. D*, 52:3003, 1995.

[8] S. Aoki et al. I=2 pion scattering length with wilson fermions. *Nucl. Phys. (Proc. Suppl.) B*, 83:241, 2000.

[9] S. Aoki et al. I=2 pion scattering length with the wilson fermions. *Phys. Rev. D*, 66:077501, 2002.

[10] C. Liu, J. Zhang, Y. Chen, and J.P. Ma. Calculating the i=2 pion scattering length using tadpole improved clover wilson action on coarse anisotropic lattices. *Nucl. Phys. B*, 624:360, 2002.

[11] P. Hasenfratz, K.J. Juge, and F. Niedermayer. New results on cut-off effects in spectroscopy with the fixed point action. *JHEP*, 0412:030, 2004.

[12] X. Du, G. Meng, C. Miao, and C. Liu. i = 2 pion scattering length with improved actions on anisotropic lattices. *Int. J. Mod. Phys. A*, 19:5609, 2004.

[13] S. Aoki et al. I=2 pion scattering length from two-pion wave functions. *Phys. Rev. D*, 71:094504, 2005.

[14] S. Aoki et al. I=2 pion scattering phase shift with wilson fermions. *Phys. Rev. D*, 67:014502, 2003.

[15] T. Yamazaki et al. I=2 ππ scattering phase shift with two flavors of o(a) improved dynamical quarks. *Phys. Rev. D*, 70:074513, 2004.

[16] Silas R. Beane, Paulo F. Bedaque, Kostas Orginos, and Martin J. Savage. I=2 pi-pi scattering from fully-dynamical mixed-action lattice qcd. *Phys. Rev. D*, 73:054503, 2006.

[17] N. Mathur, F.X. Lee, A. Alexandru, C. Bennhold, Y. Chen, S.J. Dong, T. Draper, I. Horvath, K.F. Liu, S. Tamhankar, and J.B. Zhang. A study of pentaquarks on the lattice with overlap fermions. *Phys. Rev. D*, 70:074508, 2004.

[18] Toru T. Takahashi, Takashi Umeda, Tetsuya Onogi, and Teiji Kunihiro. Search for the possible S = +1 pentaquark states in quenched lattice QCD. *Phys. Rev.*, D71:114509, 2005.

[19] F. Csikor, Z. Fodor, S. D. Katz, T. G. Kovacs, and B. C. Toth. A comprehensive search for the Theta+ pentaquark on the lattice. *Phys. Rev.*, D73:034506, 2006.

[20] N. Ishii et al. Penta-quark baryon in anisotropic lattice QCD. *Phys. Rev.*, D71:034001, 2005.
[21] Guozhan Meng and Chuan Liu. Volume dependence of spectral weights for unstable particles in a solvable model. *Phys. Rev.*, D78:074506, 2008.

[22] A. Messiah. *Quantum Mechanics*. North Holland Publishing Company, Amsterdam, Holland, 1972.