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Volume Dependence of the Energy Spectrum in Massive Quantum Field Theories

II. Scattering States

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Abstract. The low-lying energy values associated to energy eigenstates describing two stable particles enclosed in a (space-like) box of size L are shown to be expandable in an asymptotic power series of $1/L$. The coefficients in these expansions are related to the appropriate elastic scattering amplitude in a simple and apparently universal manner. At low energies, the scattering amplitude can thus be determined, if an accurate calculation of two-particle energy values is possible (by numerical simulation, for example).

1. Introduction

This paper is a continuation of [1], where I have determined the size dependence of the stable particle masses in quantum field theories enclosed in an $L \times L \times L$ box with periodic boundary conditions. The objective here is, to find out how the energy eigenstates describing two (unbound) stable particles behave in finite volume and in particular how the associated energy values vary with L. The motivation for this investigation is at least two-fold. First, in numerical simulations of lattice theories, it is helpful to have some a priori knowledge about the distribution of the low-lying energy values to perform the spectral analysis of correlation functions and to correctly interpret the energy spectrum so determined. Secondly, the formulae established in this paper relate the size dependence of the two-particle energies to the corresponding elastic scattering amplitudes and thus make the latter accessible for calculational schemes, which need a finite volume for technical reasons and which are hence unable to deals with scattering processes directly. To compute low-energy scattering amplitudes via the energy spectrum in finite volume appears to be a rather complicated way to proceed, but in the context of numerical simulations of lattice gauge theories, for example, no other practical method is presently available.

In finite volume, the particle momenta are quantized and the spectrum of energies of two-particle states with zero total momentum is therefore discrete. As $L \to \infty$, the spacing between these levels goes to zero and their density grows proportionally to the volume. An important point to note is that the level spacing is often not so small in practice. Consider for example a numerical simulation of QCD on a large lattice with $L \geqq 3$ fermi. As will be shown later, the low-lying energies W of the zero total momentum $\pi\pi$-states are then approximately equal to the free field values

$$W = 2\sqrt{m_\pi^2 + \mathbf{p}^2}, \tag{1.1}$$

where m_π denotes the physical pion mass and the (relative) pion momentum $\mathbf{p}$ is given by

$$\mathbf{p} = \frac{2\pi}{L}\mathbf{n}, \qquad \mathbf{n} \in \mathbb{Z}^3. \tag{1.2}$$

Thus, as shown by Fig. 1, the level spacing is sizeable up to very large volumes, in particular, the lowest energy value is well separated from the higher ones below (say) $L = 10$ fermi. These energy values are therefore well-defined in a practical sense and their calculation in numerical simulations should be no more difficult than the calculation of the pion mass, for example.

Consider now an arbitrary massive quantum field theory describing the physics of particles ("mesons") with spin 0 and mass m. As already mentioned, the possible energy values of two-particle states in finite volume are given by the free field expression $W = 2(m^2 + \mathbf{p}^2)^{1/2}$ plus a small correction, which is due to the meson interactions. There are two different physical processes, which contribute to this finite size energy shift. First, there are the polarization effects discussed in detail in refs. [1, 2], which involve virtual particle exchange "around the world." Secondly, the two mesons enclosed in the box interact directly, i.e. they are really in a stationary scattering state. For large L, the energy shift due to polarization effects decreases exponentially whereas the second process gives rise to corrections, which decay only as a power of $1/L$. This basic fact can easily be understood heuristically by noting that the interactions in massive quantum field theories are short ranged.

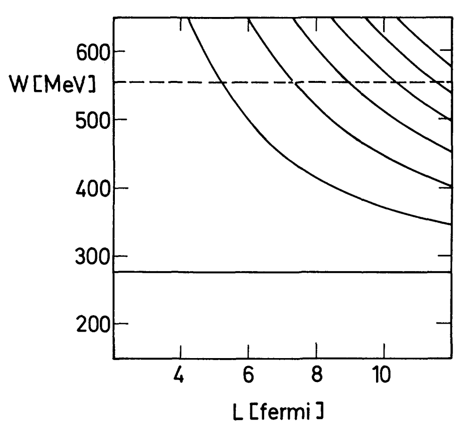

Fig. 1. Energy values of $\pi\pi$-states with zero total momentum as a function of the box size L neglecting pion interactions. The dashed line indicates the 4-pion threshold. The multiplicity of the levels shown is 1 in the channel with zero spin and isospin

Since the wave functions of the mesons are spread throughout the box, the probability for the particles to be within interaction distance is inversely proportional to the volume and the resulting energy shift is hence expected to be proportional to L^{-3}. Thus, the leading corrections to the free field energy spectrum in the two-particle sector arise from real (as opposed to virtual) scattering processes and the situation is therefore entirely different from the one considered in ref. [1], in particular, new mathematical tools will be required to prove relations such as Eq. (1.3) below.

In this paper it is shown that the individual two-particle energy values can be expanded in a power series of $1/L$ with calculable coefficients, which are simply related to the elastic meson scattering amplitude. For example, for the lowest level ($\mathbf{p}=0$), the first few terms in the expansion are given by

$$W=2m-\frac{4\pi a_0}{mL^3}\left\{1+c_1\frac{a_0}{L}+c_2\frac{a_0^2}{L^2}\right\}+O(L^{-6}), \tag{1.3}$$

$$c_1=-2.837297, \tag{1.4}$$

$$c_2=6.375183, \tag{1.5}$$

where a_0 denotes the S-wave scattering length, i.e. in terms of the S-wave scattering phase shift δ_0, we have

$$a_0=\lim_{p\to 0}\frac{1}{2ip}\left(e^{2i\delta_0}-1\right) \tag{1.6}$$

(p: magnitude of the meson momentum in the centre of mass system). Thus, as anticipated above, the leading finite size correction to the two-particle energy W is inversely proportional to the volume. The subleading terms arise from multiple scattering processes and involve the coefficients c_1 and c_2, which are related to the zeta-function of the Laplacian on a 3-dimensional torus [c_1 and c_2 are constants of the momentum lattice (1.2) in other words]. The higher terms in Eq. (1.3) depend on successively higher derivatives of the scattering amplitude at zero momentum and can be obtained quite easily if desired.

For the levels with $\mathbf{p}\neq 0$ and in more complicated situations involving particles with different masses and particles with spin, the large L expansions look similar to Eq. (1.3), in particular, the leading non-trivial term is always proportional to L^{-3}. A remarkable aspect of these expansions is that the coefficients are determined solely by the scattering phase shifts δ_l (and their derivatives) at momentum p, i.e. there is no reference to the particle interactions at other energies.

In their work on the non-ideal Bose gas almost 30 years ago, Huang and Yang [3] have already derived Eq. (1.3) in the special case of two (non-relativistic) hard spheres enclosed in a periodic box [1]. More recently, the existence of the first non-trivial term in Eq. (1.3) has also been mentioned in ref. [4] in the course of a discussion of statistical errors in quenched hadron mass calculations. The proof of

[1] I am indebted to N. Rivier for drawing my attention to this work. A small numerical discrepancy between the constants c_1, c_2 as calculated in ref. [3] and the values quoted here is due to an approximation made by Huang and Yang

Eq. (1.3) given by Huang and Yang is based on a pseudo-potential approximation to the Schrödinger equation, which is exact to the order of a_0/L considered. Although this method can probably be generalized to arbitrary short range potentials, I would not know how to carry it over to quantum field theory, because a local two-particle wave equation is not available in this case.

The large L expansions of the two-particle energy values are established here to all orders of perturbation theory in arbitrary massive quantum field theories, the philosophy concerning universality and the applicability of this method of proof being the same as in ref. [1]. Apart from Subsect. 2.7, where we shall briefly discuss the two-dimensional case, the dimensionality of space-time is always assumed to be 4. While the methods employed could easily be generalized to higher dimensions, they do not apply in dimensions 2 and 3, because the dynamical finite size energy shifts are not small compared to the free particle level splitting in these cases.

The organization of the paper is as follows. In Sect. 2, the quantum mechanical case of two (non-relativistic) bosons interacting through a potential of finite range is discussed in great detail. The basic techniques to control the volume dependence of two-particle energy values to all orders of perturbation theory are developed here and the results are illustrated by a simple numerically soluble model. It is only in Sect. 3, where the quantum field theory case is treated, that the reader is assumed to be familiar with the results and techniques of ref. [1]. As an application of the general formulae, the pion-pion and pion-nucleon system is considered in Subsect. 3.6. The paper ends with a few concluding remarks in Sect. 4 and two appendices, one discussing the zeta-function of the momentum lattice (1.2) alluded to above and the other containing the proof of a general summation formula for singular 3-dimensional momentum sums.

2. Volume Dependence of Energy Values in Quantum Mechanics

2.1. Summary of Notations

In the following subsections, details are only worked out for the case of two non-relativistic bosons ("mesons") of mass m and spin 0, which interact through a potential V of finite range. The methods used are however more generally applicable and it is not difficult to extend the results in various directions.

In infinite volume, the two-particle states are thus described by scalar wave functions $\psi(\mathbf{x}, \mathbf{y})$, where $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$ are the position space coordinates of the mesons. Bose statistics requires

$$\psi(\mathbf{x}, \mathbf{y}) = \psi(\mathbf{y}, \mathbf{x}), \tag{2.1}$$

and the scalar product is accordingly defined by

$$\langle\varphi|\psi\rangle = \tfrac{1}{2}\int d^3x d^3y\, \varphi(\mathbf{x}, \mathbf{y})^* \psi(\mathbf{x}, \mathbf{y}). \tag{2.2}$$

The Hamilton operator $\mathbb{H}$ of the system is assumed to be of the form

$$\mathbb{H} = \mathbb{H}_0 + \mathbb{V}, \tag{2.3}$$

where the action of $\mathbb{H}_0$ and $\mathbb{V}$ on wave functions ψ is given by

$$\mathbb{H}_0\psi(\mathbf{x},\mathbf{y}) = -\frac{1}{2m}(\Delta_x+\Delta_y)\psi(\mathbf{x},\mathbf{y}), \tag{2.4}$$

$$\mathbb{V}\psi(\mathbf{x},\mathbf{y}) = V(\mathbf{x}-\mathbf{y})\psi(\mathbf{x},\mathbf{y}) \tag{2.5}$$

(Δ_x, Δ_y denote the Laplace operators with respect to $\mathbf{x}$ and $\mathbf{y}$). The potential $V(\mathbf{z})$ is required to be square integrable, rotationally symmetric and of finite range, i.e.

$$V(\mathbf{z})=0 \quad \text{for} \quad |\mathbf{z}|>R\,. \tag{2.6}$$

This last assumption is made for convenience, but in what follows, a weaker condition, for example that $V(\mathbf{z})$ decays exponentially, would do just as well.

The eigenfunctions of the free Hamiltonian $\mathbb{H}_0$ are the symmetrized plane waves

$$\psi_{\mathbf{p},\mathbf{q}}(\mathbf{x},\mathbf{y}) = e^{i(\mathbf{px}+\mathbf{qy})} + e^{i(\mathbf{py}+\mathbf{qx})}, \tag{2.7}$$

which will be written as $|\mathbf{p},\mathbf{q}\rangle$ in Dirac's notation. Thus, we have

$$\mathbb{H}_0|\mathbf{p},\mathbf{q}\rangle = (\varepsilon(\mathbf{p})+\varepsilon(\mathbf{q}))|\mathbf{p},\mathbf{q}\rangle, \tag{2.8}$$

$$\varepsilon(\mathbf{p}) = \frac{\mathbf{p}^2}{2m}, \tag{2.9}$$

$$\langle\mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle = (2\pi)^6\{\delta(\mathbf{p}'-\mathbf{p})\delta(\mathbf{q}'-\mathbf{q})+\delta(\mathbf{p}'-\mathbf{q})\delta(\mathbf{q}'-\mathbf{p})\}\,. \tag{2.10}$$

Defining in-going and out-going scattering states as usual through the Møller operators, the meson scattering amplitude T_{nr}[2] is given by

$$\langle\mathbf{p}',\mathbf{q}' \text{ out } |\mathbf{p},\mathbf{q} \text{ in}\rangle = \langle\mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}\rangle - i(2\pi)^4\delta(E'-E)\delta(\mathbf{P}'-\mathbf{P})\,T_{\mathrm{nr}}(\mathbf{p}',\mathbf{q}'|\mathbf{p},\mathbf{q}),$$

where $E=\varepsilon(\mathbf{p})+\varepsilon(\mathbf{q})$ is the total energy and $\mathbf{P}=\mathbf{p}+\mathbf{q}$ the total momentum of the in-going particles[3].

With these conventions, the partial wave expansion of the scattering amplitude in the center of mass system ($\mathbf{P}=0$) reads

$$T_{\mathrm{nr}} = -\frac{8\pi}{m}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)t_l, \tag{2.12}$$

$$t_l = \frac{1}{2ip}(e^{2i\delta_l}-1), \qquad p=|\mathbf{p}|, \tag{2.13}$$

(P_l: l'th Legendre polynomial, θ: scattering angle, δ_l: scattering phase shift). Note that t_l vanishes for l odd due to Bose symmetry. The threshold parameters a_l and b_l are defined by

$$\mathrm{Re}\,t_l = p^{2l}\{a_l+p^2b_l+O(p^4)\}, \tag{2.14}$$

which agrees with the definition (1.6) of the S-wave scattering length a_0.

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[2] The subscript "nr" means "non-relativistic" and is written to distinguish T_{nr} from the relativistic amplitude T, which is normalized differently

[3] The letter W, which is used in Sect. 1 to denote the total two-particle energy, is reserved for relativistic systems

As already mentioned in the introduction, the large L expansions of the finite volume energy levels will be proved to all orders in perturbation theory, i.e. to all orders of an expansion in powers of the potential V. For the scattering amplitude T_{nr} in the centre of mass system, this expansion coincides with the Born series

$$T_{\mathrm{nr}} = \hat{V}(\mathbf{p}', \mathbf{p}) + \sum_{n=1}^{\infty} \frac{(-1)^n}{2^n} \int \frac{d^3k_1}{(2\pi)^3} \cdots \frac{d^3k_n}{(2\pi)^3}$$

$$\times \hat{V}(\mathbf{p}', \mathbf{k}_1) R_E(\mathbf{k}_1) \hat{V}(\mathbf{k}_1, \mathbf{k}_2) R_E(\mathbf{k}_2) \ldots \hat{V}(\mathbf{k}_n, \mathbf{p}), \tag{2.15}$$

$$\hat{V}(\mathbf{k}', \mathbf{k}) = \int d^3z \{ e^{-i(\mathbf{k}'-\mathbf{k})\mathbf{z}} + e^{-i(\mathbf{k}'+\mathbf{k})\mathbf{z}} \} V(\mathbf{z}), \tag{2.16}$$

$$R_E(\mathbf{k}) = \{ 2\,\varepsilon(\mathbf{k}) - E - i\varepsilon \}^{-1}. \tag{2.17}$$

In particular, for the S-wave scattering length a_0, we have

$$-\frac{8\pi}{m} a_0 = \hat{V}(\mathbf{0}, \mathbf{0}) + \sum_{n=1}^{\infty} \frac{(-1)^n}{2^n} \int \frac{d^3k_1}{(2\pi)^3} \cdots \frac{d^3k_n}{(2\pi)^3}$$

$$\times \hat{V}(\mathbf{0}, \mathbf{k}_1) \frac{m}{\mathbf{k}_1^2} \hat{V}(\mathbf{k}_1, \mathbf{k}_2) \frac{m}{\mathbf{k}_2^2} \ldots \hat{V}(\mathbf{k}_n, \mathbf{0}). \tag{2.18}$$

This concludes the discussion of the meson system in infinite volume and we now proceed to list the basic properties of the finite volume system.

The quantum mechanical states of two mesons confined to a periodic $L \times L \times L$ box are also described by wave functions $\psi(\mathbf{x}, \mathbf{y}) = \psi(\mathbf{y}, \mathbf{x})$ with $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$. The boundary conditions are taken into account by requiring

$$\psi(\mathbf{x} + \mathbf{n}L, \mathbf{y}) = \psi(\mathbf{x}, \mathbf{y}) \quad \text{for all} \quad \mathbf{n} \in \mathbb{Z}^3, \tag{2.19}$$

and the scalar product of wave functions is given by Eq. (2.2), but with integrations running over one periodicity cell only. The action of the Hamilton operator $\mathbb{H}$ on finite volume wave functions is defined as before [Eqs. (2.3)–(2.5)], where in (2.5) the potential $V(\mathbf{z})$ should be replaced by

$$V_L(\mathbf{z}) = \sum_{\mathbf{n} \in \mathbb{Z}^3} V(\mathbf{z} + \mathbf{n}L) \tag{2.20}$$

to preserve periodicity.

The plane waves (2.7) are the eigenfunctions of the free Hamiltonian $\mathbb{H}_0$ in finite volume, too, provided the momenta $\mathbf{p}$ and $\mathbf{q}$ are restricted to the discrete values (1.2). For the normalization of these states, one finds

$$\langle \mathbf{p}', \mathbf{q}' | \mathbf{p}, \mathbf{q} \rangle = L^6 \{ \delta_{\mathbf{p}', \mathbf{p}} \delta_{\mathbf{q}', \mathbf{q}} + \delta_{\mathbf{p}', \mathbf{q}} \delta_{\mathbf{q}', \mathbf{p}} \} \tag{2.21}$$

and the matrix elements of $\mathbb{V}$ in this basis are given by

$$\langle \mathbf{p}', \mathbf{q}' | \mathbb{V} | \mathbf{p}, \mathbf{q} \rangle = L^3 \delta_{\mathbf{P}', \mathbf{P}} \hat{V}(\tfrac{1}{2}(\mathbf{p}' - \mathbf{q}'), \tfrac{1}{2}(\mathbf{p} - \mathbf{q})), \tag{2.22}$$

where $\hat{V}$ is defined as before [Eq. (2.16)].

In the absence of interactions ($V = 0$) and for zero total momentum, the possible energy values of the system are

$$E = 2\varepsilon(\mathbf{p}) = \frac{4\pi^2}{mL^2} \mathbf{n}^2 \qquad (\mathbf{n} \in \mathbb{Z}^3). \tag{2.23}$$

For weakly interacting particles, ordinary perturbation theory can be applied and the spectrum is hence given by Eq. (2.23) plus small corrections. For example, using Eqs. (2.21) and (2.22), one finds for the lowest level

$$E=\frac{1}{2L^3}\hat{V}(\mathbf{0},\mathbf{0})+O(V^2). \tag{2.24}$$

Combining this result with the Born series (2.18), we have

$$E=-\frac{4\pi a_0}{mL^3}+O(V^2), \tag{2.25}$$

which already proves the large L expansion (1.3) to first order in V.

In what follows, the strategy is to write down the complete perturbation expansion of the energy levels in a tractable form and to analyze the L dependence of each term separately. As a result, one obtains a double expansion in powers of V and L^{-1}, which is not hard to regroup in the form of the desired large L expansions with coefficients expressed through the scattering amplitude.

2.2. Perturbation Theory to All Orders

High order perturbation theory can be formulated in many different ways. The aim here is to present one such possibility in a compact notation, which makes the essential structure transparent. Moreover, many of the formulae derived below will be useful in quantum field theory, too.

Using the cubic rotation symmetry, the degeneracy of the low-lying energy levels (2.23) can be lifted, and it is therefore sufficient for our purposes to consider the case of non-degenerate perturbation theory. Thus, let E_0 be an eigenvalue of $\mathbb{H}_0$ and $|\psi_0\rangle$ the corresponding eigenstate normalized to unity. For small V, one then expects that the full Hamiltonian $\mathbb{H}$ has an isolated eigenvalue E with $E=E_0+O(V)$. Define

$$F(z)=\langle\psi_0|(z-\mathbb{H})^{-1}|\psi_0\rangle. \tag{2.26}$$

This is a meromorphic function of z with simple poles at the eigenvalues of $\mathbb{H}$, in particular, there is a pole at $z=E$. Expanding in powers of V, we have

$$F(z)=(z-E_0)^{-1}+(z-E_0)^{-2}\langle\psi_0|\mathbb{V}\sum_{n=0}^{\infty}[(z-\mathbb{H}_0)^{-1}\mathbb{V}]^n|\psi_0\rangle. \tag{2.27}$$

In this form, the perturbation expansion is however not very useful, because as z gets close to E (and hence close to E_0), $(z-\mathbb{H}_0)^{-1}$ has a pole and the series explodes.

To obtain a representation, which is smooth near E, we first separate the pole at $z=E_0$ from the free propagator:

$$(z-\mathbb{H}_0)^{-1}=\frac{P_0}{z-E_0}+\frac{Q_0}{z-\mathbb{H}_0},\qquad P_0=|\psi_0\rangle\langle\psi_0|,\qquad Q_0=1-P_0. \tag{2.28}$$

Then, using the operator identity

$$A\sum_{n=0}^{\infty}[(B+C)A]^n=A'\sum_{n=0}^{\infty}(BA')^n,\qquad A'=A\sum_{n=0}^{\infty}(CA)^n, \tag{2.29}$$

with $A = \mathbb{V}$, $B = P_0/(z - E_0)$ and $C = Q_0/(z - \mathbb{H}_0)$, one gets

$$F(z) = (z - E_0 - r(z))^{-1}, \tag{2.30}$$

$$r(z) = \langle \psi_0 | \mathbb{V} \sum_{n=0}^{\infty} \left[\frac{Q_0}{z - \mathbb{H}_0} \mathbb{V} \right]^n | \psi_0 \rangle . \tag{2.31}$$

Note that the projector Q_0 excludes the eigenvalue E_0 and $r(z)$ is hence smooth in a neighborhood of E_0. It follows that (2.30) is a valid representation of $F(z)$ around E_0 and the eigenvalue E is thus determined by the implicit equation

$$E = E_0 + r(E) \tag{2.32}$$

(and the condition that $E - E_0$ is small).

In principle, Eq. (2.32) can be solved straightforwardly by inserting the perturbation series for E, expanding all entries in powers of V and equating coefficients of the same order. A more elegant way to proceed is to first expand E in powers of the function $r(z)$. To this end, it is helpful to introduce an auxiliary parameter ε as a bookkeeping device. Thus, Eq. (2.32) and the desired expansion of E are written as

$$E = E_0 + \varepsilon r(E), \tag{2.33}$$

$$E = \sum_{\nu=0}^{\infty} \varepsilon^{\nu} E_{\nu}, \tag{2.34}$$

with ε set equal to 1 at the end of the derivation. In this way one generates the solution E of Eq. (2.32) as a power series of $r(z)$.

To determine the coefficients E_ν, we now insert (2.34) into (2.33), expand in powers of ε and obtain the recursion

$$\begin{aligned} E_1 &= r_0, \\ E_{\nu+1} &= \sum_{j=1}^{\nu} r_j \sum_{l_1=1}^{\nu} \dots \sum_{l_j=1}^{\nu} \delta_{l_1+l_2+\dots+l_j,\nu} E_{l_1} E_{l_2} \dots E_{l_j}, \end{aligned} \tag{2.35}$$

where r_j is given by

$$r_j = \frac{1}{j!} \frac{\partial^j}{\partial z^j} r(z)|_{z=E_0}. \tag{2.36}$$

For example, for the next to lowest coefficients E_ν, one finds

$$E_2 = r_0 r_1, \qquad E_3 = r_0 r_1^2 + r_0^2 r_2, \tag{2.37}$$

and it would not be difficult to continue this list. Setting $\varepsilon = 1$, the resulting expansion of the energy value E thus becomes

$$\begin{aligned} E &= E_0 + \sum_{\nu=1}^{\infty} E_\nu, \\ E_\nu &= \sum_{j_1=0}^{\nu} \dots \sum_{j_\nu=0}^{\nu} C(j_1, \dots, j_\nu) r_{j_1} r_{j_2} \dots r_{j_\nu}, \end{aligned} \tag{2.38}$$

where $C(j_1, \dots, j_\nu)$ are some integer coefficients satisfying

$$C(j_1, \dots, j_\nu) = 0 \quad \text{if} \quad j_1 + j_2 + \dots + j_\nu \neq \nu - 1 \tag{2.39}$$

(an explicit expression for these coefficients exists but is not needed here).

Because $r(z)$ is of order V, only a finite number of terms in the expansion (2.38) contribute at a fixed order of V and, inserting (2.31), it would now not be difficult to write down the exact n'th order expression for the energy. For our purposes, Eq. (2.38) will however turn out to be sufficiently explicit and this last step is therefore not worked out here.

In the present approach to perturbation theory, the function $r(z)$ defined by Eq. (2.31) plays a central rôle. For the ground state level already discussed at the end of the preceding subsection, we have for example

$$r(z)=\frac{1}{2L^3}\left\{\hat{V}(\mathbf{0},\mathbf{0})+\sum_{n=1}^{\infty}\frac{(-1)^n}{2^n}L^{-3n}\sum_{\mathbf{k}_1\neq 0}\cdots\sum_{\mathbf{k}_n\neq 0}\right.$$
$$\left.\times\hat{V}(\mathbf{0},\mathbf{k}_1)R_z(\mathbf{k}_1)\hat{V}(\mathbf{k}_1,\mathbf{k}_2)R_z(\mathbf{k}_2)\ldots\hat{V}(\mathbf{k}_n,\mathbf{0})\right\}, \tag{2.40}$$

where the momenta $\mathbf{k}_j$ are summed over the lattice (1.2) and $\hat{V}$ and R_z are given by (2.16) and (2.17) (omitting $i\varepsilon$). Evidently, the Born series (2.15) and the series above are very similar, the main difference being that the momentum integrals are here replaced by sums.

To second order, Eq. (2.40) leads to

$$E=\frac{1}{2L^3}\left\{\hat{V}(\mathbf{0},\mathbf{0})-\frac{1}{2L^3}\sum_{\mathbf{k}\neq 0}\hat{V}(\mathbf{0},\mathbf{k})\frac{m}{\mathbf{k}^2}\hat{V}(\mathbf{k},\mathbf{0})+\ldots\right\}. \tag{2.41}$$

Now, at large L the momentum sum on the right-hand side may be replaced by an integral plus an error term of order L^{-1} and, recalling (2.18), the formula

$$E=-\frac{4\pi a_0}{mL^3}+O(V^2L^{-4})+O(V^3) \tag{2.25'}$$

is obtained. This example shows that for the derivation of the large L expansion of E to all orders of V and L^{-1}, a complete and explicit asymptotic formula is needed expressing the momentum sums encountered as a sum of divergent terms (in singular cases), integrals and corrections. Such a formula is presented in the following subsection and proved in Appendix B.

2.3. Summation Formulae for 3-Dimensional Momentum Sums

With the help of Poisson's summation formula (e.g. ref. [5, p. 31]), it is easy to prove the well-known result that

$$L^{-3}\sum_{\mathbf{k}}h(\mathbf{k})=\int\frac{d^3k}{(2\pi)^3}h(\mathbf{k})+O(L^{-N}) \tag{2.42}$$

for any continuous function h, which is integrable and which has integrable derivatives up to the N'th order ($N\geqq 1$). In this subsection, Eq. (2.42) is generalized to a larger class of momentum sums, involving singular functions h, such as they occur in the perturbation expansion of the finite volume energy values. Explicitly, the sums considered are of the form

$$S_q(f,\mathbf{q})=L^{-3}\sum_{\mathbf{k}}{}'\frac{f(\mathbf{k})}{(\mathbf{k}^2-\mathbf{p}^2)^q}, \tag{2.43}$$

where $\mathbf{p}=\frac{2\pi}{L}\mathbf{n}$, $\mathbf{n}\in\mathbb{Z}^3$, is a fixed external momentum, $q\geqq 1$ some integer power and the summation symbol $\sum'$ implies a sum over the lattice (1.2) excluding the points $\mathbf{k}$ with $\mathbf{k}^2=\mathbf{p}^2$. The function f is assumed to be square integrable and smooth with square integrable partial derivatives of arbitrary order. It is easy to show that these properties guarantee the absolute convergence of the sum (2.43).

Due to the singularity, the large L expansion of $S_q(f,\mathbf{p})$ does not only involve an integral over all $\mathbf{k}$ as in Eq. (2.42), but also other terms, which are proportional to the function $f(\mathbf{k})$ and its derivatives evaluated along the sphere $\mathbf{k}^2=\mathbf{p}^2$. These latter terms are multiplied by geometrical numbers, analogous to the Bernoulli numbers in Euler's sum formula, which are related to the (generalized) zeta function $Z_{lm}(s,\mathbf{n}^2)$ of the momentum lattice defined below.

To write down the large L expansion of $S_q(f,\mathbf{p})$, some further preparation is needed. First, let $Y_{lm}(\theta,\varphi)$ be the spherical harmonics with the usual normalization[4] and define Q_{lm} through

$$Q_{lm}(\mathbf{k})=\sqrt{\frac{4\pi}{2l+1}}\,k^l Y_{lm}(\theta,\varphi)\,,$$

where θ, φ are the polar angles of $\mathbf{k}$ and $k=|\mathbf{k}|$. Q_{lm} is a homogeneous polynomial of $\mathbf{k}$ of degree l. The expansion of $f(\mathbf{k})$ into spherical harmonics can then be written as

$$f(\mathbf{k})=\sum_{l=0}^{\infty}\sum_{m=-l}^{l} f_{lm}(k)\,Q_{lm}(\mathbf{k})$$

with coefficients $f_{lm}(k)$, which are smooth for $k\geqq 0$. In particular, for all l, m and arbitrary $p=|\mathbf{p}|\geqq 0$, the Taylor coefficients $f_{jlm}(p)$ defined by

$$f_{lm}(k)\underset{k\to p}{\sim}\sum_{j=0}^{\infty} f_{jlm}(p)\,(k^2-p^2)^j$$

are also smooth and could themselves be expanded, for $p\to 0$, in an asymptotic power series of p^2.

The zeta function Z_{lm} alluded to above is defined by

$$Z_{lm}(s,\mathbf{n}^2)=\sum_{\mathbf{v}\in\mathbb{Z}^3}{}' Q_{lm}(\mathbf{v})\,(\mathbf{v}^2-\mathbf{n}^2)^{-s} \tag{2.47}$$

for all $\mathbf{n}\in\mathbb{Z}^3$ and complex s with $\mathrm{Re}\,s>\frac{1}{2}(l+3)$. As before, the points $\mathbf{v}$ with $\mathbf{v}^2=\mathbf{n}^2$ are omitted in the sum and for $\mathbf{v}^2<\mathbf{n}^2$, the convention $\arg(\mathbf{v}^2-\mathbf{n}^2)=\pi$ is adopted. Note that Z_{lm} vanishes if l is odd, because $Q_{lm}(-\mathbf{v})=-Q_{lm}(\mathbf{v})$ in this case. Some properties of Z_{lm} are derived in Appendix A, in particular, it is shown there that Z_{lm} extends to a meromorphic function of s defined in the whole complex plane with simple poles at

$$s=\tfrac{3}{2}-j\,,\qquad j=0,1,2,\ldots\,, \tag{2.48}$$

---

[4] In particular, $Y_{l0}(\theta,\varphi)=\sqrt{\frac{2l+1}{4\pi}}\,P_l(\cos\theta)$, where P_l denotes the l'th Legendre polynomial normalized such that $P_l(1)=1$

Table 1. Values of the zeta function Z_{lm}. The method of calculation used is explained in Appendix A

j	$Z_{00}(j, 0)$	$Z_{00}(j, 1)$
1	− 8.91363292	− 1.21133568
2	16.53231596	23.24322188
3	8.40192397	13.05937675
4	6.94580793	13.73121437

for $l=0$ and no poles for $l \neq 0$. Z_{lm} is therefore well-defined for integer s and it is found that

$$Z_{lm}(-j, \mathbf{n}^2)=0 \quad \text{for} \quad j=1,2,3,\ldots, \tag{2.49}$$

$$Z_{lm}(0, \mathbf{n}^2)= - \sum_{\mathbf{v}^2=\mathbf{n}^2} \mathcal{Q}_{lm}(\mathbf{v}). \tag{2.50}$$

For positive integers j, $Z_{lm}(j, \mathbf{n}^2)$ must be calculated numerically, a few values being listed in Table 1 for later use.

With all the definitions ready, we now proceed to discuss the large L expansion

$$S_q(f, \mathbf{p}) \sim I_q(f, \mathbf{p}) + \sum_{j=0}^{q} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{1}{L^3} \left(\frac{2\pi}{L}\right)^{2j+l-2q} f_{jlm}(p) Z_{lm}(q-j, \mathbf{n}^2), \tag{2.51}$$

which is proved in Appendix B. For notational convenience, odd l's are included in the sum although they do not contribute (Z_{lm} vanishes). The integral $I_q(f, \mathbf{p})$ is given by

$$I_q(f, \mathbf{p}) = \lim_{\varepsilon \to 0} \int \frac{d^3k}{(2\pi)^3} \operatorname{Re}\{(\mathbf{k}^2 - \mathbf{p}^2 - i\varepsilon)^{-q}\} f(\mathbf{k}) \tag{2.52}$$

for $\mathbf{p} \neq 0$ and by

$$I_q(f, \mathbf{0}) = \frac{1}{(2q-2)!} \int \frac{d^3k}{(2\pi)^3} \frac{1}{\mathbf{k}^2} (\Delta_k)^{q-1} f(\mathbf{k}) \tag{2.53}$$

for $\mathbf{p}=0$, where Δ_k denotes the Laplacian with respect to $\mathbf{k}$. It can be shown [5] that for the class of functions f considered here, $I_q(f, \mathbf{p})$ is well-defined and smooth for $\mathbf{p} \in \mathbb{R}^3$, in particular, the Taylor expansion

$$I_q(f, \mathbf{p}) \sim \sum_{j=0}^{\infty} \binom{-q}{j} (-\mathbf{p}^2)^j I_{q+j}(f, \mathbf{0}) \tag{2.54}$$

holds as expected naively.

The large L expansion (2.51) is an expansion in powers of $1/L$ with weakly L-dependent coefficients (if $\mathbf{p} \neq 0$). It is possible to convert the expansion in a pure power series by also expanding the integral $I_q(f, \mathbf{p})$ and the coefficients $f_{jlm}(p)$ for small $\mathbf{p}$. The reason this is not done here is that the convergence properties of this power series would be rather poor, especially when $\mathbf{n}$ is not small.

Formally, the series (2.51) can be derived by inserting the expansions (2.45) and (2.46) in the sum $S_q(f, \mathbf{p})$. In each term, a power of $2\pi/L$ can then be factored out and, taking (2.49) into account, the series (2.51) is obtained [without $I_q(f, \mathbf{p})$]. This "proof" involves unregularized divergent expressions and is therefore invalid, but since it gives the right result, it is useful as a mnemonic.

2.4. Large L Expansion of the Lowest Energy Value

As discussed in Subsect. 2.2, the ground state energy E of the finite volume system is given by Eq. (2.38), where r_j are the Taylor coefficients at $z=0$ of the function $r(z)$ defined by Eq. (2.40). In particular, we have

$$r_0 = \frac{1}{2L^3}\left\{\hat{V}(\mathbf{0},\mathbf{0}) + \sum_{n=1}^{\infty} \frac{(-1)^n}{2^n} L^{-3n} \sum_{\mathbf{k}_1 \neq 0} \cdots \sum_{\mathbf{k}_n \neq 0} \right.$$
$$\left. \times \hat{V}(\mathbf{0},\mathbf{k}_1)\frac{m}{\mathbf{k}_1^2}\hat{V}(\mathbf{k}_1,\mathbf{k}_2)\frac{m}{\mathbf{k}_2^2}\ldots\hat{V}(\mathbf{k}_n,\mathbf{0})\right\}. \tag{2.55}$$

The momentum sums occurring here are multiple sums of the type $S_q(f, \mathbf{p})$ with $q=1$, $\mathbf{p}=0$ and

$$f(\mathbf{k}_1, \ldots, \mathbf{k}_n) = \hat{V}(\mathbf{0},\mathbf{k}_1)\hat{V}(\mathbf{k}_1,\mathbf{k}_2)\ldots\hat{V}(\mathbf{k}_n,\mathbf{0}).$$

It follows from the assumed properties of the potential V that f is square integrable and smooth with square integrable derivatives. For such well-behaved functions f, it is not difficult to show that the large L expansion of multiple sums is obtained simply by applying Eq. (2.51) to each sum individually. Thus, r_0 can be expanded in a power series of $1/L$ and, recalling the Born series (2.18), the first few terms are found to be

$$r_0 = -\frac{4\pi a_0}{mL^3}\left\{1 + Z_{00}(1,0)\frac{a_0}{\pi L} + \left[Z_{00}(1,0)\frac{a_0}{\pi L}\right]^2\right\} + O(L^{-6}) \tag{2.56}$$

(to *all* orders of V). Similarly, one shows that

$$r_1 = -Z_{00}(2,0)\left(\frac{a_0}{\pi L}\right)^2 + O(L^{-3}), \tag{2.57}$$

and more generally

$$r_j = O(L^{2j-4}) \tag{2.57'}$$

for $j \geqq 1$.

From the large L expansion of the coefficients r_j, we can now easily deduce the expansion of the energy value E [cf. Eqs. (2.38), (2.39)]. Noting

$$r_{j_1}r_{j_2}\ldots r_{j_\nu} = O(L^{-\nu-3}) \quad \text{if} \quad j_1+j_2+\ldots+j_\nu = \nu-1 \geqq 1, \tag{2.58}$$

it follows that at a given order of L^{-1}, only a finite number of terms contribute to the series (2.38), in particular, we have

$$E = r_0 + r_0 r_1 + O(L^{-6}). \tag{2.59}$$

Thus, we have shown that E can be expanded in an asymptotic power series of $1/L$. Moreover, combining Eqs. (2.56)–(2.59), one obtains

$$E=-\frac{4\pi a_0}{mL^3}\left\{1+c_1\frac{a_0}{L}+c_2\frac{a_0^2}{L^2}\right\}+O(L^{-6}), \tag{2.60}$$

$$c_1=\frac{1}{\pi}Z_{00}(1,0)=-2.837297, \tag{2.61}$$

$$c_2=\frac{1}{\pi^2}\{Z_{00}(1,0)^2-Z_{00}(2,0)\}=6.375183. \tag{2.62}$$

In the ground state, the mesons are moving slowly and it is therefore not surprising that the result (2.60) coincides with the relativistic formula quoted in Sect. 1 (relativistic corrections would however show up at order L^{-6}). Using the machinery developed above, the series (2.60) could easily be extended by a few more terms. Besides the scattering length a_0, these terms involve derivatives of the scattering amplitude at zero momentum such as, for example, the threshold parameter b_0.

At this point, the reader may wonder why it is that the coefficients in the large L expansion of E are expressible through the scattering amplitude and apparently do not depend on the local properties of the interaction potential, i.e. on "off-shell" quantities. The reason for this remarkable fact is that the boundary conditions are only felt when the particles are far apart. Now, within a periodicity cell, the meson wave function can be represented by a superposition of infinite volume scattering waves with energy E. Since the amplitude of these waves at large distances is proportional to the scattering amplitude, the requirement of periodicity leads to an (implicit) eigenvalue equation for E in which the dynamics of the system is only represented through the scattering amplitude at energy E. Except for the case of $1+1$-dimensional quantum mechanics, which will be discussed later, this equation is complicated and is therefore not very useful, but it does explain why E is a function of the scattering amplitude at large L (cf. ref. [3] and Subsect. 2.7).

2.5. *Volume Dependence of Higher Energy Values*

The analysis which led to the large L expansion (2.60) of the ground state energy also applies to the higher lying energy values. For simplicity, the discussion is here restricted to states, which have zero total momentum and which are invariant under the action of the full cubic rotation group $\mathcal{O}\subset O(3)$. The subspace of all these states, later referred to as the A_1^+ sector, is spanned by the vectors

$$|\mathbf{p}, A_1^+\rangle=\sum_{R\in\mathcal{O}}|R\mathbf{p}, -R\mathbf{p}\rangle, \tag{2.63}$$

where $\mathbf{p}=\frac{2\pi}{L}\mathbf{n}$ and $\mathbf{n}$ runs over all integer vectors with $n_1\geqq n_2\geqq n_3\geqq 0$. The normalization of these states is given by

$$\langle\mathbf{p}', A_1^+|\mathbf{p}, A_1^+\rangle=96\mathcal{N}(\mathbf{p})L^6\delta_{\mathbf{p}'\mathbf{p}}, \tag{2.64}$$

where $\mathcal{N}(\mathbf{p})$ denotes the number of elements of $\mathcal{O}$, which leave $\mathbf{p}$ fixed. For example, if $n_1>0$, $n_2=n_3=0$, we have $\mathcal{N}(\mathbf{p})=8$.

Because the potential V is rotationally invariant, the Hamiltonian $\mathbb{H}$ can be considered an operator acting in the A_1^+ sector. For $V=0$, the eigenstates of $\mathbb{H}$ in this sector are the basis vectors $|\mathbf{p}, A_1^+\rangle$ and the corresponding energy values are equal to $2\varepsilon(\mathbf{p})$. From the above, it is easy to show that these energy levels are not degenerate for $\mathbf{n}^2 \leqq 8$ (and also for many higher values of $\mathbf{n}^2$).

We now choose a fixed $\mathbf{p}=\frac{2\pi}{L}\mathbf{n}$ such that the basis vector $|\mathbf{p}, A_1^+\rangle$ is a non-degenerate eigenvector of $\mathbb{H}_0$ in the A_1^+ sector. The associated eigenvalue E of the full Hamiltonian can then be calculated in perturbation theory using the formalism developed in Subsect. 2.2. With $|\mathbf{p}, A_1^+\rangle$ as the unperturbed state, the function $r(z)$ defined there is given by

$$r(z)=(2\mathcal{N}(\mathbf{p})L^3)^{-1}\sum_{R\in\mathcal{O}}\left\{\hat{V}(R\mathbf{p},\mathbf{p})+\sum_{n=1}^{\infty}\frac{(-1)^n}{2^n}L^{-3n}\sum_{\mathbf{k}_1}{}'\ldots\sum_{\mathbf{k}_n}{}'\right.$$
$$\left.\times\hat{V}(R\mathbf{p},\mathbf{k}_1)R_z(\mathbf{k}_1)\hat{V}(\mathbf{k}_1,\mathbf{k}_2)R_z(\mathbf{k}_2)\ldots\hat{V}(\mathbf{k}_n,\mathbf{p})\right\}, \tag{2.65}$$

where the momenta $\mathbf{k}$ are summed over the lattice (1.2) omitting the points with $\mathbf{k}^2=\mathbf{p}^2$.

As for the ground state, the large L expansion of the energy E is obtained by first expanding the Taylor coefficients r_j of $r(z)$ defined by Eq. (2.36). According to the summation formula (2.51), the leading contribution to the coefficient r_0 at large L is simply given by replacing the momentum sums by integrals and using an $i\varepsilon$-prescription to integrate over the singularities at $\mathbf{k}^2=\mathbf{p}^2$. Thus, we have

$$r_0=(2\mathcal{N}(\mathbf{p})L^3)^{-1}\sum_{R\in\mathcal{O}}\mathcal{M}(R\mathbf{p},\mathbf{p})+O(L^{-4}), \tag{2.66}$$

$$\mathcal{M}(\mathbf{p}',\mathbf{p})=\hat{V}(\mathbf{p}',\mathbf{p})+\sum_{n=1}^{\infty}\frac{(-1)^n}{2^n}\int\frac{d^3k_1}{(2\pi)^3}\cdots\frac{d^3k_n}{(2\pi)^3}$$
$$\times\hat{V}(\mathbf{p}',\mathbf{k}_1)\,\mathrm{Re}\left\{\frac{m}{\mathbf{k}_1^2-\mathbf{p}^2-i\varepsilon}\right\}\hat{V}(\mathbf{k}_1,\mathbf{k}_2)\,\mathrm{Re}\left\{\frac{m}{\mathbf{k}_2^2-\mathbf{p}^2-i\varepsilon}\right\}\ldots\hat{V}(\mathbf{k}_n,\mathbf{p}) \tag{2.67}$$

(here and below, we assume $|\mathbf{p}'|=|\mathbf{p}|$). It is possible to express the matrix element $\mathcal{M}(\mathbf{p}',\mathbf{p})$ through the scattering amplitude T_{nr} at energy $2\varepsilon(\mathbf{p})$. To this end, one substitutes

$$\mathrm{Re}(\mathbf{k}^2-\mathbf{p}^2-i\varepsilon)^{-1}=(\mathbf{k}^2-\mathbf{p}^2-i\varepsilon)^{-1}-i\pi\delta(\mathbf{k}^2-\mathbf{p}^2) \tag{2.68}$$

and uses the rearrangement identity (2.29) to sum up those terms in the perturbation series (2.67), which combine to the scattering amplitude. After that one is left with a series, which can easily be summed by inserting the partial wave expansion (2.12), and the result then is

$$\mathcal{M}(\mathbf{p}',\mathbf{p})=-\frac{8\pi}{m}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)\frac{\mathrm{tg}\,\delta_l}{p}, \tag{2.69}$$

where $p=|\mathbf{p}|$ and θ is the angle between $\mathbf{p}$ and $\mathbf{p}'$.

With the matrix $\mathscr{M}(\mathbf{p}',\mathbf{p})$ at our disposal, it is not hard to calculate a few more terms in the large L expansion of the coefficients r_j. For the energy E, this leads to the expansion

$$E=2\varepsilon(\mathbf{p})+r_0+r_0r_1+O(L^{-6}), \tag{2.70}$$

where r_0 and r_1 are given by

$$\begin{aligned} r_0=&-\frac{4\pi}{mL^3}\sum_{l=0}^{\infty}(2l+1)\langle P_l\rangle\frac{\operatorname{tg}\delta_l}{p} \\ &\times\left\{1+Z_{00}(1,\mathbf{n}^2)\frac{\operatorname{tg}\delta_l}{\pi pL}+\left[Z_{00}(1,\mathbf{n}^2)\frac{\operatorname{tg}\delta_l}{\pi pL}\right]^2\right\}+O(L^{-6}), \end{aligned} \tag{2.71}$$

$$r_1=-\sum_{l=0}^{\infty}(2l+1)\langle P_l\rangle Z_{00}(2,\mathbf{n}^2)\left[\frac{\operatorname{tg}\delta_l}{\pi pL}\right]^2+O(L^{-3}). \tag{2.72}$$

The quantities $\langle P_l\rangle$ appearing in these equations are defined through

$$\langle P_l\rangle=\frac{1}{\mathscr{N}(\mathbf{p})}\sum_{R\in\mathcal{O}}P_l(\cos\theta_R), \tag{2.73}$$

θ_R being the angle between $\mathbf{p}$ and $R\mathbf{p}$. In particular, $\langle P_0\rangle=48/\mathscr{N}(\mathbf{p})$ and $\langle P_2\rangle=0$ for all $\mathbf{p}$.

Equation (2.70) together with (2.71), (2.72) is the final result for general $\mathbf{p}$. It shows that away from resonances (where $\operatorname{tg}\delta_l$ blows up), the corrections to the free particle energy spectrum are small and calculable for large L, provided the phase shifts are known at the energy $2\varepsilon(\mathbf{p})\simeq E$ considered. Conversely, if some finite volume energy values have been computed by independent means (by a numerical simulation, for example), the relation allows us to determine the phase shifts at these energies or at least some combinations of them.

For small $\mathbf{p}$, the partial wave expansions (2.71) and (2.72) are dominated by the S-wave contribution so that the large L expansion of the associated energy values assumes a simple form. For example, for $\mathbf{n}=(1,0,0)$, one obtains

$$E=\frac{4\pi^2}{mL^2}-\frac{12\operatorname{tg}\delta_0}{mL^2}\{1+c_1'\operatorname{tg}\delta_0+c_2'\operatorname{tg}^2\delta_0\}+O(L^{-6}), \tag{2.74}$$

$$c_1'=\frac{1}{2\pi^2}Z_{00}(1,1)=-0.061367, \tag{2.75}$$

$$c_2'=\frac{1}{4\pi^4}\{Z_{00}(1,1)^2-6Z_{00}(2,1)\}=-0.354156 \tag{2.76}$$

(the phase shift δ_0 is to be evaluated at $p=2\pi/L$).

2.6. *Numerical Study of a Simple Model*

The purpose of the present subsection is to test the large L expansions (2.60) and (2.74) in a concrete case. An important result will be that these formulae are apparently also valid in the presence of bound states, although they have only been proved in perturbation theory.

The model considered is defined by

$$V(\mathbf{z})=\begin{cases}V_0 & \text{if } |\mathbf{z}|\leqq R\,,\\ 0 & \text{otherwise}\,,\end{cases} \tag{2.77}$$

where V_0 is a constant. For this potential, the scattering phase shifts are known exactly, in particular, δ_0 is determined through

$$\operatorname{tg}(pR+\delta_0)=\frac{p}{q}\operatorname{tg}(qR)\,,\qquad q^2=p^2-mV_0 \tag{2.78}$$

(p: meson momentum in the centre of mass system). The S-wave scattering length is thus given by

$$a_0=R\left(\frac{1}{v}\operatorname{tg}v-1\right)\quad(v\leqq 0)\,,\qquad a_0=R\left(\frac{1}{v}\operatorname{tgh}v-1\right)\quad(v\geqq 0)\,, \tag{2.79}$$

where we have introduced the dimensionless parameter

$$v=\operatorname{sign}(V_0)R\sqrt{m|V_0|}\,. \tag{2.80}$$

In what follows, m and R are assumed to be fixed whereas the parameter v is considered a variable characterizing the strength of the meson interaction.

If v is negative, the potential is attractive and bound states may occur. From Eq. (2.79), one sees that the scattering length diverges every time v passes through a negative odd multiple of $\pi/2$. The number of S-wave bound states is therefore equal to n if v is in the interval $-n-\frac{1}{2}<v/\pi<-n+\frac{1}{2}$. This observation also shows that the meson interactions should be considered strong unless (say) $|v|<1$.

In finite volume, the scaled energy values

$$\hat{E}=\frac{mL^2}{4\pi^2}E \tag{2.81}$$

only depend on v and L/R. For small and moderate values of v, an accurate variational calculation of the low-lying levels in the A_1^+ sector is possible by truncating the basis (2.63) after the first N_B elements and diagonalizing the Hamiltonian $\mathbb{H}$ numerically in the subspace spanned by these vectors. I have performed such a calculation with $N_B=100$, which is sufficient to obtain results accurate to several decimal places.

In Fig. 2 the 3 lowest energy values are plotted versus v at $L/R=8$, i.e. for a box size which is reasonably large compared to the interaction radius. For $v>0$, the force between the mesons is repulsive and the energy values $\hat{E}$ are therefore slightly larger than the free particle values $\hat{E}_0$, which are equal to 0, 1 and 2 respectively. The smallness of the deviations $\Delta\hat{E}=\hat{E}-\hat{E}_0$ indicates that at this value of the box size, the asymptotic scaling law $\Delta\hat{E}\propto 1/L$ has already set in. For small negative v, the situation is similar, although, of course, the energy values are now lowered by the interaction. As v passes through $-\frac{1}{2}\pi$, the ground state turns into a bound state and the first two excited levels drop by essentially one unit. These latter states thus become the lowest finite volume scattering states in the interval $-\frac{3}{2}\pi<v<-\frac{1}{2}\pi$.

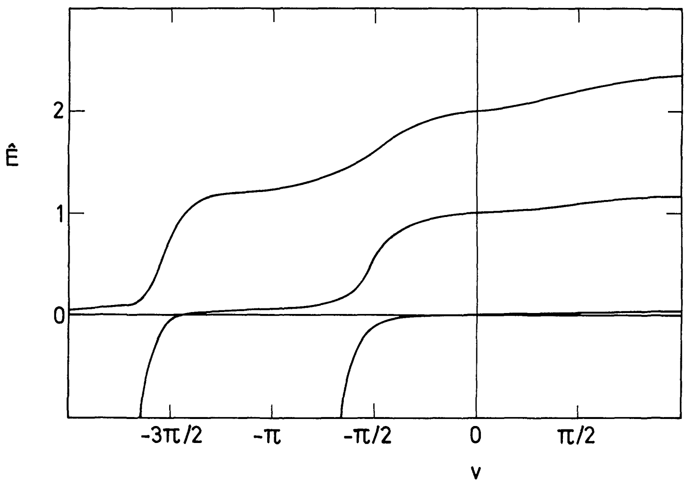

Fig. 2. Numerically calculated energy values $\hat{E}$ as a function of the parameter v for a fixed box size $L=8R$. Only the 3 lowest levels are shown

When v is further decreased, a second bound state forms at $v=-\frac{3}{2}\pi$ and the picture repeats itself.

In a larger volume, the curves in Fig. 2 change in two respects. First, the plateaus away from the transition points get even more pronounced and move closer to the integer values $\hat{E}=0,1,2$. Secondly, the transition regions near $v=-\frac{1}{2}\pi, -\frac{3}{2}\pi, \ldots$ shrink, i.e. for very large L/R, the curves essentially become step functions.

The plateaus in Fig. 2 can be understood by noting that a_0/L and $\mathrm{tg}\,\delta_0/pL$ (for small p) are small unless v is close to the transition points. The large L expansions established in the preceding subsections therefore apply and the calculated energy shifts $\Delta\hat{E}$ come out to be small thus explaining the plateaus. On the other hand, in the transition regions the energy shifts are of order 1 and the large L expansions diverge. Further analysis would therefore be required, if a quantitative understanding of the energy levels in such a resonant situation is to be achieved, too.

In places where they apply, the large L expansions (2.60) and (2.74) fit the numerically calculated energy values exceedingly well. This is shown in Fig. 3 for $v=\pi$, i.e. for a strongly repulsive potential. For smaller values of v, the agreement is even better and extends to lower values of L/R. In the presence of bound states, the expansions are apparently also valid, if one applies them to the lowest finite volume scattering states as explained above. For example, at $v=-\pi$, where there is one bound state, the quality of the fit obtained is about the same as at $v=\pi$. This confirms the expectation that the large L expansions established in this paper are universally valid, even though they have only been proved to all orders of perturbation theory.

2.7. *One-Dimensional Quantum Mechanics*

In a one-dimensional box of size L, the probability for the particles to meet is proportional to $1/L$ and the finite size energy shifts are therefore not small

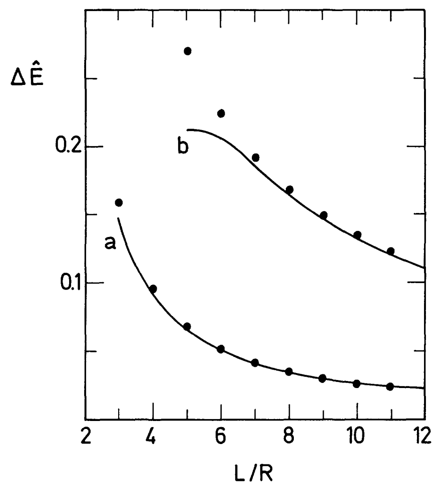

Fig. 3. Comparison of the large L expansions (2.60) (curve a) and (2.74) (curve b) with numerically calculated energy values (dots) for $v=\pi$. The energy shift $\Delta\hat{E}$ is equal to $\hat{E}-\hat{E}_0$, where $\hat{E}_0=0$ for the ground state and $\hat{E}_0=1$ for the first excited state

compared to the free particle level splitting. For this kinematical reason, the perturbative techniques developed in the preceding subsections do not apply in one dimension. The situation is however so simple that an exact relation between finite volume energy values and the scattering amplitude can be established with little effort.

The basic observation is that for zero total momentum and fixed energy E, the Schrödinger equation in infinite volume has only one solution ψ_E (respecting Bose statistics). Outside the interaction range R, this solution is given by

$$\psi_E(x,y)\propto e^{-ip|x-y|}+e^{2i\delta_0}e^{ip|x-y|}, \tag{2.82}$$

where $p=\sqrt{mE}$ is the meson momentum and $\delta_0(p)$ the scattering phase shift. Since ψ_E is unique, any finite volume eigenfunction of the Hamiltonian with energy E and zero total momentum must be proportional to ψ_E for $|x-y|<\frac{1}{2}L$. For large L, the wave function near the boundary of this region is thus given by Eq. (2.82) and the requirement of periodicity hence leads to the beautiful formula

$$e^{2i\delta_0(p)}e^{ipL}=1, \tag{2.83}$$

which relates the finite volume energy value $E=p^2/m$ to the scattering phase shift δ_0 at this energy.

Although no proof will be given in this paper, Eq. (2.83) is probably also true in $1+1$-dimensional quantum field theories up to polarization terms, which decrease exponentially as L increases. A numerical lattice calculation of the scattering phase shift at low energies should therefore be possible in these theories simply by evaluating the lowest two-particle energies for a few lattices with variable size (and fixed couplings). In particular, it would be interesting to see whether the known exact S-matrices of some "integrable" theories such as the non-linear σ-model can be reproduced in this way.

3. Volume Dependence of Two-Particle Energies in Quantum Field Theory

In quantum field theories, large L expansions of the two-particle energy values exist as in quantum mechanics, but their proof is slightly more complicated because of polarization effects. To keep the presentation as simple as possible, we here again restrict the discussion to the class of scalar quantum field theories defined at the beginning of Sect. 2 of ref. [1]. The reader is thus assumed to have read these introductory paragraphs and the notation used there is completely taken over without further reference.

For the derivation of the large L expansions, we shall make two further assumptions to avoid unnecessary technical complications, which would only obscure the essential parts of the argumentation. The first one is that the theory is invariant under the reflection $\phi(x) \to -\phi(x)$ so that correlation functions of an odd number of fields vanish. The second requirement is that the theory has a fixed ultra-violet cutoff, which is relativistically invariant and which guarantees the convergence of unsubtracted Feynman diagrams. These assumptions are not really necessary and, with some effort, the large L expansions could also be proved without them.

In what follows, the strategy is to derive a representation of the elastic scattering amplitude and of the perturbation series for finite volume energy values, which has the quantum mechanical form with a modified Bethe-Salpeter kernel in place of the potential $\hat{V}(\mathbf{k}', \mathbf{k})$. The techniques developed in Sect. 2 can then be carried over and the large L expansions are obtained as before.

3.1. Definition and Properties of the Bethe-Salpeter Kernel

The dynamics of two-particle states in the scalar quantum field theories considered here is governed by the Bethe-Salpeter (or two-particle irreducible) kernel, which will be denoted by $BS(p_1, p_2, p_3, p_4)$ in infinite volume ($p_1, \ldots, p_4$ are external euclidean 4-momenta). In perturbation theory, $BS(p_1, p_2, p_3, p_4)$ is equal to the sum of all those Feynman diagrams contributing to $G(p_1, p_2, p_3, p_4)$, which are two-particle irreducible in the (p_1, p_2)-channel, i.e. diagrams with a skeleton as in Fig. 4 are excluded.

The full connected 4-point function $G(p_1, p_2, p_3, p_4)$ can be expressed through the Bethe-Salpeter kernel by iterating the integral equation graphically represented by Fig. 5. To write down the resulting geometric series in a compact form, we introduce the following notation. First, define P, p', and p such that

$$p_1 = \tfrac{1}{2}P + p', \quad p_2 = \tfrac{1}{2}P - p', \tag{3.1}$$

$$p_3 = -(\tfrac{1}{2}P + p), \quad p_4 = -(\tfrac{1}{2}P - p). \tag{3.2}$$

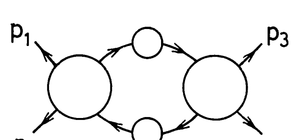

Fig. 4. Skeleton of a Feynman diagram, which is two-particle reducible in the (p_1, p_2)-channel

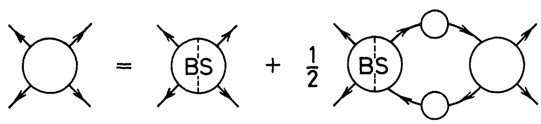

Fig. 5. Integral equation relating the Bethe-Salpeter kernel to the full connected 4-point function

Because of momentum conservation, the total momentum P flowing through the Bethe-Salpeter kernels and the two-particle propagators is always the same so that in what follows, the dependence on P is not explicitly indicated. Accordingly, we set

$$K(p', p) = BS(p_1, p_2, p_3, p_4), \tag{3.3}$$

$$G2(k) = G(\tfrac{1}{2}P + k)G(\tfrac{1}{2}P - k), \tag{3.4}$$

and the series alluded to above then reads

$$\begin{aligned} G(p_1, p_2, p_3, p_4) &= K(p', p) \\ &+ \sum_{n=1}^{\infty} \frac{1}{2^n} \int \frac{d^4k_1}{(2\pi)^4} \cdots \frac{d^4k_n}{(2\pi)^4} K(p', k_1)G2(k_1)K(k_1, k_2)G2(k_2)\ldots K(k_n, p). \end{aligned} \tag{3.5}$$

This equation resembles the Born series (2.15) for the non-relativistic scattering amplitude, but there are some important differences, in particular, the relative energies k_i^0 of the intermediate two-particle states are not restricted to the mass shell.

As a function of the total energy P_0, the 4-point function $G(p_1, \ldots, p_4)$ has a cut in the complex plane, which stems from the real two-particle intermediate states in Eq. (3.5). To exhibit this singular structure more clearly, we shall later deform the k_i^0 integration contours to pick up the contributions of the meson poles in the two-particle propagators. That there are no other singularities below the 4-particle threshold is guaranteed by

Theorem 3.1. *To all orders of perturbation theory and for arbitrary real* $\mathbf{P}$, $\mathbf{p}'$, *and* $\mathbf{p}$, *the Bethe-Salpeter kernel* $K(p', p)$ *extends to an analytic function of* P_0, p'_0, *and* p_0 *in the domain*

$$|\mathrm{Im}\, P_0| < 4m, \qquad |\mathrm{Im}\, p'_0| < m, \qquad |\mathrm{Im}\, p_0| < m. \tag{3.6}$$

Proof [5]. Let $\mathscr{D}$ be a Feynman diagram contributing to $BS(p_1, p_2, p_3, p_4)$ and let $\mathscr{G}$ be the associated abstract graph (cf. Subsect. 2.3 of ref. [1]). $\mathscr{G}$ has 4 external vertices, denoted a_1, a_2, a_3, and a_4, where the external momenta p_i leave the diagram. It is possible that some of these vertices coincide.

As in the proof of Theorem 2.3 of ref. [1], we now proceed to construct optimally distributed flows of external momentum through $\mathscr{G}$. To this end, add 2 extra vertices u, v and 8 extra lines to $\mathscr{G}$ as shown in Fig. 6. This augmented graph is

[5] The analyticity properties of the Bethe-Salpeter kernel are of course well-known from axiomatic quantum field theory (e.g. ref. [12]). A proof of Theorem 3.1 is given here for completeness and as a preparation for the proof of Theorem 3.2

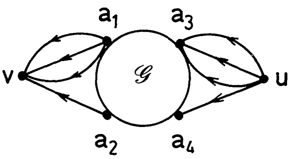

Fig. 6. Arrangement of extra vertices and lines added to the graph $\mathscr{G}$. The paths $\mathscr{P}_1, \ldots, \mathscr{P}_4$ start at u and pass through a_3 or a_4 via the extra lines connecting these vertices with u. After traversing $\mathscr{G}$, they arrive at a_1 or a_2 and end at v

3-particle irreducible between u and v, and, in view of Theorem 2.2 of ref. [1], there are therefore 4 disjoint paths $\mathscr{P}_1, \ldots, \mathscr{P}_4$ connecting u and v. The orientation of these paths is fixed by declaring u to be the initial and v the final point. For every line l in $\mathscr{G}$, define

$$[\mathscr{P}_i : l] = \begin{cases} \pm 1 & \text{if } l \in \mathscr{P}_i, \\ 0 & \text{otherwise}, \end{cases}$$

where the sign is $+1$, if the orientations of l and $\mathscr{P}_i$ coincide, and -1, if they are opposite. With the help of these orientation numbers, an integer valued flow $f_1(l)$ can be defined through

$$f_1(l) = \sum_{i=1}^{4} [\mathscr{P}_i : l].$$

By construction, f_1 is conserved at every internal vertex and the outflowing units at a_1, a_2, a_3, and a_4 are $3, 1, -3$, and -1 respectively. Furthermore, because the paths $\mathscr{P}_i$ are disjoint, we have $|f_1(l)| \leqq 1$ for all lines l in $\mathscr{G}$.

By permuting a_1 with a_2 and a_3 with a_4 in Fig. 6, further integer flows f_2, f_3, and f_4 can be constructed analogously. Consider now the momentum flow

$$k(l) = \sum_{i=1}^{4} f_i(l) q_i,$$

where $q_1, \ldots, q_4$ are arbitrary constant 4-momenta. At every internal vertex, this flow is conserved, and at the vertices $a_1, \ldots, a_4$ the outflowing momenta $p_1, \ldots, p_4$ are given by Eqs. (3.1), (3.2) with

$$\begin{aligned} \tfrac{1}{4}P &= q_1 + q_2 + q_3 + q_4, \\ p' &= q_1 + q_2 - q_3 - q_4, \\ p &= -q_1 + q_2 - q_3 + q_4. \end{aligned} \tag{3.7}$$

Moreover, we have

$$|\mathrm{Im}\, k(l)| \leqq \sum_{i=1}^{4} |\mathrm{Im}\, q_i| \quad \text{for all } l,$$

so that the singularities of the Feynman integrand of the diagram are avoided if the bound

$$\sum_{i=1}^{4} |\mathrm{Im}\, q_i| < m \tag{3.8}$$

is satisfied.

For given P, p', and p, the momenta q_i are not uniquely determined by the linear system (3.7). We may thus impose a further constraint, for example $q_1=0$. The solution of (3.7) then reads

$$q_2=\tfrac{1}{8}P+\tfrac{1}{2}p', \quad q_3=\tfrac{1}{8}P-\tfrac{1}{2}p, \quad q_4=\tfrac{1}{2}p-\tfrac{1}{2}p', \tag{3.9}$$

and the flow $k(l)$ is thus completely determined by the external momenta. The relations (3.9) and the bound (3.8) define an open complex domain $\mathbb{D}_1$ in the space of complex momenta P, p', and p. This domain contains the real momentum configurations and is convex. Moreover, by the above, $\mathbb{D}_1$ is a domain of analyticity of the Feynman integral associated to the diagram $\mathscr{D}$.

Instead of choosing $q_1=0$, we may just as well set $q_i=0$ for some $i=2,3,4$ and one then obtains a domain $\mathbb{D}_i$ of analyticity for each choice. Now we note that $\mathbb{D}_i \cap \mathbb{D}_j$ is a convex domain containing the real momentum configurations and the analytic continuations of the Feynman integral associated to $\mathscr{D}$ in the domains $\mathbb{D}_i$ and $\mathbb{D}_j$ therefore coincide on the overlap $\mathbb{D}_i \cap \mathbb{D}_j$. It follows that the Feynman integral extends to a single valued analytic function in the total domain

$$\mathbb{D}_{\mathrm{BS}}=\bigcup_{i=1}^{4} \mathbb{D}_i,$$

which contains all momenta satisfying the bound

$$|\tfrac{1}{4}\operatorname{Im}P+s'\operatorname{Im}p'|+|\tfrac{1}{4}\operatorname{Im}P+s\operatorname{Im}p|+|s'\operatorname{Im}p'+s\operatorname{Im}p|<2m$$

for some choice of signs $s', s=\pm 1$. With this explicit characterization, it is now not difficult to verify that $\mathbb{D}_{\mathrm{BS}}$ includes the domain (3.6). □

In finite volume, the Bethe-Salpeter kernel $K_L(p',p)$ is defined in exactly the same way as in infinite volume, i.e. every Feynman diagram contributing to $K(p',p)$ also contributes to $K_L(p',p)$ with all integrals over the space components of the loop momenta being replaced by sums over the lattice (1.2). It is obvious that Theorem 3.1 also applies in finite volume, and at large L the behaviour of $K_L(p',p)$ is described by

Theorem 3.2. *Suppose P_0, p_0', and p_0 are complex and satisfy the bounds* (3.6). *Then, to all orders of perturbation theory and for arbitrary (real)* $\mathbf{P}$, $\mathbf{p}'$, and $\mathbf{p}$, *we have*

$$K_L(p',p) \underset{L\to\infty}{=} K(p',p)+O(L^{-N}) \tag{3.10}$$

for all $N \geqq 1$.

Proof. Let $\mathscr{D}$ be a Feynman diagram contributing to the Bethe-Salpeter kernel and let $k(l)$ be the flow of external momentum constructed in the proof of Theorem 3.1. With this choice of momentum flow, the Feynman integrand associated to $\mathscr{D}$ is a C^∞ function of the loop momenta and the regular summation theorem (2.42) hence implies (3.10). □

Actually, using the techniques of ref. [1], it is possible to show that the difference K_L-K decays exponentially for large L, but for the present purposes, the weaker statement (3.10) is quite sufficient. In what follows, terms which vanish more rapidly than any power of $1/L$ are neglected, in particular, K_L is set equal to K without further notice.

3.2. Singularities of the Two-Particle Propagator

The elastic meson scattering amplitude is obtained from the euclidean 4-point function $G(p_1, p_2, p_3, p_4)$ by analytic continuation to purely imaginary energy components p_i^0 (cf. Subsect. 2.1 of ref. [1]). In view of Theorem 3.1, this analytic continuation presents no problem for the first term in the expansion (3.5) of the 4-point function, but the higher terms involve the two-particle propagator $G2(k)$, which gives rise to singularities in the elastic region $2m \leqq \mathrm{Im}\, P_0 < 4m$. We are thus led to study the analyticity properties of integrals of the form

$$J = \int \frac{dk_0}{2\pi} f(k_0) G2(k), \tag{3.11}$$

where $f(k_0)$ is a testfunction analytic in the strip $|\mathrm{Im}\, k_0| < m$ and $\mathbf{k}$ is real.

Lemma 3.3. *In the centre of mass system* ($\mathbf{P}=0$), *the integral* J *extends to an analytic function of* P_0 *in the region* $0 \leqq \mathrm{Im}\, P_0 < 4m$ *with a simple pole at* $P_0 = i2\omega(\mathbf{k})$ (*if* $\omega(\mathbf{k}) < 2m$)[6]. *The residue of the pole is given by*

$$J = \frac{f(0)}{(2\omega(\mathbf{k}))^2} (2\omega(\mathbf{k}) + iP_0)^{-1} + O(1). \tag{3.12}$$

Proof. It is a well-known consequence of the Källén-Lehmann representation that the single particle propagator $G(q)$ can be written as

$$G(q) = (m^2 + q^2)^{-1} + \hat{G}(q),$$

where $\hat{G}(q)$ is analytic for $q^2 > -(3m)^2$. It follows from this representation that in the centre of mass system and for $0 \leqq \mathrm{Im}\, P_0 < 4m$, the only singularities of $G2(k)$ in the strip $|\mathrm{Im}\, k_0| < m$ are simple poles at

$$k_0 = \pm(\tfrac{1}{2}P_0 - i\omega(\mathbf{k})). \tag{3.13}$$

If $\omega(\mathbf{k}) \geqq 2m$, these poles keep away from the real line and the integral J is therefore analytic in the whole strip $0 \leqq \mathrm{Im}\, P_0 < 4m$. On the other hand, if $\omega(\mathbf{k}) < 2m$, the poles approach the real axis from above and below as $\mathrm{Im}\, P_0$ grows towards $2\omega(\mathbf{k})$ and the integral develops a singularity.

To work out the singularity, we first note that (3.11) is a valid representation of J in the region $0 \leqq \mathrm{Im}\, P_0 \leqq \omega(\mathbf{k})$. Next, for $\mathrm{Im}\, P_0 = \omega(\mathbf{k})$, we shift the k_0 integration contour to the line $\mathrm{Im}\, k_0 = m'$, where m' is some mass in the interval $\frac{1}{2}\omega(\mathbf{k}) < m' < m$. Along the way one picks up a contribution from the pole at $k_0 = -\frac{1}{2}P_0 + i\omega(\mathbf{k})$, and the integral J thus becomes

$$J = \frac{f(\hat{k}_0)}{2\omega(\mathbf{k})} G(\tfrac{1}{2}P - \hat{k}) + \int_{\mathrm{Im}\, k_0 = m'} \frac{dk_0}{2\pi} f(k_0) G2(k), \tag{3.14}$$

where $\hat{k}$ is given by

$$\hat{k} = (i\omega(\mathbf{k}) - \tfrac{1}{2}P_0, \mathbf{k}). \tag{3.15}$$

As long as $\omega(\mathbf{k}) \leqq \mathrm{Im}\, P_0 < 2(m + m')$, the poles (3.13) do not cross the integration path $\mathrm{Im}\, k_0 = m'$ and the representation (3.14) hence defines an analytic function in

[6] Recall $\omega(\mathbf{k}) = \sqrt{m^2 + \mathbf{k}^2}$

this domain with a simple pole at $P_0 = i2\omega(\mathbf{k})$ coming from the first term. Since m' can be arbitrarily close to m, we have thus shown that J is analytic in the total domain $0 \leqq \mathrm{Im} P_0 < 4m$ with a pole as described by Eq. (3.12). □

If we consider $G2(k)$ a distribution on the space of test functions $f(k_0)$ which are analytic for $|\mathrm{Im}\, k_0| < m$, the statement of the lemma may be summarized by

$$G2(k) = [(2\omega(\mathbf{k}))^2 (2\omega(\mathbf{k}) + iP_0)]^{-1} 2\pi\delta(k_0) + \widehat{G2}(k), \tag{3.16}$$

where $\widehat{G2}(k)$ is a distribution analytic in the domain $0 \leqq \mathrm{Im} P_0 < 4m$. An explicit representation of $\widehat{G2}(k)$ could easily be extracted from the proof of Lemma 3.3 but is not needed in what follows. We only note that $\widehat{G2}(k)$ is also a smooth function of $\mathbf{k} \in \mathbb{R}^3$.

In finite volume, Lemma 3.3 holds literally, if we neglect corrections vanishing exponentially at large L. This follows from the observation, already made in ref. [1], that the meson self-energy $\sum_L(q)$ differs from the infinite volume self-energy $\sum(q)$ by exponentially small terms only, provided $\mathbf{q}$ is real and $|\mathrm{Im}\, q_0| < 3m$ [7]. For the derivation of the large L expansion of the low-lying two-particle energies, the finite volume two-particle propagator $G2_L(k)$ may therefore be replaced by $G2(k)$ and Eq. (3.16) may be applied as long as $0 \leqq \mathrm{Im} P_0 < 4m$.

3.3. Two-Particle Singularities of the 4-Point Function

We now use the results established in the preceding subsections to rearrange the series (3.5) in such a way that the two-particle singularities are clearly exhibited. In the end, we shall only be interested in states with zero total momentum and total energy below the 4-particle threshold. For the rest of this section, we therefore set

$$P = (iW, 0, 0, 0), \tag{3.17}$$

and assume $0 \leqq \mathrm{Re}\, W < 4m$.

According to Eq. (3.16), the two-particle propagator can be split into a singular and a regular piece as follows:

$$G2(k) = [(2\omega(\mathbf{k}))^2 (2\omega(\mathbf{k}) - W)]^{-1} 2\pi\delta(k_0) h(\mathbf{k}) + R2(k). \tag{3.18}$$

Here, $h(\mathbf{k}) \geqq 0$ denotes a smooth rotationally symmetric cutoff function satisfying

$$h(k) = \begin{cases} 1 & \text{if} \quad \omega(\mathbf{k}) < 2m, \\ 0 & \text{if} \quad \omega(\mathbf{k}) > 3m. \end{cases} \tag{3.19}$$

This auxiliary function is introduced for technical reasons to avoid a superficial ultra-violet divergence in Eqs. (3.20), (3.21) below.

If we now insert the decomposition (3.18) into Eq. (3.5) and apply the rearrangement identity (2.29), the geometric series

$$\begin{aligned} &G(p_1, p_2, p_3, p_4) \\ &\quad = \hat{K}(p', p) + \frac{1}{2} \int_{k_0 = 0} \frac{d^3k}{(2\pi)^3} \hat{K}(p', k) \frac{h(\mathbf{k})}{(2\omega(\mathbf{k}))^2 (2\omega(\mathbf{k}) - W)} \hat{K}(k, p) + \ldots \end{aligned} \tag{3.20}$$

[7] Strictly speaking, the proof of ref. [1] only applies for $|\mathrm{Im}\, q_0| \leqq m$, but by distributing the external momentum flowing through the diagram considered to 3 disjoint paths instead of only one, the argument can easily be extended

is obtained, where the new kernel $\hat{K}$ is given by

$$\hat{K}(p',p)=K(p',p)+\sum_{n=1}^{\infty}\frac{1}{2^n}\int\frac{d^4k_1}{(2\pi)^4}\cdots\frac{d^4k_n}{(2\pi)^4}$$
$$\times K(p',k_1)R2(k_1)K(k_1,k_2)R2(k_2)\ldots K(k_n,p)\,. \qquad (3.21)$$

The point of this reformulation is that $\hat{K}$ is an analytic function of W with no singularities in the strip $0 \leqq \mathrm{Re}\,W < 4m$. The two-particle cut of the 4-point function is therefore entirely due to the explicit energy denominators in Eq. (3.20). Moreover, the relative energies k_i^0 of the intermediate two-particle states have disappeared and the series (3.20) has a form, which is very similar to the non-relativistic Born series (2.15).

This similarity becomes even more pronounced, if we consider the scattering amplitude $T(\mathbf{p}', -\mathbf{p}'|\mathbf{p}, -\mathbf{p})$, which is obtained from the 4-point function by setting

$$W=2\omega(\mathbf{p})+i\varepsilon\,, \qquad (3.22)$$

and $p_0'=p_0=0$ (cf. Subsect. 2.1 of ref. [1]). Equation (3.20) then assumes the form

$$-\frac{T}{2mW}=\hat{U}_E(\mathbf{p}',\mathbf{p})+\sum_{n=1}^{\infty}\frac{(-1)^n}{2^n}\int\frac{d^3k_1}{(2\pi)^3}\cdots\frac{d^3k_n}{(2\pi)^3}$$
$$\times\hat{U}_E(\mathbf{p}',\mathbf{k}_1)R_E(\mathbf{k}_1)\hat{U}_E(\mathbf{k}_1,\mathbf{k}_2)R_E(\mathbf{k}_2)\ldots\hat{U}_E(\mathbf{k}_n,\mathbf{p})\,, \qquad (3.23)$$

where $R_E(\mathbf{k})$ is the non-relativistic resolvent (2.17) and E is defined through

$$E=\frac{\mathbf{p}^2}{m}=(W^2-4m^2)/4m\,. \qquad (3.24)$$

In contrast to the non-relativistic case, the "potential" $\hat{U}_E(\mathbf{k}',\mathbf{k})$ appearing in Eq. (3.23) is energy dependent. It is related to the kernel $\hat{K}$ by

$$\hat{U}_E(\mathbf{k}',\mathbf{k})=-\varrho(\mathbf{k}')\varrho(\mathbf{k})\hat{K}(k',k)|_{k_0'=k_0=0}\,,$$
$$\varrho(\mathbf{k})=\frac{1}{4\omega(\mathbf{k})}\sqrt{h(\mathbf{k})\,(2\omega(\mathbf{k})+W)/m}\,. \qquad (3.25)$$

From the properties of $\hat{K}$ established above, we thus infer that $\hat{U}_E(\mathbf{k}',\mathbf{k})$ is an analytic function of E and a C^∞ function of $\mathbf{k}'$ and $\mathbf{k}$ with compact support.

We finally note that if one neglects terms vanishing more rapidly than any power of L^{-1}, Eq. (3.20) is also valid in finite volume provided the integrals over the relative momenta $\mathbf{k}$ of the intermediate two-particle states are replaced by sums over the lattice (1.2). All other entries in Eq. (3.20), in particular the kernel $\hat{K}$, are the same as in infinite volume.

3.4. Perturbation Expansion of Two-Particle Energies in Finite Volume

The two-particle energy values in finite volume can be extracted from the exponential decay of correlation functions of even composite fields. A convenient choice of such operators, suitable for the calculation of energy values in the A_1^+ sector, is

$$O_{\mathbf{p}}(x_0)=\sum_{R\in\mathcal{O}}L^{-3}\int d^3x\,d^3y\,e^{-i\mathbf{p}(\mathbf{x}-\mathbf{y})}\phi(x_0,R\mathbf{x})\phi(x_0,R\mathbf{y})\,, \qquad (3.26)$$

where the notation concerning R, $\mathcal{O}$ and $\mathbf{p}$ is as in Subsect. 2.5. Note that in the presence of interactions, the relative momentum of the mesons is not conserved and $O_{\mathbf{p}}$ therefore couples to all two-particle states in the A_1^+ sector.

Now let $C_{\mathbf{p}}(x_0)$ be the (euclidean) two-point correlation function of $O_{\mathbf{p}}$ in finite volume and consider the Fourier transform

$$\tilde{C}_{\mathbf{p}}(P_0) = \int dx_0\, e^{-iP_0x_0} C_{\mathbf{p}}(x_0). \tag{3.27}$$

In the complex P_0-plane, $\tilde{C}_{\mathbf{p}}(P_0)$ is expected to have a series of poles on the imaginary axis, which correspond to the energy values we are looking for.

To locate these poles in perturbation theory, we first note that in terms of the finite volume 4-point function, we have

$$\tilde{C}_{\mathbf{p}}(P_0) = 96\mathcal{N}(\mathbf{p}) \int \frac{dp_0}{2\pi}\, G2_L(p) + \frac{48}{L^3} \sum_{R\in\mathcal{O}} \int \frac{dp'_0}{2\pi}\frac{dp_0}{2\pi}\, G2_L(p')\, G_L(p_1,p_2,p_3,p_4)\, G2_L(p), \tag{3.28}$$

where $p' = (p'_0, R\mathbf{p})$ and $p_1, \ldots, p_4$ are given by Eqs. (3.1), (3.2). As already mentioned earlier, $G2_L$ can be replaced by $G2$ and the 4-point function can be represented by the geometric series

$$G_L(p_1,p_2,p_3,p_4) = \hat{K}(p',p) + \frac{1}{2L^3}\sum_{\mathbf{k}} \left\{ \hat{K}(p',k)\, \frac{h(\mathbf{k})}{(2\omega(\mathbf{k}))^2(2\omega(\mathbf{k})+iP_0)}\, \hat{K}(k,p) \right\}_{k_0=0} + \ldots, \tag{3.29}$$

if one neglects contributions vanishing more rapidly than any power of L^{-1}. It follows from this relation and Eq. (3.16) that at any finite order of perturbation theory, $\tilde{C}_{\mathbf{p}}(P_0)$ has (multiple) poles at $P_0 = i2\omega(\mathbf{k})$ where $\mathbf{k}$ runs through the lattice (1.2). The situation is in fact exactly the same as in the non-relativistic perturbation theory discussed in Subsect. 2.2 with $\tilde{C}_{\mathbf{p}}(P_0)$ playing the rôle of the function $F(z)$. The steps needed to extract the true pole positions to all orders of perturbation theory can thus be copied from Subsect. 2.2, in particular, for each state in the A_1^+ sector, which is non-degenerate in the absence of interactions, the energy value $P_0 = iW$ is determined by an implicit equation of the type (2.32). Explicitly, for the state with $W = 2\omega(\mathbf{p})$ in lowest order, one finds

$$W = 2\sqrt{m^2 + mE}, \tag{3.30}$$

where E is the solution of

$$E = 2\varepsilon(\mathbf{p}) + r(E), \tag{3.31}$$

$$r(z) = (2\mathcal{N}(\mathbf{p})L^3)^{-1} \sum_{R\in\mathcal{O}} \left\{ \hat{U}_z(R\mathbf{p},\mathbf{p}) + \sum_{n=1}^{\infty} \frac{(-1)^n}{2^n} L^{-3n} \sum_{\mathbf{k}_1}{}' \ldots \sum_{\mathbf{k}_n}{}' \times \hat{U}_z(R\mathbf{p},\mathbf{k}_1) R_z(\mathbf{k}_1) \hat{U}_z(\mathbf{k}_1,\mathbf{k}_2) R_z(\mathbf{k}_2) \ldots \hat{U}_z(\mathbf{k}_n,\mathbf{p}) \right\} \tag{3.32}$$

(the notation is as in Subsect. 2.5).

The similarity of the result (3.31), (3.32) with the corresponding non-relativistic formulae (2.32) and (2.65) is striking, the only difference being that the potential here is energy dependent and that the parameter E is not the total energy [which is given by Eq. (3.30)]. To solve the implicit Eq. (3.31), one proceeds in exactly the same way as in Subsect. 2.2 so that these steps need not be repeated here. We have thus obtained the complete perturbation expansion of the non-degenerate levels in the A_1^+ sector and it is clear that the method would work just as well in other symmetry sectors.

3.5. Large L Expansion

The partial wave expansion of the relativistic scattering amplitude T in the centre of mass system reads

$$T = 16\pi W \sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta) t_l, \tag{3.33}$$

where t_l is again given by Eq. (2.13) and $W = 2\omega(\mathbf{p})$ is the total energy. The combination

$$\hat{T} = -\frac{T}{2mW} \tag{3.34}$$

thus has a partial wave expansion which coincides with the expansion (2.12) of the non-relativistic amplitude $T_{\rm nr}$. Moreover, the perturbation expansion (3.23) of $\hat{T}$ has exactly the same form as the Born series (2.15) with $\hat{V}$ replaced by $\hat{U}_E$. Finally, if one takes into account that the energy values in finite volume are determined by Eqs. (3.30)–(3.32), one realizes that a complete matching between the relativistic and non-relativistic formulae has been achieved. In particular, the whole large L analysis presented in Sect. 2 carries over literally and the following remarkably simple result is obtained.

Theorem 3.4. *Suppose W is a non-degenerate energy value in the A_1^+ sector. Then, up to terms of order L^{-6}, the large L expansion of W is obtained by setting $W = 2\sqrt{m^2 + mE}$ and substituting the corresponding non-relativistic large L expansion for E.*

In particular, noting

$$W = 2m + E + O(E^2), \tag{3.35}$$

and recalling Eq. (2.60), one obtains the large L expansion (1.3) of the relativistic ground state energy announced in Sect. 1. Similarly, the expansion of the next to lowest lying energy value derives from Eq. (2.74) and for the higher levels one refers to Eqs. (2.70)–(2.72). Up to the order of L^{-1} stated, the proof of Theorem 3.4 is trivial, because it makes no difference whether or not the potential which determines the function $r(z)$ is energy dependent. At higher orders, the situation is however more complicated and it is not immediately clear that the theorem still holds, although this is indicated by an explicit calculation of the order L^{-6} contribution to the ground state energy.

3.6. Application to the $\pi\pi$- and πN-System

As an illustration we here consider the case of two pions or a pion and a nucleon enclosed in a box of size L. Isospin breaking effects are neglected and the masses m_π

and m_N of the pion and the nucleon are assumed to have their physical values (i.e. $m_\pi = 139$ MeV, $m_N = 938$ MeV). In ref. [2], the finite size mass shifts of these particles due to polarization effects were estimated to be less than 1% and exponentially decreasing for $L \geqq 3$ fermi. For the large L expansions of the two-particle states to apply, the box size should therefore be at least this big.

Two-pion states have isospin $I = 0, 1$, or 2. For even isospin, the lowest state is the ground state in the A_1^+ sector and the large L expansion of the corresponding energy values W thus reads

$$W = 2\sqrt{m_\pi^2 + m_\pi E}\,, \tag{3.36}$$

$$E = -\frac{4\pi a_0^I}{m_\pi L^3}\left\{1 + c_1 \frac{a_0^I}{L} + c_2 \frac{(a_0^I)^2}{L^2}\right\} + O(L^{-6})\,, \tag{3.37}$$

where a_0^I denotes the S-wave scattering length in the channel with isospin I and the coefficients c_1, c_2 are given by Eqs. (2.61), (2.62). On the other hand, for $I = 1$ the lowest state transforms as a vector under the cubic rotation group $\mathcal{O}$ with the pions carrying one quantum of relative momentum (because of Bose statistics, two pions in an $I = 1$ state cannot be both at rest). The energy W of this state is again given by Eq. (3.36) with

$$E = \frac{4\pi^2}{m_\pi L^2} - \frac{12\,\mathrm{tg}\,\delta_1^1}{m_\pi L^2}\{1 + c_1'\,\mathrm{tg}\,\delta_1^1 + c_2'\,\mathrm{tg}^2\,\delta_1^1\} + O(L^{-6})\,, \tag{3.38}$$

where δ_1^1 denotes the scattering phase shift in the $I(J^P) = 1(1^-)$ channel at momentum $p = 2\pi L$ and the coefficients c_1', c_2' are the same as in Eq. (2.74).

The values of the scattering lengths a_0^I suggested by experiment [7] and chiral perturbation theory [8] are

$$a_0^0 = 0.3 \text{ fermi}\,, \qquad a_0^2 = -0.06 \text{ fermi}\,, \tag{3.39}$$

and for the phase shift δ_1^1, the phenomenological formula

$$\mathrm{tg}\,\delta_1^1 = 0.04\left(\frac{v^3}{1+v}\right)^{1/2} \frac{1}{1 - v/v_\varrho}\,, \qquad v = p^2/m_\pi^2\,, \qquad v_\varrho = 6.56\,, \tag{3.40}$$

appears to provide a good fit of the experimental data (cf. ref. [7, p. 96f]). With these values as input, the volume dependence of the ground state energies for $I = 0$, 1, and 2 is as shown in Fig. 7. The dynamical finite size effects on the $\pi\pi$-system are thus rather small which is no surprise in view of the small scattering lengths (3.39).

The weakness of the pion interactions at low energies is usually attributed to the Goldstone nature of these particles and a calculation of two-particle energies in lattice QCD could therefore provide a check on this aspect of the theory. To actually reproduce the curves of Fig. 7 would require a calculation of energy values on large lattices with an accuracy of about 1%, which is probably impossible to achieve in the near future. However, one does not know a priori whether the lattice pions interact weakly indeed, and to obtain at least an upper bound on the scattering lengths, a less precise computation may therefore be worthwhile.

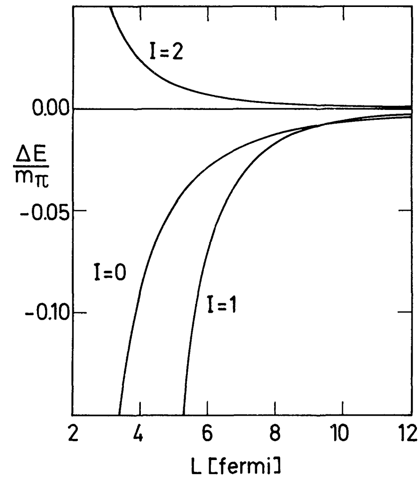

Fig. 7. Plot of the lowest $\pi\pi$-energy values for isospin $I=0, 1$, and 2 according to Eqs. (3.36)–(3.40). The energy shift ΔE is defined by $\Delta E = E - 2\varepsilon(\mathbf{p})$, where $p = 2\pi/L$ for $I=1$ and $p=0$ otherwise

The large L expansions (3.37) and (3.38) have only been proved for asymptotically large L and they do therefore not obviously apply in volumes where there are but a few two-pion levels below the 4-pion threshold (cf. Fig. 1). However, it is quite clear that for $L \gtrsim 3$ fermi the physics of slow pions in the box should not be greatly influenced by virtual many-particle states. Moreover, from experience with the simple quantum mechanical system studied in Subsect. 2.6, one concludes that the large L expansions are apparently valid, if the dynamical finite size energy shift ΔE is small compared to the free particle level splitting and if the higher order terms in the expansion are small corrections to the leading term. Both of these criteria are satisfied for all curves in Fig. 7 over the whole range of L displayed and one may therefore be confident that they are close to the true curves [if Eqs. (3.39) and (3.40) are approximately correct].

The lowest lying pion-nucleon states in the isospin $I = \frac{1}{2}, \frac{3}{2}$ sectors have positive parity and transform according to the fundamental ("spin 1/2") representation of the spin covering of the cubic group. Their energies W are given by

$$W = \sqrt{m_\pi^2 + 2\mu E} + \sqrt{m_N^2 + 2\mu E}\,, \tag{3.41}$$

$$E = -\frac{2\pi a_{0+}^I}{\mu L^3}\left\{1 + c_1 \frac{a_{0+}^I}{L} + c_2 \frac{(a_{0+}^I)^2}{L^2}\right\} + O(L^{-6})\,, \tag{3.42}$$

where μ is the reduced mass of the system and a_{0+}^I denotes the scattering length in the channel with isospin I, orbital angular momentum 0 and positive parity. The experimental values are [9]

$$a_{0+}^{1/2} = 0.24 \text{ fermi}\,, \qquad a_{0+}^{3/2} = -0.15 \text{ fermi}\,, \tag{3.43}$$

so that a plot of E versus L would look similar to Fig. 7.

We finally note that in all cases considered so far, the low-lying energy values are well separated from resonances or bound states in the same channel. For nucleon-nucleon states, the situation would be rather different, because of the existence of the deuteron which goes along with large scattering lengths [10]. Thus, in this case one is dealing with a resonance situation and finite size effects are expected to be large as was observed in the simple model of Subsect. 2.6.

4. Concluding Remarks

The relations established in this paper show that the volume dependence of the two-particle energy values is determined by the elastic scattering amplitude at these energies. An independent calculation of such energy values (by numerical simulation, for example) may therefore be expected to provide interesting qualitative information on the structure and strength of the particle interactions in the quantum field theory considered. If a very accurate calculation is feasible, one may even be able to extract the scattering phase shifts in this way. Note that one directly gets the physical scattering amplitude, in particular, no analytic continuation is required.

A study of finite size effects in a simple model such as the lattice ϕ^4-theory would of course be very useful at this stage. In doing so, the following points should be taken into account.

(a) If the basic correlation length is not much bigger than the lattice spacing "a", the large L expansions assume a form, which is slightly different from the one obtained here, because the lattice theory in infinite volume is not Lorentz invariant. In particular, one must distinguish between the rest and inertial masses of the particles. It is however not difficult to deduce the lattice large L expansions by adapting the arguments of Sect. 3 (see also ref. [11]).

(b) As long as the parameters in the Lagrangian are kept fixed and only the lattice size is varied, one need not worry about the effects of the finite ultra-violet cutoff, because these are exactly taken into account by the lattice large L expansions. However, if data from different points on the same renormalization group trajectory (points of equal low energy physics in other words) are included in the analysis, one must make sure that finite size effects are not confused with $O(a^2)$ corrections [13].

(c) As discussed in Subsect. 3.4, the two-particle energies can be determined from the exponential decay of the two-point correlation functions of the operators $O_{\mathbf{p}}$ at large times. It is not advisable to use local operators such as $\phi(x)^2$ instead of $O_{\mathbf{p}}$, because the amplitude for such operators to create a two-particle state from the vacuum is proportional to L^{-3} and is hence small in general.

An interesting feature of the large L expansions (2.70)–(2.73) of the higher energy levels is that they break down for energies near a resonance, because the coefficients in the expansion diverge. Thus, in the neighborhood of a resonance, finite size effects are strong and an energy level, which passes through a resonance as L increases, is expected to show some unusual behaviour. Eventually, this observation may lead to a practical and conceptually satisfactory characterization of resonance states in finite volume (as would be required for a meaningful calculation of the masses of unstable particles in lattice QCD, for example).

The proof of the large L expansions given in this paper does not apply in the presence of bound states, although it is quite clear from the model solved in Subsect. 2.6 that the expansions are valid in this case, too. It is difficult to dispense with the framework of Feynman diagrams in quantum field theory, but as in Sect. 3 of ref. [1], bound states may be incorporated by introducing independent interpolating fields for them. With some modifications, the proof of the large L expansions then goes through as before. In quantum mechanics, it is perhaps also possible to design a truly non-perturbative proof on the basis of a more direct analysis of the Schrödinger equation in position space as in the 1-dimensional case (cf. ref. [3]).

Appendix A: Properties of the zeta function Z_{lm}

We first show that $Z_{lm}(s, \mathbf{n}^2)$ is a meromorphic function of s with poles at $s=\frac{3}{2}-j$, $j=0,1,2,\ldots$, for $l=0$ and no singularities for $l\neq 0$. Starting from the definition (2.47), valid for $\mathrm{Re}\, s>\frac{1}{2}(l+3)$, we have

$$Z_{lm}(s, \mathbf{n}^2)=\sum_{\mathbf{v}^2<\mathbf{n}^2} \mathcal{Q}_{lm}(\mathbf{v})\,(\mathbf{v}^2-\mathbf{n}^2)^{-s}+\frac{1}{\Gamma(s)}\int_0^{\infty} dt\, t^{s-1} F_{lm}(t, \mathbf{n}^2), \tag{A.1}$$

where F_{lm} is given by

$$F_{lm}(t, \mathbf{n}^2)=\sum_{\mathbf{v}^2>\mathbf{n}^2} \mathcal{Q}_{lm}(\mathbf{v})\, e^{-t(\mathbf{v}^2-\mathbf{n}^2)}. \tag{A.2}$$

Obviously, $F_{lm}(t, \mathbf{n}^2)$ is smooth for $t>0$ and exponentially decaying for $t\to\infty$. At small t, we use Poisson's summation formula to show that

$$F_{lm}(t, \mathbf{n}^2)=-\sum_{\mathbf{v}^2\leqq\mathbf{n}^2} \mathcal{Q}_{lm}(\mathbf{v})\, e^{t(\mathbf{n}^2-\mathbf{v}^2)} + \left(\frac{\pi}{t}\right)^{3/2} e^{t\mathbf{n}^2} \sum_{\mathbf{v}} \mathcal{Q}_{lm}(i\nabla_x)\, e^{-\frac{1}{4t}(\mathbf{x}-2\pi\mathbf{v})^2}\Big|_{\mathbf{x}=0}, \tag{A.3}$$

which implies the asymptotic expansion

$$F_{lm}(t, \mathbf{n}^2) \underset{t\to 0}{\sim} \sum_{j=0}^{\infty} (A_j t^j+B_j t^{j-3/2}), \tag{A.4}$$

$$A_j=-\frac{1}{j!}\sum_{\mathbf{v}^2\leqq\mathbf{n}^2} \mathcal{Q}_{lm}(\mathbf{v})\,(\mathbf{n}^2-\mathbf{v}^2)^j, \tag{A.5}$$

$$B_j=\delta_{l0}\delta_{m0}\pi^{3/2}\frac{1}{j!}(\mathbf{n}^2)^j. \tag{A.6}$$

It follows that

$$F_{lm}^N(t, \mathbf{n}^2)=F_{lm}(t, \mathbf{n}^2)-\sum_{j=0}^{N} (A_j t^j+B_j t^{j-3/2}) \tag{A.7}$$

is of order $t^{N-1/2}$ for small t and the representation

$$Z_{lm}(s, \mathbf{n}^2)=\sum_{\mathbf{v}^2<\mathbf{n}^2} \mathcal{Q}_{lm}(\mathbf{v})\,(\mathbf{v}^2-\mathbf{n}^2)^{-s} + \frac{1}{\Gamma(s)}\left\{\int_0^1 dt\, t^{s-1}F_{lm}^N+\int_1^{\infty} dt\, t^{s-1}F_{lm}+\sum_{j=0}^{N}\left(\frac{A_j}{s+j}+\frac{B_j}{s+j-\frac{3}{2}}\right)\right\} \tag{A.8}$$

is hence valid for $\mathrm{Re}\,s > \frac{1}{2} - N$. Since N can be chosen arbitrarily large, we have thus proved that Z_{lm} extends to a meromorphic function in the whole s-plane with poles as described above [the poles at $s = -j$ are cancelled by the zeros of $1/\Gamma(s)$].

For integer $s \leqq 0$, the integrals in Eq. (A.8) do not contribute and $Z_{lm}(s, \mathbf{n}^2)$ can therefore be evaluated algebraically, the result being quoted in Eqs. (2.49) and (2.50).

For $s \geqq 1$, $Z_{lm}(s, \mathbf{n}^2)$ can be determined numerically by computing the integrals in Eq. (A.8) for $N = 1$ using any ordinary integration subroutine [rapidly convergent series representations for the integrands of the first and the second integral are provided by Eqs. (A.3) and (A.2), respectively].

Appendix B: Proof of the Large L Expansion (2.51)

The proof of Eq. (2.51) is rather lengthy and is therefore divided into several steps. In general, the strategy is to first consider simple special cases and then to gradually proceed to the more complicated cases using the results already established.

(1) We first set $\mathbf{p} = 0$ and choose

$$f(\mathbf{k}) = (\mathbf{k}^2)^j \mathcal{Q}_{lm}(\mathbf{k})\, e^{-\mathbf{k}^2}. \tag{B.1}$$

Then, it is easy to work out the right-hand side of Eq. (2.51) and the expansion to be proved thus reads

$$S_q(f, \mathbf{0}) \sim \delta_{l0}\delta_{m0} \frac{(-1)^{q'-1}}{4\pi\Gamma(q'-\frac{1}{2})} + \sum_{i=0}^{q'} \frac{1}{L^3}\left(\frac{2\pi}{L}\right)^{2i+l-2q'} \frac{(-1)^i}{i!} Z_{lm}(q'-i, 0), \tag{B.2}$$

where $q' = q - j$ (the sum is void if $q' < 0$).

To establish (B.2), we first rewrite the sum $S_q(f, \mathbf{0})$ in the form

$$S_q(f, \mathbf{0}) = \frac{1}{\Gamma(q)} \int_0^\infty dt\, t^{q-1} L^{-3} \sum_{\mathbf{k} \neq 0} (\mathbf{k}^2)^j \mathcal{Q}_{lm}(\mathbf{k})\, e^{-(t+1)\mathbf{k}^2}. \tag{B.3}$$

Next, recalling the definition (A.2) of the function F_{lm}, setting $x = (2\pi/L)^2$ and performing a simple substitution, one arrives at

$$S_q(f, \mathbf{0}) = \frac{x^{l/2-q'}}{L^3\Gamma(q)} \int_x^\infty dt (t-x)^{q-1} (-1)^j \frac{\partial^j}{\partial t^j} F_{lm}(t, 0). \tag{B.4}$$

If $j \geqq q$, partial integration now leads to

$$S_q(f, \mathbf{0}) = \frac{1}{L^3} x^{l/2-q'} (-1)^{j-q} \frac{\partial^{j-q}}{\partial t^{j-q}} F_{lm}(t, 0)|_{t=x} \tag{B.5}$$

and, using the small t expansion (cf. Appendix A)

$$F_{lm}(t, 0) = \delta_{l0}\delta_{m0} \left\{\left(\frac{\pi}{t}\right)^{3/2} - 1\right\} + O\left(e^{-\frac{\pi^2}{t}}\right), \tag{B.6}$$

one recovers (B.2).

On the other hand, if $j<q$, one has

$$S_q(f,\mathbf{0})=\frac{x^{l/2-q'}}{L^3\Gamma(q')}\int_x^\infty dt(t-x)^{q'-1}F_{lm}(t,0)\,, \tag{B.7}$$

and from (B.6) one then infers that

$$S_q(f,\mathbf{0})\sim\frac{x^{l/2-q'}}{L^3\Gamma(q')}\left\{\delta_{l0}\delta_{m0}\int_x^1 dt(t-x)^{q'-1}\left[\left(\frac{\pi}{t}\right)^{3/2}-1\right]\right.$$
$$\left.+\int_0^1 dt(t-x)^{q'-1}F^0_{lm}(t,0)+\int_1^\infty dt(t-x)^{q'-1}F_{lm}(t,0)\right\} \tag{B.8}$$

up to terms, which vanish more rapidly than any power of $1/L$ for large L. Using the representation (A.8) of the zeta function Z_{lm}, it is now a trivial exercise to evaluate all terms in Eq. (B.8) exactly. As a result, one obtains Eq. (B.2), which proves that the large L expansion (2.51) is valid in the special case considered.

(2) In this step, we again set $\mathbf{p}=0$ and assume that all partial derivatives of $f(\mathbf{k})$ up to the N'th order vanish at $\mathbf{k}=0$ for some even $N\geqq 2q$. One then has

$$f_{jlm}(0)=0\quad\text{for}\quad 2j+l\leqq N\,, \tag{B.9}$$

and, up to terms of order L^{2q-N-3}, the large L expansion (2.51) reads

$$S_q(f,\mathbf{0})=\frac{1}{(2q-2)!}\int\frac{d^3k}{(2\pi)^3}\frac{1}{\mathbf{k}^2}(\Delta_k)^{q-1}f(\mathbf{k})+O(L^{2q-N-3})\,. \tag{B.10}$$

In order to prove this relation, we note that the function

$$h(\mathbf{k})=(\mathbf{k}^2)^{-q}f(\mathbf{k}) \tag{B.11}$$

is integrable and has integrable derivatives up to the order $N-2q+3$. Thus, the ordinary summation theorem (2.42) applies and it follows that

$$S_q(f,\mathbf{0})=\int\frac{d^3k}{(2\pi)^3}\frac{1}{(\mathbf{k}^2)^q}f(\mathbf{k})+O(L^{2q-N-3})\,. \tag{B.12}$$

By using the identity

$$\Delta_k(\mathbf{k}^2)^{-q+1}=(2q-2)(2q-3)(\mathbf{k}^2)^{-q}\qquad(\mathbf{k}\neq 0)\,, \tag{B.13}$$

and partial integration, Eq. (B.12) can be matched with (B.10), and we have thus shown that the large L expansion (2.51) is also valid in the present case up to the order of L^{-1} stated. That there are no boundary terms from the partial integrations is easy to prove taking (B.9) and the square integrability of $f(\mathbf{k})$ and its derivatives into account. For example, if $q=2$, there is one partial integration needed and the contribution of the boundary at large k is proportional to

$$\lim_{R\to\infty}\int_{|\mathbf{k}|=R} d\Omega R\mathbf{k}\cdot\{f(\mathbf{k})\nabla_k(\mathbf{k}^2)^{-1}-(\mathbf{k}^2)^{-1}\nabla_k f(\mathbf{k})\}\,, \tag{B.14}$$

where Ω denotes the solid angle of $\mathbf{k}$. Now, using the Cauchy-Schwarz inequality for square integrable functions, we have

$$\left|\int_{|\mathbf{k}|=R} d\Omega f(\mathbf{k})\right|=R^{-3}\left|\int_{\mathbf{k}^2\leqq R^2} d^3k\{3f(\mathbf{k})+\mathbf{k}\cdot\nabla_k f(\mathbf{k})\}\right|\leqq C/\sqrt{R} \tag{B.15}$$

for some constant C. Similarly, one shows that

$$\left|\int_{|\mathbf{k}|=R} d\Omega \mathbf{k}\cdot \nabla_k f(\mathbf{k})\right| \leqq C'\sqrt{R}, \tag{B.16}$$

and the boundary term (B.14) is thus seen to vanish.

(3) We now combine the results of step (1) and (2) to show that the large L expansion (2.51) holds for $\mathbf{p}=0$ and arbitrary functions $f(\mathbf{k})$.

Let $N \geqq 2q$ be some even integer. Then, up to order k^N, the Taylor expansion around $\mathbf{k}=0$ of $f(\mathbf{k})$ can be rearranged in the form

$$f(\mathbf{k})=\sum_{j=0}^{N/2}\sum_{l=0}^{N-2j}\sum_{m=-l}^{l} c_{jlm}(\mathbf{k}^2)^j \mathcal{Q}_{lm}(\mathbf{k})\,e^{-\mathbf{k}^2}+f_N(\mathbf{k}), \tag{B.17}$$

where the remainder $f_N(\mathbf{k})$ is smooth and has vanishing derivatives at $\mathbf{k}=0$ up to the N'th order, i.e. f_N is a function of the type considered in step (2). Now we note that the large L expansion of $S_q(f,\mathbf{0})$ is an operation linear in f. Since we have already shown in step (1) and (2) that (2.51) applies to the functions on the right-hand side of Eq. (B.17) up to terms of order L^{2q-N-3}, it follows that (2.51) is also valid for $f(\mathbf{k})$ up to this order. Because N can be chosen arbitrarily large, (2.51) is thus completely proved for $\mathbf{p}=0$.

(4) We now proceed to consider the case $\mathbf{p}\neq 0$. In this step, the power series expansion

$$\begin{aligned} S_q(f,\mathbf{p}) \sim {} & \sum_{j=0}^{\infty}\binom{-q}{j}(-\mathbf{p}^2)^j I_{q+j}(f,\mathbf{0}) \\ & + \sum_{j=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m=-l}^{l}\frac{1}{L^3}\left(\frac{2\pi}{L}\right)^{2j+l-2q} f_{jlm}(0)\,Z_{jlm}(q,\mathbf{n}^2) \end{aligned} \tag{B.18}$$

is established and in the following step, parts of this series will be resummed to obtain (2.51). The zeta function Z_{jlm} is defined as Z_{lm}, but with an extra factor $(\mathbf{v}^2)^j$ multiplying $\mathcal{Q}_{lm}(\mathbf{v})$. In other words, using the binomial expansion, we have

$$Z_{jlm}(q,\mathbf{n}^2)=\sum_{i=0}^{j}\binom{j}{i}(\mathbf{n}^2)^{j-i}Z_{lm}(q-i,\mathbf{n}^2). \tag{B.19}$$

To prove (B.18), we choose an integer $N \geqq 1$ and decompose the sum $S_q(f,\mathbf{p})$ as follows:

$$S_q(f,\mathbf{p})=s_1+s_2+s_3+s_4, \tag{B.20}$$

$$s_1=\frac{1}{L^3}\sum_{\mathbf{k}^2<\mathbf{p}^2} f(\mathbf{k})(\mathbf{k}^2-\mathbf{p}^2)^{-q}, \tag{B.21}$$

$$s_2=\frac{1}{L^3}\sum_{0<\mathbf{k}^2\leqq\mathbf{p}^2} f(\mathbf{k})(-1)\sum_{\mu=0}^{N}\binom{-q}{\mu}(-\mathbf{p}^2)^{\mu}(\mathbf{k}^2)^{-q-\mu}, \tag{B.22}$$

$$s_3=\frac{1}{L^3}\sum_{0<\mathbf{k}^2} f(\mathbf{k})\sum_{\mu=0}^{N}\binom{-q}{\mu}(-\mathbf{p}^2)^{\mu}(\mathbf{k}^2)^{-q-\mu}, \tag{B.23}$$

$$s_4=\frac{1}{L^3}\sum_{\mathbf{p}^2<\mathbf{k}^2} f(\mathbf{k})\left\{(\mathbf{k}^2-\mathbf{p}^2)^{-q}-\sum_{\mu=0}^{N}\binom{-q}{\mu}(-\mathbf{p}^2)^{\mu}(\mathbf{k}^2)^{-q-\mu}\right\}. \tag{B.24}$$

In all these sums, $\mathbf{k}$ runs over the momentum lattice (1.2) subject to the restrictions indicated below the summation symbol. Since s_1 and s_2 are finite sums, they are trivial to expand and one obtains

$$s_i \sim \sum_{j=0}^{\infty} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{1}{L^3} \left(\frac{2\pi}{L}\right)^{2j+l-2q} f_{jlm}(0) c_{jlm}^i , \tag{B.25}$$

$$c_{jlm}^1 = \sum_{\mathbf{v}^2 < \mathbf{n}^2} (\mathbf{v}^2)^j \mathcal{Q}_{lm}(\mathbf{v}) (\mathbf{v}^2 - \mathbf{n}^2)^{-q} , \tag{B.26}$$

$$c_{jlm}^2 = - \sum_{0 < \mathbf{v}^2 \leqq \mathbf{n}^2} (\mathbf{v}^2)^j \mathcal{Q}_{lm}(\mathbf{v}) \sum_{\mu=0}^{N} \binom{-q}{\mu} (-\mathbf{n}^2)^{\mu} (\mathbf{v}^2)^{-q-\mu} \tag{B.27}$$

(here and below, $\mathbf{v}$ runs over $\mathbb{Z}^3$). Next, we note that

$$s_3 = \sum_{\mu=0}^{N} \binom{-q}{\mu} (-\mathbf{p}^2)^{\mu} S_{q+\mu}(f, \mathbf{0}) . \tag{B.28}$$

Because we have already proved (2.51) for $\mathbf{p} = 0$, it follows that

$$\begin{aligned} s_3 \sim & \sum_{\mu=0}^{N} \binom{-q}{\mu} (-\mathbf{p}^2)^{\mu} I_{q+\mu}(f, \mathbf{0}) \\ & + \sum_{j=0}^{+} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{1}{L^3} \left(\frac{2\pi}{L}\right)^{2j+l-2q} f_{jlm}(0) c_{jlm}^3 , \end{aligned} \tag{B.29}$$

$$c_{jlm}^3 = \sum_{\mu=0}^{N} \binom{-q}{\mu} (-\mathbf{n}^2)^{\mu} Z_{lm}(q+\mu-j, 0) . \tag{B.30}$$

Finally, to expand s_4 we observe that a power L^{2q} can be factored out from the bracket $\{\ldots\}$ in Eq. (B.24), the remainder being independent of L and of order $(\mathbf{v}^2)^{-q-N-1}$ for large $\mathbf{v}$ $\left(\mathbf{k} = \frac{2\pi}{L}\mathbf{v}\right)$. The sum is thus well convergent and it is easy to show (e.g. ref. [6, Sect. 8.6.3]) that the large L expansion up to terms of order $L^{2q-2N-4}$ can be obtained simply by expanding $f(\mathbf{k})$ around $\mathbf{k} = 0$. Thus, we have

$$s_4 = \sum_{j=0}^{N} \sum_{l=0}^{2N-2j} \sum_{m=-l}^{l} \frac{1}{L^3} \left(\frac{2\pi}{L}\right)^{2j+l-2q} f_{jlm}(0) c_{jlm}^4 + O(L^{2q-2N-4}) , \tag{B.31}$$

$$c_{jlm}^4 = \sum_{\mathbf{n}^2 < \mathbf{v}^2} (\mathbf{v}^2)^j \mathcal{Q}_{lm}(\mathbf{v}) \left\{ (\mathbf{v}^2 - \mathbf{n}^2)^{-q} - \sum_{\mu=0}^{N} \binom{-q}{\mu} (-\mathbf{n}^2)^{\mu} (\mathbf{v}^2)^{-q-\mu} \right\} , \tag{B.32}$$

where c_{jlm}^4 is only defined for $2j + l \leqq 2N$.

If we now collect the expansions of the four sums s_i, Eq. (B.18) is obtained up to terms of order $L^{2q-2N-4}$, provided we can show that

$$\sum_{i=1}^{4} c_{jlm}^i = Z_{jlm}(q, \mathbf{n}^2) . \tag{B.33}$$

From the explicit expressions given for the coefficients c_{jlm}^i, this relation is however easy to prove for complex q with $\mathrm{Re}\, q > j + \frac{1}{2}l + \frac{3}{2}$, and hence, by analyticity, for all q. We finally remark that N can be chosen arbitrarily large so that in fact we have established (B.18) to all orders of $1/L$.

(5) We finally note that (B.18) can be obtained from (2.51) by expanding $I_q(f, \mathbf{p})$ and $f_{jlm}(p)$ for small $\mathbf{p}$. Indeed, the first sum in (B.18) is just the Taylor expansion (2.54) of the integral $I_q(f, \mathbf{p})$ and the second sum is easily derived from the series in (2.51) by substituting

$$f_{jlm}(p) \sim \sum_{\mu=0}^{\infty} (\mathbf{p}^2)^{\mu} \binom{j+\mu}{\mu} f_{j+\mu lm}(0), \tag{B.34}$$

and using the identities (2.49) and (B.19). It follows that the large L expansion (2.51) is equivalent to (B.18) to all orders of $1/L$. Since (B.18) has already been established in step (4), we have thus proved Eq. (2.51) for arbitrary f and $\mathbf{p}$.

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