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TWO-PARTICLE STATES ON A TORUS AND THEIR RELATION TO THE SCATTERING MATRIX

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The energy spectrum of a system of two particles enclosed in a box with periodic boundary conditions is characteristic for the forces between the particles. For box sizes greater than the interaction range, and for energies below the inelastic threshold, the spectrum is shown to be determined by the scattering phases at these energies. Simple exact formulae are derived which can be used to compute the energy levels given the scattering phases or, conversely, to calculate the scattering phases if the energy spectrum is known.

1. Introduction

There is a wealth of experimental information on low-energy hadron–hadron scattering processes. Yet it has been impossible so far to compare these data with QCD, the current fundamental theory of strong interactions, except for those aspects which are determined by symmetry. In particular, some spectacular dynamical effects, such as the ρ-resonance, remain largely unexplained up to now.

In the so far most promising attempt to solve QCD at low energies one puts the theory on a lattice and computes the functional integral by numerical simulation. With regard to calculating scattering amplitudes, this method meets two fundamental difficulties. The first is that the theory lives on a *euclidean* lattice so that the real time evolution of two-particle states is not immediately accessible. Secondly, the lattices which can be simulated with the presently available computers are quite small. They are certainly too small to contain two well separated slowly moving one-particle wave packets. A direct simulation of low-energy scattering processes is therefore excluded.

For quantum field theories in 2 space-time dimensions, a general method for computing elastic scattering amplitudes has recently been proposed [3, 8] (for other ideas see refs. [10, 11]). It is based on the fact that the energy spectrum of two-particle states in a finite volume of size L with periodic boundary conditions is related to the associated scattering phase shift $\delta(k)$ in a simple manner. Since the spectrum is relatively easy to compute, using standard techniques, the phase shift

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can thus be determined. This method bypasses the difficulties mentioned above. In particular, the finite size of the lattice, initially thought to be an obstacle, is used to probe the system.

It is of course crucial for the success of the method that a simple exact formula exists which expresses the scattering phase in terms of the spectrum of two-particle states in finite volume. Explicitly, for any observed level with zero total momentum, definite internal quantum numbers and energy W, the corresponding scattering phase shift $\delta(k)$ at momentum k in the center-of-mass frame is given by

$$e^{2i\delta(k)} = e^{-ikL}, \tag{1.1}$$

where k is determined through

$$W = 2\sqrt{m^2 + k^2} \tag{1.2}$$

and m denotes the mass of the scattered particles, which I have assumed to be identical for simplicity. Eq. (1.1) holds provided W is in the elastic region and if polarization effects and scaling violations can be neglected (cf. refs. [1–3, 8]).

In 4 space-time dimensions the situation is substantially more complicated, because the rotational invariance of the system is broken by the finite spatial volume which is usually taken to be a 3-dimensional torus, i.e. a cube with linear extension L and periodic boundary conditions in all directions. It is for this reason that the derivation of eq. (1.1) cannot simply be carried over by passing to an angular momentum basis. Instead the spectrum of two-particle states is expected to depend on the scattering phases $\delta_l(k)$ for all angular momenta l which are not excluded by the cubic symmetry of the states.

The only universal formula for the connection between the scattering matrix and the spectrum of two-particle states in 4-dimensional quantum field theory so far is an expansion of the lowest levels in powers of $1/L$ [3–5], a result which has already been used to compute scattering lengths by numerical simulation [6, 7, 9]. In the present paper, a new set of relations is derived which can be regarded as the 4-dimensional analogue of eq. (1.1). To avoid inessential complications, I shall only discuss the case of two (stable) particles with spin 0 and mass m, whose dynamics can be described by a simple scalar field theory. But it is not difficult to generalize the results to any two-particle channel in an arbitrary massive quantum field theory.

To get a flavour of what has been achieved, let us suppose for a moment that all scattering phases $\delta_l(k)$ with $l = 4, 6, \dots$ are negligible in some energy range $W_1 < W < W_2$ below the inelastic threshold. Up to corrections which are exponentially small at large L, the finite volume energy spectrum can then be described by a set of simple rules. In particular, an energy value W with $W_1 < W < W_2$ belongs to the spectrum in the subspace of cubically invariant states with zero total momentum (the A_1^+ sector) if and only if the associated momentum $k > 0$, defined through eq. (1.2), satisfies one of the following two conditions.

(a) k is a solution of the equation

$$e^{2i\delta_0(k)} = \frac{\mathcal{Z}_{00}(1;q^2) + i\pi^{3/2}q}{\mathcal{Z}_{00}(1;q^2) - i\pi^{3/2}q}, \tag{1.3}$$

where

$$q = \frac{kL}{2\pi} \tag{1.4}$$

and the zeta function

$$\mathcal{Z}_{00}(s;q^2) = \frac{1}{\sqrt{4\pi}} \sum_{n\in\mathbb{Z}^3} (n^2 - q^2)^{-s} \tag{1.5}$$

is initially defined for $\mathrm{Re}\, s > 3/2$ and otherwise through analytic continuation.

(b) The parameter q defined above is equal to $|\boldsymbol{n}|$ for some non-zero integer vector $\boldsymbol{n}$. Furthermore, there is another integer vector $\boldsymbol{n}'$ with $|\boldsymbol{n}'| = |\boldsymbol{n}|$, which is not related to $\boldsymbol{n}$ by a cubic rotation/reflection. The smallest value of q with these properties is 3 [$\boldsymbol{n} = (3,0,0)$ and $\boldsymbol{n}' = (2,2,1)$ in this case]. In the free theory, this corresponds to the 9th level in the A_1^+ sector, all lower levels being non-degenerate.

The rules for the other symmetry sectors will be given later in the paper. Eq. (1.3) is the first in a sequence of compatible relations, which incorporate the phase shifts $\delta_l(k)$ for increasing angular momenta l. In this way their influence on the spectrum can be systematically controlled. For example it is possible to show that the low-lying levels in the A_1^+ sector are correctly given by eq. (1.3) [and rule (b)] up to terms which are of order L^{-11} at large L.

Although the final result is simple, its derivation is complicated. In the following, I shall first consider a non-relativistic system and work out all the details there. After that the results can be carried over to quantum field theory by invoking the effective Schrödinger equation established in refs. [3,8]. A summary of the most important formulae is given in subsects. 5.4 and 6.1. For the translation of these results to the relativistic case see sect. 7.

2. The non-relativistic model

The system studied here is exactly the same as in sect. 2 of ref. [3]. The notations employed are also the same, but to make this paper self-contained all the necessary definitions will be given below.

2.1. PROPERTIES OF THE MODEL IN INFINITE VOLUME

Consider two spinless bosons of mass m in 3-dimensional space which interact through a short-range force. The state of this system is described by a scalar wave function $\psi(\boldsymbol{x}, \boldsymbol{y})$ where $\boldsymbol{x}$ and $\boldsymbol{y}$ are the positions of the particles. In the following we are interested in states with zero total momentum so that the wave functions ψ depend only on the difference vector $\boldsymbol{r} = \boldsymbol{x} - \boldsymbol{y}$. The hamilton operator is taken to be

$$H = -\frac{1}{2\mu}\Delta + V(r), \qquad r = |\boldsymbol{r}|, \tag{2.1}$$

where Δ denotes the laplacian with respect to $\boldsymbol{r}$ and $\mu = m/2$ is the reduced mass of the system. The potential $V(r)$ is assumed to be of finite range, viz.

$$V(r) = 0 \quad \text{for} \quad r > R, \tag{2.2}$$

and we shall also take it for granted that it is smooth. This latter property saves us from unnecessary technicalities; for the validity of the final result it would be sufficient to know that the potential is square integrable.

If the particles are identical, the admissible wave functions must be even under a reflection $\boldsymbol{r} \to -\boldsymbol{r}$. To be able to discuss states with arbitrary parity, we shall therefore assume that the particles carry a flavour quantum number, such as isospin, which makes them distinguishable. No loss of generality is implied by this assumption, because it is straightforward to project onto the sectors with definite parity, at all stages of the analysis.

Elliptic regularity implies that any locally square integrable solution $\psi(\boldsymbol{r})$ of the stationary Schrödinger equation

$$H\psi = E\psi \tag{2.3}$$

is necessarily smooth (see e.g. ref. [12], theorem IX.26). The expansion in spherical harmonics

$$\psi(\boldsymbol{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm}(\theta, \varphi)\psi_{lm}(r), \tag{2.4}$$

$$\boldsymbol{r} = r(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta), \tag{2.5}$$

is hence rapidly convergent. Furthermore, the coefficients $\psi_{lm}(r)$ are smooth solutions of the radial Schrödinger equation

$$\left\{\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + k^2 - 2\mu V(r)\right\}\psi_{lm}(r) = 0, \tag{2.6}$$

where the momentum k is related to the energy E through

$$E = k^2/2\mu . \tag{2.7}$$

It does not matter here whether E is positive or negative, and we shall in the following allow k to assume any complex value.

The radial Schrödinger equation has only one linearly independent solution $u_l(r;k)$ which is bounded near the origin $r=0$. Its normalization can be fixed by imposing the boundary condition

$$\lim_{r\to 0} r^{-l} u_l(r;k) = 1 . \tag{2.8}$$

From uniqueness we then conclude that

$$\psi_{lm}(r) = b_{lm} u_l(r;k) \tag{2.9}$$

for some constants b_{lm}.

For $r > R$, the potential vanishes and the solution $u_l(r;k)$ is a linear combination of the spherical Bessel functions $j_l(kr)$ and $n_l(kr)$, viz.*

$$u_l(r;k) = \alpha_l(k) j_l(kr) + \beta_l(k) n_l(kr) . \tag{2.10}$$

The amplitudes $\alpha_l(k)$ and $\beta_l(k)$ have a number of important properties which follow straightforwardly from the radial Schrödinger equation and the normalization condition (2.8). In particular, for any given non-zero value of k, they cannot both vanish, and it is also possible to show that the combinations $k^l \alpha_l(k)$ and $k^{-l-1}\beta_l(k)$ are entire analytic functions. Furthermore, it is obvious that the symmetries

$$\alpha_l(k)^* = \alpha_l(k^*), \qquad \alpha_l(-k) = (-1)^l \alpha_l(k),$$

$$\beta_l(k)^* = \beta_l(k^*), \qquad \beta_l(-k) = (-1)^{l+1} \beta_l(k), \tag{2.11}$$

hold.

For real $k > 0$ and angular momentum l, the associated scattering phase is given by

$$e^{2i\delta_l(k)} = \frac{\alpha_l(k) + i\beta_l(k)}{\alpha_l(k) - i\beta_l(k)} . \tag{2.12}$$

It follows from the properties listed above that $e^{2i\delta_l(k)}$ is a well-defined real analytic function of k. Similarly, for $-ik > 0$ (negative real energies E), it is

* All conventions regarding Legendre polynomials, spherical harmonics and spherical Bessel functions are as in ref. [13], appendix B.

natural to introduce the phase

$$e^{2i\sigma_l(k)} = \frac{\alpha_l(k) + \beta_l(k)}{\alpha_l(k) - \beta_l(k)}, \tag{2.13}$$

which is also non-singular. $\sigma_l(k)$ is equal to $-\pi/4 \pmod \pi$ if (and only if) there is a bound state with angular momentum l at the corresponding energy. Otherwise $\sigma_l(k)$ does not have any direct physical interpretation, except that it is related to the scattering phase, analytically continued to the imaginary axis, through $\tan\sigma_l(k) = -i\tan\delta_l(k)$.

In the limit $k \to 0$, eq. (2.10) reduces to

$$u_l(r;0) = \alpha_l^0 \frac{1}{(2l+1)!!} r^l + \beta_l^0 \frac{(2l+1)!!}{2l+1} r^{-l-1}, \qquad (r > R), \tag{2.14}$$

where

$$\alpha_l^0 = \lim_{k\to 0} k^l \alpha_l(k), \qquad \beta_l^0 = \lim_{k \to 0} k^{-l-1}\beta_l(k). \tag{2.15}$$

In most instances α_l^0 does not vanish, and it is then customary to define the threshold parameters

$$a_l = \beta_l^0/\alpha_l^0. \tag{2.16}$$

In particular, a_0 is referred to as the scattering length. These parameters are important, because they determine the leading low-energy behavior of the scattering phase $\delta_l(k)$. Explicitly, from the discussion above one infers that

$$\delta_l(k) = \nu_l \pi + a_l k^{2l+1} + \mathrm{O}(k^{2l+3}) \tag{2.17}$$

for some integer ν_l.

2.2. ENERGY EIGENSTATES ON A TORUS

We now enclose the particles in a box of size $L \times L \times L$ with periodic boundary conditions. The states with zero total momentum are then described by wave functions $\psi(\boldsymbol{r})$ satisfying

$$\psi(\boldsymbol{r} + \boldsymbol{n}L) = \psi(\boldsymbol{r}) \quad \text{for all } \boldsymbol{n} \in \mathbb{Z}^3. \tag{2.18}$$

The Hamilton operator, defined by

$$H = -\frac{1}{2\mu}\Delta + V_L(\boldsymbol{r}), \qquad V_L(\boldsymbol{r}) = \sum_{\boldsymbol{n}\in\mathbb{Z}^3} V(|\boldsymbol{r} + \boldsymbol{n}L|), \tag{2.19}$$

takes into account interactions "around the world" and thus respects the periodicity of the wave functions.

H can be regarded as an elliptic hermitian differential operator, which acts on differentiable functions on a 3-dimensional torus. The spectrum of H in the corresponding space of square integrable functions is therefore purely discrete and there is a complete set of smooth eigenfunctions.

Suppose now that $\psi(\boldsymbol{r})$ is such an eigenfunction with energy $E = k^2/2\mu$, and let us assume that $L > 2R$. It is then obvious that $\psi(\boldsymbol{r})$ is a smooth periodic solution of the Helmholtz equation

$$(\Delta + k^2)\psi(\boldsymbol{r}) = 0 \tag{2.20}$$

in the "exterior region"

$$\Omega = \{\boldsymbol{r} \in \mathbb{R}^3 \mid |\boldsymbol{r} + \boldsymbol{n}L| > R \quad \text{for all } \boldsymbol{n} \in \mathbb{Z}^3\}. \tag{2.21}$$

Furthermore, for $0 \leqslant r < L/2$, the spherical components $\psi_{lm}(r)$, defined through eq. (2.4), are regular solutions of the radial Schrödinger equation (2.6). Since there is only one such solution for fixed k and l, it follows that

$$\psi_{lm}(r) = b_{lm}\{\alpha_l(k)j_l(kr) + \beta_l(k)n_l(kr)\} \tag{2.22}$$

for some constants b_{lm} and all $R < r < L/2$.

The eigenfunctions of the hamiltonian operator are actually entirely determined by their properties in the exterior region Ω. This is asserted by

Theorem 2.1. *Let $\psi(\boldsymbol{r})$ be a smooth periodic solution of the Helmholtz equation in the region Ω such that its spherical components $\psi_{lm}(r)$ satisfy eq. (2.22) for some constants b_{lm} and all $R < r < L/2$. Then there exists a unique eigenfunction of H which coincides with $\psi(\boldsymbol{r})$ on Ω.*

The proof is given in appendix A. While the theorem is of no immediate practical use, it does imply that the spectrum of H in any given energy interval $E_1 < E < E_2$ is in principle calculable when the scattering phases $\delta_l(k)$ [and $\sigma_l(k)$] are known for these energies. We only have to find all smooth solutions of the Helmholtz equation in Ω with spherical components satisfying eq. (2.22).

2.3. ANGULAR MOMENTUM CUTOFF

In the following we shall introduce an angular momentum cutoff Λ on the interaction. This may be considered as a mathematical device, which is to be removed at the end of all calculations by taking the limit $\Lambda \to \infty$. Alternatively, we may interpret Λ as a parameter, which allows us to monitor the influence of the higher scattering phases $\delta_l(k)$ on the spectrum of H. This is a useful point of view in those instances, where $\delta_l(k)$ is not known beyond some maximal value of angular momentum, a common situation when experimental data are the only source of information.

The angular momentum cutoff is introduced into the system in infinite volume by defining a modified hamiltonian H_Λ through

$$H_\Lambda = -\frac{1}{2\mu}\Delta + Q_\Lambda V(r), \tag{2.23}$$

where

$$Q_\Lambda \psi(\mathbf{r}) = \sum_{l=0}^{\Lambda} \sum_{m=-l}^{l} Y_{lm}(\theta, \varphi) \psi_{lm}(r) \tag{2.24}$$

denotes the projector on the space of wave functions with angular momenta $l \leqslant \Lambda$. Q_Λ commutes with the potential and the cutoff Hamilton operator is hence hermitian. In the same way as the original system, it describes two particles with zero total momentum and a rotationally invariant interaction of finite range R.

The interaction term in eq. (2.23) is non-local, because Q_Λ is an integral operator at fixed r. But this is of little concern for the scattering theory which can be developed without difficulty following the standard methods (Møller operators, Lippmann–Schwinger equations, etc.). It then turns out that the scattering phases are determined by the regular solution $u_l(r;k)$ of the radial Schrödinger equation as before. For all $l \leqslant \Lambda$, the latter coincides with eq. (2.6) and the scattering phases are hence exactly equal to $\delta_l(k)$, the scattering phases of the original system. For greater values of l the angular momentum cutoff comes into effect and the radial Schrödinger equation reduces to the free equation. The scattering phases of the modified system are thus equal to zero for all $l > \Lambda$.

In finite volume the cutoff hamiltonian H_Λ is defined in the obvious way by periodic repetition of the interaction term in eq. (2.23). All the statements made in subsect. 2.2, including theorem 2.1, then carry over literally.

The spectra of H and H_Λ are however not the same in general, although they can be shown to approach each other in the limit $\Lambda \to \infty$. To make this plausible, consider a non-degenerate eigenfunction $\psi(\mathbf{r})$ of H with energy E. Treating the difference $H_\Lambda - H$ as a perturbation, the first-order energy deviation ΔE is given by

$$\Delta E = c \sum_{l=\Lambda+1}^{\infty} \sum_{m=-l}^{l} \int_0^{\infty} \mathrm{d}r\, r^2 V(r) |\psi_{lm}(r)|^2, \tag{2.25}$$

where c is some constant independent of Λ. We have earlier remarked that the expansion coefficients $\psi_{lm}(r)$ go rapidly to zero (faster than any power of $1/l$) for $l \to \infty$, uniformly in the interval $0 \leqslant r \leqslant R$. ΔE is hence rapidly vanishing when the cutoff Λ is sent to infinity, thus confirming our expectation that the spectrum of H_Λ converges to the spectrum of H.

The aim in the following is to find an expression, as explicit as possible, for the finite volume energy spectrum in terms of the scattering phases. This problem will first be solved for the cutoff system. If desired the limit $\Lambda \to \infty$ can be taken after that, and one is then guaranteed to obtain the solution of the original problem.

3. Singular periodic solutions of the Helmholtz equation

As shown by theorem 2.1, the energy eigenstates of the non-relativistic model in finite volume are closely related to certain solutions of the Helmholtz equation. In sect. 4 we shall construct all these solutions for the system with an angular momentum cutoff. As a preparation towards this goal, we here discuss a class of singular solutions of the Helmholtz equation, from which all other solutions will eventually be built.

3.1. DEFINITION

In the following a function $\psi(\boldsymbol{r})$ is called a singular periodic solution of the Helmholtz equation if it has the following properties.

(i) $\psi(\boldsymbol{r})$ is a smooth function which is defined for all $\boldsymbol{r} \neq 0 \pmod L$ and which satisfies the Helmholtz equation

$$(\Delta + k^2)\psi(\boldsymbol{r}) = 0 \tag{3.1}$$

for some (possibly complex) value of k.

(ii) $\psi(\boldsymbol{r})$ is periodic with period L [eq. (2.18)].

(iii) Near the origin, $\psi(\boldsymbol{r})$ is bounded by a power of $1/r$. That is

$$\sup_{0<r<L/2} \left| r^{\Lambda+1}\psi(\boldsymbol{r}) \right| < \infty \tag{3.2}$$

for some integer Λ, which will be referred to as the degree of $\psi(\boldsymbol{r})$.

In this section all such functions are listed and some of their properties will be discussed. For values of k in the "singular set"

$$\mathcal{S} = \left\{ k \in \mathbb{R} \,\middle|\, k = \pm\frac{2\pi}{L}|\boldsymbol{n}| \quad \text{for some } \boldsymbol{n} \in \mathbb{Z}^3 \right\}, \tag{3.3}$$

the Helmholtz equation has periodic plane wave solutions, and these tend to complicate the situation. A separate treatment of these cases will therefore be necessary.

The structure of the singularity at the origin of a singular solution $\psi(\boldsymbol{r})$ of the Helmholtz equation is strongly constrained by the differential equation (3.1). To see this, first note that $\psi(\boldsymbol{r})$ is smooth for $0<r<L/2$. The expansion (2.4) in spherical harmonics hence converges rapidly and the coefficients $\psi_{lm}(r)$ satisfy the free radial Schrödinger equation. Thus there are constants b_{lm} and c_{lm} such that

$$\psi_{lm}(r)=b_{lm}k^{-l}j_l(kr)+c_{lm}k^{l+1}n_l(kr)\,. \tag{3.4}$$

Furthermore, from the bound (3.2) and the identity

$$\psi_{lm}(r)=\int \mathrm{d}\theta\,\mathrm{d}\varphi\sin\theta\,Y_{lm}(\theta,\varphi)^*\psi(\boldsymbol{r})\,, \tag{3.5}$$

one immediately infers that

$$c_{lm}=0 \quad \text{for all } l>\Lambda\,. \tag{3.6}$$

We have thus shown that

$$\psi(\boldsymbol{r})=\sum_{l=0}^{\Lambda}\sum_{m=-l}^{l}c_{lm}Y_{lm}(\theta,\varphi)k^{l+1}n_l(kr)+\hat{\psi}(\boldsymbol{r})\,, \tag{3.7}$$

where the remainder $\hat{\psi}(\boldsymbol{r})$ is a smooth solution of the Helmholtz equation in an open neighborhood of the origin $\boldsymbol{r}=0$.

3.2. GENERAL SOLUTION (REGULAR VALUES OF k)

We assume throughout this subsection that k is not contained in the singular set $\mathscr{S}$. The Helmholtz operator on the torus then has no zero modes and the Green function

$$G(\boldsymbol{r};k^2)=L^{-3}\sum_{\boldsymbol{p}\in\Gamma}\frac{\mathrm{e}^{i\boldsymbol{p}\boldsymbol{r}}}{\boldsymbol{p}^2-k^2} \tag{3.8}$$

is hence a well-defined distribution. The sum in eq. (3.8) runs over the lattice

$$\Gamma=\left\{\boldsymbol{p}\in\mathbb{R}^3\,\middle|\,\boldsymbol{p}=\frac{2\pi}{L}\boldsymbol{n}\quad\text{for some }\boldsymbol{n}\in\mathbb{Z}^3\right\} \tag{3.9}$$

and is taken in the sense of distributions. $G(\boldsymbol{r};k^2)$ is obviously periodic, and it satisfies

$$(\Delta+k^2)G(\boldsymbol{r};k^2)=-\sum_{\boldsymbol{n}\in\mathbb{Z}^3}\delta(\boldsymbol{r}+\boldsymbol{n}L)\,. \tag{3.10}$$

In particular, for all $r \neq 0$ (mod L), the Green function solves Helmholtz' equation and this implies, by elliptic regularity, that it is infinitely differentiable in this region. It is also well known that Green functions of elliptic differential operators are bounded by a power of $1/r$ near the origin. We have thus found a simple example of a singular periodic solution of the Helmholtz equation.

To determine the singularity of $G(\boldsymbol{r}; k^2)$ at the origin explicitly, first note that

$$(\Delta + k^2) n_0(kr) = -\frac{4\pi}{k}\delta(\boldsymbol{r}). \tag{3.11}$$

Invoking elliptic regularity once more, we then conclude that the difference

$$G(\boldsymbol{r}; k^2) - \frac{k}{4\pi} n_0(kr) \tag{3.12}$$

must be a smooth function in an open neighborhood of the origin. In other words, the representation (3.7) for the Green function reads

$$G(\boldsymbol{r}; k^2) = \frac{k}{4\pi} n_0(kr) + \hat{G}(\boldsymbol{r}; k^2) \tag{3.13}$$

(here and below the hat accent denotes the regular part of a function).

It is obvious that further singular solutions can be generated from the Green function by differentiating with respect to $\boldsymbol{r}$. To obtain linearly independent solutions, we should however take care that the differential operators employed do not contain terms proportional to the laplacian (Helmholtz' equation could otherwise be used to reduce the number of differentiations). This can be achieved by introducing the harmonic polynomials

$$\mathcal{Y}_{lm}(\boldsymbol{r}) = r^l Y_{lm}(\theta, \varphi) \tag{3.14}$$

and defining

$$G_{lm}(\boldsymbol{r}; k^2) = \mathcal{Y}_{lm}(\nabla) G(\boldsymbol{r}; k^2). \tag{3.15}$$

It is trivial to verify that these functions are singular periodic solutions of the Helmholtz equation of degree l.

To determine the precise form of their singularity at the origin requires more work. The crucial identity is

$$\mathcal{Y}_{lm}(\nabla) n_0(kr) = (-k)^l Y_{lm}(\theta, \varphi) n_l(kr), \tag{3.16}$$

which will be established in appendix B. From eq. (3.13) we then conclude that

$$G_{lm}(\boldsymbol{r};k^2) = \frac{(-1)^l}{4\pi} Y_{lm}(\theta,\varphi) k^{l+1} n_l(kr) + \hat{G}_{lm}(\boldsymbol{r};k^2). \tag{3.17}$$

It is clear from this result that the functions $G_{lm}(\boldsymbol{r};k^2)$ are linearly independent.

They are also complete in the sense that any singular periodic solution $\psi(\boldsymbol{r})$ of the Helmholtz equation of degree Λ is a linear combination of the functions $G_{lm}(\boldsymbol{r};k^2)$ with $l \leqslant \Lambda$. This is easy to prove. From eqs. (3.7) and (3.17) one infers that

$$\chi(\boldsymbol{r}) \stackrel{\text{def}}{=} \psi(\boldsymbol{r}) - \sum_{l=0}^{\Lambda} \sum_{m=-l}^{l} 4\pi(-1)^l c_{lm} G_{lm}(\boldsymbol{r};k^2) \tag{3.18}$$

continuously extends to a regular function at the origin. $\chi(\boldsymbol{r})$ is also periodic and a solution of the Helmholtz equation. In other words, it is a smooth periodic eigenfunction of the Laplacian with eigenvalue $-k^2$. But since we have assumed that k is not in the singular set $\mathscr{S}$, no such eigenfunction exists and we conclude that $\chi(\boldsymbol{r}) = 0$, thus proving completeness.

3.3. GENERAL SOLUTION (SINGULAR VALUES OF k)

For singular values of k, the set

$$\Gamma_k = \{\boldsymbol{p} \in \Gamma \,|\, \boldsymbol{p}^2 = k^2\} \tag{3.19}$$

is not empty and the plane waves

$$\mathrm{e}^{i\boldsymbol{pr}}, \quad \boldsymbol{p} \in \Gamma_k, \tag{3.20}$$

solve the Helmholtz equation.

Further solutions may be obtained by taking derivatives of the Green function

$$G'(\boldsymbol{r};k^2) = L^{-3} \sum_{\boldsymbol{p}\in\Gamma}{}' \frac{\mathrm{e}^{i\boldsymbol{pr}}}{\boldsymbol{p}^2 - k^2}, \tag{3.21}$$

where the primed sum implies that all momenta $\boldsymbol{p} \in \Gamma_k$ should be omitted. It is easy to show that

$$(\Delta + k^2) G'(\boldsymbol{r};k^2) = -\sum_{\boldsymbol{n}\in\mathbb{Z}^3} \delta(\boldsymbol{r} + \boldsymbol{n}L) + L^{-3} \sum_{\boldsymbol{p}\in\Gamma_k} \mathrm{e}^{i\boldsymbol{pr}}. \tag{3.22}$$

The Green function and its derivatives

$$G'_{lm}(\boldsymbol{r};k^2) = \mathscr{Y}_{lm}(\nabla) G'(\boldsymbol{r};k^2) \tag{3.23}$$

are hence not themselves singular periodic solution of the Helmholtz equation. But such functions can be constructed by forming linear combinations

$$\sum_{l=0}^{\Lambda} \sum_{m=-l}^{l} v_{lm} G'_{lm}(\boldsymbol{r}; k^2) \tag{3.24}$$

with coefficients such that

$$\sum_{l=0}^{\Lambda} \sum_{m=-l}^{l} v_{lm} i^l \mathscr{Y}_{lm}(\boldsymbol{p}) = 0 \quad \text{for all } \boldsymbol{p} \in \Gamma_k . \tag{3.25}$$

Since there are only a finite number of points in Γ_k, these conditions can always be satisfied if Λ is sufficiently large. In any case, they are just a set of equations which determine a linear subspace in the space of all possible linear combinations of the basic functions $G'_{lm}(\boldsymbol{r}; k^2)$.

The plane waves (3.20) and the linear combinations (3.24), (3.25) form a complete set of singular periodic solutions of the Helmholtz equation. To prove this, we note that eq. (3.17) remains valid if we replace G_{lm} and $\hat{G}_{lm}$ by their primed versions. For any given singular periodic solution $\psi(\boldsymbol{r})$ of degree Λ, the function

$$\chi(\boldsymbol{r}) \stackrel{\text{def}}{=} \psi(\boldsymbol{r}) - \sum_{l=0}^{\Lambda} \sum_{m=-l}^{l} v_{lm} G'_{lm}(\boldsymbol{r}; k^2), \qquad v_{lm} = 4\pi(-1)^l c_{lm}, \tag{3.26}$$

is therefore everywhere regular and periodic. Furthermore, it satisfies

$$(\Delta + k^2)\chi(\boldsymbol{r}) = -L^{-3} \sum_{\boldsymbol{p} \in \Gamma_k} e^{i\boldsymbol{p}\boldsymbol{r}} \sum_{l=0}^{\Lambda} \sum_{m=-l}^{l} v_{lm} i^l \mathscr{Y}_{lm}(\boldsymbol{p}) . \tag{3.27}$$

If we multiply this equation with $e^{-i\boldsymbol{p}\boldsymbol{r}}$ and integrate over $\boldsymbol{r}$, one immediately concludes that the coefficients v_{lm} solve the constraints (3.25). In particular, the right-hand side of eq. (3.27) vanishes and $\chi(\boldsymbol{r})$ is therefore a linear combination of the plane waves (3.20). We have thus established completeness as asserted.

3.4. EXPANSION IN SPHERICAL HARMONICS (REGULAR VALUES OF k)

We have shown in subsect. 3.2 that the general singular periodic solution of the Helmholtz equation for $k \notin \mathscr{S}$ is a (finite) linear combination of the functions $G_{lm}(\boldsymbol{r}; k^2)$. The aim here is to work out the expansion of these basis elements in spherical harmonics.

From the discussion in subsect. 3.1 and the known structure (3.17) of the singularity at the origin, one infers that

$$G_{lm}(\boldsymbol{r};k^2)=\frac{(-1)^l}{4\pi}k^{l+1}\left\{Y_{lm}(\theta,\varphi)n_l(kr)+\sum_{l'=0}^{\infty}\sum_{m'=-l'}^{l'}\mathcal{M}_{lm,l'm'}Y_{l'm'}(\theta,\varphi)j_{l'}(kr)\right\} \tag{3.28}$$

for all $0<r<L/2$. The matrix $\mathcal{M}_{lm,l'm'}$ occurring here plays a central role in the analysis of the two-particle spectrum in finite volume, and it is therefore important to compute it as explicitly as one can.

To this end it is useful to start with the simplest case, the expansion of the Green function

$$G(\boldsymbol{r};k^2)=\frac{k}{4\pi}n_0(kr)+\sum_{l=0}^{\infty}\sum_{m=-l}^{l}g_{lm}Y_{lm}(\theta,\varphi)j_l(kr). \tag{3.29}$$

In appendix D a simple relation between the coefficients g_{lm} and the zeta function $\mathcal{Z}_{lm}(s;q^2)$ is established. For complex s with $\operatorname{Re}2s>l+3$, this function is defined through

$$\mathcal{Z}_{lm}(s;q^2)=\sum_{\boldsymbol{n}\in\mathbb{Z}^3}\mathcal{Y}_{lm}(\boldsymbol{n})(\boldsymbol{n}^2-q^2)^{-s}, \tag{3.30}$$

where the convention $-\pi<\arg(\boldsymbol{n}^2-q^2)\leqslant\pi$ has been adopted. By analytic continuation it then extends to a meromorphic function in the whole complex plane. In particular, there is no singularity at $s=1$ and the announced relation is

$$g_{lm}=\frac{i^l}{\pi Lq^l}\mathcal{Z}_{lm}(1;q^2),\qquad q=\frac{kL}{2\pi}. \tag{3.31}$$

The zeta function is not expressible in terms of elementary functions, but there are well-conditioned integral representations which allow one to compute it numerically to any desired precision (appendix C).

To obtain the expansion in spherical harmonics of $G_{lm}(\boldsymbol{r};k^2)$, we apply the differential operator $\mathcal{Y}_{lm}(\nabla)$ to the series (3.29). The action of this operator on the singular term is given by eq. (3.16). The corresponding identity for the regular terms reads

$$\mathcal{Y}_{lm}(\nabla)Y_{js}(\theta,\varphi)j_j(kr)=\frac{k^l}{\sqrt{4\pi}}\sum_{l'=|j-l|}^{j+l}\sum_{m'=-l'}^{l'}C_{lm,js,l'm'}Y_{l'm'}(\theta,\varphi)j_{l'}(kr), \tag{3.32}$$

where the tensor $C_{lm,js,l'm'}$ is related to the Wigner $3j$-symbols through*

$$C_{lm,js,l'm'} = (-1)^{m'} i^{l-j+l'} \sqrt{(2l+1)(2j+1)(2l'+1)} \times \begin{pmatrix} l & j & l' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l & j & l' \\ m & s & -m' \end{pmatrix}. \tag{3.33}$$

The proof of these formulae is deferred to appendix B. Here we only note that for all values of the indices, the tensor $C_{lm,js,l'm'}$ is equal to a rational number times the square root of a positive integer.

We now collect all contributions and obtain the final result

$$\mathcal{M}_{lm,l'm'} = \frac{(-1)^l}{\pi^{3/2}} \sum_{j=|l-l'|}^{l+l'} \sum_{s=-j}^{j} \frac{i^j}{q^{j+1}} \mathcal{Z}_{js}(1;q^2) C_{lm,js,l'm'}. \tag{3.34}$$

A table of all matrix elements $\mathcal{M}_{lm,l'm'}$ with angular momenta $l, l' \leqslant 4$ is given in appendix E. As a consequence of the cubic symmetry, to be discussed later, one has the selection rules

$$\mathcal{M}_{lm,l'm'} = 0 \quad \text{if } m \neq m' \ (\mathrm{mod}\, 4) \quad \text{or} \quad l \neq l' \ (\mathrm{mod}\, 2), \tag{3.35}$$

and it is also possible to show that the identities

$$\mathcal{M}_{lm,l'm'} = \mathcal{M}_{l'm',lm} = \mathcal{M}_{l-m,l'-m'} \tag{3.36}$$

hold for arbitrary values of the indices.

3.5. EXPANSION IN SPHERICAL HARMONICS (SINGULAR VALUES OF k)

According to subsect. 3.3 there are two types of singular periodic solutions of the Helmholtz equation when k is singular. Consider first the plane wave solutions (3.20). Their expansion in spherical harmonics is given by the well-known formula

$$\mathrm{e}^{ipr} = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{l} i^l Y_{lm}(\theta_p, \varphi_p)^* Y_{lm}(\theta, \varphi) j_l(pr), \tag{3.37}$$

where θ_p and φ_p denote the polar angles of $\boldsymbol{p}$.

* The notations and sign conventions concerning Clebsch–Gordan coefficients and Wigner symbols are as in ref. [13], appendix C.

The other solutions are the linear combinations (3.24) with coefficients v_{lm} satisfying the constraints (3.25). It follows from these that

$$\sum_{l=0}^{\Lambda} \sum_{m=-l}^{l} v_{lm} G'_{lm}(\boldsymbol{r}; k^2) = \lim_{h \to k} \sum_{l=0}^{\Lambda} \sum_{m=-l}^{l} v_{lm} G_{lm}(\boldsymbol{r}; h^2). \tag{3.38}$$

The desired expansion in spherical harmonics may therefore be deduced from the expansion (3.28). In particular, if $k = 2\pi|\boldsymbol{n}|/L$ for some *non-zero* integer vector $\boldsymbol{n}$, one obtains

$$\sum_{l=0}^{\Lambda} \sum_{m=-l}^{l} v_{lm} G'_{lm}(\boldsymbol{r}; k^2) = \sum_{l=0}^{\Lambda} \sum_{m=-l}^{l} v_{lm} \frac{(-1)^l}{4\pi} k^{l+1} \Bigg\{ Y_{lm}(\theta, \varphi) n_l(kr) + \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} \mathcal{M}'_{lm,l'm'} Y_{l'm'}(\theta, \varphi) j_{l'}(kr) \Bigg\}. \tag{3.39}$$

The matrix $\mathcal{M}'_{lm,l'm'}$ in this equation is determined through the expansion

$$\mathcal{M}_{lm,l'm'} \underset{q \to |\boldsymbol{n}|}{=} \frac{1}{q^2 - \boldsymbol{n}^2} \mathcal{V}_{lm,l'm'} + \mathcal{M}'_{lm,l'm'} + \mathrm{O}(q^2 - \boldsymbol{n}^2). \tag{3.40}$$

We shall not need an explicit expression for this matrix later on, but it will be useful to know that the residue of the pole term in eq. (3.40) is given by

$$\mathcal{V}_{lm,l'm'} = -\frac{2}{\pi |\boldsymbol{n}|} \sum_{\boldsymbol{p} \in \Gamma_k} i^{l-l'} Y_{lm}(\theta_p, \varphi_p)^* Y_{l'm'}(\theta_p, \varphi_p) \tag{3.41}$$

(cf. appendix B).

For $k = 0$ the situation is somewhat special and requires a separate treatment. Note that the constraints (3.25) in this case are equivalent to $v_{00} = 0$. Accordingly, the singular solutions of the Helmholtz equation are the functions $G'_{lm}(\boldsymbol{r}; 0)$ with $l \geqslant 1$. These coincide with $G_{lm}(\boldsymbol{r}; 0)$ and from eq. (3.28) we thus deduce the expansion

$$G'_{lm}(\boldsymbol{r}; 0) = \frac{(-1)^l}{4\pi} \left(\frac{2\pi}{L} \right)^{l+1} \Bigg\{ Y_{lm}(\theta, \varphi) \frac{(2l+1)!!}{(2l+1)} \rho^{-l-1} + \sum_{l'=0}^{\infty} \sum_{m'=-l'}^{l'} \mathcal{M}^0_{lm,l'm'} Y_{l'm'}(\theta, \varphi) \frac{\rho^{l'}}{(2l'+1)!!} \Bigg\}, \tag{3.42}$$

where $\rho = 2\pi r/L$. The matrix $\mathcal{M}^{0}_{lm,l'm'}$ appearing here is defined through

$$\mathcal{M}^{0}_{lm,l'm'} = \lim_{q\to 0} q^{l+l'+1}\mathcal{M}_{lm,l'm'}, \qquad (l \geqslant 1), \tag{3.43}$$

and it would be easy to write it down explicitly in terms of zeta functions and Wigner symbols by inserting the general expression (3.34).

4. Construction of energy eigenstates

We are now well prepared to discuss the energy spectrum of the nonrelativistic model in finite volume. As explained in sect. 2, it is sufficient to consider the system with a finite angular momentum cutoff Λ, the original system being recovered in the limit $\Lambda \to \infty$. In the following, the box size L is always assumed to be greater than $2R$, and k denotes the momentum determined through eq. (2.7).

4.1. ENERGY EIGENSTATES AND SINGULAR SOLUTIONS OF THE HELMHOLTZ EQUATION

We have already remarked that the calculation of the spectrum of H_Λ in finite volume is equivalent to finding all solutions of the Helmholtz equation in the outer region Ω with some additional properties, which could be regarded as boundary conditions along the sphere $r = R$. The presence of the angular momentum cutoff now allows us to simplify the situation even further, as the following theorem shows.

Theorem 4.1. *There is a one-to-one correspondence between the eigenfunctions of H_Λ in finite volume and the singular periodic solutions $\psi(\boldsymbol{r})$ of the Helmholtz equation, which have degree Λ and whose spherical components $\psi_{lm}(r)$ satisfy eq. (2.22) for all $l \leqslant \Lambda$ and $0 < r < L/2$. The relation is that any such function restricted to Ω coincides with a unique energy eigenfunction, and vice versa.*

To determine the energy spectrum it is therefore sufficient to construct all singular periodic solutions of the Helmholtz equation of the specified type. Note that the number of conditions to be satisfied is finite and that all reference to the interaction range R has disappeared.

The proof of the theorem is simple. If we first assume that we are given a singular solution of Helmholtz' equation with properties as stated, its restriction to Ω trivially satisfies the hypotheses of theorem 2.1 and the existence of the associated eigenfunction of H_Λ is thus guaranteed.

Conversely, if we start from an energy eigenfunction $\chi(\boldsymbol{r})$, its spherical components in the interval $R < r < L/2$ satisfy

$$\chi_{lm}(r) = b_{lm} \times \begin{cases} \alpha_l(k) j_l(kr) + \beta_l(k) n_l(kr) & \text{if } l \leqslant \Lambda, \\ (2l+1)!!k^{-l} j_l(kr) & \text{otherwise.} \end{cases} \tag{4.1}$$

The desired singular solution $\psi(\boldsymbol{r})$ of Helmholtz' equation is then defined in three steps. For $\boldsymbol{r} \in \Omega$ we set $\psi(\boldsymbol{r}) = \chi(\boldsymbol{r})$. In the region $0 < r < L/2$, $\psi(\boldsymbol{r})$ is defined through the expansion (2.4), where the spherical components $\psi_{lm}(r)$ are given by the right-hand side of eq. (4.1). And, finally, in all other places $\psi(\boldsymbol{r})$ is fixed by periodicity.

The crucial point here is that the expansion in spherical harmonics, with coefficients $\psi_{lm}(r)$ as specified above, is rapidly convergent for all r in the interval $0 < r < L/2$. This is a consequence of the fact that the spherical Bessel functions $j_l(kr)$ are monotonically rising functions of r for sufficiently large l, in any fixed bounded range of r (cf. appendix A). Once the series converges for some $r = r_0$, it is hence automatically convergent for all $r \leqslant r_0$.

It is obvious that the so constructed function has all the required properties, and we have thus proved the theorem.

4.2. ENERGY SPECTRUM (REGULAR VALUES OF k)

According to sect. 3, the general singular periodic solution of the Helmholtz equation with degree Λ is given by

$$\psi(\boldsymbol{r}) = \sum_{l=0}^{\Lambda} \sum_{m=-l}^{l} v_{lm} G_{lm}(\boldsymbol{r}; k^2) \tag{4.2}$$

with arbitrary coefficients v_{lm}. Among all these functions, the energy eigenstates are those which satisfy eq. (2.22) for all $l \leqslant \Lambda$. Taking eq. (3.28) into account, this condition is equivalent to

$$b_{lm}\alpha_l(k) = \sum_{l'=0}^{\Lambda} \sum_{m'=-l'}^{l'} v_{l'm'} \frac{(-1)^{l'}}{4\pi} k^{l'+1} \mathscr{M}_{l'm',lm}, \tag{4.3}$$

$$b_{lm}\beta_l(k) = v_{lm} \frac{(-1)^l}{4\pi} k^{l+1} \tag{4.4}$$

$(l = 0, 1, \dots, \Lambda)$. The second of these equations can be used to eliminate v_{lm}. After that one is left with a homogeneous linear system for the coefficients b_{lm}. Since the number of equations is equal to the number of unknowns, a non-zero solution exists if and only if the associated determinant vanishes. This will happen for a discrete set of values of k, corresponding to the eigenvalues of H_Λ. The computation of the energy spectrum has thus been reduced to the problem of finding the zeros of the determinant of a certain k-dependent matrix.

To be able to write down this determinantal condition concisely, some further notation is needed. Let $\mathscr{H}_\Lambda$ be the space of complex vectors v with components v_{lm}, where $l = 0, 1, \dots, \Lambda$ and $m = -l, -l+1, \dots, l$. A scalar product on this space is given by

$$(v, w) = \sum_{l=0}^{\Lambda} \sum_{m=-l}^{l} v_{lm}^* w_{lm} . \tag{4.5}$$

The matrix $\mathscr{M}_{lm,l'm'}$ can obviously be regarded as a linear operator M in $\mathscr{H}_\Lambda$. Two further operators A and B may be defined through

$$[Av]_{lm} = \alpha_l(k) v_{lm}, \qquad [Bv]_{lm} = \beta_l(k) v_{lm}, \tag{4.6}$$

and from these one obtains the matrices

$$\begin{aligned} e^{2i\delta} &= (A + iB)/(A - iB), \\ e^{2i\sigma} &= (A + B)/(A - B) \end{aligned} \tag{4.7}$$

(cf. subsect. 2.1).

The condition for the existence of a non-zero solution of the linear equations (4.3) and (4.4) can now be written in the closed form

$$\det[A - BM] = 0. \tag{4.8}$$

This equation is not entirely satisfactory, because it involves the amplitudes $\alpha_l(k)$ and $\beta_l(k)$ rather than the scattering phases $\delta_l(k)$. To remove this defect, first note that all eigenvalues of H_Λ are real. The solutions k of eq. (4.8) are therefore either real or purely imaginary, depending on whether E is positive or negative. For positive and non-singular k, the determinant

$$\det[(A - iB)(M - i)] \tag{4.9}$$

is well defined and non-zero, because M is hermitian and because the eigenvalues of $A - iB$ do not vanish (cf. subsect. 2.1). It is clear then that eq. (4.8) may be divided by this factor without affecting the set of solutions.

We have thus shown that for non-singular $k > 0$, eq. (4.8) is equivalent to

$$\det[e^{2i\delta} - U] = 0, \qquad U = (M + i)/(M - i). \tag{4.10}$$

In the same way, the condition for energy eigenstates with $-ik>0$ becomes

$$\det[e^{2i\sigma}-V]=0, \qquad V=(M+1)/(M-1). \tag{4.11}$$

Where needed, both matrices U and V occurring here are unitary operators in $\mathscr{H}_1$. They are complicated but explicitly known functions of q.

4.3. ENERGY SPECTRUM (SINGULAR VALUES OF $k>0$)

We now proceed to discuss finite volume energy eigenstates with $k=2\pi|\boldsymbol{n}|/L$, where $\boldsymbol{n}$ is some *non-zero* integer vector.

In this case the general solution of Helmholtz' equation with degree Λ is given by

$$\psi(\boldsymbol{r})=\sum_{\boldsymbol{p}\in\Gamma_k} w_{\boldsymbol{p}}\, e^{i\boldsymbol{p}\boldsymbol{r}}+\sum_{l=0}^{\Lambda}\sum_{m=-l}^{l} v_{lm} G'_{lm}(\boldsymbol{r};k^2). \tag{4.12}$$

$w_{\boldsymbol{p}}$ can be chosen freely here, while the coefficients v_{lm} are constrained by eq. (3.25). Energy eigenstates are characterized by a further set of linear conditions, which can be straightforwardly derived by inserting the expansions (3.37) and (3.39) in spherical harmonics. Explicitly, they are

$$b_{lm}\alpha_l(k)=4\pi\sum_{\boldsymbol{p}\in\Gamma_k} w_{\boldsymbol{p}}\, i^l Y_{lm}(\theta_p,\varphi_p)^* + \sum_{l'=0}^{\Lambda}\sum_{m'=-l'}^{l'} v_{l'm'}\frac{(-1)^{l'}}{4\pi}k^{l'+1}\mathscr{M}'_{l'm',lm}, \tag{4.13}$$

$$b_{lm}\beta_l(k)=v_{lm}\frac{(-1)^l}{4\pi}k^{l+1}, \tag{4.14}$$

$(l=0,1,\dots,\Lambda)$.

It is obvious that a solution of these equations [and the constraint (3.25)] is obtained if we set $b_{lm}=v_{lm}=0$ and choose the coefficients $w_{\boldsymbol{p}}$ such that

$$\sum_{\boldsymbol{p}\in\Gamma_k} w_{\boldsymbol{p}}\mathscr{Y}_{lm}(\boldsymbol{p})^*=0 \quad \text{for all } l\leqslant\Lambda. \tag{4.15}$$

The plane wave

$$\psi(\boldsymbol{r})=\sum_{\boldsymbol{p}\in\Gamma_k} w_{\boldsymbol{p}}\, e^{i\boldsymbol{p}\boldsymbol{r}} \tag{4.16}$$

then has all the required properties and thus corresponds to an energy eigenstate. Such solutions always exist for any fixed cutoff Λ, because the number of points in

Γ_k will be greater than the number of equations to be satisfied for some sufficiently large k. On the other hand, if we fix k and send Λ to infinity, there will be no solutions, since the harmonic polynomials with $l \leqslant \Lambda$ eventually form a basis in the space of all functions on Γ_k.

Besides the plane waves, there are in general further solutions with $b_{lm} \neq 0$. As shown in appendix F, such solutions exist if and only if

$$\lim_{q \to |n|} \det[e^{2i\delta} - U] = 0 \tag{4.17}$$

[cf. eq. (4.10)]. As a byproduct of the proof of this statement, one finds that the operator U is not singular at $q = |n|$, i.e. the pole of the matrix M at this point cancels in the ratio (4.10). The energy values discussed in this subsection can thus be regarded as special solutions of eq. (4.10).

4.4. SUMMARY

In this section we have shown that a *non-zero* energy value $E = k^2/2\mu$ belongs to the spectrum of the cutoff Hamilton operator H_Λ if and only if one of the following conditions is satisfied.

(a) $k > 0$ is a solution of eq. (4.10). As discussed above, it does not matter whether k is singular or not.

(b) $k \neq 0$ is an element of the singular set $\mathcal{S}$ and eq. (4.15) has a non-zero solution w_p.

(c) $-ik > 0$ and k is a solution of eq. (4.11).

It is of course possible that there are eigenstates of H_Λ with energy $E = 0$ in certain instances. This is a marginal case and usually of little interest, but for completeness the conditions for their existence are derived in appendix G.

No doubt the most interesting condition is (a), which together with (b) determines the spectrum in the range $E > 0$. Eq. (4.10) can be regarded as the 4-dimensional analogue of eq. (1.1). In particular, if we are given the scattering phases in some energy interval, this relation [and (b)] allows us to compute all finite volume energy levels in that range, for all values of L greater than $2R$.

The dimension of $\mathscr{H}_\Lambda$ (and thus the rank of U) is equal to $(\Lambda + 1)^2$. At first sight, one may be led to conclude that the computation of the determinant in eq. (4.10) is rapidly becoming a practical problem when the cutoff Λ is increased. As we shall see in sect. 5, this is not true for the applications envisaged, because the matrix U can be partially diagonalized by projecting on irreducible representations of the cubic group. In the A_1^+-sector, for example, the dimension of the associated subspace is equal to 1, 2, 3, 4 for $\Lambda = 2, 4, 6, 8$, which is certainly manageable.

5. Consequences of the cubic symmetry

The finite volume systems studied in this paper are symmetric under cubic rotations and reflections. We can take advantage of this fact to considerably simplify the expressions for the energy spectrum derived in sect. 4.

5.1. REPRESENTATIONS OF THE CUBIC GROUP

The special cubic group $SO(3,\mathbb{Z})$ has 5 irreducible representations which are denoted by A_1, A_2, E, T_1 and T_2. The dimensionalities of these representations are 1, 1, 2, 3 and 3, respectively. A_1 is the trivial representation and T_1 the vector representation. The transformation matrices for the other cases can be inferred from table 1.

The irreducible representations of the full cubic group $O(3,\mathbb{Z})$ are characterized by an irreducible representation of the special cubic group and the parity $P = \pm 1$ which fixes the transformation behaviour of the states under reflections $\boldsymbol{r} \to -\boldsymbol{r}$. These representations will be denoted by A_1^+, A_1^-, and so on.

Representations of the cubic group arise naturally from representations of O(3). To discuss this connection in more detail, consider the vector space $\mathscr{H}_l$ of all homogeneous harmonic polynomials in $\boldsymbol{r} \in \mathbb{R}^3$ of degree l. The spherical harmonics $\mathscr{Y}_{lm}(\boldsymbol{r})$ with $m = -l, -l+1, \ldots, l$ form an orthonormal basis in this space. Under the action of O(3) they transform according to the irreducible representation with angular momentum l and parity $P = (-1)^l$. Explicitly, for any $R \in O(3)$ we have

$$\mathscr{Y}_{lm}(R\boldsymbol{r}) = \sum_{m'=-l}^{l} D^{(l)}_{mm'}(R)\mathscr{Y}_{lm'}(\boldsymbol{r}), \tag{5.1}$$

where the representation matrices $D^{(l)}_{mm'}(R)$ are unitary.

These matrices also define a representation of the cubic group $O(3,\mathbb{Z})$ which is reducible in most cases. For $l = 0, \ldots, 4$ the decomposition into irreducible representations is given by

$$\mathbf{0} = A_1^+ , \tag{5.2a}$$

$$\mathbf{1} = T_1^- , \tag{5.2b}$$

$$\mathbf{2} = E^+ \oplus T_2^+ , \tag{5.2c}$$

$$\mathbf{3} = A_2^- \oplus T_1^- \oplus T_2^- , \tag{5.2d}$$

$$\mathbf{4} = A_1^+ \oplus E^+ \oplus T_1^+ \oplus T_2^+ . \tag{5.2e}$$

The corresponding basis elements of $\mathscr{H}_l$ are listed in table 1.

In general we define $N(\Gamma, l)$ to be the multiplicity of the irreducible representation Γ in the decomposition of the representation space $\mathscr{H}_l$. The subspace

TABLE 1
Decomposition of $\mathcal{H}_l$ into irreducible representations Γ of the cubic group

l	Γ	Basis polynomials	Range of indices
0	A_1^+	1	
1	T_1^-	r_i	$i = 1,2,3$
2	E^+	$r_i^2 - r_j^2$	$(i,j) = (1,2),(2,3)$
2	T_2^+	$r_i r_j$	$(i,j) = (1,2),(2,3),(3,1)$
3	A_2^-	$r_1 r_2 r_3$	
3	T_1^-	$r_i^3 - \frac{3}{5} r^2 r_i$	$i = 1,2,3$
3	T_2^-	$r_i(r_j^2 - r_k^2)$	$(i,j,k) = (1,2,3),(2,3,1),(3,1,2)$
4	A_1^+	$r_1^4 + r_2^4 + r_3^4 - \frac{3}{5} r^4$	
4	E^+	$r_i^4 - r_j^4 - \frac{6}{7} r^2 (r_i^2 - r_j^2)$	$(i,j) = (1,2),(2,3)$
4	T_1^+	$r_i r_j^3 - r_i^3 r_j$	$(i,j) = (1,2),(2,3),(3,1)$
4	T_2^+	$r_i r_j^3 + r_i^3 r_j - \frac{6}{7} r^2 r_i r_j$	$(i,j) = (1,2),(2,3),(3,1)$

associated to the nth occurrence of Γ is spanned by an orthonormal basis

$$|\Gamma, \alpha; l, n\rangle, \qquad \alpha = 1, \ldots, \dim \Gamma \tag{5.3}$$

$[n = 1, 2, \ldots, N(\Gamma, l)]$. We may choose this basis such that the transformation matrices representing the action of the cubic group are independent of l and n. For $l \leqslant 4$ it is straightforward to construct such a basis from table 1 (note that the polynomials listed there are not orthonormal).

5.2. SYMMETRY PROPERTIES OF THE ZETA FUNCTION

From the transformation law eq. (5.1) and the definition eq. (3.30) of the zeta function one immediately infers that

$$\sum_{m'=-l}^{l} D_{mm'}^{(l)}(R)\, \mathcal{Z}_{lm'}(s; q^2) = \mathcal{Z}_{lm}(s; q^2) \tag{5.4}$$

for all $R \in O(3, \mathbb{Z})$. By going through the list of all group elements, we can thus obtain a set of linear relations between the zeta functions. In particular, we may choose R to be one of the reflections

$$\boldsymbol{r} \to -\boldsymbol{r}, \qquad \boldsymbol{r} \to (r_1, -r_2, r_3), \tag{5.5}$$

or a rotation by $\pi/2$ about the 3-axis. These transformations yield

$$\mathcal{Z}_{lm}(s; q^2) = 0 \quad \text{if } l \text{ is odd}, \tag{5.6}$$

$$\mathcal{Z}_{lm}(s; q^2) = \mathcal{Z}_{l-m}(s; q^2), \tag{5.7}$$

$$\mathcal{Z}_{lm}(s; q^2) = 0 \quad \text{if } m \text{ is not a multiple of } 4. \tag{5.8}$$

There are further relations which are obtained by performing rotations about the other axes. For $l \leqslant 8$ they are

$$\mathcal{Z}_{20}(s;q^2)=0\,, \tag{5.9}$$

$$\mathcal{Z}_{44}(s;q^2)=\frac{\sqrt{70}}{14}\mathcal{Z}_{40}(s;q^2)\,, \tag{5.10}$$

$$\mathcal{Z}_{64}(s;q^2)=-\frac{\sqrt{14}}{2}\mathcal{Z}_{60}(s;q^2)\,, \tag{5.11}$$

$$\mathcal{Z}_{84}(s;q^2)=\frac{\sqrt{154}}{33}\mathcal{Z}_{80}(s;q^2)\,, \tag{5.12}$$

$$\mathcal{Z}_{88}(s;q^2)=\frac{\sqrt{1430}}{66}\mathcal{Z}_{80}(s;q^2)\,. \tag{5.13}$$

For general angular momenta l, the number of linearly independent components of the zeta function $\mathcal{Z}_{lm}(s;q^2)$ is equal to $N(\mathrm{A}_1^+,l)$, the number of cubically invariant homogenous harmonic polynomials of degree l.

We finally note that the symmetries (3.35) and (3.36) of the matrix $\mathcal{M}_{lm,l'm'}$ are a straightforward consequence of eqs. (5.6)–(5.8) and the known symmetries of the Wigner 3j-symbols.

5.3. REDUCTION OF THE MATRIX $\mathcal{M}_{lm,l'm'}$

The Green function $G(r;k^2)$ is invariant under cubic transformations and its derivatives hence satisfy

$$G_{lm}(Rr;k^2)=\sum_{m'=-l}^{l} D^{(l)}_{mm'}(R)G_{lm'}(r;k^2) \tag{5.14}$$

for all $R\in \mathrm{O}(3,\mathbb{Z})$. From the expansion (3.28) in spherical harmonics we thus conclude that

$$\sum_{s=-l}^{l} D^{(l)}_{ms}(R)\mathcal{M}_{ls,l'm'}=\sum_{s'=-l'}^{l'}\mathcal{M}_{lm,l's'}D^{(l')}_{s'm'}(R)\,. \tag{5.15}$$

In other words, the matrix $\mathcal{M}_{lm,l'm'}$ transforms covariantly under the action of the cubic group.

To exploit this property it is advantageous to pass to the operator formulation introduced in subsect. 4.2. The representation matrices $D^{(l)}_{mm'}(R)$ define an operator $D(R)$ in $\mathscr{H}_\Lambda$ in the obvious way. Eq. (5.15) then simply means that $D(R)$ commutes with the operator M. A partial diagonalization of M can thus be achieved by diagonalizing $D(R)$, i.e. by projecting on the irreducible representations of the cubic group.

To this end we first note that $\mathscr{H}_\Lambda$ can be identified with the space of all harmonic polynomials of degree $l \leqslant \Lambda$ through the mapping

$$v \in \mathscr{H}_\Lambda \mapsto \sum_{l=0}^{\Lambda} \sum_{m=-l}^{l} v_{lm} \mathscr{Y}_{lm}(\boldsymbol{r}). \tag{5.16}$$

In this way the basis (5.3) becomes a basis of $\mathscr{H}_\Lambda$. It now follows from Schur's lemma that

$$\langle \Gamma, \alpha; l, n | M | \Gamma', \alpha'; l'n' \rangle = \delta_{\Gamma\Gamma'} \delta_{\alpha\alpha'} \mathscr{M}(\Gamma)_{ln,l'n'}. \tag{5.17}$$

The reduced matrix $\mathscr{M}(\Gamma)_{ln,l'n'}$ occurring here is given explicitly in appendix E for all angular momenta $l, l' \leqslant 4$.

5.4. TWO-PARTICLE STATES WITH DEFINITE CUBIC SYMMETRY

Since the Hamilton operator H_Λ is rotationally invariant, its eigenstates in finite volume come in multiplets which transform according to the irreducible representations of the cubic group. The energy spectrum in the subspace associated to a particular representation Γ can be determined straightforwardly by going through the steps in sect. 4 once more, keeping track of the transformation properties of the wave functions constructed.

As a result one finds that a *non-zero* energy value $E = k^2/2\mu$ belongs to the spectrum of H_Λ in this sector if and only if one of the following conditions is satisfied.

(a) $k > 0$ is a solution of

$$\det\left[e^{2i\delta} - U(\Gamma)\right] = 0, \tag{5.18}$$

where

$$U(\Gamma) = (M(\Gamma) + i)/(M(\Gamma) - i). \tag{5.19}$$

The operators occurring here are linear transformations of the space $\mathscr{H}_\Lambda(\Gamma)$ of all vectors v with components

$$v_{ln}, \quad l = 0, \ldots, \Lambda, \quad n = 1, \ldots, N(\Gamma, l). \tag{5.20}$$

In particular, $M(\Gamma)$ denotes the operator with matrix elements $\mathscr{M}(\Gamma)_{ln,l'n'}$ and

$$[e^{2i\delta} v]_{ln} = e^{2i\delta_l(k)} v_{ln} \tag{5.21}$$

as in sect. 4.

(b) $k = 2\pi|\boldsymbol{n}|/L$ for some non-zero integer vector $\boldsymbol{n}$ and eq. (4.15) has a nontrivial solution w_p which transforms according to the representation Γ under cubic rotations/reflections of the momentum $\boldsymbol{p}$.

(c) $-ik > 0$ and k is a solution of

$$\det\left[e^{2i\sigma} - V(\Gamma)\right] = 0, \tag{5.22}$$

where

$$V(\Gamma) = (M(\Gamma) + 1)/(M(\Gamma) - 1). \tag{5.23}$$

In addition to the energy values covered by the above rules, it is possible that $E = 0$ belongs to the spectrum of the Hamilton operator (cf. appendix G).

6. Energy spectrum in the A_1^+ sector

We now specialize to the case $\Gamma = A_1^+$ and discuss conditions (a) and (b) in more detail for $\Lambda < 6$, using the tables in appendix E. The other symmetry sectors can be worked out in the same way without difficulty.

6.1. BASIC EQUATIONS

The dimension of $\mathscr{H}_1(A_1^+)$ is equal to the number of cubically invariant harmonic polynomials with degree less than or equal to Λ. For $\Lambda < 4$ the only such polynomial is the constant and $\mathscr{H}_1(A_1^+)$ is hence one-dimensional in these cases. Eq. (5.18) then reduces to

$$e^{2i\delta_0} = \frac{m_{00} + i}{m_{00} - i}, \tag{6.1}$$

where $m_{ll'}$ is a shorthand for the matrix element $\mathscr{M}(A_1^+)_{l1,l'1}$. From table E.2 we have

$$m_{00} = \frac{1}{\pi^{3/2} q}\mathscr{Z}_{00}(1; q^2), \qquad q = \frac{kL}{2\pi}, \tag{6.2}$$

so that eq. (6.1) coincides with the result quoted in sect. 1.

When Λ is equal to 4 or 5, there are two invariant harmonic polynomials and eq. (5.18) becomes

$$\left(e^{2i\delta_0} - u_{00}\right)\left(e^{2i\delta_4} - u_{44}\right) = u_{04}^2, \tag{6.3}$$

where

$$u_{00} = \left[(m_{00} + i)(m_{44} - i) - m_{04}^2\right]/\Delta, \tag{6.4}$$

$$u_{44} = \left[(m_{00} - i)(m_{44} + i) - m_{04}^2\right]/\Delta, \tag{6.5}$$

$$u_{04} = u_{40} = -2i m_{04}/\Delta, \tag{6.6}$$

$$\Delta = (m_{00} - i)(m_{44} - i) - m_{04}^2. \tag{6.7}$$

The matrix elements m_{04} and m_{44} are given in table E.2.

Let us now briefly consider condition (b). The independent solutions w_p of eq. (4.15) with

$$w_{Rp} = w_p \quad \text{for all } R \in \mathrm{O}(3, \mathbb{Z}) \tag{6.8}$$

are not difficult to find. We first note that Γ_k decomposes into disjoint orbits $\Gamma_k^1, \dots, \Gamma_k^\nu$ under the action of the cubic group. The invariance of w_p is equivalent to the statement that

$$w_p = c_\iota \quad \text{for all } p \in \Gamma_k^\iota \tag{6.9}$$

and some constants c_ι. Eq. (4.15) thus becomes

$$\sum_{\iota=1}^{\nu} c_\iota y_{lm}^\iota = 0 \quad \text{for all } l \leqslant \Lambda, \tag{6.10}$$

where

$$y_{lm}^\iota = \sum_{p \in \Gamma_k^\iota} \mathscr{Y}_{lm}(p)^* . \tag{6.11}$$

These tensors are invariant under cubic transformations, in the same way as the zeta function is. In particular, for $l < 6$ there are only two independent components, y_{00}^ι and y_{40}^ι.

Since y_{00}^ι is just a constant times the number of points in Γ_k^ι, it is clear that eq. (6.10) has a non-zero solution, for $\Lambda < 4$, if and only if there are at least two orbits. The smallest value of q where this happens is 3. For $\Lambda = 4$ or 5 there are two conditions to be satisfied. This will always be possible if there are more than two orbits, a situation which occurs at $q = \sqrt{41}$ for the first time. There are in fact no other solutions below this value of q, as one may easily check by inspection.

6.2. QUALITATIVE DISCUSSION

We first assume that $\Lambda < 4$ and discuss the solutions of eq. (6.1). To this end it is useful to introduce the angle $\phi(q)$ through

$$\mathrm{e}^{-2i\phi} = \frac{m_{00} + i}{m_{00} - i}, \qquad \phi(0) = 0, \tag{6.12}$$

and the requirement that it depends continuously on q. $\phi(q)$ is a smoothly rising function which passes through a multiple of π when $q = |\boldsymbol{n}|$ for some integer vector $\boldsymbol{n}$ (see fig. 1). At very small q it is proportional to q^3.

Eq. (6.1) can now be written in the form

$$n\pi - \delta_0(k) = \phi(q), \qquad q = \frac{kL}{2\pi}, \tag{6.13}$$

where n is an arbitrary integer. If we fix L and suppose that $\delta_0(k)$ is known, the

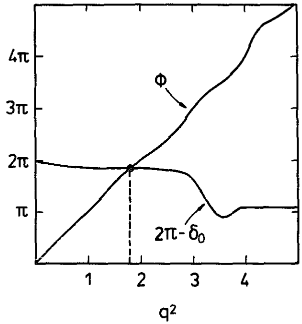

Fig. 1. Graphical solution of eq. (6.13) for $n=2$ and fixed L. Eq. (6.13) is satisfied at the point where the curves cross.

solutions of eq. (6.13) can be determined graphically. This is illustrated in fig. 1 for $n=2$ and a fictitious scattering phase $\delta_0(k)$. By running through all values of n, one obtains the complete spectrum in this way, as far as it is described by rule (a).

For $\Lambda=4$ or 5, eq. (6.1) is replaced by eq. (6.3) which is not as easy to analyse. Let us first look at this equation for the case $\delta_4(k)=0$. There are two types of solutions. One class of solutions is such that u_{44} is not equal to 1. We may then divide eq. (6.3) by the factor $1-u_{44}$ and find, after some algebra, that the condition reduces to eq. (6.1). This is, of course, the expected result.

The other type of solution occurs when

$$u_{44}=1\,. \tag{6.14}$$

The unitarity of the matrix $u_{ll'}$ then implies that u_{04} vanishes, i.e. a solution of eq. (6.14) automatically yields a solution of eq. (6.3). It is easy to check that eq. (6.14) holds if and only if k is singular and the number of orbits Γ_k^l is greater than 1. The solutions of condition (b) for $\Lambda<4$ thus become solutions of eq. (6.3) when $\Lambda=4,5$. This neatly matches with the fact that condition (b) is more restrictive for $\Lambda=4,5$.

Let us now turn to the case where $\delta_4(k)$ does not vanish. Especially at low energies the higher scattering phases are often very small (modulo π) and it is then a good approximation to treat $\delta_4(k)$ perturbatively. For the levels that have formerly been described by eq. (6.13), the first-order correction is obtained from

$$n\pi-\delta_0(k)=\phi(q)+\sigma(q)\tan\delta_4(k)\,,\qquad \sigma=\frac{m_{04}^2}{1+m_{00}^2}\,. \tag{6.15}$$

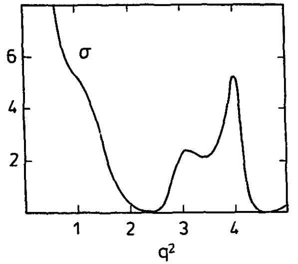

Fig. 2. Plot of the sensitivity $\sigma(q)$ [eq. (6.15)].

As shown by fig. 2, the sensitivity $\sigma(q)$ is a function with sizeable variation. In particular, for $q \to 0$ it grows proportional to $1/q^4$. This singularity does not normally cause any problem since it is cancelled by $\tan \delta_4(k)$ which is of order q^9 at small q. For all other values of q the sensitivity is finite, although it may be strongly peaked when q^2 passes through an integer.

If the scattering phase shift $\delta_4(k)$ is not close to an integer multiple of π, the spectrum must be determined from eq. (6.3) without any approximation. In this case there is no reason to expect that the result will be approximately equal to the spectrum computed by solving eq. (6.1).

Let us finally discuss the inverse problem of how to extract the scattering phases if the energy spectrum is known. In general this will be quite impossible, because the energy levels in a given sector depend on all scattering phases $\delta_l(k)$ that are not excluded by symmetry. But as is often the case, a single scattering phase dominates in the channel considered, and in these instances a computation is feasible.

Let us assume, for example, that $\delta_0(k)$ dominates in the A_1^+ sector (this will always be the case at sufficiently low energies). We may then use eq. (6.1) to compute $\delta_0(k)$ at those energies where an eigenvalue has been found. To check whether the contribution of $\delta_4(k)$ is indeed negligible, we can perform the following two tests.

First, from table E.2 one infers that $\delta_4(k)$ is the lowest scattering phase on which the spectrum in the T_1^+ sector depends. Any observed level with these quantum numbers hence allows one to compute $\delta_4(k)$ through an equation analogous to eq. (6.1) (assuming $\delta_4(k)$ dominates in the T_1^+ sector). After that the data can be inserted in eq. (6.15) to estimate the error on $\delta_0(k)$ implied by our ignorance of the higher scattering phases.

Another way to control the applicability of eq. (6.1) is to vary the box size L. If we fix k the energy $E = k^2/2\mu$ coincides with an energy eigenvalue for a sequence of values of L, including say $L = L_1$ and $L = L_2$. Accordingly we have two values q_1, q_2 of q, both of which determine the scattering phase $\delta_0(k)$ through eq. (6.1). If the results of these two calculations differ significantly, it is clear that the contribution of the higher scattering phases cannot be neglected. We may then obtain an improved estimate for $\delta_0(k)$ and a first value for $\delta_4(k)$ by inserting $q = q_1, q_2$ in eq. (6.3) and solving for the scattering phases.

6.3. LARGE-L EXPANSION

In ref. [3] it has been shown that the low-lying energy levels in the A_1^+ sector can be expanded in a power series of $1/L$ with coefficients related to the scattering phase $\delta_0(k)$.

It is almost trivial to derive these expansions from eq. (6.1). We first note that the curve representing $2\pi - \delta_0(k)$ in fig. 1 becomes flatter and eventually approaches 2π when L goes to infinity. The crossing point is hence driven to $q^2 = 2$. In general the solutions of eq. (6.13) satisfy

$$q^2 \underset{L\to\infty}{=} \boldsymbol{n}^2 + \mathrm{O}(1/L), \qquad (6.16)$$

where $\boldsymbol{n}$ is some integer vector.

For the levels described by eq. (6.1), the corrections to the leading term (6.16) can be computed as follows. We first rewrite eq. (6.1) in the form

$$\tan \delta_0(k) = \frac{\pi^{3/2} q}{\mathcal{Z}_{00}(1; q^2)}. \qquad (6.17)$$

After expanding the left- and right-hand sides of this equation in powers of k and $q - |\boldsymbol{n}|$ respectively, the desired expansion of q^2 in powers of $1/L$ is obtained straightforwardly by comparing coefficients.

As discussed in sect. 2, the behaviour of the scattering phase at low energies is given by

$$\tan \delta_0(k) = a_0 k + b_0 k^3 + \mathrm{O}(k^5). \qquad (6.18)$$

To expand the zeta function around $q^2 = \boldsymbol{n}^2$, we define a subtracted zeta function through

$$Z_{00}(s; \boldsymbol{n}^2) = \lim_{q\to|\boldsymbol{n}|} \left\{ \sqrt{4\pi}\mathcal{Z}_{00}(s; q^2) - N(\boldsymbol{n}^2 - q^2)^{-s} \right\}, \qquad (6.19)$$

where N denotes the number of integer vectors $\boldsymbol{n}'$ with $|\boldsymbol{n}'| = |\boldsymbol{n}|$. This function coincides with the zeta function introduced in ref. [3]. Now it is obvious that

$$\sqrt{4\pi}\,Z_{00}(1;q^2)=\frac{N}{n^2-q^2}+Z_{00}(1;n^2)+(q^2-n^2)Z_{00}(2;n^2)+\dots, \quad (6.20)$$

and for the asymptotic solution of eq. (6.17) one then finds

$$q^2=n^2-Nt\left\{1+tZ_{00}(1;n^2)+t^2\left[Z_{00}(1;n^2)^2-NZ_{00}(2;n^2)\right]\right\}+\mathrm{O}(1/L^4). \quad (6.21)$$

The expansion parameter t occurring here is defined through

$$t=\left\{\frac{\tan\delta_0(k)}{\pi kL}\right\}_{k=2\pi|n|/L}. \quad (6.22)$$

In particular, $t=a_0/\pi L$ for the lowest level* $n=0$.

The expansion (6.21) completely agrees with the formulae which have been derived in ref. [3] on the basis of an all order analysis of perturbation theory. The results obtained here show that the series is actually valid on a non-perturbative level and, in particular, if there are bound states.

So far we have assumed that the contribution of the higher scattering phases can be neglected at large L. The perturbative analysis of ref. [3] shows that this is correct up to terms of order L^{-4} in the expansion (6.21). Actually, the phase shifts $\delta_l(k)$ with $l\geqslant 4$ perturb the spectrum only at a much higher order. This can now be proved from eq. (6.3) which may be written in the form

$$\left[1+\frac{m_{04}^2}{m_{00}}\frac{\tan\delta_4}{1-m_{44}\tan\delta_4}\right]\tan\delta_0=\frac{1}{m_{00}}. \quad (6.23)$$

For $L\to\infty$, the square bracket is equal to 1 plus a term of order L^{-10} or L^{-8}, depending on whether n vanishes or not. The expansion (6.21) accordingly receives a contribution from $\delta_4(k)$ at order L^{-11} if $n=0$ and L^{-9} in all other cases. This underscores our general expectation that the spectrum in the A_1^+ sector is dominated by the S-wave phase shift at low energies.

* When the scattering length a_0 is positive the state with $n=0$ has negative energy at large L and thus falls under condition (c). However, for purely imaginary k eq. (5.22) is equivalent to eq. (6.17), if we insert the analytically continued scattering phase $\delta_0(k)$ and if we keep away from the zeros of $m_{00}-i$. This latter condition is satisfied for small q, and the large L expansion of the lowest level is hence given by eq. (6.21) independently of the sign of a_0.

7. Two-particle states in quantum field theory

As compared to the quantum mechanical model studied so far, there are some important new physical effects in quantum field theory which must be taken into account. The aim here is to discuss these and to explain how the relations between the scattering phases and the spectrum in finite volume can be carried over. We assume throughout that there are no massless (physical) particles in the theory considered. This part of the paper draws heavily on earlier work, especially refs. [1–3, 8], and the reader is thus referred to these publications for further details.

7.1. POLARIZATION EFFECTS

It is well known that a stable particle in quantum field theory polarizes the vacuum. The associated polarization energy is unobservable in infinite volume, since it just adds to the rest mass of the particle. But the surrounding cloud of virtual particles gives a finite extension to the particle which could be measured, in principle, by performing scattering experiments with weakly interacting test particles. In a finite volume with periodic boundary conditions the cloud is squeezed and the particle's rest mass hence depends on L. This effect has been extensively studied in the past (a partial list of references is [1, 2, 6, 7, 15]; for an introduction to the problem see ref. [16]).

The basic result is that the finite size mass shift goes to zero exponentially in the large L limit. What happens is that the finite extension of the system is felt through processes where a virtual particle is exchanged "around the world". The amplitude for such a process is exponentially suppressed, because the particle is required to travel a distance of order L along a classically forbidden path in space-time.

Not only the particle masses, but also form factors, low-energy coupling constants etc. are subject to volume-dependent polarization effects. In all these instances the underlying physical process is the same, and the associated finite size corrections are exponentially suppressed at large L [6, 7, 17].

It is quite obvious that a discussion of two-particle states and scattering wave functions in finite volume is only meaningful if polarization effects can be neglected. In the following this will always be assumed. Essentially what one requires is that the box is large enough to contain two particles together with their polarization clouds. In QCD one expects that values of L greater than about 3 fm will do. But there are no general rules as to which is the minimal acceptable box size. In each case one has to carefully study the properties of the one-particle states before one can proceed to the two-particle situation.

7.2. IDENTIFICATION OF TWO-PARTICLE STATES

In quantum field theory there are states which describe an arbitrary number of particles. Barring exceptional cases, the particle number is, however, not conserved in scattering processes. Particle counting is hence only possible if the particles are far apart from each other so that their interactions can be neglected. It is therefore not totally obvious what exactly one means by a two-particle state in finite volume.

To answer this question let us first consider the theory in infinite volume and suppose that a particular symmetry sector in the space of physical states has been selected. Specifically we are interested in states with zero total momentum, definite cubic symmetry and fixed internal quantum numbers, such as baryon number, G-parity and so on. If we look at the energy spectrum in this sector, starting from the bottom, there will first be a number of discrete energy values corresponding to the vacuum and the stable one-particle states, as far as they have the required quantum numbers. At some energy W_1 the continuous part of the spectrum begins. Initially it arises entirely from two-particle scattering states. Then, at some energy W_2, inelastic processes set in and the spectrum receives contributions from many particle states.

It is clear from these remarks that all states in infinite volume with energy W in the elastic region $W_1 \leqslant W < W_2$ are two-particle states. In a large but finite volume the continuous part of the energy spectrum is replaced by a densely spaced ladder of discrete energy eigenvalues. Some of these energy values lie in the elastic region (or just a little below if the interaction is attractive) and the associated energy eigenstates are thus referred to as the two-particle states in finite volume. Note that this merely defines what a two-particle state in finite volume is. Nothing is implied on their properties at this point except that they are certain energy eigenstates in a particular symmetry sector.

At energies above the inelastic threshold, it is in general impossible to tell the number of particles in a given energy eigenstate in finite volume. The problem is that such states describe stationary scattering processes on a torus, and in these reactions the number of particles may not be conserved if the energy is sufficiently high.

7.3. TWO-PARTICLE ENERGY SPECTRUM

We now proceed to discuss the relationship between the scattering phases and the energy spectrum of two-particle states. For simplicity we shall only consider the case of two bosons with spin 0 and mass m, whose dynamics can be described by a simple scalar field theory of the ϕ^4-type. We shall also take it for granted that the reflection symmetry $\phi \to -\phi$ is unbroken and that the single-particle states are odd under this transformation. It is not hard to generalize the results to other situations such as the pion–nucleon system.

In infinite volume the elastic scattering amplitude T can be decomposed into partial waves and the scattering phases $\delta_l(k)$ are then defined in the usual way (cf. refs. [2, 3]). An important result obtained in refs. [3, 8] is that there exists an effective Schrödinger equation which yields exactly these scattering phases when one works out the associated scattering solutions.

Explicitly, the stationary effective Schrödinger equation in the centre-of-mass frame reads

$$-\frac{1}{2\mu}\Delta\psi(\boldsymbol{r}) + \tfrac{1}{2}\int \mathrm{d}^3r'\, U_E(\boldsymbol{r},\boldsymbol{r}')\psi(\boldsymbol{r}') = E\psi(\boldsymbol{r}), \tag{7.1}$$

where the parameter E is related to the true energy W of the system through

$$W = 2\sqrt{m^2 + mE}\ . \tag{7.2}$$

The "potential" $U_E(\boldsymbol{r},\boldsymbol{r}')$ is the Fourier transform of the modified Bethe–Salpeter kernel $\hat{U}_E(\boldsymbol{k},\boldsymbol{k}')$ introduced in ref. [3]. It depends analytically on E in the range $-m < E < 3m$ and is a smooth function of the coordinates $\boldsymbol{r}$ and $\boldsymbol{r}'$, decaying exponentially in all directions*. Furthermore, the potential is rotationally invariant so that one can pass to the radial effective Schrödinger equation. The corresponding regular solution behaves exactly as in quantum mechanics, except that the large r form (2.10) only holds up to exponentially small corrections, because the potential does not strictly vanish for r greater than some radius R.

Up to polarization effects, the spectrum of two-particle states in finite volume is also described by the effective Schrödinger equation (7.1), periodically extended in the obvious way. An almost complete matching with the quantum mechanical model studied previously has thus been achieved. The essential differences are that the potential depends on E and that it does not exactly vanish for sufficiently large r. The first of these is not disturbing at all since the relation between the finite volume spectrum and the scattering phases is obtained at fixed energy.

To get around the second difference, we multiply the potential $U_E(\boldsymbol{r},\boldsymbol{r}')$ with some smooth cutoff function which vanishes if r or r' is greater than some large radius R and which is equal to 1 if both r and r' are smaller than say $0.9R$. As a result of this modification of the potential, the finite volume energy levels and the scattering phases change by terms vanishing exponentially for large R. For the analysis of the previous sections it was only required that L is greater than $2R$. In other words, we may choose R to be of order L and the errors induced by the cutoff are then exponentially decreasing with L.

We have thus established

Theorem 7.1. *Up to terms which vanish exponentially at large L, the relationship between the scattering phases and the two-particle spectrum in finite volume is exactly the same as in quantum mechanics. We only have to replace the non-relativistic energy momentum relation $E = k^2/2\mu$ by the relativistic formula $W = 2\sqrt{m^2 + k^2}$.*

* From ref. [3] it only follows that the potential falls off faster than any inverse power of r and r'. The more rapid exponential decay is obtained if we replace the cutoff function $h(\boldsymbol{k})$ introduced in sect. 3 of ref. [3] through an energy-dependent analytic expression such as $h(\boldsymbol{k}) = \exp\{(mE - \boldsymbol{k}^2)/m^2\}$.

The conditions for energy eigenstates listed in subsect. 5.4 (and sect. 6) then carry over literally.

This result supersedes theorem 3.4 of ref. [3]. It applies to any symmetry sector and to all levels in the elastic region, as discussed above. In particular, what has been said in sect. 6 about the relation between the scattering phases and the energy spectrum in the A_1^+ sector remains valid in quantum field theory. We should of course not forget that there are exponentially small corrections stemming from polarization effects and the tails of the effective potential $U_E(\boldsymbol{r}, \boldsymbol{r}')$. But the numerical experience gained so far shows that these do not cause any serious problem [6–8]. One only has to make sure that the particles studied fit into one's box without being squeezed.

8. Concluding remarks

The connection between the scattering phases and the spectrum of two-particle states on a torus established in this paper can be expected to be useful in many respects. In particular, a computation of the scattering phases through numerical simulation is certainly feasible in simple bosonic theories and perhaps also in lattice QCD, although here it seems that progress in simulation algorithms and hardware would be required for reliable results.

The most explicit formulae for the spectrum in finite volume have been obtained under the assumption that the scattering phase shifts $\delta_l(k)$ with $l \geqslant 5$ are negligible in the energy range of interest. It would not be difficult to generalize these results so as to include the contributions of the higher scattering phases up to some maximal angular momentum $\Lambda \geqslant 5$. One only has to work out the matrix $\mathscr{M}(\Gamma)_{ln,l'n'}$ for all $l, l' \leqslant \Lambda$, and this can be done algebraically on a computer, starting from the analytic expressions in subsect. 3.4.

Some of the most interesting physical effects in QCD are associated with the occurrence of unstable particles such as the ρ meson and the $\Delta(1232)$ resonance. Generally speaking the problem with resonances is that they do not correspond to some particular eigenstates of the Hamilton operator in any simple way. But it is known that they give rise to a characteristic pattern in the finite volume energy spectrum around the resonance mass [18, 16]. With the formulae derived here it will now be possible to work out in further detail what exactly these effects are. The hope is that on the basis of this analysis a practical method can be found which allows one to compute the resonance mass and perhaps its width in an unambiguous and correct manner.

The methods developed in this paper could also be applied to compute electron bands in regular crystals. In particular, the so-called muffin-tin potentials lead to eigenvalue problems of the type considered here, for wave functions on the Wigner–Seitz cell with Bloch periodic boundary conditions. Such a calculation would be quite effective, since the influence of the angular momentum cutoff Λ on the spectrum can be proved to go to zero faster than any power of Λ^{-1}.

I have benefitted from stimulating discussions with Uwe Wiese, and I would also like to thank Pierre van Baal for his enthusiastic and useful comments.

Appendix A

In this appendix theorem 2.1 is proven by showing that the function $\psi(\boldsymbol{r})$, initially defined for all $\boldsymbol{r} \in \Omega$, can be smoothly extended to a unique periodic eigenfunction of H.

It is obviously sufficient to specify the extension in the ball $r < L/2$. The spherical components $\psi_{lm}(r)$ of the function to be constructed solve the radial Schrödinger equation in this range. Taking eq. (2.22) into account, it follows that

$$\psi_{lm}(r) = b_{lm} u_l(r;k) \quad \text{for all } r < L/2. \tag{A.1}$$

The crucial step in the proof now is to show that the series

$$\psi(\boldsymbol{r}) \overset{\text{def}}{=} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm}(\theta, \varphi) \psi_{lm}(r) \tag{A.2}$$

is absolutely and uniformly convergent for $r < L/2$. If true the so-defined function $\psi(\boldsymbol{r})$ solves the Schrödinger equation in the sense of distributions, and by elliptic regularity, we then conclude that it must be a smooth eigenfunction of H. We have thus found the desired extension, and since the construction is unique, the proof of the theorem is complete.

To establish the convergence of the series (A.2), we make use of the following

Lemma A.1. *For any fixed radius r_0 and sufficiently large l, the regular solution $u_l(r;k)$ of the radial Schrödinger equation is non-negative and monotonically rising in the interval $0 \leqslant r \leqslant r_0$.*

Proof. It is well known that the function

$$v_l(r;k) = r^{-l} u_l(r;k) \tag{A.3}$$

is a solution of the integral equation

$$v_l(r;k) = 1 + \int_0^r \mathrm{d}s \, \frac{s}{2l+1} \left[(s/r)^{2l+1} - 1 \right] \left[k^2 - 2\mu V(s) \right] v_l(s;k) \tag{A.4}$$

(see e.g. ref. [14]). For any continuous function $w(r)$ on the interval $0 \leqslant r \leqslant r_0$, let us define the norm

$$\|w\| = \sup_{0 \leqslant r \leqslant r_0} |w(r)|. \tag{A.5}$$

From eq. (A.4) we then deduce that

$$\|v_l - 1\| \leqslant \frac{c_1}{l} \|v_l\| \tag{A.6}$$

for some constant c_1 independent of l. Provided $l > c_1$ it follows from this inequality that

$$\|v_l - 1\| \leqslant \frac{c_1}{l - c_1}, \tag{A.7}$$

and $v_l(r;k)$ is hence close to 1 for sufficiently large l, uniformly in the interval $0 \leqslant r \leqslant r_0$. In particular, the solution $u_l(r;k)$ is non-negative in this range.

We still have to prove that $u_l(r;k)$ is monotonically rising. From

$$v_l'(r;k) \overset{\text{def}}{=} \frac{\mathrm{d}}{\mathrm{d}r} v_l(r;k) = -\int_0^r \mathrm{d}s (s/r)^{2l+2} \left[k^2 - 2\mu V(s)\right] v_l(s;k) \tag{A.8}$$

and the boundedness of $v_l(r;k)$, one infers that there exists a constant c_2 such that

$$\|v_l'\| \leqslant c_2 \tag{A.9}$$

for all l. The square bracket in the equation

$$u_l'(r;k) = l r^{l-1} \left[v_l(r;k) + (r/l) v_l'(r;k)\right] \tag{A.10}$$

therefore converges to 1 for $l \to \infty$, uniformly in the interval $0 \leqslant r \leqslant r_0$. In particular, $u_l'(r;k)$ is non-negative for sufficiently large l and $u_l(r;k)$ is hence monotonically rising in this range. ∎

The convergence of the series (A.2) is a simple consequence of the lemma. We first remark that absolute convergence is guaranteed for all r with $R < r < L/2$, because in this range we are just expanding a given smooth function $\psi(\boldsymbol{r})$ in spherical harmonics. The lemma implies that $|\psi_{lm}(r)|$ is a monotonically rising function of r for sufficiently large l and all $r < L/2$. The convergence properties of the series therefore improve as we make r smaller, and it is hence absolutely and uniformly convergent in the whole range $0 \leqslant r \leqslant r_0$ for any $r_0 < L/2$.

Appendix B

The action of the differential operator $\mathcal{Y}_{lm}(\nabla)$ on spherical Bessel functions is described by the identities (3.16) and (3.32). The aim here is to prove these relations, using some well-known properties of the Bessel functions and the spherical harmonics.

To this end we need

Lemma B.1. *For any smooth function f(r) and all r > 0 the identity*

$$\mathcal{Y}_{lm}(\nabla)f(r)=\mathcal{Y}_{lm}(r)\left(\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right)^{l}f(r) \tag{B.1}$$

holds.

Proof. Differentiation is a local operation, and it is hence sufficient to consider the case where $f(r)$ is supported on a compact interval on the positive real axis. The Fourier transform

$$\tilde{f}(p)=\int \mathrm{d}^3r\,\mathrm{e}^{-ipr}f(r) \tag{B.2}$$

is then smooth and rapidly decaying for $p\to\infty$. It follows from this remark that

$$\mathcal{Y}_{lm}(\nabla)f(r)=\int\frac{\mathrm{d}^3p}{(2\pi)^3}\,\mathrm{e}^{ipr}i^l\mathcal{Y}_{lm}(p)\tilde{f}(p), \tag{B.3}$$

and after inserting the expansion (3.37) we get

$$\mathcal{Y}_{lm}(\nabla)f(r)=Y_{lm}(\theta,\varphi)\frac{(-1)^l}{2\pi^2}\int_0^\infty \mathrm{d}p\,p^{l+2}j_l(pr)\tilde{f}(p). \tag{B.4}$$

The identity

$$j_l(z)=z^l\left(-\frac{1}{z}\frac{\mathrm{d}}{\mathrm{d}z}\right)^l j_0(z), \tag{B.5}$$

now yields

$$\mathcal{Y}_{lm}(\nabla)f(r)=\mathcal{Y}_{lm}(r)\left(\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\right)^l\frac{1}{2\pi^2}\int_0^\infty \mathrm{d}p\,p^2j_0(pr)\tilde{f}(p). \tag{B.6}$$

The integral in this formula is independent of l and hence equal to $f(r)$. ∎

Eq. (3.16) is an immediate consequence of the lemma. We only have to set $f(r)=n_0(kr)$ and to recall that the identity (B.5) also holds if we replace $j_l(z)$ by $n_l(z)$ on both sides of the equation.

To prove eq. (3.32), we begin by noting that

$$Y_{js}(\theta,\varphi)j_j(kr)=\frac{(-i)^j}{4\pi}\int \mathrm{d}\theta_k\,\mathrm{d}\varphi_k\,\sin\theta_k\,Y_{js}(\theta_k,\varphi_k)\,\mathrm{e}^{ikr} \tag{B.7}$$

[cf. eq. (3.37)]. After acting with the differential operator $\mathcal{Y}_{lm}(\nabla)$ on this equation, one obtains an integral with an integrand proportional to the product of two spherical harmonics. It is a standard result of the representation theory of the rotation group that such a product can be expanded according to

$$Y_{lm}(\theta,\varphi)Y_{js}(\theta,\varphi)=\frac{1}{\sqrt{4\pi}}\sum_{l'=|j-l|}^{j+l}\sum_{m'=-l'}^{l'}(-i)^{l-j+l'}C_{lm,js,l'm'}Y_{l'm'}(\theta,\varphi), \tag{B.8}$$

where the tensor $C_{lm,js,l'm'}$ is given by eq. (3.33) (see e.g. ref. [13], eq. (C.17)). When this identity is inserted in the integral, one may use eq. (B.7) again and one then arrives at eq. (3.32), the desired result.

Appendix C

The zeta function $\mathcal{Z}_{lm}(s;q^2)$ introduced in subsect. 3.4 is a meromorphic function of the variable s in the whole complex plane. Its value at $s=1$ is of particular interest in this paper. The aim here is to derive an integral representation for $\mathcal{Z}_{lm}(1;q^2)$, which is suitable for numerical evaluation.

For all $t>0$ and $r\in\mathbb{R}^3$, the heat kernel $\mathcal{K}(t,r)$ of the Laplace operator on a torus with $L=2\pi$ is defined by

$$\mathcal{K}(t,r)=(2\pi)^{-3}\sum_{n\in\mathbb{Z}^3}\exp\{inr-tn^2\}. \tag{C.1}$$

An alternative representation of the kernel is

$$\mathcal{K}(t,r)=(4\pi t)^{-3/2}\sum_{n\in\mathbb{Z}^3}\exp\left\{-\frac{1}{4t}(r-2\pi n)^2\right\}. \tag{C.2}$$

The series (C.1) is rapidly convergent when t is large, while (C.2) is useful for small t. In addition to the full heat kernel, we shall also need the truncated kernel

$$\mathcal{K}^{\lambda}(t,r)=\mathcal{K}(t,r)-(2\pi)^{-3}\sum_{|n|<\lambda}\exp\{inr-tn^2\}, \tag{C.3}$$

and its derivatives

$$\mathcal{K}^{\lambda}_{lm}(t,r)=(-i)^l\mathcal{Y}_{lm}(\nabla)\mathcal{K}^{\lambda}(t,r). \tag{C.4}$$

The sum in eq. (C.3) runs over all integer vectors $\boldsymbol{n}$ in the specified range and the cutoff $\lambda > 0$ is chosen such that $\lambda^2 > \operatorname{Re} q^2$.

As long as $\operatorname{Re} 2s > l + 3$, it is obvious that

$$\mathcal{Z}_{lm}(s;q^2) = \sum_{|\boldsymbol{n}|<\lambda} \mathcal{Y}_{lm}(\boldsymbol{n})(\boldsymbol{n}^2 - q^2)^{-s} + \frac{(2\pi)^3}{\Gamma(s)} \int_0^\infty \mathrm{d}t\, t^{s-1} \mathrm{e}^{tq^2} \mathcal{K}_{lm}^{\lambda}(t, \mathbf{0}) \quad \text{(C.5)}$$

is a valid representation of the zeta function. Note that the integrand vanishes exponentially for large t. For $t \to 0$ the leading asymptotic behaviour is

$$\mathrm{e}^{tq^2} \mathcal{K}_{lm}^{\lambda}(t, \mathbf{0}) = a_{lm} t^{-3/2} + \mathrm{O}(t^{-1/2}), \qquad a_{lm} = \delta_{l0}\delta_{m0}(4\pi)^{-2}. \quad \text{(C.6)}$$

It follows from this observation that

$$\begin{aligned}\mathcal{Z}_{lm}(s;q^2) = &\sum_{|\boldsymbol{n}|<\lambda} \mathcal{Y}_{lm}(\boldsymbol{n})(\boldsymbol{n}^2 - q^2)^{-s} \\ &+ \frac{(2\pi)^3}{\Gamma(s)} \left\{ \frac{a_{lm}}{s - 3/2} + \int_0^1 \mathrm{d}t\, t^{s-1} \left[\mathrm{e}^{tq^2} \mathcal{K}_{lm}^{\lambda}(t, \mathbf{0}) - a_{lm} t^{-3/2} \right] \right. \\ &\left. + \int_1^\infty \mathrm{d}t\, t^{s-1} \mathrm{e}^{tq^2} \mathcal{K}_{lm}^{\lambda}(t, \mathbf{0}) \right\} \quad \text{(C.7)}\end{aligned}$$

for all l and all s in the half-plane $\operatorname{Re} s > 1/2$. In particular, for $s = 1$ we have

$$\begin{aligned}\mathcal{Z}_{lm}(1;q^2) = &\sum_{|\boldsymbol{n}|<\lambda} \mathcal{Y}_{lm}(\boldsymbol{n})(\boldsymbol{n}^2 - q^2)^{-1} \\ &+ (2\pi)^3 \int_0^\infty \mathrm{d}t \left[\mathrm{e}^{tq^2} \mathcal{K}_{lm}^{\lambda}(t, \mathbf{0}) - \frac{\delta_{l0}\delta_{m0}}{(4\pi)^2 t^{3/2}} \right], \quad \text{(C.8)}\end{aligned}$$

which is the desired integral representation.

The integral in eq. (C.8) can be computed numerically using standard routines. To evaluate the integrand, one makes use of the series (C.1) and (C.2), depending on whether t is greater or smaller than 1. The only potential problem is that a substantial loss of significance can occur when adding up all contributions to the zeta function, especially for large q^2. Working with extended precision numbers, it is however straightforward to obtain accurate results for say $l \leqslant 8$ and $|q| \leqslant 3$.

Appendix D

In this appendix the identity (3.31) is established. The notation introduced in appendix C is taken over. For dimensional reasons, g_{lm} must be equal to some function of q divided by L. In the following we choose units such that $L = 2\pi$.

We shall first compute the coefficient

$$g_{00} = \sqrt{4\pi}\lim_{r\to 0}\left\{G(r;k^2) - \frac{1}{4\pi r}\right\}. \tag{D.1}$$

To work out the short distance behaviour of the Green function, it is advantageous to pass to the heat kernel representation

$$G(r;k^2) = (2\pi)^{-3}\sum_{|n|<\Lambda} e^{inr}(n^2 - q^2)^{-1} + \int_0^\infty dt\, e^{tq^2}\mathscr{K}^\Lambda(t,r). \tag{D.2}$$

From the properties (C.1)–(C.3) of the heat kernel one infers that

$$\mathscr{K}^\Lambda(t,r) = (4\pi t)^{-3/2}\exp\left\{-\frac{1}{4t}r^2\right\} + \dots, \tag{D.3}$$

where the dots stand for a function which is smooth for all $t \geqslant 0$ and all r in a neighborhood of the origin. Next we note that

$$\int_0^\infty dt(4\pi t)^{-3/2}\exp\left\{-\frac{1}{4t}r^2\right\} = \frac{1}{4\pi r}. \tag{D.4}$$

Subtracting this integral from eq. (D.2), the limited $r \to 0$ can be taken straightforwardly and one then obtains

$$g_{00} = \sqrt{4\pi}\left\{(2\pi)^{-3}\sum_{|n|<\Lambda}(n^2 - q^2)^{-1} + \int_0^\infty dt\left[e^{tq^2}\mathscr{K}^\Lambda(t,0) - (4\pi t)^{-3/2}\right]\right\}. \tag{D.5}$$

This expression matches with the integral representation (C.8) of the zeta function $\mathscr{Z}_{00}(1;q^2)$ and we have thus proved eq. (3.31) for $l = 0$.

For $l \geqslant 1$ the starting point is

$$g_{lm} = (2l+1)!!\lim_{r\to 0}(kr)^{-l}\int d\theta\, d\varphi \sin\theta\, Y_{lm}(\theta,\varphi)^* G(r;k^2). \tag{D.6}$$

After inserting the heat kernel representation (D.2) for the Green function, the integral over the angles can be performed and the limit $r \to 0$ be taken. The singular term (D.3) is annihilated by the integration, because it is rotationally invariant. In all other terms we may use the identity

$$\lim_{r\to 0} r^{-l} \int \mathrm{d}\theta\, \mathrm{d}\varphi \sin\theta\, Y_{lm}(\theta,\varphi)^* \,\mathrm{e}^{i\boldsymbol{p}\boldsymbol{r}} = \frac{4\pi i^l}{(2l+1)!!} \mathcal{Y}_{lm}(\boldsymbol{p})^*, \qquad \text{(D.7)}$$

which is a straightforward consequence of eq. (3.37). In particular, together with

$$\mathcal{Y}_{lm}(\boldsymbol{p})^* = \mathcal{Y}_{lm}(\boldsymbol{p}'), \qquad \boldsymbol{p}' = (p_1, -p_2, p_3), \qquad \text{(D.8)}$$

and the cubic symmetry of the momentum lattice, eq. (D.7) leads to

$$\lim_{r\to 0} r^{-l} \int \mathrm{d}\theta\, \mathrm{d}\varphi \sin\theta\, Y_{lm}(\theta,\varphi)^* \mathcal{K}^{\lambda}(t,\boldsymbol{r}) = \frac{4\pi i^l}{(2l+1)!!} \mathcal{K}^{\lambda}_{lm}(t,\mathbf{0}). \qquad \text{(D.9)}$$

As a result of these calculations one obtains an integral formula for g_{lm}, which turns out to be identical to the right-hand side of eq. (C.8) up to an overall factor, thus proving eq. (3.31).

Appendix E

According to eq. (3.34) the matrix element $\mathcal{M}_{lm,l'm'}$ is a linear combination of the zeta functions

$$\mathcal{W}_{js} \stackrel{\text{def}}{=} \left\{\pi^{3/2}(2j+1)^{1/2} q^{j+1}\right\}^{-1} \mathcal{Z}_{js}(1;q^2) \qquad \text{(E.1)}$$

with coefficients given by eq. (3.33). The Wigner 3j-symbols occurring in this expression can be computed algebraically using Racah's formula (see e.g. ref. [13], appendix C). Table E.1 contains a complete list of the independent matrix elements with $l, l' \leqslant 4$. Matrix elements which vanish because of the selection rules (3.35) have been omitted from table E.1, and only one of the index combinations related through the symmetries (3.36) has been included.

To compute the reduced matrix elements $\mathcal{M}(\Gamma)_{ln,l'n'}$ we have to make a choice of basis $|\Gamma,\alpha;l,n\rangle$, as discussed in subsect. 5.1. It is possible to adopt a phase convention such that the reduced matrix is symmetric. A complete list of all independent (non-zero) matrix elements with $l, l' \leqslant 4$ is given in table E.2. Since $N(\Gamma, l) \leqslant 1$ for these values of l, the counting indices n and n' of the matrix elements listed are equal to 1.

TABLE E.1
Elements of the matrix $\mathcal{M}_{lm,l'm'}$ for angular momenta $l, l' \leqslant 4$

l	m	l'	m'	$\mathcal{M}_{lm,l'm'}$			
0	0	0	0	w_{00}			
1	0	1	0	w_{00}			
1	1	1	1	w_{00}			
2	0	2	0	w_{00}	$+\frac{18}{7} w_{40}$		
2	1	2	1	w_{00}	$-\frac{12}{7} w_{40}$		
2	2	2	−2		$\frac{15}{7} w_{40}$		
2	2	2	2	w_{00}	$+\frac{3}{7} w_{40}$		
3	0	1	0		$-\frac{4}{7}\sqrt{21}\, w_{40}$		
3	1	1	1		$\frac{3}{7}\sqrt{14}\, w_{40}$		
3	3	1	−1		$\frac{1}{7}\sqrt{210}\, w_{40}$		
3	0	3	0	w_{00}	$+\frac{18}{11} w_{40}$	$+\frac{100}{33} w_{60}$	
3	1	3	1	w_{00}	$+\frac{3}{11} w_{40}$	$-\frac{25}{11} w_{60}$	
3	2	3	−2		$\frac{15}{11} w_{40}$	$-\frac{70}{11} w_{60}$	
3	2	3	2	w_{00}	$-\frac{21}{11} w_{40}$	$+\frac{10}{11} w_{60}$	
3	3	3	−1		$\frac{3}{11}\sqrt{15}\, w_{40}$	$+\frac{35}{33}\sqrt{15}\, w_{60}$	
3	3	3	3	w_{00}	$+\frac{9}{11} w_{40}$	$-\frac{5}{33} w_{60}$	
4	0	0	0		$3 w_{40}$		
4	4	0	0		$\frac{3}{14}\sqrt{70}\, w_{40}$		
4	0	2	0		$-\frac{60}{77}\sqrt{5}\, w_{40}$	$-\frac{15}{11}\sqrt{5}\, w_{60}$	
4	1	2	1		$-\frac{15}{77}\sqrt{6}\, w_{40}$	$+\frac{10}{11}\sqrt{6}\, w_{60}$	
4	2	2	−2		$\frac{30}{77}\sqrt{3}\, w_{40}$	$+\frac{35}{11}\sqrt{3}\, w_{60}$	
4	2	2	2		$\frac{90}{77}\sqrt{3}\, w_{40}$	$-\frac{5}{11}\sqrt{3}\, w_{60}$	
4	3	2	−1		$\frac{15}{77}\sqrt{42}\, w_{40}$	$-\frac{10}{11}\sqrt{42}\, w_{60}$	
4	4	2	0		$\frac{30}{77}\sqrt{14}\, w_{40}$	$+\frac{15}{22}\sqrt{14}\, w_{60}$	
4	0	4	0	w_{00}	$+\frac{1458}{1001} w_{40}$	$+\frac{20}{11} w_{60}$	$+\frac{490}{143} w_{80}$
4	1	4	1	w_{00}	$+\frac{729}{1001} w_{40}$	$-\frac{1}{11} w_{60}$	$-\frac{392}{143} w_{80}$
4	2	4	−2		$\frac{1215}{1001} w_{40}$	$-\frac{42}{11} w_{60}$	$+\frac{196}{143} w_{80}$
4	2	4	2	w_{00}	$-\frac{81}{91} w_{40}$	$-2 w_{60}$	$+\frac{196}{143} w_{80}$
4	3	4	−1		$\frac{405}{1001}\sqrt{7}\, w_{40}$	$-\frac{3}{11}\sqrt{7}\, w_{60}$	$-\frac{56}{143}\sqrt{7}\, w_{80}$
4	3	4	3	w_{00}	$-\frac{243}{143} w_{40}$	$+\frac{17}{11} w_{60}$	$-\frac{56}{143} w_{80}$
4	4	4	−4				$\frac{35}{11} w_{80}$
4	4	4	0		$\frac{81}{1001}\sqrt{70}\, w_{40}$	$+\frac{6}{11}\sqrt{70}\, w_{60}$	$+\frac{7}{143}\sqrt{70}\, w_{80}$
4	4	4	4	w_{00}	$+\frac{162}{143} w_{40}$	$-\frac{4}{11} w_{60}$	$+\frac{7}{143} w_{80}$

TABLE E.2
Elements of the matrix $\mathcal{M}(\Gamma)_{ln,l'n'}$ for angular momenta $l,l' \leqslant 4$

Γ	l	l'	$\mathcal{M}(\Gamma)_{ln,l'n'}$			
A_1^+	0	0	w_{00}			
A_1^+	0	4		$\frac{6}{7}\sqrt{21}\,w_{40}$		
A_1^+	4	4	w_{00}	$+\frac{324}{143}w_{40}$	$+\frac{80}{11}w_{60}$	$+\frac{560}{143}w_{80}$
A_2^-	3	3	w_{00}	$-\frac{36}{11}w_{40}$	$+\frac{80}{11}w_{60}$	
E^+	2	2	w_{00}	$+\frac{18}{7}w_{40}$		
E^+	2	4		$-\frac{120}{77}\sqrt{3}\,w_{40}$	$-\frac{30}{11}\sqrt{3}\,w_{60}$	
E^+	4	4	w_{00}	$+\frac{324}{1001}w_{40}$	$-\frac{64}{11}w_{60}$	$+\frac{392}{143}w_{80}$
T_1^+	4	4	w_{00}	$+\frac{162}{143}w_{40}$	$-\frac{4}{11}w_{60}$	$-\frac{448}{143}w_{80}$
T_1^-	1	1	w_{00}			
T_1^-	1	3		$-\frac{4}{7}\sqrt{21}\,w_{40}$		
T_1^-	3	3	w_{00}	$+\frac{18}{11}w_{40}$	$+\frac{100}{33}w_{60}$	
T_2^+	2	2	w_{00}	$-\frac{12}{7}w_{40}$		
T_2^+	2	4		$-\frac{60}{77}\sqrt{3}\,w_{40}$	$+\frac{40}{11}\sqrt{3}\,w_{60}$	
T_2^+	4	4	w_{00}	$-\frac{162}{77}w_{40}$	$+\frac{20}{11}w_{60}$	
T_2^-	3	3	w_{00}	$-\frac{6}{11}w_{40}$	$-\frac{60}{11}w_{60}$	

Appendix F

We here discuss the solutions of the linear equations (3.25), (4.13) and (4.14). In particular, it will be shown that a solution with $b_{lm} \neq 0$ exists if and only if eq. (4.17) is satisfied.

It is useful to employ an abstract notation in the following. In subsect. 4.2 we have already introduced the vector space $\mathcal{H}_\Lambda$. Three more spaces are needed here. First note that for any fixed $\boldsymbol{p} \in \Gamma_k$, the vector y with the components

$$y_{lm} = i^l Y_{lm}(\theta_p, \varphi_p)^*, \qquad l = 0, 1, \ldots, \Lambda, \tag{F.1}$$

is an element of $\mathcal{H}_\Lambda$. The subspace spanned by all these vectors will be denoted by $\mathcal{S}$ and the associated orthogonal projector by P.

The complex vectors w with components w_p, $\boldsymbol{p} \in \Gamma_k$, form another vector space $\mathcal{W}$. The mapping

$$Y: \mathcal{W} \mapsto \mathcal{S}, \qquad (Yw)_{lm} = 4\pi \sum_{\boldsymbol{p} \in \Gamma_k} i^l Y_{lm}(\theta_p, \varphi_p)^* w_p \tag{F.2}$$

is obviously surjective, but its kernel

$$\mathscr{W}_0 = \{w \in \mathscr{W} \mid Yw = 0\} \tag{F.3}$$

is in general a non-trivial subspace of $\mathscr{W}$.

After eliminating v_{lm} through eq. (4.14), the equations to be solved can be written in the compact form

$$PBb = 0, \tag{F.4}$$

$$Ab = Yw + M'Bb, \tag{F.5}$$

where $b \in \mathscr{H}_1$ is the vector with components b_{lm}. The operators A and B are defined through eq. (4.6) and M' denotes the operator associated to the matrix $\mathscr{M}'_{lm,l'm'}$. In this language, the plane wave solutions discussed in subsect. 4.3 correspond to $b = 0$ and $w \in \mathscr{W}_0$. There are no other solutions with $b = 0$.

We now proceed to discuss the conditions for the existence of solutions with $b \neq 0$. By acting with the projectors P and $1 - P$, eq. (F.5) can be split into the components

$$Yw = PAb - PM'Bb, \tag{F.6}$$

$$(1 - P)Ab = (1 - P)M'Bb. \tag{F.7}$$

The first of these equations determines w for given b. Since Y is surjective, the existence of a solution is guaranteed. But in general it is not unique, because the kernel $\mathscr{W}_0$ may be non-trivial. This degeneracy of the solution obviously corresponds to the possibility of adding a plane wave solution.

We are then left with the problem to determine the solutions of the remaining equations (F.4) and (F.7). These two equations can be regarded as the components of

$$\{(1 - P)A - KB + iPB\}b = 0, \qquad K \overset{\text{def}}{=} (1 - P)M'(1 - P), \tag{F.8}$$

along $\mathscr{F}$ and its orthogonal complement. A non-trivial solution of eqs. (F.4) and (F.7) thus exists if and only if the condition

$$\det[(1 - P)A - KB + iPB] = 0 \tag{F.9}$$

is satisfied.

In the following we would like to show that eq. (F.9) is equivalent to eq. (4.17). To this end we first remark that

$$M \underset{q \to |n|}{=} \frac{1}{q^2 - n^2} N + M' + \mathrm{O}(q^2 - n^2), \tag{F.10}$$

where the operator N satisfies $PN = NP = N$ [cf. eqs. (3.40) and (3.41)]. Furthermore, on the subspace $\mathscr{T}$ all its eigenvalues are strictly negative and N is hence invertible there.

We now define an auxiliary operator

$$X = (q^2 - n^2)P + (1 - P) \tag{F.11}$$

and deduce that

$$\begin{aligned}\lim_{q\to|n|} U &= \lim_{q\to|n|} [(M+i)X][(M-i)X]^{-1} \\ &= [N + (M'+i)(1-P)][N + (M'-i)(1-P)]^{-1}.\end{aligned} \tag{F.12}$$

Since N is invertible on $\mathscr{T}$, the factorization

$$\begin{aligned} N &+ (M' \pm i)(1-P) \\ &= [N + K \pm i(1-P)] \times [1 + PN^{-1}PM'(1-P)],\end{aligned} \tag{F.13}$$

is possible and as a result one obtains

$$\lim_{q\to|n|} U = P + (1-P)\frac{K+i}{K-i}(1-P). \tag{F.14}$$

We have thus shown that eq. (4.17) is equivalent to

$$\det\left[e^{2i\delta} - P - (1-P)\frac{K+i}{K-i}(1-P)\right] = 0. \tag{F.15}$$

If we multiply this equation from the left with $\det(K-i)$ and from the right with $\det(A - iB)$ one recovers eq. (F.9). This establishes the desired equivalence since both factors are neither zero nor infinite.

Appendix G

For some potentials $V(r)$ and box sizes L it can happen that $E = 0$ is an eigenvalue of H_1. The existence of such eigenstates depends on whether the scattering matrix has certain properties at low energies. It is the purpose of this appendix to derive these conditions explicitly.

For $k=0$ the general solution of Helmholtz' equation with degree Λ is

$$\psi(\boldsymbol{r}) = w_0 + \sum_{l=1}^{\Lambda} \sum_{m=-l}^{l} v_{lm} G'_{lm}(\boldsymbol{r};0), \tag{G.1}$$

where w_0 and v_{lm} are arbitrary coefficients. The conditions for energy eigenstates are

$$b_{lm}\alpha_l^0 = \delta_{l0}\sqrt{4\pi}\, w_0 + \sum_{l'=1}^{\Lambda} \sum_{m'=-l'}^{l'} v_{l'm'} \frac{(-1)^{l'}}{4\pi}\left(\frac{2\pi}{L}\right)^{l'+l+1} \mathscr{M}^0_{l'm',lm}, \tag{G.2}$$

$$b_{lm}\beta_l^0 = (1-\delta_{l0}) v_{lm}\frac{(-1)^l}{4\pi} \tag{G.3}$$

$(l = 0, 1, \dots, \Lambda)$.

If the scattering length a_0 vanishes (i.e. if $\beta_0^0 = 0$), these equations have a trivial solution. We just set

$$v_{lm} = b_{lm} = 0 \quad \text{for } l = 1, 2, \dots, \Lambda,$$

$$b_{00} = \sqrt{4\pi}, \qquad w_0 = \alpha_0^0. \tag{G.4}$$

The associated wave function $\psi(\boldsymbol{r})$ is constant, and this case thus corresponds to the plane wave solutions discussed in subsect. 4.3.

There can be further solutions with $b_{00} = 0$. To obtain these, we first eliminate v_{lm} through eq. (G.3). After that we are left with an equation which determines w_0 and a linear system of equations for the coefficients b_{lm} with $1 \leqslant l \leqslant \Lambda$. A necessary and sufficient condition for the existence of solutions of this type then is that the determinant of the system vanishes.

To express this condition in a compact form it is useful to introduce the space $\mathscr{H}_\Lambda^0$ of all vectors $v \in \mathscr{H}_\Lambda$ with $v_{00} = 0$. The matrix $\mathscr{M}^0_{lm,l'm'}$ defines a linear operator M^0 in $\mathscr{H}_\Lambda^0$ and two further operators A^0 and B^0 are given by

$$[A^0 v]_{lm} = \left(\frac{2\pi}{L}\right)^{-l} \alpha_l^0 v_{lm}, \qquad [B^0 v]_{lm} = \left(\frac{2\pi}{L}\right)^{l+1} \beta_l^0 v_{lm}. \tag{G.5}$$

With the help of these notations, the condition for the existence of a solution with $b_{00} = 0$ becomes

$$\det[A^0 - B^0 M^0] = 0. \tag{G.6}$$

If the coefficients α_l^0 do not vanish, we may divide this equation by $\det A^0$ and then end up with a condition involving the threshold parameters a_l (cf. subsect.

2.1). Since M^0 is independent of L, it is clear that this equation in general has solutions for a few isolated values of L at most.

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