Nuclear Physics B364 (1991) 237–251
North-Holland

SIGNATURES OF UNSTABLE PARTICLES IN FINITE VOLUME

Martin LÜSCHER

Deutsches Elektronen-Synchroton, DESY, Notkestrasse 85, D-2000 Hamburg 52, Germany

Received 7 June 1991

Unstable particles (resonances) occur in QCD, the Higgs model and many other quantum field theories of interest. Since they are a dynamical phenomenon, showing up in scattering processes of stable particles, it is not obvious how to extract their masses from numerical simulations of the theory in euclidean space. For resonances in the elastic region, a solution to this problem is proposed here on the basis of a recently established relation between the scattering matrix in infinite volume and the two-particle energy spectrum in a periodic box.

1. Introduction

It is common practice in lattice field theory to determine the spectrum of particle masses from the exponential decay of suitable correlation functions in euclidean space. To calculate the pion mass m_π in QCD, for example, one would consider the two-point function

$$C_\pi(t) = \int \mathrm{d}^3x \, \langle \pi^a(t,\boldsymbol{x}) \pi^a(0,\boldsymbol{0}) \rangle \tag{1.1}$$

of the field

$$\pi^a = \bar{\psi}\gamma_5 \frac{\tau^a}{2} \psi, \qquad \psi = \begin{pmatrix} u \\ d \end{pmatrix}, \tag{1.2}$$

where u and d denote the up- and down-quark fields, and τ^a the isospin Pauli matrices (isospin symmetry breaking effects are neglected). One then expects that

$$C_\pi(t) \propto \mathrm{e}^{-m_\pi t} \tag{1.3}$$

at large times t, up to corrections of order $\mathrm{e}^{-3m_\pi t}$ which come from three-pion and higher intermediate states. In particular, the limit

$$m_\pi = -\lim_{t\to\infty} \frac{\partial}{\partial t} \ln C_\pi(t) \tag{1.4}$$

is reached exponentially fast and is thus suitable for numerical work.

0550-3213/91/$03.50 © 1991 – Elsevier Science Publishers B.V. All rights reserved

For this computational strategy to work out it is essential that the particle considered is stable. Only then is it possible to argue that the one-particle states make the leading contribution to the appropriate correlation functions at large times t. Resonances, on the other hand, have masses greater than the many-particle threshold in the given channel. At best they are hence dominating for some range of t before the low-energy scattering states take over.

On a more fundamental level, the problem with resonances is that they are primarily a dynamical phenomenon, which is observed in scattering processes. To compute resonance masses, one must hence be able to study particle scattering in one way or the other. This seems quite impossible in the framework of numerical simulations, because the lattices one can afford are small in physical units. In particular, the spatial sizes L of the lattices currently in use for simulations of QCD are a few fermi at most. To set up a low-energy $\pi\pi$ scattering "experiment" in such a small box is clearly inconceivable.

It has however been noted that there is a close connection between the two-particle energy spectrum in finite volume and the elastic scattering amplitude [1, 2]. The general idea then is that the latter can be inferred from the spectrum, which in turn should be accessible to numerical simulations. The practical feasibility of this programme has been demonstrated for models living in two space-time dimensions [3], and there are also some partial results on the ϕ^4-theory in four dimensions [4, 5]. In the present paper the aim is to discuss how, in principle, the properties of resonances in the elastic region can be computed along these lines. Using specific models and perturbation theory, many of the qualitative issues involved have already been clarified earlier [6–8]. The new ingredient here are the formulae of ref. [2], which allow one to address the problem quantitatively on a non-perturbative level.

To keep in touch with real physics, the ρ-resonance in QCD is taken as an example, allowing for various values of the quark masses as is the case in numerical simulations. Other resonances can be treated in the same way without additional difficulties. In sect. 2 the properties of the physical ρ-resonance are briefly discussed. The relevant results of ref. [2] are reviewed after that and in sect. 4 the spectrum of $\pi\pi$ states in finite volume is worked out. In particular, it is shown there how to determine the resonance mass if the energy spectrum is known at a few values of L.

2. Pion scattering and properties of the ρ-resonance

The theory discussed in the following is QCD with degenerate up- and down-quark masses, and an arbitrary number of heavy quarks. When formulated on a lattice, cutoff effects will be assumed to be negligible. In particular, it is taken for granted that isospin is either an exact symmetry, as for Wilson fermions, or only weakly broken. This condition is often not satisfied when one chooses to work with staggered fermions, and in these cases the analysis in this paper may not apply.

2.1. KINEMATICS

Single pion states $|p\,a\rangle$ are labelled by a momentum

$$p = (p_0, \boldsymbol{p}), \qquad p_0 = \sqrt{m_\pi^2 + \boldsymbol{p}^2}\,, \tag{2.1}$$

and an isospin index a ranging from 1 to 3. Their normalization is chosen such that

$$\langle p\,a|q\,b\rangle = \delta_{ab} 2p_0 (2\pi)^3 \delta(\boldsymbol{p} - \boldsymbol{q})\,. \tag{2.2}$$

The elastic pion scattering amplitude T_I in the channel with isospin I is defined through

$$\langle p'\,a', q'\,b' \text{ out}|p\,a, q\,b \text{ in}\rangle = \langle p'\,a', q'\,b' \text{ in} p\,a, q\,b \text{ in}\rangle$$

$$+ i(2\pi)^4 \delta(p' + q' - p - q) \sum_{I=1}^{3} Q^I_{a'b',ab} T_I\,, \tag{2.3}$$

where the isospin projectors Q^I are given by

$$Q^0_{a'b',ab} = \tfrac{1}{3}\delta_{a'b'}\delta_{ab}\,, \tag{2.4}$$

$$Q^1_{a'b',ab} = \tfrac{1}{2}(\delta_{a'a}\delta_{b'b} - \delta_{a'b}\delta_{b'a})\,, \tag{2.5}$$

$$Q^2_{a'b',ab} = \tfrac{1}{2}(\delta_{a'a}\delta_{b'b} + \delta_{a'b}\delta_{b'a}) - \tfrac{1}{3}\delta_{a'b'}\delta_{ab}\,. \tag{2.6}$$

In the centre-of-mass frame, T_I is a function of the scattering angle θ and the absolute value $k = |\boldsymbol{p}|$ of the pion momenta. It is also convenient to introduce

$$W = 2\sqrt{m_\pi^2 + k^2}\,, \tag{2.7}$$

the total energy of the scattered particles.

The partial wave expansion of T_I reads

$$T_I = 16\pi W \sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta) t_{Il}\,, \tag{2.8}$$

where $P_l(z)$ denotes the Legendre polynomial of order l (the normalization is as in ref. [12], appendix B). Bose symmetry implies that the partial waves t_{Il} vanish when $I + l$ is odd. Furthermore, if we define the scattering phase $\delta_{Il}(k)$ and the inelasticity $\eta_{ll}(k)$ through

$$t_{ll} = \frac{1}{2ik}\left(\eta_{ll}\, e^{2i\delta_{ll}} - 1\right), \qquad \eta_{ll} \geqslant 0, \tag{2.9}$$

it follows from unitarity that $\eta_{ll} = 1$ in the elastic range $2m_\pi \leqslant W < 4m_\pi$ and $\eta_{ll} \leqslant 1$ elsewhere.

2.2. THE ρ-RESONANCE

According to the Particle Data Group [9], the physical ρ-meson has quantum numbers $I^G(J^{PC}) = 1^+(1^{--})$, mass $m_\rho \simeq 770$ MeV and total width $\Gamma_\rho \simeq 150$ MeV. In almost all cases, it decays into two pions. The scattering phase $\delta_{11}(k)$ accordingly passes through $\pi/2$ at the resonance energy, which corresponds to a pion momentum k equal to

$$k_\rho = \tfrac{1}{2}\sqrt{m_\rho^2 - 4m_\pi^2}\,. \tag{2.10}$$

The effective range formula

$$\frac{k^3}{W}\cot\delta_{11} = a + bk^2 \tag{2.11}$$

is in fact known to fit the experimental data quite well, if the parameters a and b are chosen such that

$$\delta_{11} = \frac{\pi}{2}, \qquad \frac{\partial\delta_{11}}{\partial k} = \frac{8k_\rho}{m_\rho\Gamma_\rho} \qquad \text{at } k = k_\rho. \tag{2.12}$$

This amounts to

$$a = -bk_\rho^2 = \frac{4k_\rho^5}{m_\rho^2\Gamma_\rho}\,. \tag{2.13}$$

(The effective range theory for pion scattering is discussed in more detail in ref. [10]. For an analysis of the experimental pion phase shifts see ref. [11], for example.)

A simple phenomenological description of the decay $\rho \to \pi\pi$ is provided by the interaction lagrangian

$$\mathscr{L}_{\text{int}} = g_{\rho\pi\pi}\epsilon_{abc}\rho_\mu^a\pi^b\partial^\mu\pi^c\,. \tag{2.14}$$

The ρ-meson field ρ_μ^a and the pion field π^a occuring here are effective fields with canonical kinetic terms. To first order in the coupling $g_{\rho\pi\pi}$, this model gives

$$\Gamma_\rho = \frac{(g_{\rho\pi\pi})^2}{6\pi} \cdot \frac{k_\rho^3}{m_\rho^2}, \tag{2.15}$$

from which one infers

$$g_{\rho\pi\pi} \simeq 6.0, \tag{2.16}$$

a rather large value.

2.3. QUARK MASS DEPENDENCE OF $\delta_{11}(k)$

As already mentioned in sect. 1, we shall also study the spectrum of QCD at quark masses larger than their physical values. In particular, we shall be interested in situations where the ρ-resonance is in the elastic energy range. The scattering phase $\delta_{11}(k)$ is then not known, but it is likely that the effective range formula (2.11), with parameters determined through eq. (2.12), continues to be a good approximation. Furthermore, it seems reasonable to assume that the effective coupling $g_{\rho\pi\pi}$ is only weakly dependent on the quark mass so that the ρ-width is still given by eqs. (2.15) and (2.16). We are then left with a scattering phase $\delta_{11}(k)$, which is completely determined once m_ρ/m_π and the pion mass are specified. The latter just sets the scale, while m_ρ^2/m_π^2 is roughly inversely proportional to the quark mass.

In the following the phase shift defined in this way will be referred to as the phenomenological scattering phase. It is only needed for the purpose of illustration and no claim is made that it coincides with the true pion phase shift in QCD.

3. Pions in the femto-universe

A term originally introduced by Bjorken [13], the femto-universe here denotes a four-dimensional world with spatial extension L in the range between say 2 and 10 fermi. More specifically, space is assumed to be a torus, i.e. a cubic box with periodic boundary conditions in all directions. This little world is what can be simulated on a computer, and the question then is how to deduce the properties of hadrons in infinite volume from such computations.

3.1. POLARIZATION EFFECTS

Since the pion is an extended object roughly one fermi wide, it will be slightly squeezed when placed in the box. In particular, the energy $\epsilon(p)$ of a pion with momentum p must be expected to differ from its energy in infinite volume. The effect is known to decrease exponentially at large L,

$$\epsilon(p) = \sqrt{m_\pi^2 + p^2} + \mathrm{O}(\mathrm{e}^{-m_\pi L}), \tag{3.1}$$

reaching a level of less than 2 percent of the pion mass for box sizes $L > 1.5 \times m_\pi^{-1}$ [14, 15].

In the framework of effective pion models, finite-size effects of the type just described arise from virtual pion exchange around the femto-universe. They are present in all physical situations considered below and are referred to as polarization effects. Being related to classically forbidden processes, they are exponentially suppressed at large L. For this reason they will be neglected in the following, but in any numerical work it would be important to check on the size of these corrections, especially in the case of single pion states.

3.2. TWO-PION STATES

When considering states of two pions in the femto-universe, it is crucial to note that the quantum of momentum in this little world is given by

$$\Delta p = 2\pi/L = 1240\ \mathrm{MeV}/L\ [\mathrm{fm}]. \tag{3.2}$$

The energy spectrum of the theory below say $4m_\pi$ is hence far from being continuous. In every sector with definite quantum numbers, one rather has a sequence of discrete levels that are separated by energy gaps of the order of 100 MeV.

Of particular interest in the following are the energy eigenstates with zero total momentum, energies W in the elastic region $2m_\pi < W < 4m_\pi$ and the same quantum numbers as the ρ-meson. In particular, they are required to have even G-parity, isospin $I = 1$ and no other flavour. And they should transform as a vector (the representation T_1^-) under reflections and cubic rotations of space. The collection of all these energy eigenstates will be referred to as the ρ-sector.

3.3. ENERGY SPECTRUM AND PION PHASE SHIFTS

If the pions would not interact, the possible $\pi\pi$ energy values W in the ρ-sector would be given by

$$W = 2\sqrt{m_\pi^2 + k^2}\,, \tag{3.3}$$

where $k = \Delta p|\boldsymbol{n}|$ and $\boldsymbol{n}$ runs through all integer vectors such that $0 < k < \sqrt{3}\,m_\pi$. The basic result of ref. [2] is that the true energy spectrum is still given by eq. (3.3), but with k being a solution of a complicated non-linear equation which involves the pion scattering phases $\delta_{1l}(k)$.

To write it down, let us first assume that all scattering phases $\delta_{1l}(k)$ with $l \geqslant 3$ vanish in the elastic region. The equation then reads

$$n\pi - \delta_{11}(k) = \phi(q), \qquad n \in \mathbb{Z}, \qquad q = \frac{kL}{2\pi}, \tag{3.4}$$

where $\phi(q)$ is a known kinematical function, whose properties are discussed in appendix A. For fixed L, eq. (3.4) has a finite number of solutions k in the range $0 < k < \sqrt{3}\, m_\pi$, and the corresponding energy values W, defined through eq. (3.3), are precisely the energies of the states in the ρ-sector*.

To the author's knowledge the physical pion scattering phase $\delta_{13}(k)$ has not been measured at low energies. It is presumably very small there, since the lightest observed resonance with quantum numbers $I^G(J^{PC}) = 1^+(3^{--})$, the $\rho_3(1690)$, is far above the inelastic threshold. In the simple ρ exchange model with interaction (2.14), one indeed finds that $\delta_{13}(k) < 1°$ for all energies around and below the ρ-mass. Under these conditions its influence on the energy spectrum in the ρ-sector may be treated as a small perturbation. To first order, eq. (3.4) then gets replaced by

$$n\pi - \delta_{11}(k) = \phi(q) + \tfrac{4}{9}\sigma(q)\tan\delta_{13}(k)\,, \tag{3.5}$$

where the sensitivity $\sigma(q)$ is another kinematical function defined in appendix A. If one inserts the scattering phase $\delta_{13}(k)$ computed from ρ-exchange, the correction term in eq. (3.5) is in most cases less than a percent of $\phi(q)$. Corrections of a few percent are found when m_ρ is close to $2m_\pi$ and if k is large.

The influence of the higher scattering phases can be discussed similarly, but since these are even smaller than $\delta_{13}(k)$, it is unlikely that they lead to a noticeable effect.

4. Signatures of the ρ-resonance

In the following the working hypotheses is made that the spectrum in the ρ-sector is accurately described by eq. (3.4), i.e. that the influence of the higher scattering phases is negligible. As discussed above, one has reason to expect that this assumption is justified down to a level of a fraction of a degree – an accuracy far sufficient for the analysis of numerical data.

Eq. (3.4) may be read in two ways. We may first insert the phenomenological scattering phase (2.11) and work out the solutions of the equation. This will give us the "expected" energy spectrum in the ρ-sector. Or else we may assume that one or the other energy level has been computed through numerical simulation. Eq. (3.4) then yields the scattering phase $\delta_{11}(k)$ at the corresponding values of k.

4.1. EXPECTED ENERGY SPECTRUM IN THE ρ-SECTOR

For physical values of m_π, m_ρ and Γ_ρ, the predicted energy spectrum in the ρ-sector is shown in fig. 1. Since the phenomenological scattering phase is small

* There are further levels with $q \geqslant \sqrt{5}$ which we do not discuss here, because they are above the inelastic threshold for box sizes $L < (20/3)^{1/2}\pi \times m_\pi^{-1}$, i.e. for $L < 11$ fm.

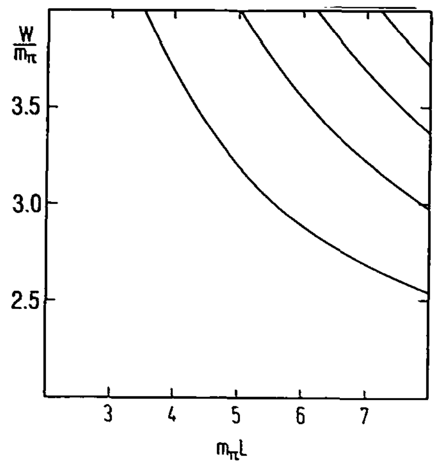

Fig. 1. Expected energy spectrum in the ρ-sector for physical values of $m_\mp$, m_ρ and Γ_ρ.

below the inelastic threshold (a few degrees at most), the spectrum is practically as if the pions would not interact at all. The maximal deviation from the free pion levels is less than 11 MeV, an effect which is surely hard to detect in any numerical simulation.

A more interesting result is obtained when the up- and down-quark mass is large enough for the ρ-mass to move below the inelastic threshold (see fig. 2a). The most

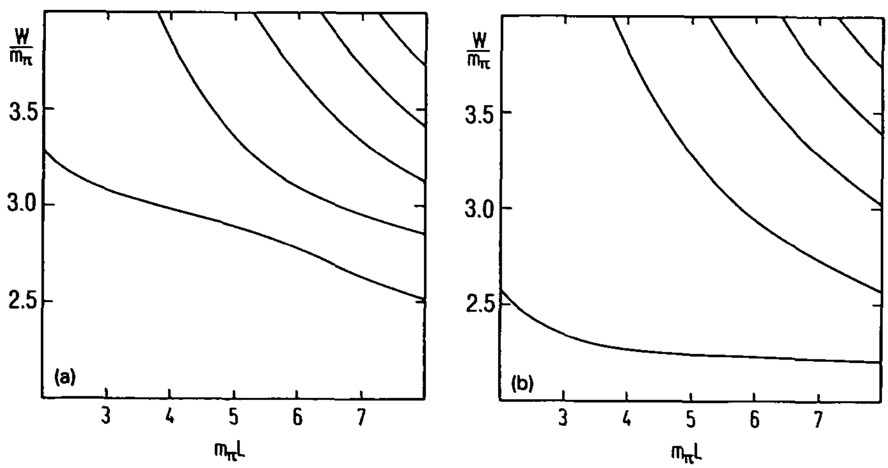

Fig. 2. Expected energy spectrum in the ρ-sector for (a) $m_\rho/m_\mp = 3$ and (b) $m_\rho/m_\mp = 2.2$. In both cases the ρ-meson width is assumed to be given by eqs. (2.15) and (2.16). This amounts to $\Gamma_\rho/m_\mp = 0.30$ and $\Gamma_\rho/m_\mp = 0.038$, respectively.

obvious difference compared to fig. 1 is that at all values of L there is one more level below the inelastic threshold. This is in accord with the naive expectation that the ρ corresponds to an additional state which mixes with the two-pion states. The figure also shows that all levels vary substantially with L. In particular, there are no pronounced plateaus at the ρ-mass, as one would expect for a very narrow resonance [6–8].

At even smaller values of m_ρ/m_π, the lowest level looks more and more like a stable particle state (see fig. 2b). The reason for this behaviour is that the available phase space for ρ-decay becomes small and eventually vanishes at threshold. Effectively one thus has a narrow width case, with a flat plateau at the resonance energy extending up to values of L greater than $8 \times m_\pi^{-1}$.

4.2. DETERMINATION OF THE ρ-MASS FROM SIMULATION DATA

Let us now assume that some energy values in the ρ-sector have been computed through numerical simulation on a few lattices with fixed bare coupling and quark masses. Via eq. (3.3), each measured energy value W corresponds to some momentum k, and the scattering phase $\delta_{11}(k)$ at these momenta is then determined by eq. (3.4). With sufficient data one will in this way be able to trace out the complete phase shift in the elastic region. If the ρ-resonance is below the inelastic threshold, a fit of the data with a Breit–Wigner or effective range formula then allows one to estimate the resonance energy and width, taking eq. (2.12) as the definition of these two quantities.

Alternatively, by varying L one may directly search for the point, where $\delta_{11}(k)$ passes through $\pi/2$. This happens when q [the parameter introduced in eq. (3.4)] satisfies

$$\phi(q) = (n - \tfrac{1}{2})\pi \tag{4.1}$$

for some integer n. The complete list of solutions of this equation in the range $0 \leqslant q \leqslant 3$ is given in appendix A. Once this point is found, the resonance width may be determined from the identity

$$\Gamma_\rho = -\frac{8k_\rho^2}{q\phi'(q)} \cdot \frac{\gamma}{4k_\rho^2 + m_\rho\gamma}, \qquad \gamma = L\frac{\partial W}{\partial L}, \tag{4.2}$$

which is a straightforward consequence of eq. (3.4) and the definition (2.12) of the ρ-width. For a very narrow resonance, the calculation of the slope γ may however turn out to be impractical, because it may be impossible to compute the energy values in the ρ-sector with the necessary statistical accuracy. The best one can achieve in this case is an upper bound on the width.

4.3. RESONANCE AMPLITUDES

When computing the energy spectrum in the ρ-sector through numerical simulation, one proceeds as in the case of the pion mass calculation outlined in sect. 1. That is, one chooses some fields with the right quantum numbers and works out their correlation matrix at large times t. The desired energy values can then be read off from the eigenvalues of the matrix (see ref. [3], appendix A, for the relevant technical lemma).

Two-pion states can be created from the vacuum by acting with operators of the type

$$\mathcal{O}_k^a(t,x) = \int d^3z f_k(z)\epsilon_{abc}\pi^b(t,x+z)\pi^c(t,x), \tag{4.3}$$

where $f_k(z)$ is some periodic wave function, which transforms according to the representation T_1^- of the cubic group. All levels in the ρ-sector can eventually be reached by these operators. The states with energies close the ρ-mass are special, however, because they have an enhanced projection on the states generated from the vacuum by local operators. The computation of this part of the spectrum may hence be facilitated by including such operators in the correlation matrix.

To illustrate the point, let us consider the correlation function

$$C_\rho(t) = \int d^3x \langle j_k^a(t,x) j_k^a(0,\mathbf{0})\rangle \tag{4.4}$$

of the isospin current

$$j_\mu^a = \bar{\psi}\gamma_\mu \frac{\tau^a}{2}\psi. \tag{4.5}$$

This operator has the same quantum numbers as the ρ-meson, and all energies $W_\alpha < 4m_\pi$ appearing in the finite-volume spectral representation

$$C_\rho(t) = \sum_{\alpha=1}^{\infty} A_\alpha e^{-W_\alpha t} \tag{4.6}$$

hence come from intermediate states $|\alpha\rangle$ in the ρ-sector.

If $|\alpha\rangle$ is a state well below the resonance energy, it describes two weakly interacting pions in the femto-universe. The probability that both of them are close to the origin is proportional to L^{-6}. Since it is only then that a non-zero overlap with the state $j_k^a(0,\mathbf{0})|0\rangle$ is obtained, it follows that the amplitude

$$A_\alpha = L^3 |\langle 0|j_k^a(0,\mathbf{0})|\alpha\rangle|^2 \tag{4.7}$$

is of order L^{-3}. (It is straightforward to confirm this qualitative argumentation in the free pion theory, where the isospin current is given by $j_\mu^a = \epsilon_{abc}\pi^b\partial_\mu\pi^c$.)

For the levels close to the resonance energy, the situation is different. To see this let us first imagine that the coupling $g_{\rho\pi\pi}$ between the ρ-resonance and the two-pion states is switched off. The ρ would then be stable and the amplitude A_α of the corresponding state would be of order 1. When the coupling is turned on, the former resonance state mixes with the nearby two-pion states. The mixing is usually small, except when a two-pion level happens to cross the resonance energy [6]. In that case the associated amplitudes just rotate into each other so that both levels will in general have an appreciable amplitude. The upshot then is that the off-resonance states are suppressed relative to the states around the resonance mass. The energies of the latter should hence be comparatively easy to extract from the current correlation function.

Further support for this conclusion comes from the spectral representation of the current correlation function in infinite volume,

$$C_\rho(t) = \int_{2m_\pi}^{\infty} \mathrm{d}W \varrho(W) \mathrm{e}^{-Wt}. \tag{4.8}$$

Up to a kinematical factor, the spectral density $\varrho(W)$ coincides with the total cross section for $\mathrm{e}^+\mathrm{e}^- \to$ hadrons, where the final state is required to have isospin $I = 1$. As is well known [16], the ρ-resonance shows up in these processes through a broad peak, which may be roughly represented by the Breit–Wigner formula

$$\varrho(W) \simeq \frac{3k^3}{8\pi^2 W} \cdot \frac{m_\rho^2}{(W - m_\rho)^2 + \frac{1}{4}\Gamma_\rho^2}. \tag{4.9}$$

When this expression is inserted in the spectral integral (4.8), one finds that $C_\rho(t)$ is dominated by the states around the ρ-peak for all times t that are not too large compared to m_ρ^{-1}, but large enough to suppress the contribution of the high-energy states.

5. Conclusions

The ideas discussed in this paper provide a conceptually satisfactory basis to approach the problem of resonances in lattice field theory. So far the method only applies to resonances in the elastic region, and its practical feasibility has not yet been demonstrated. To study the technical issues involved, it would certainly be useful to experiment with a simple test case, such as the linear σ-model, before one turns to the physically more relevant theories.

If the resonance considered is very narrow, it may be difficult to extract its width from the two-particle energy spectrum in finite volume, unless the latter can be determined very accurately. In this situation it is probably better to try to compute the relevant phenomenological coupling constants directly from three point correlation functions. The theoretical problem of how to pass to the desired on-shell matrix elements has, however, not been solved up to now.

Appendix A

A.1. ZETA FUNCTIONS

Let $\boldsymbol{r}$ be a vector in $\mathbb{R}^3$ and r, θ, φ its polar coordinates. A complete set of homogenous harmonic polynomials in $\boldsymbol{r}$ is given by

$$\mathscr{Y}_{lm}(\boldsymbol{r}) = r^l Y_{lm}(\theta, \varphi), \tag{A.1}$$

where $l = 0, 1, 2, \ldots$ and $m = -l, -l+1, \ldots, l$. The functions $Y_{lm}(\theta, \varphi)$ are the usual spherical harmonics, with phases and normalizations chosen as in ref. [12], appendix B. In particular, $Y_{00}(\theta, \varphi) = 1/\sqrt{4\pi}$.

The generalized zeta functions $\mathscr{Z}_{lm}(s; q^2)$ of the cubic lattice are meromorphic functions of s in the whole complex plane. For $\mathrm{Re}\, 2s > l + 3$, they are defined through the convergent series

$$\mathscr{Z}_{lm}(s; q^2) = \sum_{\boldsymbol{n} \in \mathbb{Z}^3} \mathscr{Y}_{lm}(\boldsymbol{n}) (\boldsymbol{n}^2 - q^2)^{-s} \tag{A.2}$$

and elsewhere through analytic continuation (in eq. (A.2) the phase convention $-\pi < \arg(\boldsymbol{n}^2 - q^2) \leqslant \pi$ is adopted). An efficient way to evaluate the zeta functions numerically is described in ref. [2], appendix C.

A.2. DISCUSSION OF THE ANGLE $\phi(q)$

For all $q \geqslant 0$, the angle $\phi(q)$ is determined by

$$\tan \phi(q) = -\frac{\pi^{3/2} q}{\mathscr{Z}_{00}(1; q^2)}, \qquad \phi(0) = 0, \tag{A.3}$$

and the requirement that it depends continuously on q. For $q^2 \geqslant 0.1$, $\phi(q)$ is very nearly equal to πq^2 (see table A.1). The numbers listed there are exact to the precision stated. For intermediate values of q^2, quadratic interpolation will in general yield sufficiently accurate results.

TABLE A.1
Values of the angle $\phi(q)$ in the range $0.1 \leqslant q^2 \leqslant 9.0$

q^2	$\phi/\pi q^2$	q^2	$\phi/\pi q^2$	q^2	$\phi/\pi q^2$
0.1	1.1100	3.1	1.0083	6.1	0.9933
0.2	1.1352	3.2	1.0098	6.2	0.9856
0.3	1.1091	3.3	1.0063	6.3	0.9773
0.4	1.0779	3.4	1.0000	6.4	0.9688
0.5	1.0503	3.5	0.9924	6.5	0.9601
0.6	1.0283	3.6	0.9850	6.6	0.9515
0.7	1.0121	3.7	0.9791	6.7	0.9429
0.8	1.0021	3.8	0.9766	6.8	0.9345
0.9	0.9981	3.9	0.9814	6.9	0.9262
1.0	1.0000	4.0	1.0000	7.0	0.9182
1.1	1.0071	4.1	1.0318	7.1	0.9104
1.2	1.0178	4.2	1.0540	7.2	0.9030
1.3	1.0292	4.3	1.0594	7.3	0.8959
1.4	1.0382	4.4	1.0558	7.4	0.8892
1.5	1.0422	4.5	1.0481	7.5	0.8831
1.6	1.0408	4.6	1.0387	7.6	0.8777
1.7	1.0345	4.7	1.0286	7.7	0.8734
1.8	1.0247	4.8	1.0185	7.8	0.8706
1.9	1.0128	4.9	1.0088	7.9	0.8705
2.0	1.0000	5.0	1.0000	8.0	0.8750
2.1	0.9872	5.1	0.9924	8.1	0.8857
2.2	0.9751	5.2	0.9867	8.2	0.8982
2.3	0.9645	5.3	0.9838	8.3	0.9055
2.4	0.9563	5.4	0.9847	8.4	0.9072
2.5	0.9512	5.5	0.9902	8.5	0.9058
2.6	0.9508	5.6	0.9985	8.6	0.9030
2.7	0.9564	5.7	1.0050	8.7	0.8994
2.8	0.9686	5.8	1.0071	8.8	0.8957
2.9	0.9852	5.9	1.0050	8.9	0.8921
3.0	1.0000	6.0	1.0000	9.0	0.8889

In the small-q^2 range, $\phi(q)$ is roughly proportional to q^3. The function

$$\phi_0(q) = \arctan \frac{2\pi^2 q^3}{1+x}, \tag{A.4}$$

$$x = 8.91363\, q^2 - 16.5323\, q^4 - 8.402\, q^6 - 6.95\, q^8, \tag{A.5}$$

gives an accurate numerical representation there, with

$$|1 - \phi_0(q)/\phi(q)| < 4 \times 10^{-5} \tag{A.6}$$

for all $q^2 \leqslant 0.1$.

TABLE A.2
Solutions q_n of eq. (A.7) in the range $0 \leqslant q \leqslant 3$

n	q_n	$\phi'(q_n)$
1	0.6877	4.0280
2	1.2007	8.3454
3	1.6208	10.7651
4	1.8806	8.5345
5	2.0620	16.4027
6	2.3532	21.5301
7	2.6826	6.3787
8	2.8789	23.4860

For each integer $n \geqslant 1$, the equation

$$\phi(q) = \left(n - \tfrac{1}{2}\right)\pi \tag{A.7}$$

has a unique solution $q = q_n$, which is given in table A.2 together with the first derivative of $\phi(q)$ at this point.

A.3. PROPERTIES OF THE SENSITIVITY $\sigma(q)$

The sensitivity $\sigma(q)$ is defined through

$$\sigma(q) = \frac{12}{7q^4} \cdot \frac{\mathscr{Z}_{40}(1;q^2)^2}{\pi^3 q^6 + q^4 \mathscr{Z}_{00}(s;q^2)^2}. \tag{A.8}$$

$\sigma(q)$ is non-negative and smooth for all $q > 0$. The function varies appreciably with peaks at the points where the zeta functions are singular. In the range $0 < q^2 \leqslant 9$ the bound

$$\sigma(q) \leqslant \frac{7}{q^4} + \frac{6}{(q^2-4)^2 + 1} \tag{A.9}$$

holds.

References

[1] M. Lüscher, Commun. Math. Phys. 105 (1986) 153
[2] M. Lüscher, Nucl. Phys. B354 (1991) 531
[3] M. Lüscher and U. Wolff, Nucl. Phys. B339 (1990) 222
[4] I. Montvay and P. Weisz, Nucl. Phys. B290 [FS20] (1987) 327
[5] Ch. Frick, K. Jansen, J. Jersák, I. Montvay, P. Seuferling and G. Münster, Nucl. Phys. B331 (1990) 515

[6] U. Wiese, Nucl. Phys. B (Proc. Suppl.) 9 (1989) 609

[7] M. Lüscher, Selected topics in lattice field theory, Lectures given at Les Houches (1988), *in* Fields, strings and critical phenomena, ed. E. Brézin and J. Zinn-Justin (North-Holland, Amsterdam, 1989)

[8] T.A. DeGrand, Phys. Rev. D43 (1991) 2296

[9] M. Aguilar-Benitez et al. (Particle Data Group), Phys. Lett. B239 (1990)

[10] L.S. Brown and R.L. Goble, Phys. Rev. Lett. 20 (1968) 346

[11] P. Estabrooks and A.D. Martin, Nucl. Phys. B79 (1974) 301

[12] A. Messiah, Quantum mechanics, Vols. I, II (North Holland, Amsterdam, 1965)

[13] J.D. Bjorken, Elements of quantum chromodynamics, *in* Proc. Summer Institute on Particle physics, ed. Anne Mosher, SLAC report 224 (1980)

[14] M. Lüscher, On a relation between finite-size effects and elastic scattering processes, Lecture given at Cargèse (1983), *in* Progress in gauge field theory, ed. G. 't Hooft et al. (Plenum, New York, 1984)

[15] M. Lüscher, Commun. Math. Phys. 104 (1986) 177

[16] B.H. Wiik and G. Wolf, Electron–positron interactions, Springer Tracts in Modern Physics, Vol. 86 (Springer, Berlin, 1979)