Instituto de Física
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Quantum Scattering Phenomena in Higher Dimensions

Volta Redonda

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"Postulates are based on assumption and adhered to by faith. Nothing in the Universe can shake them."

— Isaac Asimov; I, Robot

Abstract

In this thesis we study quantum scattering theory in $\mathcal{N}$ spacial dimensions. The study of theoretical, non-relativistic quantum scattering of a single particle reduces to the solutions of Lippmann–Schwinger equations. Those are integral equations, and to solve them exactly, the integrand must be a product, where every function is a function of only one variable; in this case, we say the function is separable. Therefore, we must find a completely separable Green's function, and also to have a potential that is also separable. As for the means to find such Green's function in $\mathcal{N}$ dimensions, we develop a general formula for the $\mathcal{N}$-dimensional Green's function in any orthogonal, rotational coordinate system, in which the Helmholtz equation is completely separable. Having acquiring such a formula, we proceed to solve Lippmann–Schwinger equation in two four-dimensional problems and one six-dimensional problem. We study the wavefunctions and their associated scattering amplitudes and cross-sections. For this end, we plot graphics of the scattering cross-sections, which help us visualize and interpret the physics of quantum scatterings.

Usually, when studying scattering by a potential boundary-wall we introduce three quantities: the scattering amplitude, the reflection and the transmission amplitudes. They help us understand the probabilities related to how much of a wavefunction gets reflected or transmitted upon interaction with this potential. However, having only three quantities — the scattering amplitude and the transmission and reflection amplitudes — might not reveal everything about the system. Therefore, we introduce a little-known formula for a quantity known as the quantum refraction index, as a function of momentum and the scatterers density in a medium and investigate its behavior. To help with this investigation, we plot graphics of the quantum refraction index associated with those systems and give interpretations of our results.

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Chapter 1

Introduction

Scattering phenomena were first studied by Lord Rayleigh [1] and are part of our day-to-day life – electromagnetic scattering of visible light [2] makes us see the blue sky, green grass, celestial bodies at night, and air scattering allows us to hear music, to talk, to tell stories. Not only that, scattering of electromagnetic waves revolutionized, for example, medicine, with the discovery of X-rays and the development of radiotherapy. When considering matter waves, it immediately comes to mind the Rutherford scattering experiment. This experiment, established the foundations of nuclear physics, which today is the driving force behind green energy, nuclear medicine [3] and (rather unfortunately) warfare. When we explore particle physics, as yet another example, we enter the realm of Quantum Field Theory, which is a relativistic quantum mechanical theory. Scattering is one of the only ways, at least so far, that we can use to investigate what happens in the atomic and subatomic scales, and this equation is fundamental for these studies. Scattering of particles is our way of produce particles showers, to study the physics of interactions, to see inside the atomic nucleus and find the quarks, gluons, and if we are with enough energy, even quark-gluon plasma, the same material there was ”right after” the very Big Bang. Also, ever since 2015, with the detection of gravitational-waves, there is hope and research for gravitational-waves astronomy [4–10]. Gravitational waves are waves produced and transmitted by the very fabric of space-time. These investigations will most certainly take into account effects due to scattering by strong and weak gravitational fields, as we observe the deepest secrets of the Cosmos.

Another instance in which scattering phenomena appears is when we consider another type of matter scattering, the quantum scattering phenomena [11]. These phenomena can be achieved mathematically when we consider $E > |V|$ in the Schrödinger equation. While it might easy to solve the Schrödinger equation for one particle having a single interaction with the potential in this case, a very important question disturbs us: how to keep tabs on the possible multiple interactions of the wave function with the potential using only Schrödinger's equation? Of course, there are techniques for when the potential is spherically symmetric, namely, partial-wave analysis or the well-known Born approximation, but in nature things are not usually symmetric. Then, what if our potential is not spherically symmetric?

In order to keep track of multiple scattering processes we could invoke Huygens' principle. It is quite interesting that Huygens' principle is not correct for classical optics — which is precisely the subject it was proposed to explain — and it works perfectly well for quantum mechanical waves [12, 13]. The key point is the time derivative of classical wave equation (2^{nd}), and the time derivative of quantum mechanical wave equation which is first order. Huygens' principle establishes that a wave front impinging upon each point of a given target produce a secondary spherical wave, and, these secondary waves interfere at each point of space producing a new wave front and so forth. This interpretation is not clear when we formulate a scattering problem using the Schrödinger equation. In fact, Schrödinger equation governs the quantum dynamics from a local point of view. Said in other, equivalent words, it is a mathematical relation between quantities and their derivatives evaluated a given point of space. To keep track of multiple scattering it is better to model the problem from the global point of view.

This is achieved if we formulate the scattering problem using the Lippmann–Schwinger equation [14], which is a Fredholm integral equation of the second kind [15]. Integral equations by themselves are a challenging subject, however, when applied to scattering problems they allow us to interpret multiple scattering just as Huygens' principle states. An incident wave interacts with a potential in a given point and propagates to another point. The resulting wave is a superposition — an integral calculated over the target coordinates — of all the contributions.

Numerical solutions of the Lippmann–Schwinger are difficult to obtain since they demand hefty calculations and powerful computers. *Approximate* solutions can be calculated using partial-wave method for low energies. In fact, in the partial-wave technique one expands the final wavefunction in a convenient basis of eigenfunctions. The coefficients of each eigenfunction depend on certain phase-shifts δ_l. In practical problems one calculates just two or three of them. For high-energy problems the most suitable method to study *approximately* scattering problems is the Born approximation. In this case, it is possible to relate each term of Born approximation to a given process, e.g., there is a contribution that keeps track of the particle hitting the target once, another contribution accounts for the particle hitting the target twice and so forth. However, as long as the first order Born approximation is not so difficult to calculate, second and higher order corrections become more and more complicated.

Exact solutions, in principle, are valid for every energy range — including the intermediary energy range where neither partial-wave nor Born approximation work well [3] — and can be used to calculate differential as well as total cross-sections. The exact final wavefunction could also be used to investigate the complex angular momenta structure [16] of the problem and they could be used to visualize the scattering problem by plotting the probability density $|\psi(x, y, z)|^2$.

However, as far as we know exact solutions of the Lippmann–Schwinger are scarce. In 2018, Maioli and Schmidt [17] presented the first analytical solution of the Lippmann–Schwinger for the scattering of a plane-wave by a circular boundary-wall [18] — which are potentials written in terms of distributions [19] which are defined along curves or surfaces. Later on, the same authors and Azado and de Jesus studied several other geometries such as: elliptical [20], spherical [21], spheroidal [22]; as well as scattering problems formulated in non-Euclidean spaces such as the Poincaré disk and Poincaré upper half-plane [23]. These solutions serve as a basis for studies of more complicated problems involving two potentials [24] as well as multiple scattering.

The outline for this thesis is the following: in chapter 2, we present a brief introduction to quantum scattering theory. In the first section, we present the wavefunction formalism up to the scattering cross-section. We go further by showing the Lippmann–Schwinger equation, and an expression for calculating the scattering amplitude. In the second section, we present the formal theory of quantum scattering. We do so using the Møller operators, and consequently, we use them to define the $S-$operator. Using this operator, we present an equation relating the scattering amplitude with the $T-$operator. Once again, but with other techniques, we show how the differential cross-section is related to the scattering amplitudes. We advance, introducing the optical theorem, and the birth of Lippmann–Schwinger equation via the formal theory of quantum scattering. At last, we define the quantum refraction index (formally known [25] as the Bohr–Peierls–Placzek relation) using the optical theorem and the fact that the $S-$operator conserves energy.

In chapter 3, we show the conditions under which the Helmholtz equation is separable in $\mathcal{N}$ dimensions. Next, we propose a Green's function for any $\mathcal{N}$-dimensional, orthogonal, rotational coordinate system, which can be applied to extend the original 11 coordinate system showed by Moon and Spencer [26–28]. Our objective is to apply this Green's function to solve the Lippmann–

Schwinger equation in $\mathcal{N}$ dimensions. Therefore, we calculated the free Green's function in a $\mathcal{N}$-dimensional hyperspherical coordinate system, first solving the free Helmholtz equation with spherical symmetry in order to find a closed-form solution, and later finding a bilinear expansion for the same Green's function. To find this expansion, we constructed a set of $\mathcal{N} - 2$ angular functions using harmonic polynomials. These functions are eigenfunctions of the square of the orbital angular momentum operator, $\mathbf{L}^2$. Upon doing so, we constructed a Green's function using the aforementioned general formula. Using this bilinear expansion, we show a familiar Gegenbauer type expression for Hankel's function [29,30]. We conclude this chapter by showing the equivalence between our constructed solution and the usual way of obtaining the Green's function, that is, by solving a partial differential equation.

In chapter 4, we solve the Lippmann–Schwinger equation for three different systems: the first is the scattering of a scalar particle by a 4-dimensional boundary-wall, represented as a hyperspherical potential. The second is again the scattering of a scalar particle by a 4-dimensional hyperspherical potential, but this time, we define a region we call a Dirac medium, or a Dirac sphere. This region is a solid sphere. Each point within and on the surface of this sphere holds a delta function. In this case, there arises the need for using reflection and transmission coefficients, because of the nature of the potential. The third system is the scattering of two non-interacting scalar particles by a three-dimensional boundary-wall, mathematically written as a spherical potential. This time, we are dealing with two particles, each with three degrees of freedom, whence it follows that we need to use a six-dimensional hyperspherical coordinate system to deal with this case. After solving each Lippmann–Schwinger equation, we present the wavefunction, the scattering amplitude, and therefore the differential and total cross-sections. Moreover, we reveal the quantum refraction index for each case, and also add graphics of the cross-sections and quantum refraction indexes.

Finally, in chapter 5, we present a summary of our conclusions and some perspectives into future investigations.

Chapter 2

A Brief Introduction to Quantum Scattering Theory

In this chapter we study the fundamental concepts concerning the non-relativistic quantum scattering theory. We begin with the local formulation — governed by the Schrödinger equation — and outline how to obtain the scattering amplitude and the cross-section via wavefunction formalism. Then we move to the global formulation, which on its turn, is governed by the Lippmann–Schwinger equation. In both approaches one models the scattering in the same way: a projectile impinges upon a target, the interaction takes place and then the projectile is scattered to infinity. We review the key concepts of such model: S and T operators as well as Møller operators. Finally, we arrive at the Lippmann–Schwinger in the position representation and calculate the quantum refraction index for matter waves.

2.1 The wavefunction formalism

In this approach to scattering phenomena, we solve Schrödinger equation while concerned with the continuous part of the energy eigenvalues. To do so, the first step is to define $\mathbf{r_1}$ as the position of the impinging particle and $\mathbf{r_2}$ as the position of the source of potential. Let us assume the following about the system: it is not relativistic, there is no emission nor absorption, there is no spin, the internal states of the particles remain unchanged, and the potentials are such that $V = V(\mathbf{r_1} - \mathbf{r_2})$. In fact, we can always work in the center of mass reference frame, and that's how we are going to proceed. Moreover, our potential has finite range, i.e., it is a *localized potential*. What this means is that $V(\mathbf{r_1} - \mathbf{r_2})$ is defined only for $\mathbf{r_1} - \mathbf{r_2} \leq a$, where a is the range of this potential. In other words, $V(\mathbf{r_1} - \mathbf{r_2}) = 0$ if $\mathbf{r_1} - \mathbf{r_2} > a$.

When a plane wave impinges upon our target, and the potential has a finite range a such that, *far away* from the potential, i.e., $r >> a$, the wavefunction has energy

$$E = \frac{\hbar^2 k^2}{2m} \ .$$

With this energy, and with the change $\mathbf{r} = \mathbf{r_1} - \mathbf{r_2}$, the time-independent Schrödinger's equation for the free-particle reads

$$-\frac{\hbar^2}{2m}(\nabla^2 + k^2)\psi = 0 \ , \tag{2.1}$$

whose solutions are

$$\psi(\mathbf{r}) = e^{\pm i\mathbf{k}\cdot\mathbf{r}} \tag{2.2}$$

with $k = |\mathbf{k}|$ as the wave number. Because we are using a localized potential, that is noticeable only if $r < a$, equation (2.2) might as well represent an incoming wave that will hit our target. The outgoing wave, when $r >> a$, is the result of the interaction between our incoming wave and the potential, so we expect it to be scattered in all directions, thus being a *spherical wave*, and it is written

$$\frac{e^{ikr}}{r}$$

such that probability is conserved. So as r grows bigger, the numerator oscillates, but the whole fraction goes to zero. But this scattered wave might not be *uniformly* scattered in every direction – it may depend upon the direction in which we choose to make a measurement. So, adding an angular factor to our scattered wave, we have

$$\psi_{scatt}(\mathbf{r}) = f_{\mathbf{k}}(\hat{\mathbf{r}})\frac{e^{ikr}}{r}. \tag{2.3}$$

Now, far away from our potential, the wavefunction should have contributions of the incoming (2.2) and the outgoing waves (because the target is small when compared to the plane wave, only a very small fraction of it gets in fact scattered). In order to account for the fact that the scattered wave vanishes when $r \to \infty$, we use the convention that the incoming wave is the one that travels from $-\infty$ to $+\infty$ as $t \to \infty$ and write the total wavefunction at $r >> a$ as

$$\psi(\mathbf{r}) \approx e^{i\mathbf{k}\cdot\mathbf{r}} + f_{\mathbf{k}}(\hat{\mathbf{r}})\frac{e^{ikr}}{r}. \tag{2.4}$$

The funtion $f_{\mathbf{k}}(\hat{\mathbf{r}})$, henceforth also referred as $f(\theta, \phi)$, is called *scattering amplitude*. In quantum mechanics, it is directly related to the probability of finding a particle in a given direction through another quantity called *differential cross section*, which is a way of quantify the number of particles per solid angle per unit of time. In fact, this quantity is well defined, and it is the *area* through which the flux of particles is the same as the flux through a solid angle $\Omega(\theta, \phi)$. On the other hand, in classical physics, this quantity is related to the probability that a specific process takes place.

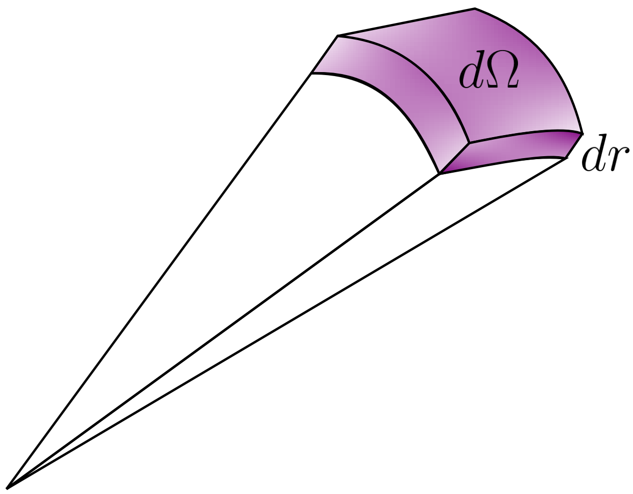

Figure 2.1: Solid angle $d\Omega$.

So, we simply calculate

$$d\sigma = \frac{\text{number of particles scattered } \textit{to} \text{ a solid angle } d\Omega \text{ at } (\theta, \phi) \text{ per unit time}}{\text{incoming flux or number of particles hitting the target per area per unit time}} \tag{2.5}$$

It is easy to calculate the denominator. The *probability current* or *probability flux* is

$$\mathbf{j}(\mathbf{r}, t) = \frac{\hbar}{2mi} \left[\psi^*_{inc} \vec{\nabla} \psi_{inc} - \psi_{inc} \vec{\nabla} \psi^*_{inc} \right] \tag{2.6}$$

and it describes the flow of probability of finding a particle at $(\mathbf{r}, t)$ per unit area per unit time. Our incident wave function is a plane, so

$$\mathbf{j}(\mathbf{r}, t) = \frac{\hbar}{2mi} \left[e^{-i\mathbf{k}\cdot\mathbf{r}} (i\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} - e^{i\mathbf{k}\cdot\mathbf{r}} (-i\mathbf{k}) e^{-i\mathbf{k}\cdot\mathbf{r}} \right] = \frac{\hbar \mathbf{k}}{m} \ . \tag{2.7}$$

For the numerator, the number of particles inside the volume

$$dv = r^2 dr \ d\Omega$$

at any given time should be

$$dn = \rho dv = |\psi_{scatt}|^2 dr \; d\Omega = \left| f(\theta, \phi) \frac{e^{ikr}}{r} \right|^2 dr \; d\Omega \tag{2.8}$$

where $\rho = |\psi_{scatt}|^2$ is the probability density of finding the scattered wave function in that region. Now, the particles need a time dt to travel the distance dr with a velocity u, as in

$$dt = \frac{dr}{u} = \frac{dr}{p/m} = \frac{dr}{\hbar k/m} \tag{2.9}$$

Thus, the number of particles scattered *to* a solid angle $d\Omega$ at (θ, ϕ) per unit time is simply

$$\frac{dn}{dt} = \frac{\hbar k}{m} |f(\theta, \phi)|^2 d\Omega \tag{2.10}$$

Substituting (2.7) and (2.10) into (2.5), we get immediately

$$d\sigma = \frac{dn}{dt} \frac{1}{|\mathbf{j}(\mathbf{r}, t)|} = \frac{\cancel{\hbar k}}{\cancel{m}} |f(\theta, \phi)|^2 d\Omega \cdot \frac{1}{\frac{\cancel{\hbar k}}{\cancel{m}}} = |f(\theta, \phi)|^2 d\Omega \; . \tag{2.11}$$

This is called *the differential cross-section*, and often it gets slightly rewritten as

$$\frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2 \tag{2.12}$$

One may be tempted to integrate this differential quantity. This is exactly how we define the *total cross-section*:

$$\sigma = \int d\sigma = \int |f(\theta, \phi)|^2 \; d\Omega. \tag{2.13}$$

It appears as if this scattering amplitude function is an essential mathematical object to our purposes, so how do we calculate it? We would need to solve the interacting Schrödinger equation

$$-\frac{\hbar^2}{2m}(\nabla^2 + k^2)\psi + V(\mathbf{r})\psi = 0 \; , \tag{2.14}$$

and then take the limit $r \to \infty$ to find an expression similar to (2.4), to identify the scattering amplitude. In general though, we can not: the calculations become so hard so quickly that the only solutions are numerical, through computational analysis. There is a known general solution for for the case $V = V(r)$, which is called *the partial-wave solution*, but it works only for central potentials, like Coulomb or Yukawa. These solutions are expansions series using eigenfunctions of the hamiltonian in (2.14), and they are indeed *the* solutions when we are working with central potentials. However, the potentials we consider in this work are local, with defined range, and are not central. We define them as [18]

$$V(\mathbf{r}) = \int \gamma(r', \Omega')\delta^{(\mathcal{N})}(\mathbf{r} - \mathbf{r}')\ d^{\mathcal{N}}r', \tag{2.15}$$

where the integral is taken over a hyper-volume dictated by the geometry of the problem, and $\gamma(r', \Omega')$ effectively gives us "how much" deltas exist in a unit volume, thus being the scatterers density. So despite the success and power of partial-wave analysis, it will not be of help as we go forward. The solutions we seek for (2.14) will also be written as a series of eigenfunctions of the hamiltonian, but will work for a broader scope of potentials. In chapter 4 we show how to find such wavefunctions using our potentials.

2.1.1 Integral equations

Lets solve Schrödinger's equation, but first, we set

$$V(\mathbf{r}) = -\frac{\hbar^2}{2m}U(\mathbf{r}). \tag{2.16}$$

Now, equation (2.14) can be written as

$$\nabla^2\psi + k^2\psi = -U(\mathbf{r})\psi(\mathbf{r}). \tag{2.17}$$

Note that the left hand side (l.h.s.) is the Helmholtz equation, but the right hand side (r.h.s.), as it stands, pose difficulties. If we shift our interpretation of the r.h.s. and consider the product as a non-homogeneous term, then we may use the fact that the solution for a partial differential equation (P.D.E.) is

$$\psi(\mathbf{r}) = \psi_h(\mathrm{r}) + \psi_p(\mathbf{r}), \tag{2.18}$$

that is, it is the sum of the solution of the homogenous equation ψ_h plus the particular solution, the one that actually solves (2.17). The homogenous solution ψ_h is known, it is equation (2.2):

$$\psi_h(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{2.19}$$

To find ψ_p, we can think about the Green's function related to equation (2.17), which is the solution of

$$(\nabla^2 + k^2)G(\mathbf{r}|\mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}'). \tag{2.20}$$

The vector $\mathbf{r}'$ represents one point on the source of potential, and $\mathbf{r}$ is the point in space, or in other words, it represents where is the observer. After solving equation (2.20), the solution (2.18) translates to

$$\psi(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}} - \int_{V'} dV' \; G(\mathbf{r}|\mathbf{r}')U(\mathbf{r}')\psi(\mathbf{r}'). \tag{2.21}$$

This is the Lippmann–Schwinger equation in position basis, and it is the most important equation in quantum scattering theory. Now, we actually can solve equation (2.20), and the solutions are given in detail in chapter 3 for any number of degrees of freedom. Moreover, we solve equation (2.21) in chapter 4 using methods of integral equations [15]. For now, we can use the well-known solutions in three-dimensions for equation (2.20) to explore one final aspect of Lippmann–Schwinger equation:

$$G^{\pm}(\mathbf{r}|\mathbf{r}') = \frac{e^{\pm ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r} - \mathbf{r}'|}. \tag{2.22}$$

Substituting the incoming Green's function (which is the one with + sign) in (2.22) into (2.21) reveals

$$\psi(\mathbf{r}) = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{1}{4\pi}\int_{V'} dV' \; \frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} U(\mathbf{r}')\psi(\mathbf{r}'), \tag{2.23}$$

and if we were to estimate its behavior when $r \gg r'$, we would use the fact that

$$|\mathbf{r} - \mathbf{r}'| \approx r - \hat{n}\cdot\mathbf{r}'.$$

which is perfectly fine to use in the phase when the magnitude $|\mathbf{r} - \mathbf{r}'|$ is not comparable to k. In the denominator, it is no problem to set $|\mathbf{r} - \mathbf{r}'| \approx r$. Therefore,

$$\begin{aligned}\psi(\mathbf{r}) &\approx \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}} - \frac{1}{4\pi}\int_{V'} dV' \; \frac{e^{ik(r-\hat{n}\cdot\mathbf{r}')}}{r} U(\mathbf{r}')\psi(\mathbf{r}') \\ &\approx \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{k}\cdot\mathbf{r}} + \left[-\frac{1}{4\pi}\int_{V'} dV' \; e^{-i\mathbf{k}\cdot\mathbf{r}'} U(\mathbf{r}')\psi(\mathbf{r}')\right] \frac{e^{ikr}}{r}\end{aligned} \tag{2.24}$$

The realization that (2.4) is of the form (2.24) makes us conclude that

$$f_{\mathbf{k}}(\hat{\mathbf{r}}) = -\frac{1}{4\pi}\int_{V'} dV' \; e^{-i\mathbf{k}\cdot\mathbf{r}'} U(\mathbf{r}')\psi(\mathbf{r}'). \tag{2.25}$$

This is a formula to calculate the scattering amplitude $f_{\mathbf{k}}(\hat{\mathbf{r}})$, which looks like an integral equation, but is not, because it is enough for us to know $\psi(\mathbf{r})$ in order to solve this expression. Is it possible to find an *approximation* to the scattering amplitude? Yes, if we know an approximation to the wavefunction. Looking again at (2.21), we notice that it may be interpreted as *recursive* equation, that is, we could insert $\psi(\mathbf{r})$ inside itself and iterate, indefinitely. This iterative series, which is made of the infinite summation of integrals, is know as *the Born series*. References [31] and [32] have great introductions to this subject.

2.2 The operator formalism

In a scattering experiment, what give us information about the system are the incoming wavefunction and the scattered wavefunction. Usually, we are concerned with an incoming plane-wave and an outgoing wavefunction that is a sum between a plane-wave and a scattered spherical wave. But again, the contribution of the spherical wave goes to zero as we get farther away form the scattering region, or from our potential. Thus, when we use time to characterize a wavefunction, we see that asymptotically, the incoming wave is

$$\lim_{t\to-\infty} |\psi\rangle = |\psi_{\text{in}}\rangle \tag{2.26}$$

and the outgoing wave is

$$\lim_{t\to+\infty} |\psi\rangle = |\psi_{\text{out}}\rangle \ . \tag{2.27}$$

This might not always be the case of course. For example, the particle could enter a blackhole, and then there would not be an outgoing wavefunction. Or the particle could produce a bound state if it interacted with an atom, but here we are considering only elastic scattering states, so we do not need to worry. For what comes next, we use the Rydberg units of measure, in which $\hbar = 2m^* = 1$, where m^* is the mass of the particle.

2.2.1 One particle scattering by a potential

The hamiltonian operator is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\mathbf{r}) = \hat{H}_0 + \hat{V}(\mathbf{r}). \tag{2.28}$$

Using this hamiltonian, we know that the solution for Schrödinger's equation is

$$\hat{U}(t) = e^{-it\hat{H}}. \tag{2.29}$$

We can write the solution for the free Schrödinger equation as

$$\hat{U}_0(t) = e^{-it\hat{H}_0} \tag{2.30}$$

Suppose that $\hat{U}(t)\left|\psi\right\rangle$ describes an scattering experiment. As $t \to \pm\infty$, we impose

$$\hat{U}(t)\left|\psi\right\rangle \xrightarrow[t\to-\infty]{} \hat{U}_0(t)\left|\psi_{\text{in}}\right\rangle, \tag{2.31}$$

$$\hat{U}(t)\left|\psi\right\rangle \xrightarrow[t\to+\infty]{} \hat{U}_0(t)\left|\psi_{\text{out}}\right\rangle. \tag{2.32}$$

Equations (2.31) and (2.32) are related when $t = 0$ via the *asymptotic condition*[1]

$$\hat{U}(t)\left|\psi\right\rangle - \hat{U}_0(t)\left|\psi_{\text{in}}\right\rangle \xrightarrow[t\to-\infty]{} 0 \tag{2.33}$$

and its analog equation for $\left|\psi_{\text{out}}\right\rangle$, which reads

$$\hat{U}(t)\left|\psi\right\rangle - \hat{U}_0(t)\left|\psi_{\text{out}}\right\rangle \xrightarrow[t\to+\infty]{} 0. \tag{2.34}$$

The Møller operators and the S-operator

When we multiply (2.31) by the left with $\hat{U}^\dagger(t)$, we get

$$\left|\psi\right\rangle - \hat{U}^\dagger(t)\hat{U}_0(t)\left|\psi_{\text{in}}\right\rangle \xrightarrow[t\to-\infty]{} 0. \tag{2.35}$$

Now, we can **define** the Møller operators as

$$\hat{\Omega}_\pm \coloneqq \lim_{t\to\mp\infty} \hat{U}^\dagger(t)\hat{U}_0(t) = \lim_{t\to\mp\infty} e^{i\hat{H}t}e^{-i\hat{H}_0 t}. \tag{2.36}$$

Although these operators are not unitary, in general, here we are interested only in those that are. The matters of convergence of equation (2.35), the existence conditions for Møller operators, and deeper analysis may be found in [11]. If we calculate the derivative of (2.36),

$$\frac{d}{dt}\hat{U}^\dagger(t)\hat{U}_0(t) = ie^{i\hat{H}t}(\hat{H} - \hat{H}_0)e^{-i\hat{H}_0 t} = i\hat{U}^\dagger(t)\hat{V}\hat{U}_0(t), \tag{2.37}$$

[1] More details about the asymptotic condition, including its proof, can be found in reference [11].

we see that we can write the product as an integral of its derivative. Upon product with a ket by the right, we get

$$d\left(\hat{U}^\dagger(t)\hat{U}_0(t)\right)|\psi\rangle = i\ dt\ \hat{U}^\dagger(t)\hat{V}\hat{U}_0(t)\,|\psi\rangle \tag{2.38}$$

or, integrating between $0 < t < \infty$,

$$\hat{U}^\dagger(t)\hat{U}_0(t)\,|\psi\rangle = |\psi\rangle + i\int_0^\infty dt'\ \hat{U}^\dagger(t')\hat{V}\hat{U}_0(t')\,|\psi\rangle \tag{2.39}$$

We write the state vector in equation (2.31) and (2.32) as

$$\begin{aligned} |\psi\rangle &= \lim_{t\to-\infty} \hat{U}^\dagger(t)\hat{U}_0(t)\,|\psi_{\text{in}}\rangle = \hat{\Omega}_+\,|\psi_{\text{in}}\rangle \\ |\psi\rangle &= \lim_{t\to+\infty} \hat{U}^\dagger(t)\hat{U}_0(t)\,|\psi_{\text{out}}\rangle = \hat{\Omega}_-\,|\psi_{\text{out}}\rangle \end{aligned} \tag{2.40}$$

For our intents and purposes, this means that

$$\hat{\Omega}_-\,|\psi_{\text{out}}\rangle = \hat{\Omega}_+\,|\psi_{\text{in}}\rangle \tag{2.41}$$

and clearly, multiplying with $\hat{\Omega}_-^\dagger$ by the left, we get

$$|\psi_{\text{out}}\rangle = \hat{\Omega}_-^\dagger\hat{\Omega}_+\,|\psi_{\text{in}}\rangle \tag{2.42}$$

whence we define the *S-operator* as

$$\boxed{\hat{S} \coloneqq \hat{\Omega}_-^\dagger\hat{\Omega}_+}. \tag{2.43}$$

It transpires from definition (2.36) that

$$\hat{H}\hat{\Omega}_\pm = \hat{\Omega}_\pm\hat{H}_0. \tag{2.44}$$

To see why, lets take a positive real variable τ, for which

$$\begin{aligned} e^{i\hat{H}\tau}\hat{\Omega}_\pm &= e^{i\hat{H}\tau}\lim_{t\to\mp\infty} e^{i\hat{H}t}e^{-i\hat{H}_0 t} \\ &= \lim_{t\to\mp\infty} e^{i\hat{H}(t+\tau)}e^{-i\hat{H}_0 t} \\ &= \underbrace{\lim_{t\to\mp\infty} e^{i\hat{H}(t+\tau)}e^{-i\hat{H}_0(t+\tau)}}_{\text{Møller operators}} e^{i\hat{H}_0\tau} \\ &= \hat{\Omega}_\pm e^{i\hat{H}_0\tau}. \end{aligned}$$

Now, we must simple take a derivative with respect to τ and taking the limit $\tau \to 0$, to get

$$\frac{d}{d\tau}\left(e^{i\hat{H}\tau}\hat{\Omega}_{\pm}\right) = \frac{d}{d\tau}\left(\hat{\Omega}_{\pm}e^{i\hat{H}_0\tau}\right) \xrightarrow[\tau\to 0]{} i\hat{H}\cancelto{1}{e^{i\hat{H}\tau}}\hat{\Omega}_{\pm} = i\hat{H}_0\hat{\Omega}_{\pm}\cancelto{1}{e^{i\hat{H}_0\tau}}$$

which is equation (2.44). Since this relation is true, and since we work with those Møller operators that are subject to

$$\hat{\Omega}_{\pm}^{\dagger}\hat{\Omega}_{\pm} = \mathbb{1},$$

equation (2.44) may be rewritten as

$$\hat{\Omega}_{\pm}^{\dagger}\hat{H}\hat{\Omega}_{\pm} = \hat{H}_0. \tag{2.45}$$

Therefore,

$$\begin{aligned}
[\hat{S},\hat{H}_0] &= \hat{S}\hat{H}_0 - \hat{H}_0\hat{S} \\
&= \hat{\Omega}_{-}^{\dagger}\hat{\Omega}_{+}\hat{H}_0 - \hat{H}_0\hat{S} \\
&= \hat{\Omega}_{-}^{\dagger}\hat{H}\hat{\Omega}_{+} - \hat{H}_0\hat{S} \\
&= \hat{H}_0\hat{\Omega}_{-}^{\dagger}\hat{\Omega}_{+} - \hat{H}_0\hat{S} \\
&= \hat{H}_0\hat{S} - \hat{H}_0\hat{S} \\
&= 0.
\end{aligned} \tag{2.46}$$

Thus, $\hat{S}$ conserves energy, that is, the energy of $|\psi_{\text{in}}\rangle$ is equal to the energy of $|\psi_{\text{out}}\rangle$:

$$\langle\psi_{\text{in}}|\,\hat{H}_0\,|\psi_{\text{in}}\rangle = \langle\psi_{\text{in}}|\,\hat{S}^{\dagger}\hat{S}\hat{H}_0\,|\psi_{\text{in}}\rangle = \langle\psi_{\text{in}}|\,\hat{S}^{\dagger}\hat{H}_0\hat{S}\,|\psi_{\text{in}}\rangle = \langle\psi_{\text{out}}|\,\hat{H}_0\,|\psi_{\text{out}}\rangle\,,$$

where we used the fact that $\hat{S}^{\dagger}\hat{S} = \mathbb{1}$. Since the free hamiltonian and the S-matrix commute, one can easily diagonalize them simultaneously, provided that one of them has a continuous spectrum, which is the case of $\hat{H}_0$. Moreover, in momentum-space, the matrix elements $\langle p'|\,\hat{S}\,|p\rangle$ satisfy

$$\langle p'|[\hat{H}_0,\hat{S}]\,|p\rangle = \Big(E_{p'} - E_p\Big)\,\langle p'|\hat{S}\,|p\rangle = 0 \tag{2.47}$$

which implies that $\langle p'|\,\hat{S}\,|p\rangle$ is zero everywhere except when $E_{p'} = E_p$, where E_p is the energy eigenvalue associated with the eigenstate $|p\rangle$, and $E_{p'}$ is the energy eigenvalue associated with the eigenstate $|p'\rangle$. Thus, one writes

$$\langle p'|\hat{S}\,|p\rangle = \delta(E_{p'} - E_p) \times (\text{remainder}). \tag{2.48}$$

This translates the conservation of energy in momentum-space representation. Now, to find this remainder, one sets

$$\hat{S} = \mathbb{1} + \hat{R}, \tag{2.49}$$

where $\mathbb{1}$ represents no interaction and $\hat{R}$ represents interaction. Now it is the element $\langle p'|\hat{R}\,|p\rangle$ who carries the delta factor $\delta(E_{p'} - E_p)$. Consequently, the momentum-space matrix element of the S-operator representation reads

$$\langle p'|\hat{S}\,|p\rangle = \delta(\mathbf{p'} - \mathbf{p}) - 2\pi i \delta(E_{p'} - E_p) \times t(\mathbf{p'}, \mathbf{p}) \tag{2.50}$$

What is the meaning of this equation? And what is this $t(\mathbf{p'}, \mathbf{p})$? The first term is just the amplitude for the particle to travel without interacting. The second term is the amplitude that is scattered. Looking closely, we gather that $\hat{S}$ conserving energy means nothing for the momentum components – they may change once scattering happens. Because of this, the factor $t(\mathbf{p'}, \mathbf{p})$ is a smooth function. Moreover, it is only defined for $E_{p'} = E_p$. In other words, the function $t(\mathbf{p'}, \mathbf{p})$ exists only when $p^2 = p'^2$, thus being called *T-matrix on the energy shell* or even *on-shell T-matrix*. We **define** the *scattering amplitude* as:

$$f(\mathbf{p'}, \mathbf{p}) = -(2\pi)^2 m\; t(\mathbf{p'}, \mathbf{p}) \tag{2.51}$$

2.2.2 Quantum cross-section

The wavefunction $\langle p|\psi_{\text{out}}\rangle$ determines the probability of finding the particle with momentum $\mathbf{p}$ long after the scattering occurred. So the probability we find the particle with momentum $\mathbf{p}$ at $d\Omega$, about the direction $\hat{\mathbf{p}}$, is

$$P(d\Omega) = d\Omega \int_0^\infty |\psi_{\text{out}}(\mathbf{p})|^2 p^2 dp. \tag{2.52}$$

As we can see, we are not interested in a specific magnitude of momentum, only the direction. Suppose we have an incoming particle with state vector $|\psi_{\text{in}}\rangle = |\phi\rangle$, and that a scattering experiment is made where wave packets differ *randomly* from state $|\phi\rangle$ by a factor[2] $\boldsymbol{\rho}$, such that a typical wave packet is represented by

$$\phi_\rho(\mathbf{p}) = e^{-i\boldsymbol{\rho}\cdot\mathbf{p}}\phi(\mathbf{p}).$$

[2] Remember, the generator of translation is the momentum operator [32].

What this means is simple. If our $|\psi_{\text{in}}\rangle$ is such that it travels in the direction of the geometric centre of our target, $e^{-i\boldsymbol{\rho}\cdot\mathbf{p}}\phi(\mathbf{p})$ will hit the target in a distance ρ from the said centre.

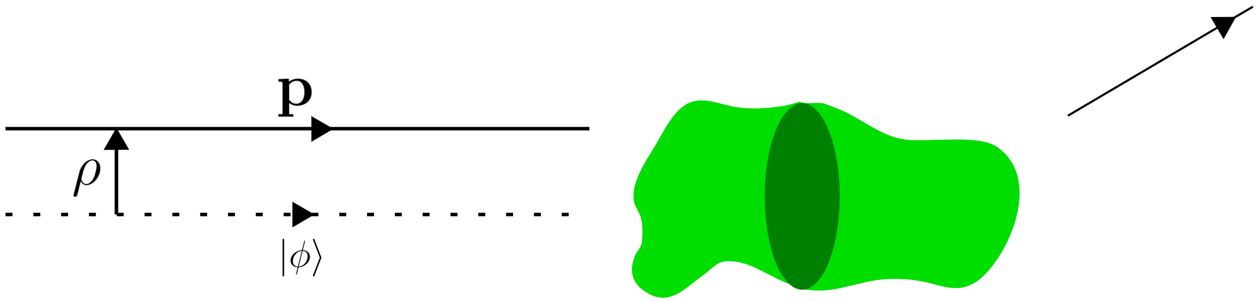

Figure 2.2: Scattering of wave packets.

After many experiments with random $\boldsymbol{\rho}$, the number of scattered particles to $d\Omega$ is

$$N_{\text{scatt}}(d\Omega) = \sum_j P(d\Omega) \approx \int n_{\text{in}} P(d\Omega) d^2\rho = n_{\text{in}}\Sigma(d\Omega) \tag{2.53}$$

where n_{in} is the number of incident particles per unit area, and Σ is our newly defined cross-sectional area of the target, or in other words, it is the effective *size* of the target. This cross-sectional area should be proportional to the scattering cross-section, such that

$$\Sigma(d\Omega) = \frac{d\sigma}{d\Omega} \cdot d\Omega. \tag{2.54}$$

Equations (2.42) and (2.43) reveal

$$|\psi_{\text{out}}\rangle = \hat{S}\,|\psi_{\text{in}}\rangle\,, \tag{2.55}$$

and consequently,

$$\langle p|\psi_{\text{out}}\rangle = \int \langle p|\,\hat{S}|p'\rangle\langle p'\,|\psi_{\text{in}}\rangle\, d^3p' = \psi_{\text{out}}(\mathbf{p}). \tag{2.56}$$

Equation (2.56), in its turn, together with (2.50) and (2.52), tell us

$$\psi_{\text{out}}(\mathbf{p}) = \psi_{\text{in}}(\mathbf{p}) + \frac{i}{2m}\int \delta(E_p - E_{p'}) f(\mathbf{p},\mathbf{p}')\psi_{\text{in}}(\mathbf{p}')d^3p'. \tag{2.57}$$

If we choose

$$\psi_{\text{in}}(\mathbf{p}) = e^{-i\boldsymbol{\rho}\cdot\mathbf{p}}\phi(\mathbf{p})$$

and assume we are observing far away from the incidence direction in an angle $d\Omega$, what follows is

$$\psi_{\text{out}}(\mathbf{p}) = \frac{i}{2\pi m}\int \delta(E_p - E_{p'}) f(\mathbf{p},\mathbf{p}') e^{-i\boldsymbol{\rho}\cdot\mathbf{p}'}\phi(\mathbf{p}')d^3p', \tag{2.58}$$

and finally,

$$\Sigma = \frac{d\Omega}{(2\pi)^2 m^2}\int d^2\rho \int_0^\infty dp\, p^2 \int d^3p' \int d^3p'' \Big[\delta(E_p - E_{p'})\delta(E_p - E_{p''}) f(\mathbf{p},\mathbf{p}') f^*(\mathbf{p},\mathbf{p}'') \times e^{-i\boldsymbol{\rho}\cdot(\mathbf{p}'-\mathbf{p}'')}\phi(\mathbf{p}')\phi(\mathbf{p}'')\Big]. \tag{2.59}$$

To simplify this humongous equation, first realize that

$$\int d^2\rho\, e^{-i\boldsymbol{\rho}\cdot(\mathbf{p}'-\mathbf{p}'')} = (2\pi)^2\delta^{(2)}(\mathbf{p}'_\perp - \mathbf{p}''_\perp),$$

because the integral is in the plane where $\boldsymbol{\rho}$ lies, so we are only interested in the components of $\mathbf{p}'$ and $\mathbf{p}''$ in that plane, that is perpendicular to the incident direction $\mathbf{p}_0$, which means that the notation $\mathbf{p}''_\perp$ represents a perpendicular projection or component of a vector $\mathbf{p}''$ in relation to $\mathbf{p}_0$. It is easy to see that

$$\delta(E_p - E_{p''}) = \delta(E_{p'} - E_{p''}), \tag{2.60}$$

because we have two delta functions. One of them will be different from zero only if $E_p = E_{p'}$, and the other will be only if $E_p = E_{p''}$. But then, it is logical to conclude that $\delta(E_p - E_{p''}) = \delta(E_{p'} - E_{p''})$. Using the properties

$$\delta(ax) = \frac{\delta(x)}{|a|} \tag{2.61}$$

and

$$\delta(x^2 - a^2) = \frac{\delta(x-a) + \delta(x+a)}{2a}, \tag{2.62}$$

one has

$$\delta(E_{p'} - E_{p''}) = 2m\delta(p'^2 - p''^2) = \frac{m}{p''}[\delta(p' - p'') + \delta(p' + p'')] \tag{2.63}$$

This delta function, in its turn, is only concerned with the components that are parallel to the direction $\mathbf{p}_0$, and since we are taking the integrals in spherical coordinates, there won't be a negative component of $\mathbf{p}'$. Therefore, we write

$$2m\delta(p'^2 - p''^2) = \frac{m}{p''_{\parallel}}\delta(p'_{\parallel} - p''_{\parallel}), \tag{2.64}$$

and additionally,

$$\frac{m}{p''_{\parallel}}\delta(p'_{\parallel} - p''_{\parallel})\delta^{(2)}(\mathbf{p}'_{\perp} - \mathbf{p}''_{\perp}) = \frac{m}{p''_{\parallel}}\delta^{(3)}(\mathbf{p}' - \mathbf{p}''),$$

where $p''_{\parallel}$ is the magnitude of parallel component of $\mathbf{p}''$ in relation to the incident momentum $\mathbf{p}_0$. Because of this, equation (2.59) becomes

$$\begin{aligned}
\Sigma(d\Omega) &= \frac{d\Omega}{m}\int_0^{\infty} dp\, p^2 \int d^3p'\delta(E_p - E_{p'})f(\mathbf{p},\mathbf{p}')\phi(\mathbf{p}')\int d^3p''\frac{1}{p''_{\parallel}}\delta^{(3)}(\mathbf{p}' - \mathbf{p}'')f^*(\mathbf{p},\mathbf{p}'')\phi(\mathbf{p}'') \\
&= \frac{d\Omega}{m}\int_0^{\infty} dp\, p^2 \int d^3p'\frac{1}{p'_{\parallel}}\delta(E_p - E_{p'})|f(\mathbf{p},\mathbf{p}')|^2|\phi(\mathbf{p}')|^2 \\
&= \frac{d\Omega}{m}\int_0^{\infty} dp\, p^2 \int d^3p'\frac{1}{p'_{\parallel}}\frac{m}{p'}[\delta(p-p') + \delta(p+p')]|f(\mathbf{p},\mathbf{p}')|^2|\phi(\mathbf{p}')|^2 \\
&= d\Omega\int d^3p'\frac{p'}{p'_{\parallel}}|f(\mathbf{p},\mathbf{p}')|^2|\phi(\mathbf{p}')|^2,
\end{aligned}$$

where we used $p = p'$. However, this integral is different from zero only in a very small region where $\phi(\mathbf{p}')$ is indeed different from zero. In this region, $f(\mathbf{p},\mathbf{p}')$ is an insignificant constant, so we can replace $\mathbf{p}' \to \mathbf{p}_0$, to get [11]

$$\Sigma(d\Omega) = d\Omega|f(\mathbf{p},\mathbf{p}_0)|^2 \cancelto{1}{\int d^3p'|\phi(\mathbf{p}')|^2} = d\Omega|f(\mathbf{p},\mathbf{p}_0)|^2 \tag{2.65}$$

which is what we expected from the cross-section. Thus, equation (2.54) reveals

$$\frac{d\sigma}{d\Omega} = |f(\mathbf{p},\mathbf{p}_0)|^2, \tag{2.66}$$

which is the familiar result for the quantum differential cross-section, just like (2.12).

2.2.3 The Optical Theorem

Now, we must explain a fundamental relationship, known as **the optical theorem**. Recall that

$$\hat{S} = \mathbb{1} + \hat{R}. \tag{2.49}$$

Equation (2.55) implies that $\hat{S}$ is unitary (because of conservation of energy, as we saw). Therefore,

$$\mathbb{1} = \hat{S}^{\dagger}\hat{S} = (\mathbb{1} + \hat{R}^{\dagger})(\mathbb{1} + \hat{R}) = \mathbb{1} + \hat{R} + \hat{R}^{\dagger} + \hat{R}^{\dagger}\hat{R} \Longrightarrow \hat{R} + \hat{R}^{\dagger} = -\hat{R}^{\dagger}\hat{R}. \tag{2.67}$$

Upon calculating the matrix elements, we get

$$\langle p'|\hat{R}\,|p\rangle + \langle p'|\hat{R}^\dagger\,|p\rangle = -\int d^3p'' \langle p'|\hat{R}^\dagger|p''\rangle\langle p''|\hat{R}^\dagger|p\rangle. \tag{2.68}$$

As we've seen from equations (2.50) and (2.51),

$$\langle p'|\hat{R}\,|p\rangle = -2\pi i\delta(E_{p'} - E_p)t(\mathbf{p}',\mathbf{p}) = \frac{i}{2\pi m}\delta(E_{p'} - E_p)f(\mathbf{p}',\mathbf{p}), \tag{2.69}$$

and since $\langle p'|\hat{R}^\dagger\,|p\rangle = \langle p'|\hat{R}\,|p\rangle^*$, we can factor out a delta function, obtaining from (2.68)

$$f(\mathbf{p}',\mathbf{p}) - f(\mathbf{p},\mathbf{p}')^* = \frac{i}{2\pi m}\int d^3p''\delta(E_p - E_{p''})f(\mathbf{p}'',\mathbf{p}')^* f(\mathbf{p}'',\mathbf{p}) \tag{2.70}$$

Setting $\mathbf{p} = \mathbf{p}'$, we can solve the integral using the same delta properties (2.61) and (2.62), to get

$$\text{Im}\{f(\mathbf{p},\mathbf{p})\} = \frac{p}{4\pi}\int d\Omega''|f(\mathbf{p}'',\mathbf{p})|^2 \tag{2.71}$$

or yet

$$\text{Im}\{f(\mathbf{p},\mathbf{p})\} = \frac{p}{4\pi}\sigma(\mathbf{p}) \tag{2.72}$$

Equations (2.71) and (2.72) are known as the optical theorem, and constitute an important relation between the attenuation factor $f(\mathbf{p},\mathbf{p})$ and the effective area of the scatterer. The function $f(\mathbf{p},\mathbf{p})$ is known as *forward scattering amplitude*, for the angle between the arguments is zero.

2.2.4 Green's operator and Lippmann-Schwinger equation

Using the definitions

$$\hat{H}_0 = \frac{\hat{p}^2}{2m}$$

and

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V}(\mathbf{r}) = \hat{H}_0 + \hat{V}(\mathbf{r}),$$

one may define two associated operators, which can be interpreted as the *inverse operators of the hamiltonians*:

$$G_0(z) = \frac{1}{z\mathbb{1} - \hat{H}_0}, \tag{2.73}$$

and

$$G(z) = \frac{1}{z\mathbb{1} - \hat{H}}. \tag{2.74}$$

Of course, these operators exist as long as z is not an eigenvalue of $\hat{H}_0$ and $\hat{H}$ respectively. This makes the operators to be not analytic in general because of the singularities in $z \in \mathbb{R}^+$.

At first glance, one may find, justifiably, that the operator $G(z)$ is way more difficult to work with than $G_0(z)$. In such a case, it should be useful to have an equation relating both operators. Contemplating the identity

$$A^{-1} = B^{-1} + B^{-1}(B - A)A^{-1},$$

one readly sees that taking $A = z - \hat{H}$ and $B = z - \hat{H}_0$, one finds

$$\begin{gathered} G(z) = G_0(z) + G_0(z)VG(z) \\ \text{or} \\ G_0(z) = G(z) + G(z)VG_0(z). \end{gathered} \tag{2.75}$$

These are known as the *resolvent equations* or *Lippmann-Schwinger* equations for the Green's operator. Of course, $G_0(z)$ is known and it is diagonal in the momentum representation. In fact, it looks like

$$G_0(z)\left|p\right\rangle = \frac{1}{z - \hat{H}_0}\left|p\right\rangle = \frac{1}{z - E_p}\left|p\right\rangle. \tag{2.76}$$

While it is good to know that the Green's operators are subject to an equation, one may argue that it would be better to have an equation that covers the spacial evolution of our state kets. Let us recall equation (2.39):

$$\hat{U}^\dagger(t)\hat{U}_0(t)\left|\psi\right\rangle = \left|\psi\right\rangle + i\int_0^\infty dt'\ \hat{U}^\dagger(t')\hat{V}\hat{U}_0(t')\left|\psi\right\rangle. \tag{2.39}$$

If $\left|\psi_{\text{in}}\right\rangle = \left|\phi\right\rangle$, then $\left|\psi\right\rangle = \hat{\Omega}_+\left|\psi_{\text{in}}\right\rangle = \hat{\Omega}_+\left|\phi\right\rangle = \left|\phi_+\right\rangle$. Similarly, if $\left|\psi_{\text{out}}\right\rangle = \left|\phi\right\rangle$, then $\left|\psi\right\rangle = \hat{\Omega}_-\left|\psi_{\text{out}}\right\rangle = \hat{\Omega}_-\left|\phi\right\rangle = \left|\phi_-\right\rangle$. Using this and taking the hint of equations (2.40), we get

$$\lim_{t\to\infty}\hat{U}^\dagger(t)\hat{U}_0(t)\left|\phi\right\rangle = \hat{\Omega}_-\left|\phi\right\rangle = \left|\phi_-\right\rangle = \left|\phi\right\rangle + i\int_0^\infty dt'\ \hat{U}^\dagger(t')\hat{V}\hat{U}_0(t')\left|\phi\right\rangle \tag{2.77}$$

Since the any absolutely convergent integral allows the introduction of a convergence factor $e^{-\epsilon\tau}$, we have,

$$
\begin{aligned}
|\phi_-\rangle &= |\phi\rangle + i \lim_{\epsilon\to 0^+} \int_0^\infty dt' \; e^{-\epsilon t'} \hat{U}^\dagger(t')\hat{V}\hat{U}_0(t')\,|\phi\rangle \\
&= |\phi\rangle + i \lim_{\epsilon\to 0^+} \int_0^\infty dt' \; e^{-i(E_p - i\epsilon - \hat{H})t'} \hat{V}\mathbb{1}\,|\phi\rangle \\
&= |\phi\rangle + i \lim_{\epsilon\to 0^+} \int d^3p \int_0^\infty dt' \; e^{-i(E_p - i\epsilon - \hat{H})t'} \hat{V}\,|p\rangle\,\langle p|\phi\rangle \\
&= |\phi\rangle + i \lim_{\epsilon\to 0^+} \int d^3p \int_0^\infty dt' \; (-i)(E_p - i\epsilon - \hat{H})^{-1}\hat{V}\,|p\rangle\,\langle p|\phi\rangle \\
&= |\phi\rangle + i \lim_{\epsilon\to 0^+} \int d^3p \int_0^\infty dt' \; G(E_p - i\epsilon)\hat{V}\,|p\rangle\,\langle p|\phi\rangle\,.
\end{aligned}
\tag{2.78}
$$

This is an integral equation for $|\phi_-\rangle$ in momentum basis, and it there exists an analogous equation for $|\phi_+\rangle$:

$$
|\phi_+\rangle = |\phi\rangle + i \lim_{\epsilon\to 0^+} \int d^3p \int_0^\infty dt' \; G(E_p + i\epsilon)\hat{V}\,|p\rangle\,\langle p|\phi\rangle\,. \tag{2.79}
$$

In general,

$$
|\phi_\pm\rangle = |\phi\rangle + i \lim_{\epsilon\to 0^+} \int d^3p \int_0^\infty dt' \; G(E_p \pm i\epsilon)\hat{V}\,|p\rangle\,\langle p|\phi\rangle\,. \tag{2.80}
$$

It is wise to define a ket

$$
|p_\pm\rangle = \hat{\Omega}_\pm\,|p\rangle\,, \tag{2.81}
$$

where

$$
\hat{H}\,|p_\pm\rangle = E_p\,|p_\pm\rangle\,,
$$

and

$$
|\phi_\pm\rangle = \int d^3p \; \phi(\mathbf{p})\,|p_\pm\rangle = \hat{\Omega}_\pm \int d^3p \; \phi(\mathbf{p})\,|p_\pm\rangle
$$

If we multiply (2.80) by the left with a complete set, in order to expand $|\phi_\pm\rangle$ in momentum space, we get

$$
\int d^3p \; \phi(\mathbf{p})\,|p_\pm\rangle = \int d^3p \; \phi(\mathbf{p})[|p\rangle + G(E_p \pm i0)\hat{V}\,|p\rangle], \tag{2.82}
$$

where we took the limit $\epsilon \to 0^+$, and since this equation is true for any function $\phi(\mathbf{p})$, one can see that in general

$$|p_\pm\rangle = |p\rangle + G(E_p \pm i0)\hat{V}\,|p\rangle\,. \tag{2.83}$$

One can define a new operator, called *T-operator*:

$$\hat{T}(z) = \hat{V} + \hat{V}\hat{G}(z)\hat{V} \tag{2.84}$$

Upon multiplication by the left with $\hat{G}_0(z)$,

$$\hat{G}_0(z)\hat{T}(z) = \underbrace{\left(\hat{G}_0(z)\hat{V} + \hat{G}_0(z)\hat{V}\hat{G}(z)\right)}_{\text{Lippmann–Schwinger equation}}\hat{V} = \hat{G}(z)\hat{V}. \tag{2.85}$$

There is an analogous equation:

$$\hat{T}(z)\hat{G}_0(z) = \hat{V}\hat{G}(z). \tag{2.86}$$

Then, if we use (2.84) together with (2.85), we find a Lippmann–Schwinger equation for the T-operator:

$$\hat{T}(z) = \hat{V} + \hat{V}\hat{G}_0(z)\hat{T}(z) \tag{2.87}$$

In equation (2.84), we multiply by the right with $|p\rangle$, and use (2.83), to get

$$T(E_p \pm i0)\,|p\rangle = [\hat{V} + \hat{V}\hat{G}(E_p \pm i0)\hat{V}]\,|p\rangle \tag{2.88}$$

$$= \hat{V}[1 + \hat{G}(E_p \pm i0)\hat{V}]\,|p\rangle \tag{2.89}$$

$$= \hat{V}\,|p_\pm\rangle\,. \tag{2.90}$$

We rewrite equation (2.83) using (2.85) and use (2.88), to get

$$\begin{aligned} |p_\pm\rangle &= |p\rangle + G(E_p \pm i0)\hat{V}\,|p\rangle \\ &= |p\rangle + \hat{G}_0(E_p \pm i0)\hat{T}(E_p + i0)\,|p\rangle \\ &= |p\rangle + \hat{G}_0(E_p \pm i0)\hat{V}\,|p_\pm\rangle \end{aligned} \tag{2.91}$$

This is the Lippmann–Schwinger equation for the state ket $|p_\pm\rangle$, and it is of crucial importance for the development of this work. One can use this equation in position basis, to find an integral equation:

$$\psi_{\mathbf{p}}(\mathbf{r}) = \langle r|p_{\pm}\rangle = \langle r|p\rangle + \langle r|\,\hat{G}_0(E_p \pm i0)\hat{V}|r'\rangle\langle r'|p_{\pm}\rangle \tag{2.92}$$

$$= \phi_{\mathbf{p}}(\mathbf{r}) + \int d^3r' G(\mathbf{r}|\mathbf{r}')V(\mathbf{r}')\psi_{\mathbf{p}}(\mathbf{r}') \tag{2.93}$$

This is the form of Lippmann–Schwinger's equation we will use in this work.

2.2.5 Quantum refraction index

Before we continue, a new quantity will be defined, to help us get information about a potential.

Say an experimental physicist measures the differential cross-section of a quantum-scattering experiment – this physicist would have multiple real numbers, and the average between those would give the differential cross section. While it is possible to interpret these numbers by themselves and extract information about the system, we can also define a number that tells us the deviation between the direction of propagation of the original impinging plane-wave and the final spherical-wave. In the 1940's, physicists introduced the concept of a *quantum refractive index* [33, 34], and many authors have redefined it throughout the years; for example, see [35–38]. One can find a valid expression for this quantum refraction index as follows: when a plane-wave traveling forwardly with wave vector $\mathbf{k}_0$ encounters a region containing a uniform refractive medium at $|\mathbf{r}| = 0$, we expect that, at a great distance $|\mathbf{r}| = R$ (now away from the region), we have

$$\psi = e^{ik_0R}e^{i\phi NR}e^{-\sigma NR}. \tag{2.94}$$

Here, $\sigma = \sigma_T/2$, and σ_T is the total cross-section. ϕ determines the attenuation of the wavefunction, manifested as a phase shift, and N is the scatterers density inside the region of scattering. But we also need to have a plane-wave at a far distance $|\mathbf{r}| = R$, so we can say that the new wave number is proportional to k_0, i.e.,

$$\psi = e^{ink_0R} \tag{2.95}$$

When we compare (2.94) with (2.95), we get

$$n = 1 + \frac{N}{k_0}(\phi + i\sigma) \tag{2.96}$$

According to the optical theorem,

$$\sigma = \frac{2\pi}{k}\,\mathrm{Im}(f(0)) \tag{2.97}$$

and

$$\phi = \frac{2\pi}{k}\,\text{Re}(f(0)). \tag{2.98}$$

Here, we chose to represent the forward scattering amplitude as $f(0)$ for the purpose of simplifying the notation. The meaning is still the same, it is the scattering of a wavefunction whose angle of incidence is $\theta = 0$ with respect to the horizontal plane. Substituting, we get

$$n = 1 + \frac{2\pi N}{k_0}\frac{f(0)}{k}. \tag{2.99}$$

Champenois, on the other hand, defines the quantum refraction index [39] as

$$n = 1 + 2\pi N\left(\frac{m_p + m_t}{m_t}\right)\left\langle\frac{f(k_r)}{k_p^2}\right\rangle. \tag{2.100}$$

Definition (2.100) is identical to (2.99) when $m_t \gg m_p$. In (2.99), N is the number of scatterers per unit volume, m_p is the particle's mass, m_t is the target's mass, k_r is the wave number of the impinging particle, measured in the center of mass reference frame, and k_p is the wave number of the particle, in its own reference frame. The quantity between brackets $\langle\ldots\rangle$ means the average over all values. Note that we said N is the number of scatterers per unit volume. Let us recall the definition of our potential (2.15):

$$V(\mathbf{r}) = \int \gamma(r', \Omega')\delta^{(\mathcal{N})}(\mathbf{r} - \mathbf{r}')\; d^{\mathcal{N}}r', \tag{2.15}$$

Upon comparison of (2.15) with (2.99) and (2.100), one concludes realizes that

$$N = \gamma(r', \Omega').$$

Using Born's approximation, we consider the system in the target's reference frame, and we make $m_t \gg m_p$, such that

$$n \approx 1 + 2\pi\gamma(r', \Omega')\left\langle\frac{f(k_r)}{k_p^2}\right\rangle. \tag{2.101}$$

Notice that Champenois takes the average of a number of values for the scattering amplitude. In this work, we do not need to worry about the average for three reasons — because our impinging wave is always a plane-wave, in the Born approximation the scatterer has a fixed position in space, and, as we'll see, we consider the scatterer's density to be constant, which aligns with spherical symmetry to help in our calculations. The quantum refraction index is also known as Bohr–Peierls–Placzek relation, after a 1939 paper [25]. Next, we see one technique that allows us to use all of this to actually obtain a wavefunction.

Parts of the following chapter have appeared on the previously published article listed below. I have permission from my co-authors/publishers to use the work listed below in my dissertation/thesis:

M. E. Pereira and A. G. M. Schmidt, Few-Body Systems **63**, 25 (2022)

Chapter 3

The $\mathcal{N}$-dimensional Green's Function of a free particle

In order to formulate a scattering problem in terms of the Lippmann–Schwinger equation we need to know the free particle Green's function. Additionally, our technique to solve the referred integral equation relies on two facts: (i) the possibility of expanding the Green's function in terms of some suitable eigenfunctions. Such infinite series was proved to be uniformly convergent. And, (ii) using a boundary-wall potential, which we generalize to $N-$dimensions. In this chapter we calculate thoroughly the free Green's function for the Helmholtz equation that has a radial-like coordinate in generalized curvilinear coordinates.

3.1 Separability of Helmholtz's equation in $\mathcal{N}$ generalized curvilinear coordinates

Moon and Spencer [26,27] showed that in three dimensions, Helmholtz's equation can be separated in 11 coordinate systems. In all those cases, Helmholtz's equation takes the form

$$\left\{\frac{1}{h_1h_2h_3}\left[\frac{\partial}{\partial\xi_1}\left(\frac{h_2h_3}{h_1}\frac{\partial}{\partial\xi_1}\right)+\frac{\partial}{\partial\xi_2}\left(\frac{h_1h_3}{h_2}\frac{\partial}{\partial\xi_2}\right)+\frac{\partial}{\partial\xi_3}\left(\frac{h_1h_2}{h_3}\frac{\partial}{\partial\xi_3}\right)\right]+k^2\right\}\psi=0. \tag{3.1}$$

Here, $\boldsymbol{\xi}$ is a three-dimensional vector in any coordinate system, and h_i are the *scale factors* [40]. The scale factors can be interpreted as the unit vectors in any coordinate system, which look like

$$h_i=\frac{\partial\boldsymbol{\xi}}{\partial\xi_i}\Bigg/\left|\frac{\partial\boldsymbol{\xi}}{\partial\xi_i}\right|=\frac{\partial\hat{\boldsymbol{\xi}}}{\partial\xi_i} \tag{3.2}$$

Therefore, the metric tensor associated with this coordinate system must have a diagonal matrix representation if the system is orthogonal. Since this is the case we are interested in, our metric tensor, whose components are

$$g_{ij} = \frac{\partial \hat{\boldsymbol{\xi}}}{\partial \xi_i} \cdot \frac{\partial \hat{\boldsymbol{\xi}}}{\partial \xi_j}, \tag{3.3}$$

becomes, in fact,

$$g_{ii} = \frac{\partial \hat{\boldsymbol{\xi}}}{\partial \xi_i} \cdot \frac{\partial \hat{\boldsymbol{\xi}}}{\partial \xi_i} = g_{ij}\delta_{ij} = \left(\frac{\partial \hat{\boldsymbol{\xi}}}{\partial \xi_i}\right)^2 = h_i^2. \tag{3.4}$$

Then, it is trivial to calculate the determinant of such a matrix, and we use the simplified notation

$$\det(g) = g = h_1^2 h_2^2 h_3^2. \tag{3.5}$$

Equation (3.1) transmutes to

$$\left[\frac{1}{\sqrt{g}} \sum_{i=1}^{3} \frac{\partial}{\partial \xi_i} \left(\frac{\sqrt{g}}{g_{ii}} \frac{\partial}{\partial \xi_i}\right) + k^2\right] \psi = 0. \tag{3.6}$$

If we consider more than three dimensions, then the number of terms in 3.5) increases. Let us consider the case of $\mathcal{N}$ dimensions. Since we want the system to be orthogonal, (3.4) still holds, and the determinant of the metric tensor (3.5) gets a natural extension. Now, it is

$$\det(g) = g = h_1^2 h_2^2 h_3^2 \dots h_{\mathcal{N}}^2 = \prod_{i=1}^{\mathcal{N}} h_i^2. \tag{3.7}$$

Helmholtz's equation (3.1) now in $\mathcal{N}$ dimensions, becomes

$$\left[\frac{1}{\sqrt{g}} \sum_{i=1}^{\mathcal{N}} \frac{\partial}{\partial \xi_i} \left(\frac{\sqrt{g}}{g_{ii}} \frac{\partial}{\partial \xi_i}\right) + k^2\right] \psi = 0. \tag{3.8}$$

It is identical to (3.6) except for the limits in the summation. Assume that

$$\psi(\xi_1, \dots, \xi_{\mathcal{N}}) = U_1(\xi_1) \dots U_{\mathcal{N}}(\xi_{\mathcal{N}}).$$

This brings about

$$\frac{1}{\sqrt{g}} \sum_{i=1}^{\mathcal{N}} \frac{\partial}{\partial \xi_i} \left\{\frac{\sqrt{g}}{g_{ii}} \frac{\partial}{\partial \xi_i} \left[U_1(\xi_1) \dots U_{\mathcal{N}}(\xi_{\mathcal{N}})\right]\right\} + k^2 U_1(\xi_1) \dots U_{\mathcal{N}}(\xi_{\mathcal{N}}) = 0,$$

which can be simplified to give

$$\sum_{i=1}^{\mathcal{N}} \frac{1}{U_i(\xi_i)} \frac{\partial}{\partial \xi_i} \left[\frac{\sqrt{g}}{g_{ii}} \frac{dU_i(\xi_i)}{d\xi_i} \right] + k^2 \sqrt{g} = 0. \tag{3.9}$$

For this equation to be separable, we propose that

$$\begin{cases} \frac{\sqrt{g}}{g_{11}} & = f_1(\xi_1) F_1(\xi_2, \dots, \xi_{\mathcal{N}}) \\ \quad \vdots & \\ \frac{\sqrt{g}}{g_{\mathcal{N}\mathcal{N}}} & = f_{\mathcal{N}}(\xi_{\mathcal{N}}) F_{\mathcal{N}}(\xi_1, \dots, \xi_{\mathcal{N}-1}) \end{cases}, \tag{3.10}$$

where the functions F_i are functions of all the coordinates except ξ_i. Now, equation (3.9) gives rise to

$$\sum_{i=1}^{\mathcal{N}} \frac{F_i(\xi_j)}{U_i(\xi_i)} \frac{d}{d\xi_i} \left(f_i \frac{dU_i(\xi_i)}{d\xi_i} \right) + k^2 \sqrt{g} = 0, \tag{3.11}$$

with $i \neq j$. We seem to be only twisting and manipulating the equations without getting in any place new. However, notice that the functions F_i, because they come from the metric tensor, must depend exclusively on the geometry of the coordinate system. The functions U_i depend also on the boundary conditions imposed by each problem and they may depend on the eigenvalues (for instance, $Y_l^m(\theta, \phi)$ can be taken as a function of the indexes ℓ and m, which are directly connected to its eigenvalues). The eigenvalues α_i, on their turn, depend on the boundary conditions. But how do they look like? Since we do not know this answer beforehand, let us make an assumption: $\alpha_1 = k^2$, and the rest of them can be worked on later, with the condition that they might vary smoothly. This condition gives us the freedom to take a derivative of equation (3.11) taking each α_i as a variable. Opening the summation in equation (3.11) results in

$$\frac{F_1}{U_1} \left(\frac{df_1}{d\xi_1} \frac{dU_1(\xi_1)}{d\xi_1} + f_1 \frac{d^2 U_1(\xi_1)}{d\xi_1^2} \right) + \frac{F_2}{U_2} \left(\frac{df_2}{d\xi_2} \frac{dU_2(\xi_2)}{d\xi_2} + f_2 \frac{d^2 U_2(\xi_2)}{d\xi_2^2} \right) + \ldots + k^2 \sqrt{g} = 0.$$

Proceeding to taking the derivatives with respect to α_i, we find:

To α_1,

$$F_1 \frac{\partial}{\partial \alpha_1} \left[\frac{1}{U_1} \left(\frac{df_1}{d\xi_1} \frac{dU_1}{d\xi_1} + f_1 \frac{d^2 U_1}{d\xi_1^2} \right) \right] + F_2 \frac{\partial}{\partial \alpha_1} \left[\frac{1}{U_2} \left(\frac{df_2}{d\xi_2} \frac{dU_2}{d\xi_2} + f_2 \frac{d^2 U_2}{d\xi_2^2} \right) \right] + \ldots + \sqrt{g} = 0.$$

We find a similar equation for α_2,

$$F_1 \frac{\partial}{\partial \alpha_2} \left[\frac{1}{U_1} \left(\frac{df_1}{d\xi_1} \frac{dU_1}{d\xi_1} + f_1 \frac{d^2 U_1}{d\xi_1^2} \right) \right] + F_2 \frac{\partial}{\partial \alpha_2} \left[\frac{1}{U_2} \left(\frac{df_2}{d\xi_2} \frac{dU_2}{d\xi_2} + f_2 \frac{d^2 U_2}{d\xi_2^2} \right) \right] + \ldots + 0 = 0.$$

The last term on the left hand side is zero because $k^2 = \alpha_1$ and $\sqrt{g}$, as we've seen, only depends on the geometry of the system, not the boundary conditions of each problem. Therefore, one can take $\mathcal{N}$ derivatives, and they will result in a system of equations, namely

$$\begin{aligned} f_1 F_1 \Phi_{11}(\xi_1) + f_2 F_2 \Phi_{21}(\xi_2) + \ldots + f_{\mathcal{N}} F_{\mathcal{N}} \Phi_{\mathcal{N}1}(\xi_{\mathcal{N}}) &= \sqrt{g} \\ f_1 F_1 \Phi_{12}(\xi_1) + f_2 F_2 \Phi_{22}(\xi_2) + \ldots + f_{\mathcal{N}} F_{\mathcal{N}} \Phi_{\mathcal{N}2}(\xi_{\mathcal{N}}) &= 0 \\ &\vdots \\ f_1 F_1 \Phi_{1\mathcal{N}}(\xi_1) + f_2 F_2 \Phi_{2\mathcal{N}}(\xi_2) + \ldots + f_{\mathcal{N}} F_{\mathcal{N}} \Phi_{\mathcal{N}\mathcal{N}}(\xi_{\mathcal{N}}) &= 0. \end{aligned} \tag{3.12}$$

Here, we defined

$$\Phi_{ij}(\xi_i) = \frac{-1}{f_i(\xi_i)} \frac{\partial}{\partial \alpha_j} \left[\frac{1}{U_i} \frac{d}{d\xi_i} \left(f_i \frac{dU_i(\xi_i)}{d\xi_i} \right) \right], \tag{3.13}$$

and using this Φ_{ij} one may write equation (3.11) as

$$\sum_{i=1}^{\mathcal{N}} f_i F_i \Phi_{ij} + k^2 \sqrt{g} = 0. \tag{3.14}$$

Equation (3.12) is easily solved by Cramer's method[1]. For that, we define a new matrix, called *Stäckel matrix*:

$$\mathcal{S} = \begin{pmatrix} \Phi_{11} & \Phi_{12} & \cdots & \Phi_{1\mathcal{N}} \\ \Phi_{21} & \Phi_{22} & \cdots & \Phi_{2\mathcal{N}} \\ \vdots & \vdots & \ddots & \vdots \\ \Phi_{\mathcal{N}1} & \Phi_{\mathcal{N}2} & \cdots & \Phi_{\mathcal{N}\mathcal{N}} \end{pmatrix} \tag{3.15}$$

If we want a solution, we need to have $\det(\mathcal{S}) = \mathcal{S} \neq 0$. Thus, we have defined the *Stäckel determinant*[2], and with it, we write the solution for (3.12) as

$$f_i F_i = \frac{\sqrt{g}}{\mathcal{S}} M_{i1}, \tag{3.16}$$

where M_{i1} is the co-factor of the element Φ_{i1}. When we juxtapose (3.16) and (3.10), it is inevitable to conclude that

[1] If one needs to remind oneself about the Cramer's method, also known as Cramer's rule, one may read, for instance, David Poole's *Linear Algebra: A Modern Introduction*, 2nd ed., Brooks Cole (2005).

[2] For more insight into the Stäckel matrices, see [26, 27].

$$\frac{\sqrt{g}}{g_{ii}} = \frac{\sqrt{g}}{\mathcal{S}} M_{i1} \Rightarrow \boxed{g_{ii} = \frac{\mathcal{S}}{M_{i1}}}. \tag{3.17}$$

This is the first separability condition, and of course, there is a second one. On the grounds of iteration of equation (3.16), it results

$$\frac{\sqrt{g}}{g_{ii}} = \frac{f_1 F_1}{M_{11}} = \frac{f_2 F_2}{M_{22}} = \ldots = \frac{f_{\mathcal{N}} F_{\mathcal{N}}}{M_{\mathcal{N}\mathcal{N}}},$$

which is true only if

$$\boxed{\frac{\sqrt{g}}{\mathcal{S}} = \prod_{i=1}^{\mathcal{N}} f_i(\xi_i)}. \tag{3.18}$$

Equation (3.18) is the *Robertson condition*, and is otherwise known as the second separability condition [41]. This condition is reasonable, due to the fact that $\sqrt{g}$ is already a product.

Conditions (3.17) and (3.18) are necessary for Helmholtz equation (3.9) to be separable. Are they sufficient, though?

According to them,

$$\frac{\sqrt{g}}{g_{ii}} = \left(\prod_{i=1}^{\mathcal{N}} f_i(\xi_i) \right) M_{i1}. \tag{3.19}$$

Substituting this into (3.9), one faces

$$\sum_{i=1}^{\mathcal{N}} \frac{1}{U_i(\xi_i)} \frac{\partial}{\partial \xi_i} \left[M_{i1} \prod_{i=1}^{\mathcal{N}} f_i(\xi_i) \frac{dU_i}{d\xi_i} \right] + k^2 g_{ii} M_{i1} \prod_{i=1}^{\mathcal{N}} f_i(\xi_i) g_{ii} = 0.$$

Hence, upon simplification,

$$\sum_{i=1}^{\mathcal{N}} \frac{M_{i1} \prod_{j=1}^{\mathcal{N}} f_j(\xi_j)/f_i(\xi_i)}{U_i(\xi_i)} \frac{\partial}{\partial \xi_i} \left[f_i \frac{dU_i}{d\xi_i} \right] + k^2 g_{ii} M_{i1} \prod_{i=1}^{\mathcal{N}} f_i(\xi_i) g_{ii} = 0,$$

whereupon, after dividing by $\sqrt{g}$,

$$\sum_{i=1}^{\mathcal{N}} \frac{1}{g_{ii} f_i U_i} \frac{\partial}{\partial \xi_i} \left[f_i \frac{dU_i}{d\xi_i} \right] + k^2 = 0. \tag{3.20}$$

What to make of this? Recall that the determinant of Stäckel's matrix can be written as

$$\mathcal{S} = \sum_{i=1}^{\mathcal{N}} \Phi_{i1} M_{i1}, \tag{3.21}$$

and as a consequence,

$$1 = \sum_{i=1}^{\mathcal{N}} \Phi_{i1} \frac{M_{i1}}{\mathcal{S}} = \sum_{i=1}^{\mathcal{N}} \frac{\Phi_{i1}}{g_{ii}}. \tag{3.22}$$

If that is so, one can make a naive linear combination, as to write

$$\alpha_1 = \alpha_1 \sum_{i=1}^{\mathcal{N}} \frac{\Phi_{i1}}{g_{ii}} + \alpha_2 \sum_{i=1}^{\mathcal{N}} \frac{\Phi_{i2}}{g_{ii}} + \ldots + \alpha_{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} \frac{\Phi_{i\mathcal{N}}}{g_{ii}}, \tag{3.23}$$

given that

$$\sum_{i=1}^{\mathcal{N}} \Phi_{kj} M_{km} = \mathcal{S} \delta_{jm}.$$

Bearing that in mind, it transpires from equations (3.20) that

$$\sum_{i=1}^{\mathcal{N}} \frac{1}{g_{ii}} \left[\frac{1}{f_i U_i} \frac{d}{d\xi_i} \left(f_i \frac{dU_i}{d\xi_i} \right) + \sum_{j=1}^{\mathcal{N}} \alpha_j \Phi_{ij}(\xi_i) \right] = 0.$$

Insofar as it must be valid for every g_{ii}, we attain

$$\boxed{\frac{1}{f_i U_i} \frac{d}{d\xi_i} \left(f_i \frac{dU_i}{d\xi_i} \right) + \sum_{j=1}^{\mathcal{N}} \alpha_j \Phi_{ij}(\xi_i) = 0}, \tag{3.24}$$

which is the Helmholtz equation, completely separated [26, 27, 41].

3.2 The Green's Function for Helmholtz's Equation in generalized curvilinear $\mathcal{N}$-dimensional coordinates

The $\mathcal{N}$-dimensional Helmholtz's equation can be separated, resulting in equation (3.24). In what comes next, we will work with a set of rotational coordinate systems. What this means is that our results will be valid for any $\mathcal{N}$ dimensional extension of those original 11 coordinate systems developed by Moon and Spencer, in which Helmholtz equation is completely separable. With that in mind, let us determine ξ_1 to be used as a radial-like coordinate, and assume that there exists a function $W_p(\xi_2, \xi_3, \ldots, \xi_{\mathcal{N}})$, subject to

$$W_p(\xi_2, \xi_3, \ldots, \xi_{\mathcal{N}}) = U_{2m_2}(\xi_2) U_{3m_3}(\xi_3) \cdots U_{\mathcal{N}m_{\mathcal{N}}}(\xi_{\mathcal{N}}) \ , \tag{3.25}$$

where the m_i index may represent any necessary set of indexes. We demand that these functions $W_p(\xi_2, \xi_3, \ldots, \xi_{\mathcal{N}})$ obey the following orthonormality condition:

$$\int \cdots \int W_q^*(\xi_2, \xi_3, \ldots, \xi_{\mathcal{N}}) W_p(\xi_2, \xi_3, \ldots, \xi_{\mathcal{N}}) \rho(\xi_2, \xi_3, \ldots, \xi_{\mathcal{N}}) d\xi_2 d\xi_3 \cdots d\xi_{\mathcal{N}} = \delta_{pq} \ , \tag{3.26}$$

where ρ is a weight function, and in which the indexes p and q can represent any necessary set of indexes that we may need. Since we have an orthonormal basis, we can write the Green's function in the form

$$G^{(\mathcal{N})}(\vec{\xi}|\vec{\xi}') = \sum_q U_{1q}(\xi_1|\xi_1') B_q(\xi_2', \xi_3', \ldots, \xi_{\mathcal{N}}') W_q(\xi_2, \xi_3, \ldots, \xi_{\mathcal{N}}) \ , \tag{3.27}$$

where the index q again represents any set of necessary indexes and the functions B_q are functions that depend upon the angles in the source vector ξ'. We will proceed the calculation of the B_q functions first, as follows. The Green's function obeys

$$\sum_{i=1}^{\mathcal{N}} \frac{M_{i1}}{f_i S} \frac{\partial}{\partial \xi_i} \left(f_i \frac{\partial G}{\partial \xi_i} \right) + k^2 G = -\frac{\delta^{\mathcal{N}}(\vec{\xi} - \vec{\xi}')}{h_1 h_2 \cdots h_{\mathcal{N}}} \ . \tag{3.28}$$

According to equation (3.24), the following equallity holds

$$\frac{1}{f_i U_i} \frac{d}{d\xi_i} \left(f_i \frac{dU_i}{d\xi_i} \right) = -\sum_{j=1}^{\mathcal{N}} \alpha_j \Phi_{ij}(\xi_i), \tag{3.29}$$

so if we are interested in finding the B_q functions, we want to investigate the action of the Helmholtz's operator in the W_q functions. Therefore, using the definition (3.25), equation (3.24) becomes

$$\sum_{i=2}^{\mathcal{N}} \frac{1}{f_i} \frac{\partial}{\partial \xi_i} \left(f_i \frac{\partial W_q}{\partial \xi_i} \right) = -W_q \sum_{\substack{j=1 \\ i=2}}^{\mathcal{N}} \alpha_j \Phi_{ij}(\xi_i) \ , \tag{3.30}$$

so we need to figure out what exactly the left hand side (l.h.s) of equation (3.30) does to our functions W_q. To do that, we divide equation (3.30) by $g_{ii} = \frac{\mathcal{S}}{M_{i1}}$, and remembering that

$$\begin{aligned} \mathcal{S}\delta_{1m} &= \sum_{\ell m} M_{\ell m} \Phi_{\ell m} = M_{1m}\Phi_{1m} + M_{2m}\Phi_{2m} + \cdots + M_{\mathcal{N}m}\Phi_{\mathcal{N}m} \\ &= M_{1m}\Phi_{1m} + \sum_{\ell=2}^{\mathcal{N}} M_{\ell m}\Phi_{\ell m} \ , \end{aligned}$$

we conclude that

$$\mathcal{S}\delta_{1m} - M_{1m}\Phi_{1m} = \sum_{\ell=2}^{\mathcal{N}} M_{\ell m}\Phi_{\ell m} \tag{3.31}$$

and we have

$$\sum_{i=2}^{\mathcal{N}} \frac{M_{i1}}{\mathcal{S}} \frac{1}{f_i} \frac{\partial}{\partial \xi_i} \left(f_i \frac{\partial W_q}{\partial \xi_i} \right) = -W_q \sum_{\substack{j=1 \\ i=2}}^{\mathcal{N}} \frac{M_{i1}}{\mathcal{S}} \alpha_{jq} \Phi_{ij}(\xi_i)$$
$$= -\frac{W_q}{\mathcal{S}} \sum_{j=1}^{\mathcal{N}} \alpha_{jq} \sum_{i=2}^{\mathcal{N}} M_{i1} \Phi_{ij}(\xi_i) = -\frac{W_q}{\mathcal{S}} \sum_{j=1}^{\mathcal{N}} \alpha_{jq} \left[\mathcal{S} \delta_{1m} - M_{1m} \Phi_{1m} \right]$$
$$= -\frac{\alpha_{1q} \mathcal{S} W_q}{\mathcal{S}} + \frac{M_{11}}{\mathcal{S}} W_q \sum_{j=1}^{\mathcal{N}} \alpha_{jq} \Phi_{1j} = -k^2 W_q + \frac{M_{11}}{\mathcal{S}} W_q \sum_{j=1}^{\mathcal{N}} \alpha_{jq} \Phi_{1j} \ . \tag{3.32}$$

Now, we multiply equation (3.32) by $U_{1q} B_q$ and sum under q, obtaining the result of applying Helmholtz's operator on the W_q functions:

$$\sum_{i=2}^{\mathcal{N}} \frac{M_{i1}}{\mathcal{S}} \frac{1}{f_i} \frac{\partial}{\partial \xi_i} \left[f_i \frac{\partial}{\partial \xi_i} \left(\sum_q U_{1q} B_q W_q \right) \right] = -k^2 \sum_q U_{1q} B_q W_q$$
$$+ \frac{M_{11}}{\mathcal{S}} \sum_{j=1}^{\mathcal{N}} \Phi_{1j} \left(\sum_q \alpha_{jq} U_{1q} B_q W_q \right) \ . \tag{3.33}$$

To see how equation (3.33) helps us getting our function B_q, we substitute equation (3.27) into (3.28), getting

$$\sum_q B_q W_q \frac{M_{11}}{\mathcal{S}} \left[\frac{1}{f_1} \frac{d}{d\xi_1} \left(f_1 \frac{dU_{1q}}{d\xi_1} \right) \right] + \sum_{i=2}^{\mathcal{N}} \frac{M_{i1}}{\mathcal{S}} \frac{1}{f_i} \frac{\partial}{\partial \xi_i} \left[f_i \frac{\partial}{\partial \xi_i} \left(\sum_q U_{1q} B_q W_q \right) \right]$$
$$+ k^2 \sum_q U_{1q} B_q W_q = -\frac{\delta^{\mathcal{N}}(\vec{\xi} - \vec{\xi}')}{h_1 h_2 \cdots h_{\mathcal{N}}} \ . \tag{3.34}$$

We do not despair, because noting that the second and third terms of the l.h.s. of equation (3.34) are just equation (3.33), we realize that what we actually have is

$$\sum_q B_q W_q \frac{M_{11}}{\mathcal{S}} \left[\frac{1}{f_1} \frac{d}{d\xi_1} \left(f_1 \frac{dU_{1q}}{d\xi_1} \right) + U_{1q} \sum_{j=1}^{\mathcal{N}} \alpha_{jq} \Phi_{1j} \right] = -\frac{\delta^{\mathcal{N}}(\vec{\xi} - \vec{\xi}')}{h_1 h_2 \cdots h_{\mathcal{N}}} \ , \tag{3.35}$$

and the expression between brackets is just an equation of the first coordinate. Therefore, if we rewrite the Stäckel determinant using the first and second separability conditions

$$g_{ii} = \frac{\mathcal{S}}{M_{ii}}$$
$$\frac{g}{\mathcal{S}} = f_1(\xi_1) f_2(\xi_2) \cdots f_{\mathcal{N}}(\xi_{\mathcal{N}}) \ ,$$

we will have

$$\frac{M_{11}}{\mathcal{S}} = \frac{M_{11}(\xi_2, \ldots \xi_{\mathcal{N}}) f_1(\xi_1) f_2(\xi_2) \cdots f_{\mathcal{N}}(\xi_{\mathcal{N}})}{h_1 h_2 \cdots h_{\mathcal{N}}} \ , \tag{3.36}$$

so upon using expression (3.36) and the orthogonality condition (3.26) in equation (3.35), we find

$$D_{\xi_1}\left[U_{1q}\right] B_q(\xi_2', \xi_3', \ldots, \xi_{\mathcal{N}}') = -\frac{\delta(\xi_1 - \xi_1')}{f_1(\xi_1)} \frac{W_q^*(\xi_2', \xi_3', \ldots, \xi_{\mathcal{N}}') \rho(\xi_2', \xi_3', \ldots, \xi_{\mathcal{N}}')}{M_{11}(\xi_1', \xi_2', \ldots \xi_{\mathcal{N}}') f_2(\xi_2') \cdots f_{\mathcal{N}}(\xi_{\mathcal{N}}')} \ , \tag{3.37}$$

where

$$D_{\xi_1}\left[U_{1q}\right] = \frac{1}{f_1} \frac{d}{d\xi_1}\left(f_1 \frac{dU_{1q}}{d\xi_1}\right) + U_{1q} \sum_{j=1}^{\mathcal{N}} \alpha_{jq} \Phi_{1j} \ .$$

If we compare the quantities in both sides of equation (3.37), we will realize that

$$\boxed{B_q(\xi_2', \xi_3', \ldots, \xi_{\mathcal{N}}') = \frac{W_q^*(\xi_2', \xi_3', \ldots, \xi_{\mathcal{N}}') \rho(\xi_2', \xi_3', \ldots, \xi_{\mathcal{N}}')}{M_{11}(\xi_2', \ldots \xi_{\mathcal{N}}') f_2(\xi_2') \cdots f_{\mathcal{N}}(\xi_{\mathcal{N}}')}} \ . \tag{3.38}$$

Now there is only the equation relative to the ξ_1 coordinate, that is,

$$\frac{1}{f_1} \frac{d}{d\xi_1}\left(f_1 \frac{dU_{1q}}{d\xi_1}\right) + U_{1q} \sum_{j=1}^{\mathcal{N}} \alpha_{jq} \Phi_{1j} = -\frac{\delta(\xi_1 - \xi_1')}{f_1(\xi_1)} \ , \tag{3.39}$$

but that is just a Helmholtz's equation in one dimension for a Green's Function. Hence, if the solutions for the associated homogeneous differential equation are $y_{1q}(\xi_1)$ and $y_{2q}(\xi_2)$, we know that [40]

$$U_{1q}(\xi_1|\xi_1') = -\frac{y_{1q}(\xi_{1<}) y_{2q}(\xi_{1>})}{\mathcal{W}(y_{1q}(\xi_1), y_{2q}(\xi_1)) f_1(\xi_1)\Big|_{\xi_1'}} \ , \tag{3.40}$$

where $\xi_> = \max(\xi, \xi')$ and $\xi_< = \min(\xi, \xi')$. Finally, using equation (3.40) and the two separability conditions, is easy to see that

$$\boxed{G^{(\mathcal{N})}(\vec{\xi}|\vec{\xi}') = -\frac{(h_1(\xi_i'))^2}{\sqrt{g(\xi_i')}} \rho(\xi_j') \sum_q \frac{y_{1q}(\xi_{1<}) y_{2q}(\xi_{1>})}{\mathcal{W}(y_{1q}(\xi_1), y_{2q}(\xi_1))\Big|_{\xi_1'}} W_q^*(\xi_j') W_q(\xi_j)} \ , \tag{3.41}$$

this is the Green's function for the Helmholtz equation written in generalized curvilinear coordinates.

3.3 An expansion for Green's Function in hyper-spherical coordinates

We have yet to find the necessary functions in order to make use of equation (3.41). In the next pages, we will solve this conundrum in two different ways. First, we will *construct* a solution that solves [43] the free Helmholtz equation completely, using harmonic polynomials. Second, we will calculate an unambiguous differential equation, that will left the reader no doubt about the validity of the first solution.

3.3.1 The construction method

Consider Helmholtz's equation for a function ψ

$$\nabla^2\psi + k^2\psi = 0 \ , \tag{3.42}$$

where we made $\vec{r} \neq \vec{r}\,'$. Of course, when $k = 0$, we have Laplace's differential equation

$$\nabla^2\psi = 0 \ , \tag{3.43}$$

so we can postulate that solutions of Laplace's differential equation relate to solutions of Helmholtz's equation. Using $\mathcal{N}$-hyperspherical coordinates, we see that equation (3.42) reads

$$\begin{aligned}
&\frac{1}{r^{\mathcal{N}-1}}\frac{\partial}{\partial r}\left(r^{\mathcal{N}-1}\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin^{\mathcal{N}-2}\theta_1}\frac{\partial}{\partial\theta_1}\left(\sin^{\mathcal{N}-2}\theta_1\frac{\partial\psi}{\partial\theta_1}\right) + \dots \\
&+\frac{1}{r^2\sin^2\theta_1\cdots\sin^2\theta_{\mathcal{N}-3}\sin\theta_{\mathcal{N}-2}}\frac{\partial}{\partial\theta_{\mathcal{N}-2}}\left(\sin\theta_{\mathcal{N}-2}\frac{\partial\psi}{\partial\theta_{\mathcal{N}-2}}\right) \\
&+\frac{1}{r^2\sin^2\theta_1\cdots\sin^2\theta_{\mathcal{N}-3}\sin^2\theta_{\mathcal{N}-2}}\frac{\partial^2\psi}{\partial\phi^2} + k^2\psi = 0 \ .
\end{aligned} \tag{3.44}$$

Let us identify $\Lambda^2_{(\mathcal{N})}$ as the *generalized angular momentum operator*, which is

$$\begin{aligned}
-\Lambda^2_{(\mathcal{N})} =&\frac{1}{\sin^{\mathcal{N}-2}\theta_1}\frac{\partial}{\partial\theta_1}\left(\sin^{\mathcal{N}-2}\theta_1\frac{\partial}{\partial\theta_1}\right) + \dots \\
&+\frac{1}{\sin^2\theta_1\cdots\sin^2\theta_{\mathcal{N}-3}\sin\theta_{\mathcal{N}-2}}\frac{\partial}{\partial\theta_{\mathcal{N}-2}}\left(\sin\theta_{\mathcal{N}-2}\frac{\partial}{\partial\theta_{\mathcal{N}-2}}\right) \\
&+\frac{1}{\sin^2\theta_1\cdots\sin^2\theta_{\mathcal{N}-3}\sin^2\theta_{\mathcal{N}-2}}\frac{\partial^2}{\partial\phi^2} \ ,
\end{aligned} \tag{3.45}$$

such that the Helmholtz's equation will look like

$$\left[\frac{1}{r^{\mathcal{N}-1}}\frac{\partial}{\partial r}\left(r^{\mathcal{N}-1}\frac{\partial}{\partial r}\right)+k^2-\frac{\Lambda^2_{(\mathcal{N})}}{r^2}\right]\psi=0 \tag{3.46}$$

and Laplace's equation will be, setting $k=0$,

$$\left[\frac{1}{r^{\mathcal{N}-1}}\frac{\partial}{\partial r}\left(r^{\mathcal{N}-1}\frac{\partial}{\partial r}\right)-\frac{\Lambda^2_{(\mathcal{N})}}{r^2}\right]\psi=0\ . \tag{3.47}$$

It is easy to see that the k^2 makes the radial part of equations (3.46) and (3.47) to be different, while the generalized angular momentum operator remains the same. Now, we know nothing about the solutions of equation (3.46), but we do know the fundamental solution of the Green's function analogue of equation (3.47),

$$\nabla^2\psi=\left[\frac{1}{r^{\mathcal{N}-1}}\frac{\partial}{\partial r}\left(r^{\mathcal{N}-1}\frac{\partial}{\partial r}\right)-\frac{\Lambda^2_{(\mathcal{N})}}{r^2}\right]\psi=-\delta\left(\vec{x}-\vec{x}'\right) \tag{3.48}$$

which is simply

$$\psi(\mathbf{r},\mathbf{r}')=\frac{1}{|\mathbf{r}-\mathbf{r}'|^{\mathcal{N}-2}}=\frac{1}{r_>^{\mathcal{N}-2}}\sum_{\lambda=0}^{\infty}\left(\frac{r_<}{r_>}\right)^{\lambda}C^{\alpha}_{\lambda}(\mathbf{u}\cdot\mathbf{u}')\ , \tag{3.49}$$

that is, the solution of Laplace's equation in $\mathcal{N}$-hyperspherical coordinates is proportional to a linear combination of Gegenbauer polynomials, where we introduced the unit vectors

$$\mathbf{u}\equiv\frac{1}{r}\left(r_1,r_2,\ldots,r_{\mathcal{N}}\right)\equiv\frac{\mathbf{r}}{r}$$
$$\mathbf{u}'\equiv\frac{1}{r'}\left(r'_1,r'_2,\ldots,r'_{\mathcal{N}}\right)\equiv\frac{\mathbf{r}'}{r'}$$

and

$$2\alpha=\mathcal{N}-2 \tag{3.50}$$

So we have our solution, which completely solves equation (3.48). Now one may ask, 'how does it helps solving equation (3.46)?', to which a good answer would be to use equation (3.49) with $r<r'$, such that

$$\psi(\mathbf{r},\mathbf{r}')=\frac{1}{|\mathbf{r}-\mathbf{r}'|^{\mathcal{N}-2}}=\frac{1}{r'^{\mathcal{N}-2}}\sum_{\lambda=0}^{\infty}\left(\frac{r}{r'}\right)^{\lambda}C^{\alpha}_{\lambda}(\mathbf{u}\cdot\mathbf{u}')\ . \tag{3.51}$$

Since this is a solution of (3.47) because $r<r'$, we substitute (3.51) into that equation, to get

$$\nabla^2 \left(\frac{1}{|\mathbf{r} - \mathbf{r}'|^{\mathcal{N}-2}} \right) = \sum_{\lambda=0}^{\infty} \frac{1}{r'^{\lambda+\mathcal{N}-2}} \nabla^2 \left[r^\lambda C_\lambda^\alpha(\mathbf{u} \cdot \mathbf{u}') \right] = 0 \ . \tag{3.52}$$

Considering that r' is not zero, each term of the sum must be zero, but

$$\nabla^2 \left[r^\lambda C_\lambda^\alpha(\mathbf{u} \cdot \mathbf{u}') \right] = \left[\frac{1}{r^{\mathcal{N}-1}} \frac{\partial}{\partial r} \left(r^{\mathcal{N}-1} \frac{\partial}{\partial r} \right) - \frac{\Lambda^2_{(\mathcal{N})}}{r^2} \right] r^\lambda C_\lambda^\alpha(\mathbf{u} \cdot \mathbf{u}') \tag{3.53}$$

and

$$\frac{1}{r^{\mathcal{N}-1}} \frac{\partial}{\partial r} \left(r^{\mathcal{N}-1} \frac{\partial}{\partial r} \right) r^\lambda = \lambda(\lambda + \mathcal{N} - 2) r^{\lambda-2} \tag{3.54}$$

such that

$$\left[\Lambda^2_{(\mathcal{N})} - \lambda(\lambda + \mathcal{N} - 2) \right] C_\lambda^\alpha(\mathbf{u} \cdot \mathbf{u}') = 0 \ . \tag{3.55}$$

What this means is that the Gegenbauer's polynomials are eigenfunctions of the generalized angular momentum operator, with eigenvalues $\lambda(\lambda + \mathcal{N} - 2)$. We introduce the *hyperspherical harmonics* Y

$$C_\lambda^\alpha(\mathbf{u} \cdot \mathbf{u}') = \sum_\mu a_{\lambda,\mu}(\mathbf{u}) Y_{\lambda,\mu}(\mathbf{u}') \ , \tag{3.56}$$

with $a(\mathbf{u})$ being the coefficients of the expansion. The reason why we can write the Gegenbauer's polynomial this way is explained in detail by Avery and Avery [43]. The polynomial is a function of a scalar quantity, so it must be invariant under rotations of the coordinate system, so

$$R C_\lambda^\alpha(\mathbf{u} \cdot \mathbf{u}') = C_\lambda^\alpha(\mathbf{u} \cdot \mathbf{u}') \tag{3.57}$$

and also

$$\sum_\mu a_{\lambda,\mu}(R^{-1}\mathbf{u}) Y_{\lambda,\mu}(R^{-1}\mathbf{u}') = \sum_\mu a_{\lambda,\mu}(\mathbf{u}) Y_{\lambda,\mu}(\mathbf{u}') \ , \tag{3.58}$$

where R is, clearly, the rotation matrix. Writing the hyperspherical harmonic as

$$Y_{\lambda,\mu}(R^{-1}\mathbf{u}') = \sum_{\mu'} Y_{\lambda,\mu'}(\mathbf{u}') D^\lambda_{\mu',\mu}(R) \tag{3.59}$$

and imposing onto the hyperspherical harmonics to be orthogonal, the transformation matrix must be unitary, so

$$\sum_{\mu} D^{\lambda *}_{\mu'',\mu}(R) D^{\lambda}_{\mu',\mu}(R) = \delta_{\mu'',\mu'} \ .$$

The coefficients a must then obey the inverse transformation law, in order for C^{α}_{λ} to be invariant. Therefore,

$$a_{\lambda,\mu}(R^{-1}\mathbf{u}) = \sum_{\mu''} a_{\lambda,\mu''}(\mathbf{u}) D^{\lambda *}_{\mu'',\mu}(R). \tag{3.60}$$

Now equations (3.57) and (3.58) are true as we wanted, and to see why, consider

$$\begin{aligned}
RC^{\alpha}_{\lambda}(\mathbf{u}\cdot\mathbf{u}') &= \sum_{\mu} a_{\lambda,\mu}(R^{-1}\mathbf{u}) Y_{\lambda,\mu}(R^{-1}\mathbf{u}') \\
&= \sum_{\mu}\sum_{\mu''} a_{\lambda,\mu''}(\mathbf{u}) D^{\lambda *}_{\mu'',\mu}(R) Y_{\lambda,\mu'}(\mathbf{u}') D^{\lambda}_{\mu',\mu}(R) \\
&= \sum_{\mu''} a_{\lambda,\mu''}(\mathbf{u}) Y_{\lambda,\mu'}(\mathbf{u}') \delta_{\mu'',\mu'} \\
&= \sum_{\mu'} a_{\lambda,\mu'}(\mathbf{u}) Y_{\lambda,\mu'}(\mathbf{u}') \\
&= C^{\alpha}_{\lambda}(\mathbf{u}\cdot\mathbf{u}').
\end{aligned}$$

Taking the complex conjugate of (3.60), we can compare it to (3.59), we see that they obey the same transformation law under rotations, so

$$a_{\lambda,\mu}(\mathbf{u}) = K_{\lambda} Y^{*}_{\lambda,\mu}(\mathbf{u}),$$

where K_{λ} is some constant. Therefore, our Gegenbauer's polynomial is written

$$C^{\alpha}_{\lambda}(\mathbf{u}\cdot\mathbf{u}') = K_{\lambda} \sum_{\mu} Y^{*}_{\lambda,\mu}(\mathbf{u}) Y_{\lambda,\mu}(\mathbf{u}'), \tag{3.61}$$

which is a generalization for the well known addition theorem for the spherical harmonics. Using the orthogonality condition

$$\int d\Omega_{\mathcal{N}} Y^{*}_{p,q}(\mathbf{u}) Y_{p',q'}(\mathbf{u}) = \delta_{p,p'}\delta_{q,q'}, \tag{3.62}$$

we can calculate the constant K_{λ}. Setting $\mathbf{u} = \mathbf{u}'$ in (3.61), integrating this expression over a solid angle $d\Omega$ and using condition (3.62), we get

$$\int d\Omega_{\mathcal{N}}\ C^{\alpha}_{\lambda}(1) = K_{\lambda}\sum_{\mu}\int d\Omega_{\mathcal{N}}\ Y^{*}_{\lambda,\mu}(\mathbf{u})Y_{\lambda,\mu}(\mathbf{u}) = K_{\lambda}\sum_{\mu}\delta_{\lambda,\lambda}\delta_{\mu,\mu} = K_{\lambda}\sum_{\mu}1. \tag{3.63}$$

There's still a need to calculate both the Gegenbauer's polynomial and that summation of ones, which gives us the number of degenerate states. Upon expansion of the series (3.49), we find that the firsts polynomials are

$$\begin{aligned}
C^{\alpha}_{0}(\cos\theta) &= 1\\
C^{\alpha}_{1}(\cos\theta) &= 2\alpha\cos\theta\\
C^{\alpha}_{2}(\cos\theta) &= 2\alpha(\alpha+1)\cos^{2}\theta-\alpha\\
C^{\alpha}_{3}(\cos\theta) &= \frac{4}{3}\alpha(\alpha+1)(\alpha+2)\cos^{3}\theta-2\alpha(\alpha+1)\cos\theta\\
&\vdots
\end{aligned} \tag{3.64}$$

Remembering the definition of the α index at equation (3.50), we have

$$\begin{aligned}
C^{\alpha}_{0}(1) &= 1\\
C^{\alpha}_{1}(1) &= \mathcal{N}-2\\
C^{\alpha}_{2}(1) &= \frac{(\mathcal{N}-1)(\mathcal{N}-2)}{2}\\
C^{\alpha}_{3}(1) &= \frac{\mathcal{N}(\mathcal{N}-1)(\mathcal{N}-2)}{3\cdot 2}\\
&\vdots
\end{aligned}$$

and then finally

$$\begin{aligned}
C^{\alpha}_{0}(1) &= \frac{(0+\mathcal{N}-3)!}{(\mathcal{N}-3)!0!}\\
C^{\alpha}_{1}(1) &= \frac{(1+\mathcal{N}-3)!}{(\mathcal{N}-3)!1!}\\
C^{\alpha}_{2}(1) &= \frac{(2+\mathcal{N}-3)!}{(\mathcal{N}-3)!2!}\\
C^{\alpha}_{3}(1) &= \frac{(3+\mathcal{N}-3)!}{(\mathcal{N}-3)!3!}\\
&\vdots\\
C^{\alpha}_{\lambda}(1) &= \frac{(\lambda+\mathcal{N}-3)!}{(\mathcal{N}-3)!\lambda!}
\end{aligned} \tag{3.65}$$

There is still one piece left, the number of degenerate states. In our coordinate system, we have only one azimuthal angle, so in three dimensions

$$\sum_{\mu} 1 = \sum_{m=-\ell}^{\ell} 1 = 2\ell + 1 \tag{3.66}$$

In four dimensions,

$$\sum_{\mu} 1 = \sum_{\ell=0}^{\lambda} 2\ell + 1 = (\lambda + 1)^2 \tag{3.67}$$

In five dimensions,

$$\sum_{\mu} 1 = \sum_{\ell=0}^{\lambda} (\ell + 1)^2 = \frac{\lambda(\lambda+1)(\lambda+2)}{6} + \lambda(\lambda+1) + \lambda + 1 = \frac{1}{6}\frac{(2\lambda+3)(\lambda+2)!}{\lambda!} \tag{3.68}$$

In six dimensions,

$$\sum_{\mu} 1 = \sum_{\ell=0}^{\lambda} \frac{(2\ell+3)(\ell+2)!}{6\ \ell!} = \frac{1}{12}\frac{(\lambda+2)(\lambda+3)!}{\lambda!} \tag{3.69}$$

In seven dimensions,

$$\sum_{\mu} 1 = \sum_{\ell=0}^{\lambda} \frac{(\ell+2)(\ell+3)!}{12\ \ell!} = \frac{1}{120}\frac{(2\lambda+5)(\lambda+4)!}{\lambda!} \tag{3.70}$$

So in general,

$$\sum_{\mu} 1 = \frac{(\mathcal{N}+2\lambda-2)(\mathcal{N}+\lambda-3)!}{(\mathcal{N}-2)!\lambda!} \tag{3.71}$$

In possession of equations (3.63), (3.65) and (3.71), it is easy to see that

$$\int d\Omega_{\mathcal{N}} \frac{(\lambda+\mathcal{N}-3)!}{(\mathcal{N}-3)!\lambda!} = K_\lambda \frac{(\mathcal{N}+2\lambda-2)(\mathcal{N}+\lambda-3)!}{(\mathcal{N}-2)!\lambda!}$$

The integration over the solid angle $d\Omega_{\mathcal{N}}$ is just the surface area of a hypersphere of $\mathcal{N}-1$ dimensions with unit radius, so

$$\frac{2\pi^{\mathcal{N}/2}}{\Gamma\left(\frac{\mathcal{N}}{2}\right)} \frac{(\lambda+\mathcal{N}-3)!}{(\mathcal{N}-3)!\lambda!} = K_\lambda \frac{(\mathcal{N}+2\lambda-2)(\mathcal{N}+\lambda-3)!}{(\mathcal{N}-2)!\lambda!}$$

that is,

$$K_\lambda = \frac{\mathcal{N}-2}{\mathcal{N}+2\lambda-2} \cdot \frac{2\pi^{\mathcal{N}/2}}{\Gamma\left(\frac{\mathcal{N}}{2}\right)} \tag{3.72}$$

What about normalization of the Gegenbauer's polynomials? It is as follows:

$$\begin{aligned}
&\int d\Omega_s\; C_\lambda^\alpha(\mathbf{u}\cdot\mathbf{u}')C_{\lambda'}^\alpha(\mathbf{u}'\cdot\mathbf{u}'') \\
&= \int d\Omega_{\mathcal{N}} \left[K_\lambda \sum_\mu Y_{\lambda,\mu}^*(\mathbf{u})Y_{\lambda,\mu}(\mathbf{u}')\right]\left[K_{\lambda'} \sum_{\mu'} Y_{\lambda',\mu'}^*(\mathbf{u})Y_{\lambda',\mu'}(\mathbf{u}'')\right] \\
&= \delta_{\lambda,\lambda'} K_\lambda K_{\lambda'} \sum_\mu Y_{\lambda,\mu}^*(\mathbf{u}')Y_{\lambda,\mu}(\mathbf{u}'') \\
&= K_\lambda C_\lambda^\alpha(\mathbf{u}'\cdot\mathbf{u}'')
\end{aligned} \tag{3.73}$$

We just need to set $\mathbf{u}' = \mathbf{u}''$ to get

$$\int d\Omega_{\mathcal{N}}\; \left|C_\lambda^\alpha(\mathbf{u}\cdot\mathbf{u}')\right|^2 = K_\lambda C_\lambda^\alpha(1) \tag{3.74}$$

but as it happens, we have just calculated the K_λ constant. Introducing

$$u_{\mathcal{N}} = \cos\theta \Longleftrightarrow d\Omega_{\mathcal{N}} = (\sin\theta)^{\mathcal{N}-2}\; d\theta d\Omega_{\mathcal{N}-1} \tag{3.75}$$

equation (3.74) becomes

$$\int d\Omega_{\mathcal{N}}\; \left|C_\lambda^\alpha(u_{\mathcal{N}})\right|^2 = \int d\Omega_{\mathcal{N}-1} \int_0^\pi d\theta\; (\sin\theta)^{\mathcal{N}-2} \left|C_\lambda^\alpha(\cos\theta)\right|^2 \tag{3.76}$$

however, the left hand side is just equation (3.74) and the integral over the solid angle is the surface area of a hypersphere of $\mathcal{N}-1$ dimensions, so

$$\frac{\mathcal{N}-2}{\mathcal{N}+2\lambda-2} \cdot \frac{2\pi^{\mathcal{N}/2}}{\Gamma\left(\frac{\mathcal{N}}{2}\right)} \cdot \frac{(\lambda+\mathcal{N}-3)!}{\lambda!(\mathcal{N}-3)!} = \frac{2\pi^{(\mathcal{N}-1)/2}}{\Gamma\left(\frac{\mathcal{N}-1}{2}\right)} \int_0^\pi d\theta\; (\sin\theta)^{\mathcal{N}-2} \left|C_\lambda^\alpha(\cos\theta)\right|^2 \tag{3.77}$$

Therefore, the normalization constant (squared) of the Gegenbauer's polynomials is

$$\boxed{\int_0^\pi d\theta\; (\sin\theta)^{\mathcal{N}-2} \left|C_\lambda^\alpha(\cos\theta)\right|^2 = \sqrt{\pi}\frac{\Gamma\left(\frac{\mathcal{N}-1}{2}\right)(\mathcal{N}-2)(\mathcal{N}-3+\lambda)!}{\Gamma\left(\frac{\mathcal{N}}{2}\right)(\mathcal{N}-2+2\lambda)(\mathcal{N}-3)!\lambda!}} \tag{3.78}$$

Notice that the *weight function* [40] for the integration of *one* Gegenbauer's polynomial is a sine function; for $\mathcal{N}-2$ it becomes

$$\rho(\theta_1, \ldots, \theta_{\mathcal{N}-2}) = \prod_{j=1}^{\mathcal{N}-2} (\sin\theta_j)^{\mathcal{N}-j} \tag{3.79}$$

Let us get back to our most important function, the hyperspherical harmonic, whose shape is still unknown. In three dimensions,

$$Y = Y_\ell^m(\theta, \phi) = N e^{im\phi} P_\ell^m(\cos\theta) = N \frac{h_m(x, y)}{r^l} P_\ell^m(z) \tag{3.80}$$

with

$$h_m(x, y) = (x + iy)^m \tag{3.81}$$

which follows directly from de Moivre's formula. Since the Gegenbauer's polynomial is a solution for Laplace's differential equation with fixed r, so it must be the hyperspherical harmonics Y. Therefore, the h_m functions are *harmonic polynomials*. Let us generalize the spherical harmonics to higher dimensions.

Harmonic Polynomials and The Hyperspherical Harmonics

A polynomial f_n is *homogeneous* and of order n if and only if

$$\sum_{j=1}^{\mathcal{N}} x_j \frac{\partial f_n}{\partial x_j} = n f_n \tag{3.82}$$

We can define *harmonic functions* H_s as homogeneous functions that satisfy Laplace's differential equation

$$\nabla^2 H_s = 0 \tag{3.83}$$

The *harmonic polyomials*, which we will represent as h_s throughout this text and are also subject to equation (3.83), are a special case of the harmonic functions. To see that a homogeneous polynomial f_n can be written as

$$f_n = h_n + r^2 h_{n-2} + r^4 h_{n-4} + \ldots \tag{3.84}$$

where r is some hyperradius, consider

$$\nabla^2 \left(r^\beta f_s\right) = r^\beta \nabla^2 f_s + \beta(\beta + \mathcal{N} + 2s - 2) r^{\beta-2} f_s \tag{3.85}$$

If this function $r^\beta f_s$ is homogeneous and harmonic, equation (3.83) tells us that

$$\nabla^2 \left(r^\beta h_s \right) = \beta(\beta + \mathcal{N} + 2s - 2) r^{\beta-2} h_s \tag{3.86}$$

Applying the laplacian operator ν times to the function f_n, we get

$$\nabla^{2\nu} f_n = \sum_{k=\nu}^{\lfloor n/2 \rfloor} \frac{(2k)!!}{(2k-2\nu)!!} \frac{(\mathcal{N} + 2n - 2k - 2)!!}{(\mathcal{N} + 2n - 2k - 2\nu - 2)!!} r^{2k-2\nu} h_{n-2k} \tag{3.87}$$

Let $h_s(x_1, \ldots, x_{\mathcal{N}-1})$ be a harmonic polynomial of order s, independent of $x_\mathcal{N}$. In this case,

$$\nabla^2 h_s = \nabla'^2 h_s = 0 \tag{3.88}$$

with ∇'^2 being a generalized laplacian operator in $\mathcal{N} - 1$ dimensions

$$\nabla^2 = \nabla'^2 + \frac{\partial^2}{\partial x_\mathcal{N}^2} \tag{3.89}$$

Multiplying h_s by $x_\mathcal{N}^{n-s}$, with $n \geq s$, and applying the laplacian operator k times, we get

$$\nabla^{2k} \left(x_\mathcal{N}^{n-s} h_s(x_1, \ldots, x_{\mathcal{N}-1}) \right) = \frac{\partial^{2k}}{\partial x_\mathcal{N}^{2k}} x_\mathcal{N}^{n-s} h_s = \frac{(n-s)!}{(n-s-2k)!} x_\mathcal{N}^{n-s-2k} h_s \tag{3.90}$$

If $n = 2\nu$, we find

$$\nabla^n f_n = n!! \frac{(\mathcal{N} + n - 2)!!}{(\mathcal{N} - 2)!!} h_0 \to h_0 = \frac{(\mathcal{N} - 2)!!}{n!!\, (\mathcal{N} + n - 2)!!} \nabla^n f_n \tag{3.91}$$

Using equations (3.84) and (3.91), it's possible (though not very amusing; see [43]) to show that

$$h_n = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{(-1)^k\ (\mathcal{N} + 2n - 2k - 4)!!}{(2k)!!\ (\mathcal{N} + 2n - 4)!!} r^{2k}\ \nabla^{2k} f_n \tag{3.92}$$

Surely, if

$$f_n = x_\mathcal{N}^{n-s} h_s(x_1, \ldots, x_{\mathcal{N}-1}) \tag{3.93}$$

we make $n \to n - s$ and get

$$h_n = O_n[f_n] = \sum_{k=0}^{\lfloor (n-s)/2 \rfloor} \left[\frac{(-1)^k\ (\mathcal{N} + 2n - 2k - 4)!!}{(2k)!!\ (\mathcal{N} + 2n - 4)!!} \frac{(n-s)!}{(n-s-2k)!} r^{2k} x_\mathcal{N}^{n-s-2k} \right] \times h_s(x_1, \ldots, x_{\mathcal{N}-1}) \tag{3.94}$$

which is an outward projection of the harmonic polynomial of highest order within f_n, hence we called it $O_n[f_n]$. There are some terms that are independent on k, so we can rewrite the last expression to get

$$h_n = \frac{(n-s)!}{(\mathcal{N}+2n-4)!!} r^{n-s} h_s(x_1, \ldots, x_{\mathcal{N}-1}) \times \sum_{k=0}^{\lfloor (n-s)/2 \rfloor} \left[\frac{(-1)^k \; (\mathcal{N}+2n-2k-4)!!}{(2k)!! \; (n-s-2k)!} \left(\frac{x_{\mathcal{N}}}{r}\right)^{n-s-2k} \right] \quad (3.95)$$

We see through equations (3.64) that

$$C_\lambda^\alpha(\mathbf{u}\cdot\mathbf{u}') = \sum_{k=0}^{\lfloor \lambda/2 \rfloor} \frac{(-1)^k \; (\mathcal{N}+2\lambda-2k-4)!!}{(2k)!! \; (\lambda-2k)! \; (\mathcal{N}-4)!!} (\mathbf{u}\cdot\mathbf{u}')^{\lambda-2k} \quad (3.96)$$

Using (3.50), we see that $\mathcal{N} = 2(\alpha+1)$. So the changes

$$\alpha \to \alpha + s$$

$$\lambda \to n - s$$

are equivalent to

$$\mathcal{N} \to \mathcal{N} + 2s$$

$$2\lambda \to 2(n-s)$$

and

$$(\mathcal{N}+2\lambda-2k-4)!! \to (\mathcal{N}+2n-2k-4)!!$$

which immediately brings about

$$C_{n-s}^{\alpha+s}\left(\frac{x_{\mathcal{N}}}{r}\right) = \sum_{k=0}^{\lfloor (n-s)/2 \rfloor} \frac{(-1)^k \; (\mathcal{N}+2n-2k-4)!!}{(2k)!! \; (n-s-2k)! \; (\mathcal{N}+2s-4)!!} \left(\frac{x_{\mathcal{N}}}{r}\right)^{n-s-2k} \quad (3.97)$$

Comparing (3.97) with (3.95), we finally conclude that

$$h_n = \frac{(n-s)! \; (\mathcal{N}+2s-4)!!}{(\mathcal{N}+2n-4)!!} r^{n-s} h_s(x_1, \ldots, x_{\mathcal{N}-1}) C_{n-s}^{\alpha+s}\left(\frac{x_{\mathcal{N}}}{r}\right) \quad (3.98)$$

is of the same form as (3.80). Therefore, if we wish to create a set of orthonormal hyperspherical harmonics in some number of dimensions $\mathcal{N}$, we start with such a set in $(\mathcal{N}-1)$-dimensional space.

In three dimensions, the orthonormal hyperspherical harmonics are the familiar $Y_{\ell,m}(\theta,\phi)$, so if $\mathcal{N}=4$, we have

$$h_\ell(x_1,x_2,x_3) = r_{(3)}^\ell Y_{\ell,m}(\theta,\phi) \tag{3.99}$$

where the subscript represents the number of dimensions in which we are taking the hyperradius, so

$$r_{(3)}^2 = x_1^2 + x_2^2 + x_3^2$$

From equation (3.98), we see that

$$h_\lambda \propto r_{(4)}^{\lambda-\ell} r_{(3)}^\ell h_\ell(x_1,x_2,x_3) C_{\lambda-\ell}^{1+\ell}\left(\frac{x_4}{r_{(4)}}\right) \tag{3.100}$$

In the last equation,

$$r_{(4)}^2 = x_1^2 + x_2^2 + x_3^2 + x_4^2 = r_{(3)}^2 + x_4^2$$

Defining the angle χ by

$$\cos\chi = \frac{x_4}{r_{(4)}}$$

we get

$$1 = \left(\frac{r_{(3)}}{r_{(4)}}\right)^2 + \cos^2\chi \rightarrow \sin\chi = \frac{r_{(3)}}{r_{(4)}}$$

Dividing equation (3.100) by $r_{(4)}^\lambda$, we obtain

$$Y_{\lambda,\ell,m}(\chi,\theta,\phi) \propto \sin^\ell\chi C_{\lambda-\ell}^{1+\ell}\left(\frac{x_4}{r_{(4)}}\right) Y_{\ell,m}(\theta,\phi) \tag{3.101}$$

In general, if a set of functions satisfy

$$\left[\Lambda_{\mathcal{N}-1}^2 - \ell(\ell+\mathcal{N}-3)\right] Y_{\ell,\mu}(\Omega_{\mathcal{N}-1}) = 0$$

then there is a set of functions

$$Y_{\lambda,\ell,\mu}(\Omega_\mathcal{N}) \propto \left(\frac{r_{(\mathcal{N}-1)}}{r_{(\mathcal{N})}}\right)^\ell C_{\lambda-\ell}^{\alpha+\ell}\left(\frac{x_\mathcal{N}}{r_{(\mathcal{N})}}\right) Y_{\ell,\mu}(\Omega_{\mathcal{N}-1}) \tag{3.102}$$

which satisfies

$$\left[\Lambda_\mathcal{N}^2 - \lambda(\lambda+\mathcal{N}-2)\right] Y_{\lambda,\ell,\mu}(\Omega_\mathcal{N}) = 0 \tag{3.103}$$

Equations (3.102) and (3.103) suggests that a the hyperspherical harmonics can be expressed as[3]

$$\boxed{Y_{\mu_1,\mu_2,\ldots}(u_1,u_2,\ldots) = N_{\lambda,\mu}\; e^{im\phi} \prod_{j=1}^{\mathcal{N}-2} (\sin\theta_j)^{\mu_{j+1}} C^{\alpha_j+\mu_{j+1}}_{\mu_j-\mu_{j+1}}(\cos\theta_j)} \tag{3.104}$$

where we defined

$$2\alpha_j = \mathcal{N} - j - 1 \tag{3.105}$$

and where the angles $\theta_1,\ldots,\theta_{\mathcal{N}-2}$ are defined by

$$\begin{aligned}
x_{\mathcal{N}} &= r\cos\theta_1 \\
x_{\mathcal{N}-1} &= r\sin\theta_1\cos\theta_2 \\
x_{\mathcal{N}-2} &= r\sin\theta_1\sin\theta_2\cos\theta_3 \\
&\vdots \\
x_2 &= r\sin\theta_1\cdots\sin\theta_{\mathcal{N}-2}\cos\phi \\
x_1 &= r\sin\theta_1\cdots\sin\theta_{\mathcal{N}-2}\sin\phi
\end{aligned} \tag{3.106}$$

and also indexes μ_j are integers subject to

$$\mu_1 \geq \mu_2 \geq \cdots \geq |\mu_{\mathcal{N}-1}|\,. \tag{3.107}$$

It is easy to find the value of the normalization constant. To do so, we multiply (3.104) by it's complex conjugate and integrate over the solid hyperangle. The integration over ϕ is trivial and yields 2π, while the integration over all the other angles is already set by equation (3.78), so upon due change of indexes, we get

$$\boxed{N^{-2}_{\lambda,\mu} = 2\pi \prod_{j=1}^{\mathcal{N}-2} \frac{\sqrt{\pi}\,\Gamma(\alpha_j+\mu_{j+1}+\frac{1}{2})(\alpha_j+\mu_{j+1})(2\alpha_j+\mu_{j+1}+\mu_j-1)!}{\Gamma(\alpha_j+\mu_{j+1}+1)(\mu_j-\mu_{j+1})!(\alpha_j+\mu_j)(2\alpha_j+2\mu_{j+1}-1)!}} \tag{3.108}$$

The Green's Function

To construct the Green's function using equation (3.41), we first calculate the scale factors and the metric tensor. They are written with the coordinates defined by (3.106) so it is trivial to calculate the scale factors (3.2). They shall take the form

[3] It's possible that there is still some doubt as to if this solution really works for equation (3.103). Indeed, we didn't "actually solve" an equation, we created some function which appears to work as a solution. See next section for proof that it works.

$$
\begin{aligned}
h_1 &= 1 \\
h_2 &= r \\
h_3 &= r\sin\theta_1 \\
&\vdots \\
h_i &= r\sin\theta_1\cdots\sin\theta_{i-2} \\
&\vdots \\
h_{\mathcal{N}-1} &= r\sin\theta_1\cdots\sin\theta_{\mathcal{N}-3} \\
h_{\mathcal{N}} &= r\sin\theta_1\cdots\sin\theta_{\mathcal{N}-2}
\end{aligned}
\tag{3.109}
$$

and

$$
\begin{aligned}
&g_{ii} = h_i^2 \ ; \\
&\sqrt{g} = h_1 h_2 \cdots h_{\mathcal{N}} = r^{\mathcal{N}-1}\sin^{\mathcal{N}-2}\theta_1 \sin^{\mathcal{N}-3}\theta_1 \cdots \sin^2\theta_{\mathcal{N}-3}\sin\theta_{\mathcal{N}-2} \ .
\end{aligned}
\tag{3.110}
$$

To go further, we need to use equations (3.46), (3.104) and (3.103). Indeed, since

$$
\Lambda^2_{\mathcal{N}} Y_{\lambda,\ell,\mu}(\Omega_{\mathcal{N}}) = \lambda(\lambda+\mathcal{N}-2) Y_{\lambda,\ell,\mu}(\Omega_{\mathcal{N}})
$$

equation (3.46) for the radial part g of Green's function $G^{(\mathcal{N})}(\mathbf{x}|\mathbf{r}')$ becomes

$$
\left[\frac{1}{r^{\mathcal{N}-1}}\frac{\partial}{\partial r}\left(r^{\mathcal{N}-1}\frac{\partial}{\partial r}\right) + k^2 - \frac{\lambda(\lambda+\mathcal{N}-2)}{r^2}\right] g = 0 \tag{3.111}
$$

which is equivalent to

$$
\frac{d^2 g}{dr^2} + \frac{(\mathcal{N}-1)}{r}\frac{dg}{dr} + \left[k^2 - \frac{\lambda(\lambda+\mathcal{N}-2)}{r^2}\right] g = 0 \tag{3.112}
$$

The change

$$
g(r) = r^{1-n/2} y(r) \tag{3.113}
$$

transforms this differential equation into

$$
\frac{d^2 y}{dr^2} + \frac{1}{r}\frac{dy}{dr} + \left\{k^2 - \frac{[\lambda(\lambda+\mathcal{N}-2) + (\frac{\mathcal{N}}{2}-1)^2]}{r^2}\right\} y = 0 \tag{3.114}
$$

that is, a Bessel's differential equation of order

$$
\sigma^2 = \lambda(\lambda+\mathcal{N}-2) + \left(\frac{\mathcal{N}}{2}-1\right)^2 \tag{3.115}
$$

whose solutions are well known:

$$g(r) = r^{1-n/2} Z_\sigma(kr) \tag{3.116}$$

In this notation, Z represents some combination of Bessel's functions[4]. Since we want the Green's function to be well-behaved when $r \to \infty$ and when $r \to 0$, we choose

$$Z_\sigma(kr) = AJ_\sigma(kr) + BH_\sigma^{(1)}(kr) \tag{3.117}$$

with A and B real constants. The function $J_\sigma(x)$ is called Bessel's function of order σ, $H_\sigma^{(1)}(x)$ is Hankel's function of the first order, with order σ and they can be used to represent the solution of equation (3.114). The wronskian associated with this choice is [29, 45]

$$W[r^{1-n/2} J_\sigma(kr), r^{1-n/2} H_\sigma^{(1)}(kr)](r) = \frac{2ir^{1-\mathcal{N}}}{\pi} \tag{3.118}$$

This quantity clearly doesn't vanish (except at $r \to \infty$), since $\mathcal{N} \geq 3$. Upon substitution of (3.98), (3.117), (3.118) and (3.108), as well as the scale factors (3.109), the metric tensor (3.110) and the weight function (3.79) in (3.41), we get [46]

$$\begin{aligned} G^{(\mathcal{N})}(\mathbf{r}|\mathbf{r}') = \frac{i\pi}{2} \sum_q \Bigg\{ & \frac{J_\sigma(kr_<)H_\sigma^{(1)}(kr_>)}{(r_< r_>)^{\mathcal{N}/2-1}} \frac{e^{i\mu_{\mathcal{N}-1}(\phi-\phi')}}{2\pi} \\ & \times \prod_{j=1}^{\mathcal{N}-2} \left[\frac{(\sin\theta_j \cdot \sin\theta_j')^{\mu_{j+1}} C_{\mu_j-\mu_{j+1}}^{\alpha_j+\mu_{j+1}}(\cos\theta_j) C_{\mu_j-\mu_{j+1}}^{\alpha_j+\mu_{j+1}}(\cos\theta_j')}{\frac{\sqrt{\pi}\Gamma(\alpha_j+\mu_{j+1}+\frac{1}{2})(\alpha_j+\mu_{j+1})(2\alpha_j+\mu_{j+1}+\mu_j-1)!}{\Gamma(\alpha_j+\mu_{j+1}+1)(\mu_j-\mu_{j+1})!(\alpha_j+\mu_j)(2\alpha_j+2\mu_{j+1}-1)!}} \right] \Bigg\} \end{aligned} \tag{3.119}$$

To be convinced of the validity of expansion (3.119), let us choose some $\mathcal{N}$, say $\mathcal{N} = 3$ in order to recover a well-known result. In this case, $j - 1 = 1$, and $\alpha_j = 1/2$, which means that equation (3.129) reduces to the associated Legendre equation, since $a^2 \to \mu_j(\mu_j + 1)$ and $b^2 \to \mu_{j+1}^2$. As is well-known from the theory of spherical harmonics $-m \leq \ell \leq m$, so we identify $\ell \to \mu_1$ and $m \to \mu_2$. Upon using the well-known identity

$$C_{\ell-m}^{(1/2+m)}(x) = \frac{(-1)^m \; m! \; 2^m}{(2m)!} (1-x^2)^{-m/2} P_\ell^m(x), \tag{3.120}$$

where $x = \cos\theta$, our angular function becomes

$$(1-x^2)^{m/2} C_{\ell-m}^{(1/2+m)}(x) = \frac{(-1)^m \; m! \; 2^m}{(2m)!} P_\ell^m(x) \tag{3.121}$$

and (3.115) will be simply

$$\sigma_{\mu_1,(3)} = \mu_1 + \frac{1}{2} = \ell + \frac{1}{2}. \tag{3.122}$$

[4]The first instance of notation that we were able to find is due to Arnold Sommerfeld [44].

Calculating the remaining constants we recover the familiar bilinear expansion [15] of the Green's function

$$\begin{aligned} G^{(3)}(\mathbf{r}|\mathbf{r}') &= \frac{i\pi}{2\sqrt{r_< r_>}} \sum_{\ell,m} J_{\ell+\frac{1}{2}}(kr_<) H^{(1)}_{\ell+\frac{1}{2}}(kr_>) Y^m_\ell(\theta,\phi) Y^{m*}_\ell(\theta',\phi') \\ &= ik \sum_{\ell,m} j_\ell(kr_<) h^{(1)}_\ell(kr_>) Y^m_\ell(\theta,\phi) Y^{m*}_\ell(\theta',\phi'), \end{aligned} \tag{3.123}$$

in fact, the above expression was the workhorse for a previous paper [21] where the authors studied the scattering of a plane wave by a spherical shell with an arbitrary coupling strength. Adjusting the coupling strength function, they were able to investigate the scattering by a hemisphere, a spherical cap, and a Janus particle.

3.3.2 The differential equation method

If at this point one is still not convinced that equation (3.104) is the solution of equation (3.103), we can proceed as follows: we know that Helmholtz's equation in hyperspherical coordinates can be written as

$$\begin{aligned} & r^2\left(\frac{\partial^2\psi}{\partial r^2} + \frac{\mathcal{N}-1}{r}\frac{\partial\psi}{\partial r}\right) + \frac{1}{\sin^{\mathcal{N}-2}\theta_1}\frac{\partial}{\partial\theta_1}\left(\sin^{\mathcal{N}-2}\theta_1\frac{\partial\psi}{\partial\theta_1}\right) + \dots \\ &+ \frac{1}{\sin^2\theta_1\cdots\sin^2\theta_{\mathcal{N}-3}\sin\theta_{\mathcal{N}-2}}\frac{\partial}{\partial\theta_{\mathcal{N}-2}}\left(\sin\theta_{\mathcal{N}-2}\frac{\partial\psi}{\partial\theta_{\mathcal{N}-2}}\right) \\ &+ \frac{1}{\sin^2\theta_1\cdots\sin^2\theta_{\mathcal{N}-3}\sin^2\theta_{\mathcal{N}-2}}\frac{\partial^2\psi}{\partial\phi^2} + k^2r^2\psi = 0 \end{aligned} \tag{3.124}$$

We substitute the *ansatz*

$$\psi(r,\theta_1,\dots,\theta_{\mathcal{N}-2},\phi) = R(r)\Phi(\phi)\prod_{j=1}^{\mathcal{N}-2}\Theta_j(\theta_j) \tag{3.125}$$

and get

$$\begin{aligned}
&\frac{r^2}{R}\left(\frac{d^2R}{dr^2}+\frac{\mathcal{N}-1}{r}\frac{dR}{dr}\right)+\frac{1}{\Theta_1\sin^{\mathcal{N}-2}\theta_1}\frac{d}{d\theta_1}\left(\sin^{\mathcal{N}-2}\theta_1\frac{d\Theta_1}{d\theta_1}\right)\\
&+\frac{1}{\Theta_2\sin^{\mathcal{N}-3}\theta_2\sin^2\theta_1}\frac{d}{d\theta_2}\left(\sin^{\mathcal{N}-3}\theta_2\frac{d\Theta_2}{d\theta_2}\right)\\
&+\dots\\
&+\frac{1}{\Theta_{\mathcal{N}-3}\sin^2\theta_1\cdots\sin^2\theta_{\mathcal{N}-3}}\frac{d}{d\theta_{\mathcal{N}-2}}\left(\sin^2\theta_{\mathcal{N}-3}\frac{d\Theta_{\mathcal{N}-3}}{d\theta_{\mathcal{N}-3}}\right)\\
&+\frac{1}{\Theta_{\mathcal{N}-2}\sin^2\theta_1\cdots\sin^2\theta_{\mathcal{N}-3}\sin\theta_{\mathcal{N}-2}}\frac{d}{d\theta_{\mathcal{N}-2}}\left(\sin\theta_{\mathcal{N}-2}\frac{d\Theta_{\mathcal{N}-2}}{d\theta_{\mathcal{N}-2}}\right)\\
&+\frac{1}{\Phi\sin^2\theta_1\cdots\sin^2\theta_{\mathcal{N}-3}\sin^2\theta_{\mathcal{N}-2}}\frac{d^2\Phi}{d\phi^2}+k^2r^2=0\ .
\end{aligned} \tag{3.126}$$

The solution for ϕ is obvious,

$$\Phi_m(\phi)=e^{im\phi} \tag{3.127}$$

The equations for θ_j are simple for $j-1=1$, but not so much for the other ones, since those equations' eigenvalues are unknown. In fact, we have no reason to assume that all the eigenvalues associated with the polar angles are of the form $\ell(\ell+1)$. Since $1\le j-1\le\mathcal{N}-2$, let's make the change

$$m^2\to b^2 \tag{3.128}$$

such that the polar equations become

$$\frac{d^2\Theta}{d\theta^2}+(j-1)\cot\theta\frac{d\Theta}{d\theta}+\left[a^2-\frac{b^2}{\sin^2\theta}\right]\Theta=0 \tag{3.129}$$

where we omitted the indexes for simplicity, and a^2 is the unknown eigenvalue. If

$$\begin{aligned}
&x=\cos\theta\\
&a^2\to\mu_j(\mu_j+2\alpha_j)\\
&b^2\to\mu_{j+1}(\mu_{j+1}+2\alpha_{j+1})
\end{aligned} \tag{3.130}$$

the change

$$\Theta(x)=(1-x^2)^{\mu_{j+1}/2}M(x) \tag{3.131}$$

translates into

$$(1-x^2)\frac{d^2M}{dx^2}-(2\alpha_{j+1}+j)x\frac{dM}{dx}+\Bigg[\mu_j(\mu_j+2\alpha_j)-\mu_{j+1}$$
$$+\frac{x^2(\mu_{j+1}+j-2)\mu_{j+1}-(\mu_{j+1}+2\alpha_{j+1})\mu_{j+1}}{1-x^2}\Bigg]M=0 \quad (3.132)$$

But by definition, $2\alpha_j = \mathcal{N} - j - 1$, that is, $2\alpha_{j+1} = 2\alpha_j - 1$. This means, implicitly, that we make $j \to \mathcal{N} - j$. The result is

$$(1-x^2)\frac{d^2M}{dx^2}-[1+2(\alpha_j+\mu_{j+1})]x\frac{dM}{dx}+(\mu_j-\mu_{j+1})(\mu_j-\mu_{j+1}+2\alpha_j)M=0 \quad (3.133)$$

which is a Gegenbauer's differential equation when $\alpha \to \alpha_j + \mu_{j+1}$ and $\lambda \to \mu_j - \mu_{j+1}$. Now, what is left is the radial equation, which takes the form of a Bessel's differential equation. That concludes our proof.

3.4 A closed-form solution for the Green's Function of Helmholtz's Equation for the free particle in hyper-spherical coordinates

In the previous section, we found an eigenfunction (bilinear) expansion for our Green's Function. Now, we ask ourselves if we can obtain a closed-form solution for equation (3.44). In other words, is it possible to sum equation (3.119)? While it may seem hard to execute this sum, we can take a different approach. Because of spherical symmetry, a free-particle only has one degree of freedom – the radial-like one. Consequently, Helmholtz's equation for Green's function of a free particle is [42]

$$\frac{\partial^2 G}{\partial r^2}+\frac{\mathcal{N}-1}{r}\frac{\partial G}{\partial r}+k^2G=-\delta(r-r') \quad (3.134)$$

Using the *ansatz*

$$G\left(\mathbf{r}|\mathbf{r}'\right)=r^{1-\mathcal{N}/2}g(r), \quad (3.135)$$

one finds

$$\frac{\partial G}{\partial r}=\left(1-\frac{\mathcal{N}}{2}\right)r^{-\mathcal{N}/2}g(r)+r^{1-\mathcal{N}/2}\frac{dg}{dr}$$

and

$$\frac{\partial^2 G}{\partial r^2} = \left(1-\frac{\mathcal{N}}{2}\right)\left[\left(-\frac{\mathcal{N}}{2}\right) r^{-\mathcal{N}/2-1} g(r) + r^{-\mathcal{N}/2}\frac{dg}{dr}\right] + \left(1-\frac{\mathcal{N}}{2}\right) r^{-\mathcal{N}/2}\frac{dg}{dr} + r^{1-\mathcal{N}/2}\frac{d^2 g}{dr^2}$$
$$= r^{1-\mathcal{N}/2}\frac{d^2 g}{dr^2} + 2\left(1-\frac{\mathcal{N}}{2}\right) r^{-\mathcal{N}/2}\frac{dg}{dr} + \left(-\frac{\mathcal{N}}{2}\right)\left(1-\frac{\mathcal{N}}{2}\right) r^{-\mathcal{N}/2-1} g(r).$$

Upon substitution, we have

$$r^{1-\mathcal{N}/2}\frac{d^2 g}{dr^2} + 2\left(1-\frac{\mathcal{N}}{2}\right) r^{-\mathcal{N}/2}\frac{dg}{dr} + \left(-\frac{\mathcal{N}}{2}\right)\left(1-\frac{\mathcal{N}}{2}\right) r^{-\mathcal{N}/2-1} g(r)$$
$$+\left(\frac{\mathcal{N}-1}{r}\right)\left[\left(1-\frac{\mathcal{N}}{2}\right) r^{-\mathcal{N}/2} g(r) + r^{1-\mathcal{N}/2}\frac{dg}{dr}\right] + k^2 r^{1-\mathcal{N}/2} g(r) = -\delta(r-r'),$$

and so

$$r^{1-\mathcal{N}/2}\frac{d^2 g}{dr^2} + \left[\left(\frac{\mathcal{N}-1}{r}\right) r^{1-\mathcal{N}/2} + 2\left(1-\frac{\mathcal{N}}{2}\right) r^{-\mathcal{N}/2}\right]\frac{dg}{dr}$$
$$+\left[\left(\frac{\mathcal{N}-1}{r}\right)\left(1-\frac{\mathcal{N}}{2}\right) r^{-\mathcal{N}/2} + k^2 r^{1-\mathcal{N}/2} + \left(-\frac{\mathcal{N}}{2}\right)\left(1-\frac{\mathcal{N}}{2}\right) r^{1-\mathcal{N}/2}\right] g = -\delta(r-r').$$

Working on those brackets and parentheses, and factoring out the $r^{1-\mathcal{N}/2}$ terms, we find

$$r^{1-\mathcal{N}/2}\left\{\frac{d^2 g}{dr^2} + \frac{1}{r}\frac{dg}{dr} + \left[k^2 - \frac{\left(\frac{\mathcal{N}}{2}-1\right)^2}{r^2}\right] g\right\} = -\delta(r-r'),$$

and if we make $r' = 0$ and $r \neq r'$, we have a Bessel's equation of order $\frac{\mathcal{N}}{2} - 1$

$$\frac{d^2 g}{dr^2} + \frac{1}{r}\frac{dg}{dr} + \left[k^2 - \frac{\left(\frac{\mathcal{N}}{2}-1\right)^2}{r^2}\right] g = 0,$$

whose solutions are Hankel's functions. Hence, our *ansatz* (3.135) becomes

$$G\left(\mathbf{r}|\mathbf{r}' = \mathbf{0}\right) = A r^{1-\mathcal{N}/2} H^{(2)}_{\frac{\mathcal{N}}{2}-1}(kr) + B r^{1-\mathcal{N}/2} H^{(1)}_{\frac{\mathcal{N}}{2}-1}(kr). \tag{3.136}$$

Here, we adopt the time convention $e^{-i\omega t}$ and we assume $Im(k) > 0$, and so $A = 0$. To find B, we consider non-homogeneous Dirichlet's boundary conditions, as follows. Beginning with equation (3.134), we integrate over a $\mathcal{N}$-dimensional volume, obtaining

$$\int_V \nabla^2 G \; d^{\mathcal{N}}v + k^2 \int_V G \; d^{\mathcal{N}}v = -1.$$

Using the divergence theorem,

$$\int_V \nabla^2 G \; d^{\mathcal{N}}v = \int_V \vec{\nabla} \cdot \left(\vec{\nabla} G\right) \; d^{\mathcal{N}}v = \int_S \left(\vec{\nabla} G\right) \cdot \hat{n} \; d^{\mathcal{N}-1}s = \int_S \frac{\partial G}{\partial r} \; d^{\mathcal{N}-1}s$$

which means

$$\int_S \frac{\partial G}{\partial r} \; d^{\mathcal{N}-1}s + \int_V G \; d^{\mathcal{N}}v = -1$$

The boundary conditions will impose

$$\int_V G \; d^{\mathcal{N}}v = 0$$

that is,

$$\boxed{\int_S \frac{\partial G}{\partial r} \; d^{\mathcal{N}-1}s = -1}. \tag{3.137}$$

It is easy but not trivial to show that given ϵ as the radius of a $\mathcal{N}$-sphere, it's area is

$$S_{\mathcal{N}-1}(\epsilon) = \frac{2\pi^{\mathcal{N}/2}\epsilon^{\mathcal{N}-1}}{\Gamma\left(\frac{\mathcal{N}}{2}\right)} \tag{3.138}$$

Then, using the chain rule for the r derivative, equation (3.137) becomes

$$\lim_{\epsilon \to 0} \left[S_{\mathcal{N}-1} B \left(\left(1 - \frac{\mathcal{N}}{2}\right) \epsilon^{-\mathcal{N}/2} H^{(1)}_{\frac{\mathcal{N}}{2}-1}(k\epsilon) + k\epsilon^{1-\mathcal{N}/2} \frac{d}{d(kr)} H^{(1)}_{\frac{\mathcal{N}}{2}-1}(kr)\Big|_{r=\epsilon} \right) \right] = -1 \tag{3.139}$$

Using the asymptotic expansion

$$H^{(1)}_{\nu}(x) \approx -i \frac{(\nu-1)!}{\pi} \left(\frac{2}{x}\right)^{\nu} \; ,$$

we have

$$H^{(1)}_{\frac{\mathcal{N}}{2}-1}(k\epsilon) \approx -i \frac{\Gamma(\frac{\mathcal{N}}{2}-1)}{\pi} \left(\frac{2}{k\epsilon}\right)^{\frac{\mathcal{N}}{2}-1} \tag{3.140}$$

and

$$\frac{d}{d(kr)} H^{(1)}_{\frac{\mathcal{N}}{2}-1}(kr)\Big|_{r=\epsilon} \approx i \frac{\left(\frac{\mathcal{N}}{2}-1\right)\Gamma(\frac{\mathcal{N}}{2}-1)}{2\pi} \left(\frac{2}{k\epsilon}\right)^{\mathcal{N}/2} \tag{3.141}$$

Bringing equation (3.139) together with (3.140) and (3.141) will give us

$$\lim_{\epsilon\to 0}\left[S_{\mathcal{N}-1}B\left(\left(1-\frac{\mathcal{N}}{2}\right)\epsilon^{-\mathcal{N}/2}(-i)\frac{\Gamma(\frac{\mathcal{N}}{2}-1)}{\pi}\left(\frac{2}{k\epsilon}\right)^{\frac{\mathcal{N}}{2}-1} + k\epsilon^{1-\mathcal{N}/2}i\frac{\left(\frac{\mathcal{N}}{2}-1\right)\Gamma(\frac{\mathcal{N}}{2}-1)}{2\pi}\left(\frac{2}{k\epsilon}\right)^{\mathcal{N}/2}\right)\right]=-1 \quad (3.142)$$

According to equation (3.137) and the properties of the gamma function,

$$\frac{iB}{\pi}\frac{2\pi^{\mathcal{N}/2}(\frac{\mathcal{N}}{2}-1)\Gamma\left(\frac{\mathcal{N}}{2}-1\right)}{\Gamma\left(\frac{\mathcal{N}}{2}\right)}\left[2\left(\frac{2}{k}\right)^{\mathcal{N}/2-1}\right]=4iB\left(\frac{2\pi}{k}\right)^{\mathcal{N}/2-1}=-1$$

Hence,

$$B=\frac{i}{4}\left(\frac{k}{2\pi}\right)^{\mathcal{N}/2-1} \quad (3.143)$$

and our solution (3.136) becomes, with $A=0$,

$$G\left(\mathbf{r}|\mathbf{r}'=\mathbf{0}\right)=\frac{i}{4}\left(\frac{k}{2\pi r}\right)^{\mathcal{N}/2-1}H^{(1)}_{\frac{\mathcal{N}}{2}-1}(kr)\ .$$

Finally, if we agree to make the generalization $r\to|\mathbf{r}-\mathbf{r}'|$ we write

$$\boxed{G^{(\mathcal{N})}\left(\mathbf{r}|\mathbf{r}'\right)=\frac{i}{4}\left(\frac{k}{2\pi|\mathbf{r}-\mathbf{r}'|}\right)^{\mathcal{N}/2-1}H^{(1)}_{\frac{\mathcal{N}}{2}-1}(k|\mathbf{r}-\mathbf{r}'|)} \quad (3.144)$$

For the Green's function to be unique, it has to be equal to (3.119). It is convenient to rewrite this equation here, for comparison:

$$G^{(\mathcal{N})}(\mathbf{r}|\mathbf{r}')=\frac{i\pi}{2}\sum_q\left\{\frac{J_\sigma(kr_<)H^{(1)}_\sigma(kr_>)}{(r_<r_>)^{\mathcal{N}/2-1}}\frac{e^{i\mu_{\mathcal{N}-1}(\phi-\phi')}}{2\pi} \times\prod_{j=1}^{\mathcal{N}-2}\left[\frac{(\sin\theta_j\cdot\sin\theta_j')^{\mu_{j+1}}C^{\alpha_j+\mu_{j+1}}_{\mu_j-\mu_{j+1}}(\cos\theta_j)C^{\alpha_j+\mu_{j+1}}_{\mu_j-\mu_{j+1}}(\cos\theta_j')}{\frac{\sqrt{\pi}\Gamma(\alpha_j+\mu_{j+1}+\frac{1}{2})(\alpha_j+\mu_{j+1})(2\alpha_j+\mu_{j+1}+\mu_j-1)!}{\Gamma(\alpha_j+\mu_{j+1}+1)(\mu_j-\mu_{j+1})!(\alpha_j+\mu_j)(2\alpha_j+2\mu_{j+1}-1)!}}\right]\right\} \quad (3.119)$$

Equating (3.144) and (3.119), and simplifying constant factors, we get an *Gegenbauer expansion* for the Hankel function

$$
\frac{H^{(1)}_{\frac{\mathcal{N}}{2}-1}(k|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|^{\frac{\mathcal{N}}{2}-1}} = \left(\frac{2\pi}{kr_< r_>}\right)^{\frac{\mathcal{N}}{2}-1} \sum_q \Bigg\{ J_\sigma(kr_<) H^{(1)}_\sigma(kr_>) e^{i\mu_{\mathcal{N}-1}(\phi-\phi')} \\
\times \prod_{j=1}^{\mathcal{N}-2} \left[\frac{(\sin\theta_j \cdot \sin\theta'_j)^{\mu_{j+1}} C^{\alpha_j+\mu_{j+1}}_{\mu_j-\mu_{j+1}}(\cos\theta_j) C^{\alpha_j+\mu_{j+1}}_{\mu_j-\mu_{j+1}}(\cos\theta'_j)}{\frac{\sqrt{\pi}\Gamma(\alpha_j+\mu_{j+1}+\frac{1}{2})(\alpha_j+\mu_{j+1})(2\alpha_j+\mu_{j+1}+\mu_j-1)!}{\Gamma(\alpha_j+\mu_{j+1}+1)(\mu_j-\mu_{j+1})!(\alpha_j+\mu_j)(2\alpha_j+2\mu_{j+1}-1)!}} \right] \Bigg\} \quad (3.145)
$$

This expansion can and will be used as we consider some applications of the results acquired in this chapter, as we'll see in the next pages.

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M. E. Pereira and A. G. M. Schmidt, Few-Body Systems **63**, 25 (2022)

Chapter 4

Scattering Phenomena in $\mathcal{N}$-dimensions

In this chapter we apply the methodology we developed in the previous chapter — where we obtained an exact expression for the free particle Green's function and its eigenfunction expansion — to scattering problems. Namely, we investigate the scattering of a plane-wave by: (i) a four-dimensional spherical shell; (ii) a four-dimensional sphere filled with Dirac delta functions; and (iii) a six-dimensional spherical shell. We exactly solve the Lippmann–Schwinger for these problems, calculate the differential and total cross-sections, as well as the quantum refractive index.

4.1 Applications in quantum scattering phenomena

In order for us to put equation (3.41) in use, let us consider three systems [46], (i) scattering in a four-dimensional hyperspherical boundary-wall potential [22] , (ii) scattering in a four-dimensional potential distributed in a hyperspherical region, and (iii) scattering in a six-dimensional hyperspherical boundary-wall potential. In all cases, we use the potential defined by [18], which can be explored to suit a number of systems.

4.1.1 One-particle scattering in 4D

Suppose one has some unit vector $\hat{\mathbf{r}}$ defined as [47]

$$\hat{\mathbf{r}} = (\sin\omega\sin\theta\cos\phi, \sin\omega\sin\theta\sin\phi, \sin\omega\cos\theta, \cos\omega) \tag{4.1}$$

where the angles θ and ϕ are the well known spherical angles and this new angle ω an extra angle, ranging from 0 to π as θ does. The importance of this coordinate system stems from the fact that this is the coordinate system Fock used in 1935 to solve the hydrogen atom problem [43]. It is easy to see that, if $\mathcal{N} = 4$, equation (3.119) is simply

$$G^{(4)}(\mathbf{r}|\mathbf{r}') = \frac{i\pi}{2}\sum_q \left\{ \frac{J_\sigma(kr_<)H_\sigma^{(1)}(kr_>)}{(r_<r_>)^{4/2-1}} \frac{e^{i\mu_{4-1}(\phi-\phi')}}{2\pi} \right. \\ \left. \times \prod_{j=1}^{4-2} \left[\frac{(\sin\theta_j \cdot \sin\theta_j')^{\mu_{j+1}} C_{\mu_j-\mu_{j+1}}^{\alpha_j+\mu_{j+1}}(\cos\theta_j) C_{\mu_j-\mu_{j+1}}^{\alpha_j+\mu_{j+1}}(\cos\theta_j')}{\frac{\sqrt{\pi}\Gamma(\alpha_j+\mu_{j+1}+\frac{1}{2})(\alpha_j+\mu_{j+1})(2\alpha_j+\mu_{j+1}+\mu_j-1)!}{\Gamma(\alpha_j+\mu_{j+1}+1)(\mu_j-\mu_{j+1})!(\alpha_j+\mu_j)(2\alpha_j+2\mu_{j+1}-1)!}} \right] \right\} \tag{4.2}$$

and we get, for $\theta_1 = \omega$ and $\theta_2 = \theta$,

$$G^{(4)}(\mathbf{r}|\mathbf{r}') = \frac{i\pi}{2}\sum_q \left\{ \frac{J_\sigma(kr_<)H_\sigma^{(1)}(kr_>)}{r_<r_>} \frac{e^{i\mu_3(\phi-\phi')}}{2\pi} \right. \\ \times \left[\frac{(\sin\omega \cdot \sin\omega')^{\mu_2} C_{\mu_1-\mu_2}^{\alpha_1+\mu_2}(\cos\omega) C_{\mu_1-\mu_2}^{\alpha_1+\mu_2}(\cos\omega')}{\frac{\sqrt{\pi}\Gamma(\alpha_1+\mu_2+\frac{1}{2})(\alpha_1+\mu_2)(2\alpha_1+\mu_2+\mu_1-1)!}{\Gamma(\alpha_1+\mu_2+1)(\mu_1-\mu_2)!(\alpha_1+\mu_1)(2\alpha_1+2\mu_2-1)!}} \right] \\ \left. \times \left[\frac{(\sin\theta \cdot \sin\theta')^{\mu_3} C_{\mu_2-\mu_3}^{\alpha_2+\mu_3}(\cos\theta) C_{\mu_2-\mu_3}^{\alpha_2+\mu_3}(\cos\theta')}{\frac{\sqrt{\pi}\Gamma(\alpha_2+\mu_3+\frac{1}{2})(\alpha_2+\mu_3)(2\alpha_2+\mu_3+\mu_2-1)!}{\Gamma(\alpha_2+\mu_3+1)(\mu_2-\mu_3)!(\alpha_2+\mu_2)(2\alpha_2+2\mu_3-1)!}} \right] \right\} \tag{4.3}$$

Labeling, for the sake of convention, $\mu_3 \equiv m$, and $\mu_2 \equiv \ell$, and using equation (3.105) to calculate $2\alpha_1 = 2$, $2\alpha_2 = 1$, we get

$$G^{(4)}(\mathbf{r}|\mathbf{r}') = \frac{i\pi}{2}\frac{1}{r_<r_>}\sum_q \left\{ J_\sigma(kr_<)H_\sigma^{(1)}(kr_>) \frac{e^{im(\phi-\phi')}}{2\pi} \right. \\ \times \left[\frac{(\sin\omega \cdot \sin\omega')^{\ell} C_{\mu_1-\ell}^{1+\ell}(\cos\omega) C_{\mu_1-\ell}^{1+\ell}(\cos\omega')}{\frac{\sqrt{\pi}\Gamma(1+\ell+\frac{1}{2})(1+\ell)(2+\ell+\mu_1-1)!}{\Gamma(1+\ell+1)(\mu_1-\ell)!(1+\mu_1)(2+2\ell-1)!}} \right] \\ \left. \times \left[\frac{(\sin\theta \cdot \sin\theta')^{m} C_{\ell-m}^{\frac{1}{2}+m}(\cos\theta) C_{\ell-m}^{\frac{1}{2}+m}(\cos\theta')}{\frac{\sqrt{\pi}\Gamma(\frac{1}{2}+m+\frac{1}{2})(\frac{1}{2}+m)(1+m+\ell-1)!}{\Gamma(\frac{1}{2}+m+1)(\ell-m)!(\frac{1}{2}+\ell)(1+2m-1)!}} \right] \right\} \tag{4.4}$$

Using the well-known [48] relation

$$C_{\ell-m}^{\frac{1}{2}+m}(x) = (-1)^m \frac{(1-x^2)^{-\frac{m}{2}} m! 2^m}{(2m)!} P_\ell^m(x) \tag{4.5}$$

as well as three properties of the gamma function, namely

$$\Gamma(n) = (n-1)! \ , \tag{4.6}$$

$$\Gamma(z+1) = z\Gamma(z) \ , \tag{4.7}$$

$$\Gamma\left(z+\frac{1}{2}\right) = 2^{1-2z}\sqrt{\pi}\frac{\Gamma(2z)}{\Gamma(z)} \ , \tag{4.8}$$

we get

$$\begin{aligned} G^{(4)}(\mathbf{r}|\mathbf{r}') = \frac{i\pi}{2}\sum_{n,\ell,m} N_{n,\ell}^2 \frac{J_{n+\ell+1}(kr_<)}{r_<}\frac{H^{(1)}_{n+\ell+1}(kr_>)}{r_>} \\ \times (\sin\omega\sin\omega')^\ell C_n^{\ell+1}(\cos\omega)C_n^{\ell+1}(\cos\omega')Y_\ell^m(\theta,\phi)Y_\ell^{m*}(\theta',\phi'), \end{aligned} \tag{4.9}$$

where we made the changes $\mu_1 \to n$ and

$$N_{n\ell}^2 = \frac{\Gamma(\ell+2)(n-\ell)!(n+1)(2\ell+1)!}{\sqrt{\pi}\Gamma(\ell+\frac{3}{2})(\ell+1)(\ell+n+1)!} \tag{4.10}$$

Using yet again equation (3.144) to find out the result of the summation in equation (4.9), we get, for $\mathcal{N} = 4$,

$$G^{(4)}(\mathbf{r}|\mathbf{r}') = \frac{ik}{8\pi}\frac{H_1^{(1)}(k|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|} \tag{4.11}$$

With the intention of finding the expansion for a plane wave, we make $r' \to \infty$ and use a well-known formula. For a large argument z, the Hankel function is approximately [45]

$$H_\nu^{(1)}(z) = \sqrt{\frac{2}{\pi z}}\exp\left\{i\left[z-\left(\nu+\frac{1}{2}\right)\frac{\pi}{2}\right]\right\} \tag{4.12}$$

Since $r' \to \infty$, $|\mathbf{r}-\mathbf{r}'| \approx r' - \hat{\mathbf{n}}\cdot\mathbf{r}$, with $\hat{\mathbf{n}}$ being a unit vector, our closed-form Green's function reads

$$G^{(4)}(\mathbf{r}|\mathbf{r}'\to\infty) \approx \frac{ik}{8\pi}\frac{\sqrt{2/\pi}}{\sqrt{k(r'-\hat{\mathbf{n}}\cdot\mathbf{r})}}\frac{e^{ik(r'-\hat{\mathbf{n}}\cdot\mathbf{r})}e^{-i3\pi/2}}{r'-\hat{\mathbf{n}}\cdot\mathbf{r}} \tag{4.13}$$

However, the fact that $r' \to \infty$ makes $r \approx 0$. We will make this substitution except in the exponential, because of the rapid oscillations. Moving on, and using Euler's formula for complex numbers, we get

$$G^{(4)}(\mathbf{r}|\mathbf{r}'\to\infty) = \frac{ik}{8\pi}\frac{1}{\sqrt{kr'\pi}}\frac{e^{ikr'}e^{-i\mathbf{k}\cdot\mathbf{r}}}{r'}(-1+i) \tag{4.14}$$

Similar approach (i.e., asymptotic evaluation of Hankel's function) for the series expansion (4.9) gives rise to

$$G^{(4)}(\mathbf{r}|\mathbf{r}' \to \infty) = \frac{i\pi}{2} \sum_{n,\ell,m} N_{n,\ell}^2 \frac{J_{n+\ell+1}(kr)}{r} \frac{(-i)^{n+\ell}}{\sqrt{\pi}} \frac{e^{ikr'}}{r'\sqrt{kr'}}(-1+i) \\ \times (\sin\omega\sin\omega')^\ell C_n^{\ell+1}(\cos\omega) C_n^{\ell+1}(\cos\omega') Y_l^m(\theta,\phi) Y_l^{m*}(\theta',\phi') \tag{4.15}$$

Upon comparison, we find that

$$e^{-i\mathbf{k}\cdot\mathbf{r}} = \frac{4\pi^2}{k} \sum_{n,\ell,m} \Bigg[N_{n,\ell}^2 (-i)^{n+\ell} \frac{J_{n+\ell+1}(kr)}{r} \\ \times (\sin\omega\sin\omega')^\ell C_n^{\ell+1}(\cos\omega) C_n^{\ell+1}(\cos\omega') Y_l^m(\theta,\phi) Y_l^{m*}(\theta',\phi') \Bigg] \tag{4.16}$$

or, taking the complex conjugate, we find the plane-wave expansion

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{4\pi^2}{k} \sum_{n,\ell,m} \Bigg[i^{n+\ell} N_{n,\ell}^2 \frac{J_{n+\ell+1}(kr)}{r} \\ \times (\sin\omega\sin\omega')^\ell C_n^{\ell+1}(\cos\omega) C_n^{\ell+1}(\cos\omega') Y_l^{m*}(\theta,\phi) Y_l^{m}(\theta',\phi') \Bigg] \tag{4.17}$$

Let us now return to r' being comparable to r. Using the potential

$$V(\mathbf{r}') = \int_S \gamma(s,t,u) \frac{\delta(r'-r_0)\delta(\omega'-s)\delta(\theta'-t)\delta(\phi'-u)}{r'^3 \sin^2\omega' \sin\theta'}\ dS \tag{4.18}$$

and the surface element

$$dS = r_0^3 \sin^2 s \sin t\ dsdtdu \tag{4.19}$$

we get

$$V(\mathbf{r}') = \frac{r_0^3 \delta(r'-r_0)}{r'^3 \sin^2\omega' \sin\theta'} \int_S \gamma(s,t,u)\delta(\omega'-s)\delta(\theta'-t)\delta(\phi'-u)\ \sin^2 s \sin t\ dsdtdu \tag{4.20}$$

With all these elements in place, the normalized Lippmann-Schwinger equation

$$\psi(\mathbf{r}) = \varphi(\mathbf{r}) + A\int_{V'} G(\mathbf{r}|\mathbf{r}')V(\mathbf{r}')\psi(\mathbf{r}')d\tau' \tag{2.21}$$

results in

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{i\pi A r_0^3}{2} \sum_{n,\ell,m} \Bigg\{ N_{n,\ell}^2 \int_{V'} d^4r' \Bigg[\frac{J_{n+\ell+1}(kr_<)}{r_<} \frac{H^{(1)}_{n+\ell+1}(kr_>)}{r_>} \frac{\delta(r'-r_0)}{r'^3}$$
$$\times (\sin\omega\sin\omega')^\ell C_n^{\ell+1}(\cos\omega) C_n^{\ell+1}(\cos\omega') Y_\ell^m(\theta,\phi) Y_\ell^{m*}(\theta',\phi')$$
$$\times \int_S dsdtdu\ \sin^2 s\sin t\ \gamma(s,t,u) \frac{\delta(\omega'-s)}{\sin^2\omega'} \frac{\delta(\theta'-t)}{\sin\theta'} \delta(\phi'-u)\psi(r',\omega',\theta',\phi') \Bigg]\Bigg\} \quad (4.21)$$

The integration with the primed variables using $d^4r' = r'^3 \sin^2\omega' \sin\theta'$, ultimately, does nothing but apply the filtration properties of Dirac's delta function, giving us

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{i\pi A r_0^3}{2} \sum_{n,\ell,m} \Bigg[N_{n,\ell}^2 \frac{J_{n+\ell+1}(kr_<)}{r_<} \frac{H^{(1)}_{n+\ell+1}(kr_>)}{r_>} (\sin\omega)^\ell C_n^{\ell+1}(\cos\omega) Y_\ell^m(\theta,\phi)$$
$$\times \int_S dsdtdu\ \sin^2 s\sin t\ \gamma(s,t,u) C_n^{\ell+1}(\sin s)^\ell(\cos s) Y_\ell^{m*}(t,u)\psi(r_0,s,t,u) \Bigg] \quad (4.22)$$

which of course also changes the definition of $r_<(r_>)$. Now we have

$$r_< = \min(r, r_0)$$
$$r_> = \max(r, r_0)$$

Equation (4.22) is almost complete. To solve it, let us consider the simple case

$$\boxed{\gamma(s,t,u) = \gamma_0 = \text{const.}}$$

The simple case of constant distribution

Writing

$$a_{n,\ell,m}(r_0) = \int_0^\pi \int_0^\pi \int_0^{2\pi} dsdtdu\ \sin^2 s\sin t\ (\sin s)^\ell C_n^{\ell+1}(\cos s) Y_\ell^{m*}(t,u)\psi(r_0,s,t,u) \quad (4.23)$$

then equation (4.22) becomes

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{i\pi A\gamma_0 r_0^3}{2} \sum_q N_{n,\ell}^2 a_{n,\ell,m}(r_0) \frac{J_{n+\ell+1}(kr_<)}{r_<} \frac{H^{(1)}_{n+\ell+1}(kr_>)}{r_>} (\sin\omega)^\ell C_n^{\ell+1}(\cos\omega) Y_\ell^m(\theta,\phi) \quad (4.24)$$

and now is easy to see $a_{n,\ell,m}(r_0)$ as coefficients for the expansion of our wavefunction; so, in this perspective, there is just one piece missing from the solution needed. Thus, in order to calculate these coefficients, let us proceed as usual and use the orthogonality properties of these spherical angular functions. Recalling the expansion for the plane-wave (4.17) and multiplying the latter equation by

$$(\sin\omega)^{\ell'+2} C_{n'}^{\ell'+1}(\cos\omega) Y_{\ell'}^{m'*}(\theta,\phi)\sin\theta$$

and integrating on the surface of a 3-sphere, we get

$$a_{n,\ell,m}(r) = \frac{4\pi^2}{k}\sum_q \Bigg[N_{n,\ell}^2 i^{n+\ell}\frac{J_{n+\ell+1}(kr)}{r}(\sin\widetilde{\omega})^\ell C_n^{\ell+1}(\cos\widetilde{\omega}) Y_\ell^{m*}(\widetilde{\theta},\widetilde{\phi}) \\ \times \int_0^\pi\int_0^\pi\int_0^{2\pi} d\omega\sin^2\omega d\theta\sin\theta d\phi\; (\sin\omega)^{2\ell}\left|C_n^{\ell+1}(\cos\omega)\right|^2 Y_\ell^m(\theta,\phi) Y_\ell^{m*}(\theta,\phi)\Bigg] \\ + \frac{i\pi A\gamma_0 r_0^3}{2}\frac{J_{n+\ell+1}(kr_<)}{r_<}\frac{H_{n+\ell+1}^{(1)}(kr_>)}{r_>} a_{n,\ell,m}(r_0) \quad (4.25)$$

Since

$$\int_0^\pi\int_0^\pi\int_0^{2\pi} d\omega\sin^2\omega d\theta\sin\theta d\phi\; (\sin\omega)^{2\ell}\left|C_n^{\ell+1}(\cos\omega)\right|^2 Y_\ell^m(\theta,\phi) Y_\ell^{m*}(\theta,\phi) = \frac{1}{N_{n,\ell}^2} \quad (4.26)$$

our coefficient (4.25) becomes

$$a_{n,\ell,m}(r) = \frac{4\pi^2}{k} i^{n+\ell}\frac{J_{n+\ell+1}(kr)}{r}(\sin\widetilde{\omega})^\ell C_n^{\ell+1}(\cos\widetilde{\omega}) Y_\ell^{m*}(\widetilde{\theta},\widetilde{\phi}) \\ + \frac{i\pi A\gamma_0 r_0^3}{2}\frac{J_{n+\ell+1}(kr_<)}{r_<}\frac{H_{n+\ell+1}^{(1)}(kr_>)}{r_>} a_{n,\ell,m}(r_0) \quad (4.27)$$

Evaluating in $r = r_0$ and isolating $a_{n,\ell,m}(r_0)$ conduce to

$$a_{n,\ell,m}(r_0) = \frac{\frac{4\pi^2 i^{n+\ell}}{k}\frac{J_{n+\ell+1}(kr_0)}{r_0}(\sin\widetilde{\omega})^\ell C_n^{\ell+1}(\cos\widetilde{\omega}) Y_\ell^{m*}(\widetilde{\theta},\widetilde{\phi})}{1 - \frac{i\pi A\gamma_0 r_0^3}{2}\frac{J_{n+\ell+1}(kr_0)}{r_0}\frac{H_{n+\ell+1}^{(1)}(kr_0)}{r_0}} \quad (4.28)$$

Therefore, the wavefunction we were searching is

$$
\psi(\mathbf{r}) = \frac{4\pi^2}{k} \sum_{n,\ell,m} \Bigg[i^{n+\ell} N_{n,\ell}^2 \frac{J_{n+\ell+1}(kr)}{r}
$$

$$
\times (\sin\omega \sin\omega')^\ell C_n^{\ell+1}(\cos\omega) C_n^{\ell+1}(\cos\omega') Y_l^{m*}(\theta,\phi) Y_l^m(\theta',\phi') \Bigg]
$$

$$
+ \frac{2i\pi^3 A\gamma_0 r_0^3}{k} \sum_{n,\ell,m} \left\{ N_{n,\ell}^2 \left[\frac{i^{n+\ell} \frac{J_{n+\ell+1}(kr_0)}{r_0} (\sin\widetilde{\omega})^\ell C_n^{\ell+1}(\cos\widetilde{\omega}) Y_\ell^{m*}(\widetilde{\theta},\widetilde{\phi})}{1 - \frac{i\pi A\gamma_0 r_0^3}{2} \frac{J_{n+\ell+1}(kr_0)}{r_0} \frac{H_{n+\ell+1}^{(1)}(kr_0)}{r_0}} \right] \right.
$$

$$
\left. \times \frac{J_{n+\ell+1}(kr_<)}{r_<} \frac{H_{n+\ell+1}^{(1)}(kr_>)}{r_>} (\sin\omega)^\ell C_n^{\ell+1}(\cos\omega) Y_\ell^m(\theta,\phi) \right\} \quad (4.29)
$$

where the angles with tilde denote the angle of incidence of the plane wave.

4.1.2 Scattering Amplitudes, Cross-Sections, and the refraction index

There are several methods to calculate both differential and total cross-sections. The two most well-known are Born approximation, and partial-wave analysis [3, 11]. One of them is suitable for high-energy physical processes, and the other is suitable for low-energy physical processes. Admittedly, it is difficult to go beyond the second Born approximation or to calculate high-order corrections using the partial-wave analysis. Furthermore, as we've established, our potentials do not admit partial-wave analysis as it is usually taught. Here, since we have the exact form of the wavefunction, we investigate its behavior when $kr \to \infty$. Using Hankel's function asymptotic expansion (4.12) we can calculate the asymptotic behavior of the wavefunction (4.29) and compare with the limit,

$$
\lim_{kr\to\infty} \psi(r,\omega,\theta,\phi) = e^{ikr} + f_4(\omega,\theta,\phi)\frac{e^{ikr}}{r^{3/2}}. \quad (4.30)
$$

One readily obtains an exact expression for the scattering amplitude

$$
f_4(\omega,\theta,\phi) = \gamma_0 A R^{5/2} e^{-i\pi/4} \sum_{n,\ell,m} (-i)^{n+\ell} a_{n\ell m}(R) N_{n\ell}^2 (\sin\omega)^\ell C_n^{(\ell+1)}(\cos\omega) Y_\ell^m(\theta,\phi) j_{n+\ell+1/2}(kR), \quad (4.31)
$$

and using the orthogonality properties of the spherical harmonics and the associated Gegenbauer functions (3.78) it is straightforward to calculate the total cross-section,

$$
\sigma_4 = \gamma_0^2 A^2 R^5 \sum_{n,\ell,m} N_{n\ell}^2 \left|a_{n\ell m}(R)\right|^2 j_{n+\ell+1/2}^2(kR). \quad (4.32)
$$

Now, we present the quantum refraction index (2.101) for this system:

$$n = 1 + \frac{2\pi\gamma_0^2 R^{5/2} e^{-i\pi/4}}{k^2} \times \sum_{n,\ell,m} (-i)^{n+\ell} \sqrt{\frac{2\ell+1}{4\pi}} a_{n\ell m}(R) N_{n\ell}^2 (\sin\omega)^\ell C_n^{(\ell+1)}(\cos\omega) j_{n+\ell+1/2}(kR) \quad (4.33)$$

Since we used a constant coupling function and we are calculating the index using a hyperspherical coordinate system, there exists a spherical symmetry, which allow us to ignore the average calculation in (2.101). In order to investigate the behavior of these quantities — as well as to gain insight about the physical problem — it is interesting to plot them. So, in practical terms, one needs to truncate the series. Considering that $j_\ell(z) \to 0$, when $\ell > z$, we may use just a few terms of the series for low wave number. Also, to plot the differential cross section $d\sigma_4/d\Omega = \left|f_4(\omega,\theta,\phi)\right|^2$, it is easier to use cartesian coordinates $r = \sqrt{x^2+y^2+z^2+w^2}$, $\theta = \arccos\left(z/\sqrt{x^2+y^2+z^2}\right)$, $\phi = \arctan(y/x)$, and $\omega = \arccos(w/r)$, labeling the four axis Ox, Oy, Oz, Ow. Then we need to fix one of them, say, $w = 0$. Doing so, $d\sigma_4/d\Omega$ will depend on three variables x, y, z and its value can be presented in a color scale. In Figure 4.1 we present the differential cross section, with $w = 0$, from three distinct point-of-views when a plane wave impinges upon the four-dimensional spherical shell along Oz direction. We see the drastic influence that the choice for the $\tilde{\omega}$ angle inflicts upon the differential cross-section. In Figure 4.2 we change the incident wave direction to Ow and we plot the differential cross section considering $\omega = 0$, i.e, the Oz direction.

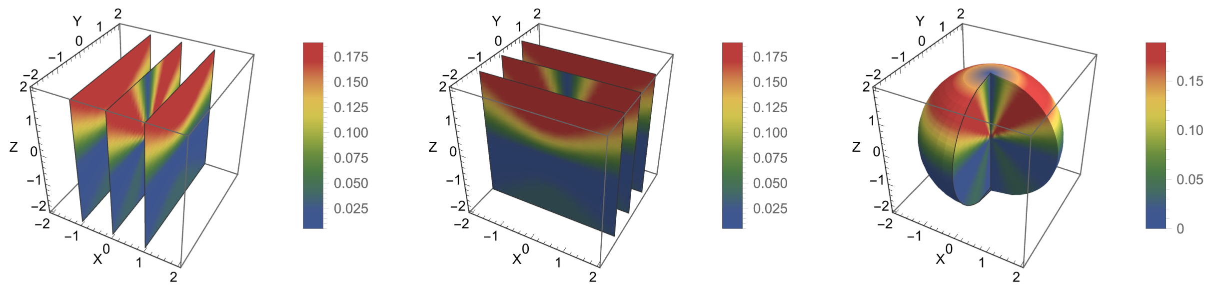


Figure 4.1: Plot of differential cross-section $d\sigma_4/d\Omega$ for the scattering of a plane wave, incident along Oz direction namely $(\widetilde{\omega}, \widetilde{\theta}, \widetilde{\phi}) = (\pi/2, 0, 0)$, with $k = 5$ and $\gamma_0 = 50$. In the left and middle figures we plot $d\sigma_4/d\Omega$ in a color scale, along stacked planes along X and Y directions, respectively. In the right figure we present the same quantity plotted along a center cut sphere, all of them with $w = 0$. Hypersphere radius is $R = 1$, we truncate the series at $n = 6$ and use atomic units where $\hbar = 2m^* = 1/2$.

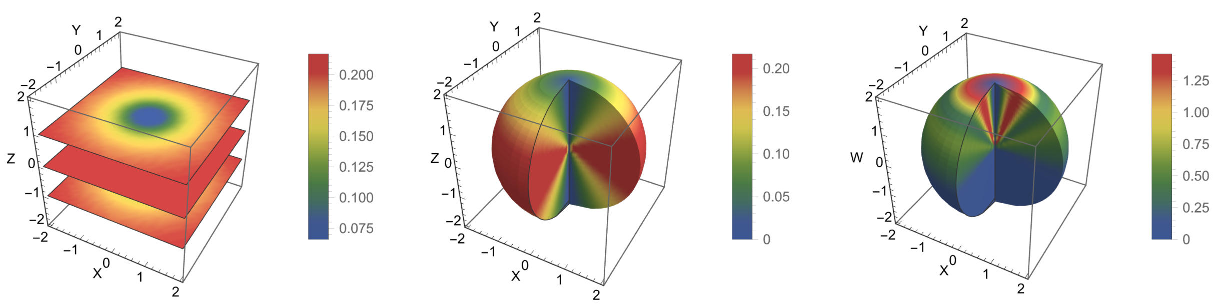


Figure 4.2: Plot of differential cross-section $d\sigma_4/d\Omega$ for the scattering of a plane wave, incident along Ow direction namely $(\widetilde{\omega}, \widetilde{\theta}, \widetilde{\phi}) = (0, 0, 0)$, with $k = 5$ and $\gamma_0 = 50$. In the left figure we plot $d\sigma_4/d\Omega$ in a color scale, along stacked planes along Z direction taking $w = 0$. In the middle and right figures we plot the same quantity plotted along center cut spheres with $w = 0$, and $z = 0$, respectively. Hypersphere radius is $R = 1$, we truncate the series at $n = 6$ and use atomic units where $\hbar = 2m^* = 1/2$.

The total cross-section is a function of the incident momentum $\vec{k}$ as well as the coupling constant γ_0, so it is a simple task to plot a surface $\sigma_4(\gamma_0, k)$ when we define the incident plane wave direction $(\widetilde{\omega}, \widetilde{\theta}, \widetilde{\phi})$. In Figure (4.3) we plot the total cross-section (4.32) as a function of k and γ_0. Observe that, in the left box, there are three regions where σ_4 is large. In the right box, there are five regions where the combination of the values of the coupling constant and the wavenumber results in a significant increase in the value of the total cross-section. This helps to reveal the meaning of the total scattering cross-section — it is proportional to the probability of scattering in any direction. For some sets of γ_0 and $\vec{k}$, the total cross-section is very small.

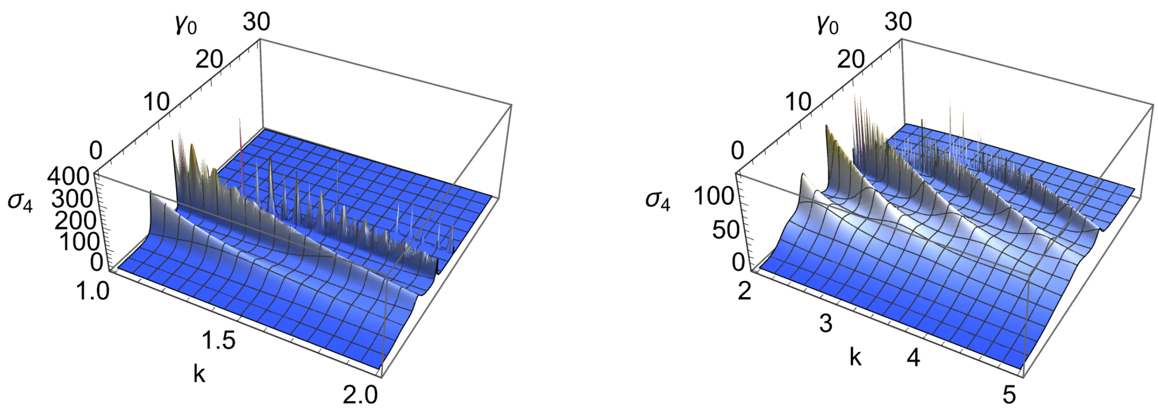
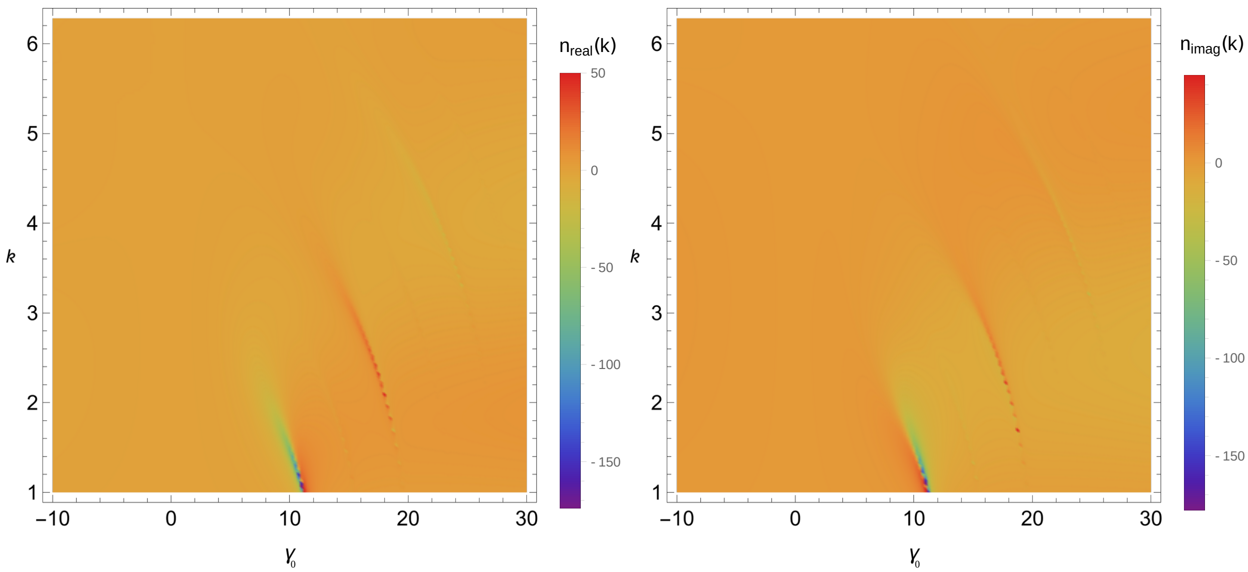


Figure 4.3: Plot of total cross-section σ_4 for the scattering of a plane wave, incident along Ow direction namely $(\widetilde{\omega}, \widetilde{\theta}, \widetilde{\phi}) = (0, 0, 0)$, as a function of k and γ_0. Observe that there are certain curves — relationships between γ_0 and k — which yield a higher total cross section. We split the figure in two parts to produce a better visualization of the ripples of the right figure. Hypersphere radius is $R = 1$, we truncate the series at $n = 6$ and use atomic units where $\hbar = 2m^* = 1/2$.

In what follows, we show the behavior of the quantum refraction index (4.33) in Figure (4.4), with fixed ω. We use color map, and show n as a function of the wave number k and γ_0 varying linearly. We choose arbitrarily $\omega = \pi/2$.



(a) Re(n)

(b) Im(n)

Figure 4.4: Real and imaginary parts of the quantum refraction index, where we set $\omega = \pi/2$. Here the angles θ and ϕ are set to zero, to represent the forward scattering amplitude.

The intricate pattern of peaks and valleys is a result of the scattering amplitude (4.31). One may set γ varying linearly because we choose $\gamma_0 = \text{const}$ previously. There are sets of points (γ_0, k) which allows the wavefunction to scatter, while most of the other values for these quantities makes the scattering event not to take place. The impinging plane-wave could not have enough momentum and/or the target could have such a strong coupling factor that renders the scattering of the wavefunction impossible.

4.2 Scattering by a 4D Dirac Hypersphere

There are essentially two possible choices for hyper-spherical coordinates in four spatial dimensions [47]. In one of them, there are two radial coordinates and two angular coordinates. The second one has a single radial variable and three angular variables. The latter can also be used to investigate the interaction between two bodies in a plane.

We can apply the same methodology of the previous section not for a four-dimensional spherical shell but for a solid hypersphere. More than letting the Dirac delta run along a given surface S, we consider a hypersphere filled with Dirac delta functions and call such a region a *Dirac medium*. To model such solid hypersphere, with radius R, we introduce the potential,

$$V_4(r',\omega',\theta',\phi') = \int_0^R \int_0^\pi \int_0^\pi \int_0^{2\pi} \gamma(v,s,t,u) \frac{\delta(r'-v)\delta(\omega'-s)\delta(\theta'-t)\delta(\phi'-u)}{J}\, dV', \qquad (4.34)$$

where $dV' = v^3 \sin^2 s \sin t \; ds\; dt\; du\; dv$ and J is the Jacobian. Substituting the potential V_4 into the Lippmann–Schwinger equation and integrating over the primed variables we obtain,

$$\begin{aligned} \psi(r,\omega,\theta,\phi) &= \varphi(r,\omega,\theta,\phi) + \frac{A\pi i}{2} \sum_{n,\ell,m} N^2_{n,\ell} (\sin\omega)^\ell C_n^{(\ell+1)}(\cos\omega) Y_\ell^m(\theta,\phi) \int_0^R \int_0^\pi \int_0^\pi \int_0^{2\pi} \\ &\quad \gamma(v,s,t,u) v^3 \frac{J_{n+\ell+1}(kr_<)}{r_<} \frac{H^{(1)}_{n+\ell+1}(kr_>)}{r_>} (\sin s)^{\ell+2} C_n^{(\ell+1)}(\cos s) \sin t \\ &\quad \times Y_\ell^{m*}(t,u) \psi(v,s,t,u)\; du\; dt\; ds\; dv. \end{aligned} \qquad (4.35)$$

This is a Lippmann–Schwinger equation of Volterra type [15, 45]. Here, once again we use the notation $r_< = \min(r,r')$ and $r_> = \max(r,r')$ and after integration over r' one must take $r_< = \min(r,v)$ and $r_> = \max(r,v)$. Again, $N^2_{n\ell}$ is given by (4.10). Indeed, the Lippmann–Schwinger equation reformulated as a Volterra Lippmann–Schwinger equation was studied by Kouri [49] in the context of the quantum inverse scattering theory [50]. Therein, Kouri *et al* transformed the Fredholm Lippmann–Schwinger equation into a Volterra Lippmann–Schwinger equation, and this transformation brought several advantages, such as uniform and absolute convergence as well as the possibility of solving the inverse problem exactly.

4.2.1 Exterior Domain

Let us commence with the wavefunction valid at the region $r > R$ since it is simpler to obtain. In this domain $r_< = v$ and $r_> = r$ thus, the above integral equation suggests the definition of a coefficient,

$$\begin{aligned} \alpha_{n\ell m} &= \int_0^R dv\; v^2 \int_0^\pi ds \int_0^\pi dt \int_0^{2\pi} du\; \gamma(v,s,t,u) J_{n+\ell+1}(kv) (\sin s)^{\ell+2} C_n^{(\ell+1)}(\cos s) \\ &\quad \times Y_\ell^{m*}(t,u) \sin t\; \psi(v,s,t,u)\;, \end{aligned} \qquad (4.36)$$

observing that due to the integrations over primed variables we have now $r_< = \min(r,v)$ and $r_> = \max(r,v)$. The wavefunction reads,

$$\psi_{ext}(r,\omega,\theta,\phi) = \varphi(r,\omega,\theta,\phi) + \frac{A\pi i}{2} \sum_{n,\ell,m} \alpha_{n\ell m} N^2_{n,\ell} (\sin\omega)^\ell C_n^{(\ell+1)}(\cos\omega) Y_\ell^m(\theta,\phi) \frac{H^{(1)}_{n+\ell+1}(kr)}{r}. \qquad (4.37)$$

For simplicity we take a constant coupling strength, i.e., let us consider $\gamma(r,\omega,\theta,\phi)=\gamma_0$. Then equation (4.36) can be written as,

$$\alpha_{n\ell m}=\gamma_0 A_{n\ell m}, \tag{4.38}$$

where, of course

$$A_{n\ell m}=\int_0^R dv\, v^2\int_0^\pi ds\,\int_0^\pi dt\,\int_0^{2\pi} du\; J_{n+\ell+1}(kv)(\sin s)^{\ell+2}C_n^{(\ell+1)}(\cos s)Y_\ell^{m*}(t,u)\sin t\;\psi(v,s,t,u)\;,$$

thus, evaluating the above wavefunction at $r=R$, multiplying it by,

$$r^2 J_{n'+\ell'+1}(kr)(\sin\omega)^{\ell'+2}C_{n'}^{(\ell'+1)}(\cos\omega)Y_{\ell'}^{m'*}(\theta,\phi), \tag{4.39}$$

where n',ℓ' and m' are integer numbers in the physically allowed domain, we integrate over the hypersphere to obtain an equation for $A_{n\ell m}$ which can be easily solved,

$$A_{n\ell m}=\frac{c_{n\ell m}}{1-\dfrac{\gamma_0\pi A i}{2}I_{n\ell}}, \tag{4.40}$$

where we set

$$I_{n\ell}=\int_0^R dr\; rJ_{n+\ell+1}(kr)H^{(1)}_{n+\ell+1}(kr), \tag{4.41}$$

and $c_{n\ell m}$ are the plane wave partial-wave like coefficients,

$$c_{n'\ell'm'}=\int_0^R\int_0^\pi\int_0^\pi\int_0^{2\pi}\varphi(r,\omega,\theta,\phi)r^2J_{n'+\ell'+1}(kr)(\sin\omega)^{\ell'}C_{n'}^{(\ell'+1)}(\cos\omega)Y_{\ell'}^{m'}(\theta,\phi)d\phi\; d\theta\; d\omega\; dr, \tag{4.42}$$

which on their turn can be calculated easily if one consider φ to be a plane wave (4.17) with wavenumber $\mathbf{k}=k(\cos\tilde\phi\sin\tilde\theta\sin\tilde\omega,\sin\tilde\phi\sin\tilde\theta\sin\tilde\omega,\cos\tilde\theta\sin\tilde\omega,\cos\tilde\omega)$, breeding

$$c_{n'\ell'm'}=(\sin\tilde\omega)^{\ell'}C_{n'}^{(\ell'+1)}(\cos\tilde\omega)Y_{\ell'}^{m'*}(\tilde\theta,\tilde\phi)\int_0^R dr\; rJ^2_{n'+\ell'+1}(kr). \tag{4.43}$$

The beseeched wavefunction, valid in the exterior domain $r>R$, is given by the substitution of (4.38), (4.40) and (4.43) into (4.37).

4.2.2 Interior Domain

For the interior domain $r<R$, in equation (4.35), we will split the domain into two. When we take a shell with radius $r<R$, there will be inner shells such that $0\le v\le r$ and outer shells such that

$r \leq v \leq R$. So, the integral equation (4.35) becomes,

$$\begin{aligned}\psi(r,\omega,\theta,\phi) &= \varphi(r,\omega,\theta,\phi) + \frac{A\pi i}{2}\sum_{n,\ell,m} N_{n,\ell}^2 (\sin\omega)^\ell C_n^{(\ell+1)}(\cos\omega) Y_\ell^m(\theta,\phi) \\ &\times \int_0^\pi \int_0^\pi \int_0^{2\pi} \sin t\, (\sin s)^{\ell+2} C_n^{(\ell+1)}(\cos s) Y_\ell^{m*}(t,u)\, du\, dt\, ds \\ &\times \left\{ \int_0^r + \int_r^R \right\} \gamma(v,s,t,u) \frac{J_{n+\ell+1}(kr_<)}{r_<} \frac{H_{n+\ell+1}^{(1)}(kr_>)}{r_>} \psi(v,s,t,u) v^3\, dv,\end{aligned} \tag{4.44}$$

in the first integral $r_< = v, r_> = r$ and, in the second one $r_< = r, r_> = v$. This time, equation (4.44) begs for the definitions

$$\begin{aligned}\mathcal{R}_{n\ell m}(r) &= \int_r^R dv\, v^2 \int_0^\pi ds \int_0^\pi dt \int_0^{2\pi} du\, \gamma(v,s,t,u) H_{n+\ell+1}^{(1)}(kv) (\sin s)^{\ell+2} C_n^{(\ell+1)}(\cos s) \\ &\times Y_\ell^{m*}(t,u) \sin t\, \psi(v,s,t,u)\ ,\end{aligned} \tag{4.45}$$

and

$$\begin{aligned}\mathcal{T}_{n\ell m}(r) &= \int_0^r dv\, v^2 \int_0^\pi ds \int_0^\pi dt \int_0^{2\pi} du\, \gamma(v,s,t,u) J_{n+\ell+1}(kv) (\sin s)^{\ell+2} C_n^{(\ell+1)}(\cos s) \\ &\times Y_\ell^{m*}(t,u) \sin t\, \psi(v,s,t,u)\ ,\end{aligned} \tag{4.46}$$

which in turn can be interpreted as position-dependent *reflection* and *transmission amplitudes*, respectively[1]. The interior wavefunction now looks like

$$\begin{aligned}\psi_{int}(r,\omega,\theta,\phi) &= \varphi(r,\omega,\theta,\phi) + Aik\sqrt{\frac{\pi}{2}} \sum_{n,\ell,m} \alpha_{n\ell m} N_{n,\ell}^2 (\sin\omega)^\ell C_n^{(\ell+1)}(\cos\omega) Y_\ell^m(\theta,\phi) \\ &\times \left[\mathcal{R}_{n\ell m}(r) \frac{j_{n+\ell+1/2}(kr)}{\sqrt{kr}} + \mathcal{T}_{n\ell m}(r) \frac{h_{n+\ell+1/2}^{(1)}(kr)}{\sqrt{kr}} \right].\end{aligned} \tag{4.47}$$

Said in other, equivalent words, at the interior domain we have a superposition of waves — originated by the incident plane wave — which, on its turn, undergoes multiple reflections at the inner shells and they are represented by the spherical Bessel functions; there are also waves that undergo multiple transmissions at the inner shells and we represent them by the spherical Hankel functions. We also notice, from (4.45) and (4.46), that once the wave reaches the last shell, $r = R$, the reflection amplitude $\mathcal{R}_{n\ell m}(R) = 0$. The transmission amplitude vanishes at the hypersphere center, i.e., $\mathcal{T}_{n\ell m}(0) = 0$.

[1]For an one-dimensional introduction to the transmission and reflection amplitudes, see, for example, Merzbacher [31].

In the special case we are studying, the coupling strength $\gamma(\cdot) = \gamma_0$ is constant so equations (4.45) and (4.46) take simpler forms, and we represent them now as (notice the change in the font style):

$$\mathcal{R}_{n\ell m}(r) = \gamma_0 R_{n\ell m}(r), \qquad \mathcal{T}_{n\ell m}(r) = \gamma_0 T_{n\ell m}(r). \tag{4.48}$$

With the objective to calculate these functions we follow the technique outlined in the previous subsection. Thus, we multiply (4.47) by,

$$r^2 J_{n'+\ell'+1}(kr)(\sin\omega)^{\ell'+2} C_{n'}^{(\ell'+1)}(\cos\omega) Y_{\ell'}^{m'*}(\theta,\phi), \tag{4.49}$$

and integrate over the three angular variables and over r from r'' to R and write the result in terms of spherical Bessel and Hankel functions,

$$\begin{aligned} R_{n\ell m}(r'') &= f_{n\ell m}(r'') + \gamma_0 Aik \int_{r''}^{R} dr\, r^2 h^{(1)}_{n+\ell+1/2}(kr) \Big[R_{n\ell m}(r) j_{n+\ell+1/2}(kr) \\ &\quad + T_{n\ell m}(r) h^{(1)}_{n+\ell+1/2}(kr) \Big]. \end{aligned} \tag{4.50}$$

Next, we apply the same idea to find an equation for the transmission amplitude functions, obtaining

$$\begin{aligned} T_{n\ell m}(r'') &= g_{n\ell m}(r'') + \gamma_0 Aik \int_{0}^{r''} dr\, r^2 j_{n+\ell+1/2}(kr) \Big[R_{n\ell m}(r) j_{n+\ell+1/2}(kr) \\ &\quad + T_{n\ell m}(r) h^{(1)}_{n+\ell+1/2}(kr) \Big]. \end{aligned} \tag{4.51}$$

the above equations (4.50) and (4.51) are Volterra integral equations [51], so to solve the scattering problem at the interior domain, we must tackle a system of coupled Volterra equations. While one may say it seems like a formidable task, we do not give up. Instead, we can transform these equations into more familiar first-order ordinary differential equations. To this end, we simply differentiate (4.50) and (4.51) with respect to r'' to come upon

$$\begin{aligned} \frac{dR_{n\ell m}(r'')}{dr''} &= \frac{df_{n\ell m}(r'')}{dr''} - \gamma_0 Aik h^{(1)}_{n+\ell+1/2}(kr'') \Big[R_{n\ell m}(r'') j_{n+\ell+1/2}(kr'') \\ &\quad + T_{n\ell m}(r'') h^{(1)}_{n+\ell+1/2}(kr'') \Big] (r'')^2, \end{aligned} \tag{4.52}$$

and

$$\begin{aligned} \frac{dT_{n\ell m}(r'')}{dr''} &= \frac{dg_{n\ell m}(r'')}{dr''} + \gamma_0 Aik j_{n+\ell+1/2}(kr'') \Big[R_{n\ell m}(r'') j_{n+\ell+1/2}(kr'') \\ &\quad + T_{n\ell m}(r'') h^{(1)}_{n+\ell+1/2}(kr'') \Big] (r'')^2, \end{aligned} \tag{4.53}$$

where we set, for economy,

$$\frac{df_{n\ell m}(r)}{dr} = -8\pi i^{n+\ell} r^3 (\sin\tilde{\omega})^\ell C_n^{(\ell+1)}(\cos\tilde{\omega}) Y_\ell^{m*}(\tilde{\theta},\tilde{\phi})\; j^2_{n+\ell+1/2}(kr), \tag{4.54}$$

and

$$\frac{dg_{n\ell m}(r)}{dr} = 8\pi i^{n+\ell} r^3 (\sin\tilde{\omega})^\ell C_n^{(\ell+1)}(\cos\tilde{\omega}) Y_\ell^{m*}(\tilde{\theta},\tilde{\phi})\; j_{n+\ell+1/2}(kr) h^{(1)}_{n+\ell+1/2}(kr). \tag{4.55}$$

These expressions are so because we had

$$\begin{aligned} f_{n\ell m}(r) &= \int_r^R dv\; v^2 \int_0^\pi ds \int_0^\pi dt \int_0^{2\pi} du\; \gamma(v,s,t,u) H^{(1)}_{n+\ell+1}(kv)(\sin s)^{\ell+2} C_n^{(\ell+1)}(\cos s) \\ &\quad \times Y_\ell^{m*}(t,u) \sin t\; \varphi(v,s,t,u)\;, \end{aligned} \tag{4.56}$$

and

$$\begin{aligned} g_{n\ell m}(r) &= \int_0^r dv\; v^2 \int_0^\pi ds \int_0^\pi dt \int_0^{2\pi} du\; \gamma(v,s,t,u) J_{n+\ell+1}(kv)(\sin s)^{\ell+2} C_n^{(\ell+1)}(\cos s) \\ &\quad \times Y_\ell^{m*}(t,u) \sin t\; \varphi(v,s,t,u)\;, \end{aligned} \tag{4.57}$$

where we did suppress the primes. Now, it is an almost effortless task to solve the system composed by equations (4.52)-(4.55) using Mathematica 12.3.1.

We plot in Figure (4.5) the square modulus of the first two non-vanishing reflection and transmission functions for a plane wave impinging upon the hypersphere along Oz-direction. Observe that reflection vanishes at $r = R$ as well as transmission also vanishes when $r = 0$. Also, the reflection function increases when the wavefunction penetrates the hypersphere, while the transmission function reaches maxima around $r = 0.4R$ and around $r = 0.7R$.

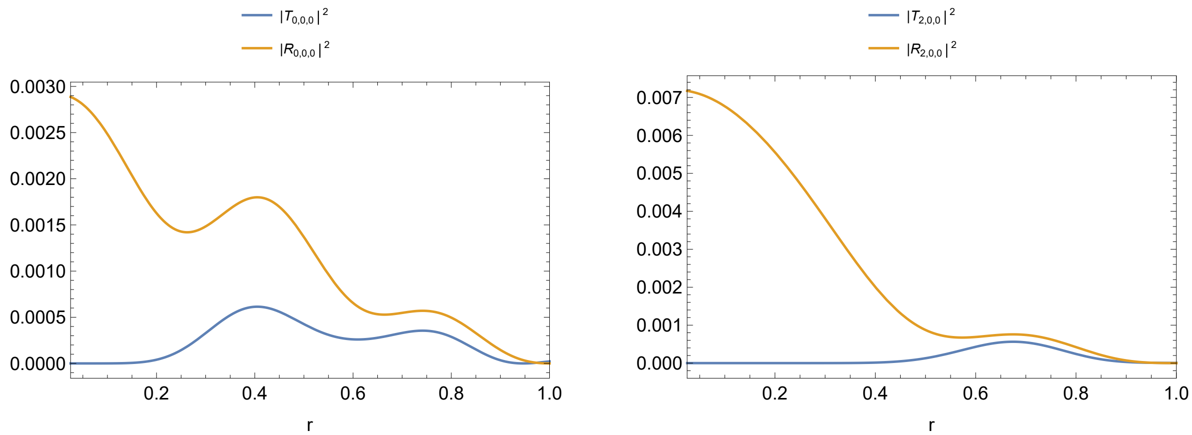


Figure 4.5: Plot of position-dependent reflection and transmission functions given by equations (4.45) and (4.46), respectively. The incident wave propagates along Oz direction namely $(\tilde{\omega}, \tilde{\theta}, \tilde{\phi}) = (\pi/2, 0, 0)$, with $k = 2\pi$ and $\gamma_0 = 100$. In the left figure we plot $|R_{000}|^2$ and $|T_{000}|^2$. In the right we plot $|R_{200}|^2$ and $|T_{200}|^2$. We take $R = 1$ and truncate the series at $n = 6$ and we use atomic units where $\hbar = 2m^* = 1/2$.

We see, rather alarmingly, that $|R_{000}|^2 + |T_{000}|^2 \neq 1$. Why is that? Because we are only considering one set of quantum numbers, namely, $(0, 0, 0)$. The summation throughout all quantum numbers yields the probability conserving result $|R|^2 + |T|^2 = 1$.

4.2.3 Scattering Amplitudes and Cross Section

We can also calculate straightforwardly — using (4.12) — the scattering amplitude for four-dimensional Dirac hypersphere, attaining

$$f_4(\omega, \theta, \phi) = \gamma_0 A \sqrt{\frac{\pi}{2k}} e^{-i\pi/4} \sum_{n,\ell,m} (-i)^{n+\ell} A_{n\ell m} N_{n\ell}^2 (\sin\omega)^\ell C_n^{(\ell+1)}(\cos\omega) Y_\ell^m(\theta, \phi), \tag{4.58}$$

as well as the total cross-section,

$$\sigma_{4s} = \frac{\gamma_0^2 A^2 \pi}{2k} \sum_{n,\ell,m} N_{n\ell}^2 \left|A_{n\ell m}\right|^2. \tag{4.59}$$

We can, once again, calculate the quantum refraction index (2.101). As in the case of the hyper-spherical shell, we use spherical symmetry to facilitate our calculations. The quantum refraction index is

$$n = 1 + \frac{2\pi\sqrt{\pi}\gamma_0^2 A e^{-i\pi/4}}{k^2\sqrt{2k}} \sum_{n,\ell,m} (-i)^{n+\ell} \sqrt{\frac{2\ell+1}{4\pi}} A_{n\ell m} N_{n\ell}^2 (\sin\omega)^\ell C_n^{(\ell+1)}(\cos\omega). \tag{4.60}$$

We plot in Figure 4.6 the square modulus of the scattering amplitude $f_4(\omega, \theta, \phi)$ for an incident plane wave impinging upon the four-dimensional Dirac hypersphere along Oz taking $w = 0$.

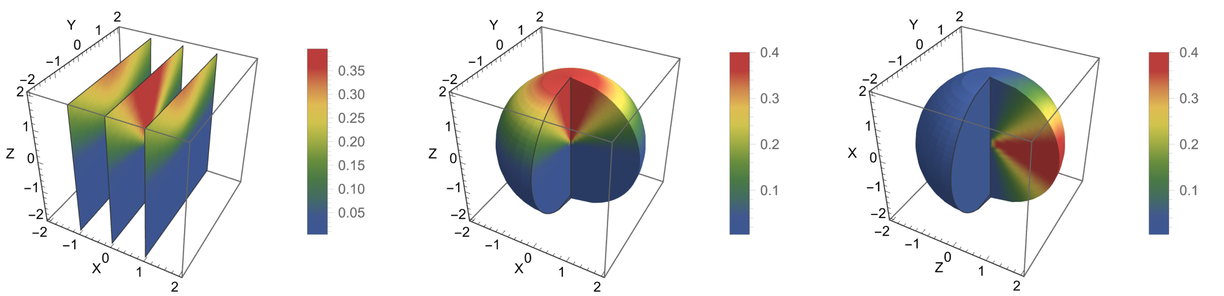


Figure 4.6: Plot of differential cross section $d\sigma_4/d\Omega$ for the scattering of a plane wave by a four-dimensional Dirac hypersphere. The incident wave propagates along Oz direction namely $(\tilde{\omega}, \tilde{\theta}, \tilde{\phi}) = (\pi/2, 0, 0)$, with $k = 5$ and $\gamma_0 = 50$. In the left figure we plot $d\sigma_4/d\Omega$ in a color scale, along stacked planes in the X direction. In the middle and right figures we present the same quantity plotted along a center cut sphere with $w = 0$. We take $R = 1$ and truncate the series at $n = 6$ and we use atomic units where $\hbar = 2m^* = 1/2$.

In Figure 4.7 we illustrate the dependence of the total cross-section, given by equation (4.59), as a function of the wavenumber k and the coupling constant γ_0. In the left box, we selected k to be the first four zeros of $j_{1/2}$, and in the right box, the wavenumber is one of the first four zeros of $j_{3/2}$. Observe that there are certain values of γ_0 which produce sharp peaks and increases the total cross-section, e.g., when $k = \pi$ and $\gamma_0 = 44$ (left blue curve); as well as $k = 4.493$ and $\gamma_0 = 59$ (right blue curve).

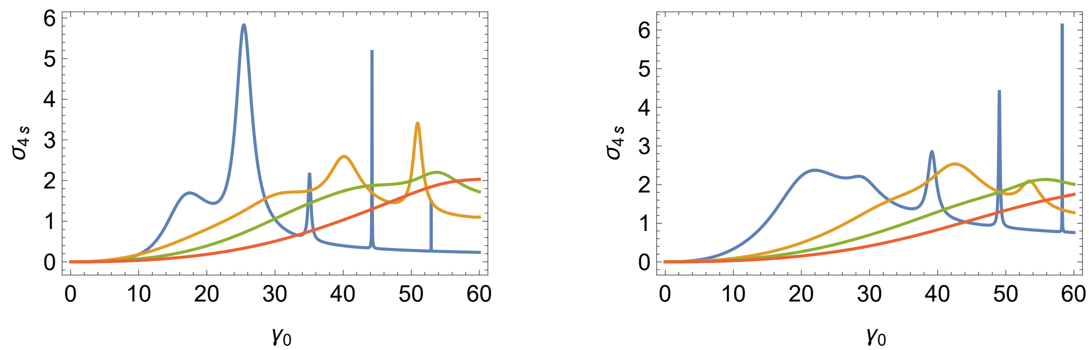
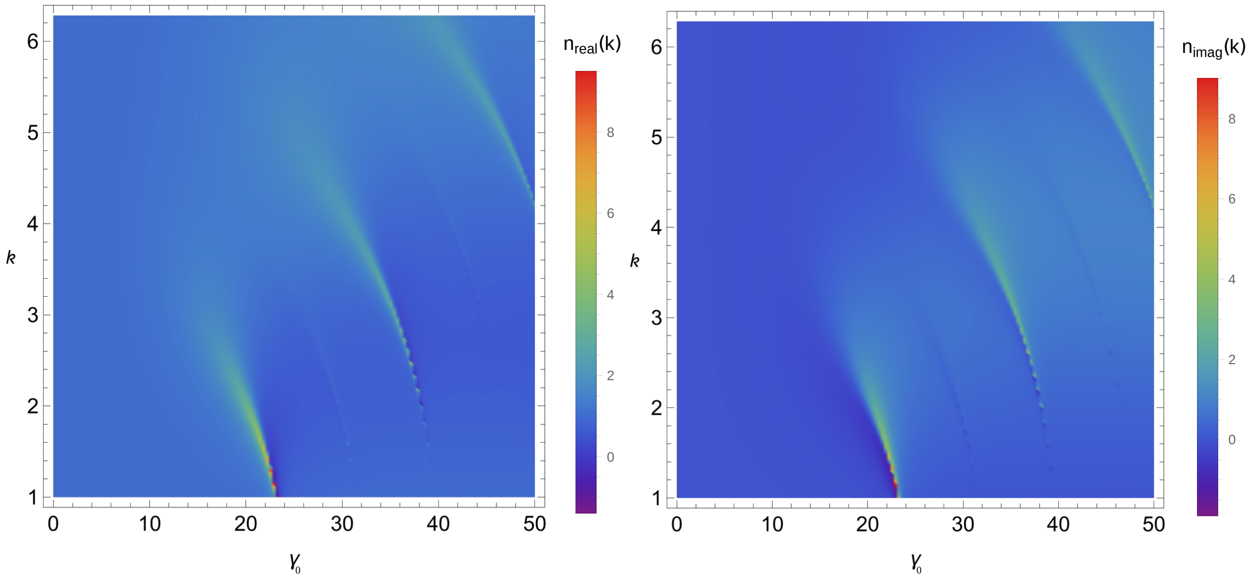


Figure 4.7: Plot of total cross section σ_{4s} for the scattering of a plane wave by a four-dimensional Dirac hypersphere, incident along Oz direction namely $(\tilde{\omega}, \tilde{\theta}, \tilde{\phi}) = (\pi/2, 0, 0)$. In the left figure we plot four curves $\sigma_{4s} = \sigma_{4s}(\gamma_0)$ taking the wave number to be a zero of $j_{1/2}$, namely, $k = \pi, 2\pi, 3\pi$ and 4π (blue, yellow, green and red, respectively). Observe that there are certain values of γ_0 which produce a sharp peak. In the right box we also plot four curves $\sigma_{4s} = \sigma_{4s}(\gamma_0)$ now taking the wave number to be a zero of $j_{3/2}$, namely, $4.493; 7.725; 10.904; 14.066$ (blue, yellow, green and red, respectively). We take $R = 1$ and truncate the series at $n = 12$ and we use atomic units where $\hbar = 2m^* = 1/2$.

In Figure 4.8 we reveal the quantum refraction index with color map, shown as a function of the wave number and γ varying linearly. We set arbitrarily $\omega = \pi/2$.



(a) Re(n) (b) Im(n)

Figure 4.8: Real and imaginary parts of the quantum refraction index, with $\omega = \pi/2$. The other two angles, θ and ϕ are zero, due to the forward scattering amplitude.

We show the real and imaginary parts of the quantum refraction index n. It is a combination of values of γ_0 and k that produces the maxima points we see in lighter colors at the peaks, which makes us recall figure 4.3. This daedal relation between n, γ_0 and k produces those circular-like patterns. As for the physical meaning of this mysterious quantity n, one may see that depending on the value of γ_0 in relation to k, which apparently obey a circular-like function, we can maximize (or minimize) the probability of detecting the wavefunction after the scattering event, if we are able to fine-tune γ_0. Bear in mind the fact that here γ_0 varies linearly, but it is a special case. One may conceive a situation where n is an arbitrary function of γ_0, in which event the real and imaginary parts of n would possibly look very different.

4.3 Scattering in a two-particle system

Let us consider two particles 1 and 2, with arbitrary positions $\mathbf{r_1}$ and $\mathbf{r_2}$. Since the positions are arbitrary, let $\mathbf{r_1} \,//\, \hat{\mathbf{j}}$ and $\mathbf{r_2} \,//\, \hat{\mathbf{i}}$. In this way, we can construct an orthogonal coordinate system – a 6-dimensional hyper-spherical coordinate system.

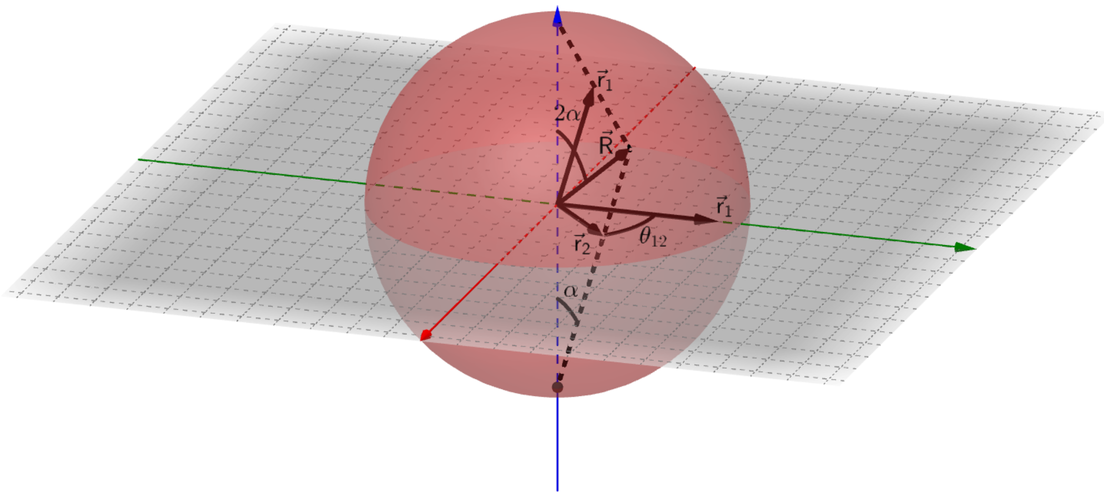


Figure 4.9: Illustration of a 3D sphere with an additional angle α.

Looking at Figure 4.9, we are led to define not only a distance

$$r = R \coloneqq \sqrt{r_1^2 + r_2^2} \tag{4.61}$$

but also a angle α subject to

$$\cos\alpha \coloneqq \frac{r_1}{r} \tag{4.62}$$

such that the points $r_1 = (x_1, y_1, z_1)$ and $r_2 = (x_2, y_2, z_2)$ can be written

$$\begin{cases} x_1 = r_1 \sin\theta_1 \cos\phi_1 = r\cos\alpha \sin\theta_1 \cos\phi_1 \\ y_1 = r_1 \sin\theta_1 \sin\phi_1 = r\cos\alpha \sin\theta_1 \sin\phi_1 \\ z_1 = r_1 \cos\theta_1 = r\cos\alpha\cos\theta_1 \end{cases} \tag{4.63}$$

$$\begin{cases} x_2 = r_2 \sin\theta_2 \cos\phi_2 = 2\sin\alpha \sin\theta_2 \cos\phi_2 \\ y_2 = r_2 \sin\theta_2 \sin\phi_2 = r\sin\alpha \sin\theta_2 \sin\phi_2 \\ z_2 = r_2 \cos\theta_2 = r\sin\alpha\cos\theta_2 \end{cases} \tag{4.64}$$

The scale factors are easily calculated using the definition

$$h_i^2 = \sum_{j=1}^{\mathcal{N}} \left(\frac{\partial x_j}{\partial \xi_i} \right)^2 \tag{4.65}$$

where $i = \{r, \alpha, \theta_1, \phi_1, \theta_2, \phi_2\}$ and ξ is a generic variable, to be specified by the said index. Calculating, we get

$$\begin{aligned} h_r &= 1 \\ h_\alpha &= r \\ h_{\theta_1} &= r\cos\alpha \\ h_{\phi_1} &= r\cos\alpha\sin\theta_1 \\ h_{\theta_2} &= r\sin\alpha \\ h_{\phi_2} &= r\sin\alpha\sin\theta_2 \end{aligned} \tag{4.66}$$

such that

$$\sqrt{g} = \prod_i h_i = r^5 \cos^2\alpha \sin^2\alpha \sin\theta_1 \sin\theta_2 \tag{4.67}$$

In order to find the Green's function, we must solve the 6-dimensional Helmholtz equation

$$(\nabla_1^2 + \nabla_2^2 + k^2)\psi = 0 \tag{4.68}$$

which can be rewritten simply as

$$\frac{1}{\sqrt{g}} \sum_{i=1}^{6} \frac{\partial}{\partial \xi_i} \left(\frac{\sqrt{g}}{g_{ii}} \frac{\partial \psi}{\partial \xi_i} \right) + k^2 \psi = 0 \tag{4.69}$$

Using equations (4.66), we get

$$\begin{aligned} \frac{1}{r^5}\frac{\partial}{\partial r}\left(r^5 \frac{\partial\psi}{\partial r}\right) &+ \frac{1}{r^2\cos^2\alpha\sin^2\alpha}\frac{\partial}{\partial\alpha}\left(\cos^2\alpha\sin^2\alpha\frac{\partial\psi}{\partial\alpha}\right) \\ &+ \frac{1}{r^2\cos^2\alpha\sin\theta_1}\frac{\partial}{\partial\theta_1}\left(\sin\theta_1\frac{\partial\psi}{\partial\theta_1}\right) + \frac{1}{r^2\cos^2\alpha\sin^2\theta_1}\frac{\partial^2\psi}{\partial\phi_1^2} \\ &+ \frac{1}{r^2\cos^2\alpha\sin\theta_2}\frac{\partial}{\partial\theta_1}\left(\sin\theta_2\frac{\partial\psi}{\partial\theta_2}\right) + \frac{1}{r^2\cos^2\alpha\sin^2\theta_2}\frac{\partial^2\psi}{\partial\phi_2^2} + k^2\psi = 0 \end{aligned} \tag{4.70}$$

which sugests us the following *ansatz*

$$\psi(r, \alpha, \theta_1, \theta_2, \phi_1, \phi_2) = R(r)A(\alpha)Y_{\ell_1}^{m_1}(\theta_1, \phi_1)Y_{\ell_2}^{m_2}(\theta_2, \phi_2) \tag{4.71}$$

Consequently, equation (4.70) evolves to

$$\frac{1}{r^5 R}\frac{d}{dr}\left(r^5\frac{dR}{dr}\right)+k^2 + \frac{1}{r^2}\left\{\frac{1}{A\cos^2\alpha\sin^2\alpha}\frac{d}{d\alpha}\left(\cos^2\alpha\sin^2\alpha\frac{dA}{d\alpha}\right)-\left[\frac{\ell_1(\ell_1+1)}{\cos^2\alpha}+\frac{\ell_2(\ell_2+1)}{\sin^2\alpha}\right]\right\}=0 \quad (4.72)$$

The latter is separated if there is a constant B such that

$$\frac{1}{r^5 R}\frac{d}{dr}\left(r^5\frac{dR}{dr}\right)+k^2-\frac{B}{r^2}=0 \quad (4.73a)$$

$$\frac{1}{A\cos^2\alpha\sin^2\alpha}\frac{d}{d\alpha}\left(\cos^2\alpha\sin^2\alpha\frac{dA}{d\alpha}\right)-\left[\frac{\ell_1(\ell_1+1)}{\cos^2\alpha}+\frac{\ell_2(\ell_2+1)}{\sin^2\alpha}\right]+B=0 \quad (4.73b)$$

Upon simple manipulation, (4.73) yields

$$\frac{d^2R}{dr^2}+\frac{5}{r}\frac{dR}{dr}+\left[k^2-\frac{B}{r^2}\right]R=0 \quad (4.74a)$$

$$\frac{1}{\cos^2\alpha\sin^2\alpha}\frac{d}{d\alpha}\left(\cos^2\alpha\sin^2\alpha\frac{dA}{d\alpha}\right)-\left[\frac{\ell_1(\ell_1+1)}{\cos^2\alpha}+\frac{\ell_2(\ell_2+1)}{\sin^2\alpha}+B\right]A=0 \quad (4.74b)$$

It is easy to see that B is the eigenvalue of the angular equation in (4.74b). To solve the equation for the angular function, one possibility is to substitute

$$z=\sin^2\alpha \quad (4.75)$$

which naturally produces

$$\frac{dA}{d\alpha}=\frac{dA}{dz}\frac{dz}{d\alpha}=2\sin\alpha\cos\alpha\frac{dA}{dz}=2\sqrt{z}\sqrt{1-z}\frac{dA}{dz}$$

and then

$$\begin{aligned}\frac{d^2A}{d\alpha^2}&=\frac{d}{d\alpha}\left(\frac{dA}{d\alpha}\right)=2\sqrt{z}\sqrt{1-z}\frac{d}{dz}\left(2\sqrt{z}\sqrt{1-z}\frac{dA}{dz}\right)\\&=4\sqrt{z}\sqrt{1-z}\left[\frac{d}{dz}(\sqrt{z}\sqrt{1-z})\frac{dA}{dz}+\sqrt{z}\sqrt{1-z}\frac{d^2A}{dz^2}\right]\\&=4\sqrt{z}\sqrt{1-z}\left[\left(\frac{\sqrt{1-z}}{2\sqrt{z}}-\frac{\sqrt{z}}{2\sqrt{1-z}}\right)\frac{dA}{dz}+\sqrt{z}\sqrt{1-z}\frac{d^2A}{dz^2}\right]\\&=\left[\frac{4(1-z)}{2}-\frac{4z}{2}\right]\frac{dA}{dz}+4z(1-z)\frac{d^2A}{dz^2}\\&=4z(1-z)\frac{d^2A}{dz^2}+(2-4z)\frac{dA}{dz}.\end{aligned}$$

Working out the derivatives in (4.74b) brings about

$$\frac{d^2A}{d\alpha^2} + 2(\cot\alpha - \tan\alpha)\frac{dA}{d\alpha} - \left[\frac{\ell_1(\ell_1+1)}{\cos^2\alpha} + \frac{\ell_2(\ell_2+1)}{\sin^2\alpha} + B\right] A = 0$$

which, transforming the variable α to z, gives

$$4z(1-z)\frac{d^2A}{dz^2} + (6-12z)\frac{dA}{dz} + \left[B - \frac{\ell_1(\ell_1+1)}{1-z} - \frac{\ell_2(\ell_2+1)}{z}\right] A. \tag{4.76}$$

To go further, we must perform a couple more changes of variables. The first one is to set

$$A(z) = z^{\ell_2/2}(1-z)^{\ell_1/2}y(z)$$

leading to a hypergeometric equation

$$z(1-z)\frac{d^2y}{dz^2} + \left[\frac{3}{2} + \ell_2 - (\ell_1+\ell_2+3)\,z\right]\frac{dy}{dz} + \left(B - \ell_1^2 - \ell_2^2 - 4\ell_1 - 4\ell_2 - \frac{\ell_1\ell_2}{2}\right)\frac{y}{4} = 0 \tag{4.77}$$

and the second one is

$$z = \frac{1-t}{2},$$

transforming the angular equation for α into

$$(1-t^2)\frac{d^2y}{dt^2} + \left[\ell_1 - \ell_2 - (\ell_1+\ell_2+3)\,t\right]\frac{dy}{dt} + \frac{1}{4}\left(B - \ell_1^2 - \ell_2^2 - 4\ell_1 - 4\ell_2 - 2\ell_1\ell_2\right) y = 0. \tag{4.78}$$

Equation (4.78) is a Jacobi differential equation if

$$B = (\ell_1+\ell_2+2n+4)(\ell_1+\ell_2+2n) = (\ell_1+\ell_2+2n+2)^2 - 4 \tag{4.79}$$

where n is a natural number. Thus, the angular function shall be

$$A(\alpha) = N_{\ell_1,\ell_2,n}(\sin\alpha)^{\ell_2}(\cos\alpha)^{\ell_1}P_n^{(\ell_1+1/2,\ell_2+1/2)}(\cos 2\alpha). \tag{4.80}$$

However, realizing we can write (see Appendix)

$$P_n^{(a,b)}(x) = {}_2F_1\left(-n, n+a+b+1; a+1; \frac{1-x}{2}\right) \tag{4.81}$$

our solution for the equation for α is

$$A(\alpha) = N_{\ell_1,\ell_2,n}(\cos\alpha)^{\ell_1}(\sin\alpha)^{\ell_2}{}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2\alpha\right) \tag{4.82}$$

the normalization factor $N_{\ell_1,\ell_2,n}$ now reads

$$N_{\ell_1,\ell_2,n} = \sqrt{\frac{\Gamma(n+\ell_2+3/2)(\ell_1+\ell_2+2n+2)(\ell_1+\ell_2+n+1)!}{n![\Gamma(\ell_2+3/2)]^2\Gamma(\ell_1+n+3/2)}} \tag{4.83}$$

What is left now is to determine the radial function. This is an easy task, since substitution of (4.79) into equation (4.74a) gives

$$\frac{d^2R}{dr^2} + \frac{5}{r}\frac{dR}{dr} + \left[k^2 - \frac{(\ell_1+\ell_2+2n+2)^2-4}{r^2}\right]R = 0 \tag{4.84}$$

whose solutions can be written as

$$\begin{aligned} R_1(r) &= \frac{J_{\ell_1+\ell_2+2n+2}(kr)}{r^2} \\ R_2(r) &= \frac{H^{(1)}_{\ell_1+\ell_2+2n+2}(kr)}{r^2} \end{aligned} \tag{4.85}$$

and the associated wronskian determinant [45] is

$$\mathcal{W}[R_1, R_2](r) = \frac{2i}{\pi r^5} \tag{4.86}$$

Using equation (3.41) and substituting (4.66), (4.67), (4.80), (4.83) and the spherical harmonics sugested by (4.71) into it, we get the six-dimensional hyperspherical Green's function for the free-particle

$$\begin{aligned} G^{(6)}(\mathbf{r}|\mathbf{r}') = \frac{i\pi}{2}\sum_q \Bigg[& \frac{\Gamma(n+\ell_2+3/2)(\ell_1+\ell_2+2n+2)(\ell_1+\ell_2+n+1)!}{n![\Gamma(\ell_2+3/2)]^2\Gamma(\ell_1+n+3/2)} \\ & \times \frac{J_{\ell_1+\ell_2+2n+2}(kr_<)}{r_<^2}\frac{H^{(1)}_{\ell_1+\ell_2+2n+2}(kr_>)}{r_>^2} Y^{m_1}_{\ell_1}(\theta_1,\phi_1)Y^{*m_1}_{\ell_1}(\theta_1',\phi_1')Y^{m_2}_{\ell_2}(\theta_2,\phi_2)Y^{*m_2}_{\ell_2}(\theta_2',\phi_2') \\ & \times (\sin\alpha)^{\ell_2}(\cos\alpha)^{\ell_1}{}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2\alpha\right) \\ & \times (\sin\alpha')^{\ell_2}(\cos\alpha')^{\ell_1}{}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2\alpha'\right)\Bigg] \end{aligned} \tag{4.87}$$

with $r_> \equiv \max(r, r')$ and $r_< \equiv \min(r, r')$. [2]

[2] Compare with equation (12.3.92), found in *Methods of Theoretical Physics* Part II, p. 1732, by Philip McCord Morse, Herman Feshbach. The Jacobi polynomials used here are also called *shifted Jacobi polynomials*.

Now consider the Lippmann-Schwinger equation

$$\psi(\mathbf{r}) = \varphi(\mathbf{r}) + A\int_{V'} G(\mathbf{r}|\mathbf{r}')V(\mathbf{r}')\psi(\mathbf{r}')d\tau' \tag{4.88}$$

where A is a constant. Suppose

$$V(\mathbf{r}') = \int_S dS\left[\frac{\delta(r'-r_0)\delta(\alpha'-w)\delta(\theta_1'-u_1)\delta(\phi_1'-v_1)\delta(\theta_2'-u_2)\delta(\phi_1'-v_2)}{r'^5\sin^2\alpha'\cos^2\alpha'\sin\theta_1'\sin\theta_2'} \times\gamma(u_1,u_2,v_1,v_2,w)\right] \tag{4.89}$$

such that (4.88) becomes

$$\psi(\mathbf{r}) = \varphi(\mathbf{r}) + A\int_{V'}\int_S dS\, d\tau'\, G(\mathbf{r}|\mathbf{r}')\,\frac{\delta(r'-r_0)\delta(\alpha'-w)\delta(\theta_1'-u_1)\delta(\phi_1'-v_1)\delta(\theta_2'-u_2)\delta(\phi_1'-v_2)}{r'^5\sin^2\alpha'\cos^2\alpha'\sin\theta_1'\sin\theta_2'} \times\gamma(u_1,u_2,v_1,v_2,w)\psi(\mathbf{r}') \tag{4.90}$$

Upon substitution of the Green function (4.87) into the latter expression translates to

$$\begin{aligned}\psi(\mathbf{r}) = \varphi(\mathbf{r}) + \frac{i\pi A}{2}\int_{V'}\int_S dSd\tau'\sum_q &\left[\frac{\Gamma(n+\ell_2+3/2)(\ell_1+\ell_2+2n+2)(\ell_1+\ell_2+n+1)!}{n![\Gamma(\ell_2+3/2)]^2\Gamma(\ell_1+n+3/2)}\right.\\ &\times\frac{J_{\ell_1+\ell_2+2n+2}(kr_<)}{r_<^2}\frac{H^{(1)}_{\ell_1+\ell_2+2n+2}(kr_>)}{r_>^2}Y^{m_1}_{\ell_1}(\theta_1,\phi_1)Y^{*m_1}_{\ell_1}(\theta_1',\phi_1')Y^{m_2}_{\ell_2}(\theta_2,\phi_2)Y^{*m_2}_{\ell_2}(\theta_2',\phi_2')\\ &\times(\sin\alpha)^{\ell_2}(\cos\alpha)^{\ell_1}{}_2F_1\left(-n,n+\ell_1+\ell_2+2;\ell_2+\frac{3}{2};\sin^2\alpha\right)\\ &\left.\times(\sin\alpha')^{\ell_2}(\cos\alpha')^{\ell_1}{}_2F_1\left(-n,n+\ell_1+\ell_2+2;\ell_2+\frac{3}{2};\sin^2\alpha'\right)\right]\\ &\frac{\delta(r'-r_0)\delta(\alpha'-w)\delta(\theta_1'-u_1)\delta(\phi_1'-v_1)\delta(\theta_2'-u_2)\delta(\phi_1'-v_2)}{r'^5\sin^2\alpha'\cos^2\alpha'\sin\theta_1'\sin\theta_2'}\gamma(u_1,u_2,v_1,v_2,w)\psi(\mathbf{r}')\end{aligned} \tag{4.91}$$

Now, we use the elements of integration

$$d\tau' = r'^5\sin^2\alpha'\cos^2\alpha'\sin\theta_1'\sin\theta_2' dr'd\alpha d\theta_1 d\theta_2 d\phi_1 d\phi_2$$

$$dS = r_0^5\sin^2 w\cos^2 w\sin u_1\sin u_2 dwdu_1du_2dv_1dv_2$$

to simplify and integrate the primed variables. Since there are delta functions involved, we get

$$\psi(\mathbf{r}) = \varphi(\mathbf{r}) + \frac{i\pi A r_0^5}{2} \sum_q \left[\frac{\Gamma(n+\ell_2+3/2)(\ell_1+\ell_2+2n+2)(\ell_1+\ell_2+n+1)!}{n![\Gamma(\ell_2+3/2)]^2\Gamma(\ell_1+n+3/2)} \right]$$
$$\times \frac{J_{\ell_1+\ell_2+2n+2}(kr_<)}{r_<^2} \frac{H^{(1)}_{\ell_1+\ell_2+2n+2}(kr_>)}{r_>^2} Y_{\ell_1}^{m_1}(\theta_1,\phi_1) Y_{\ell_2}^{m_2}(\theta_2,\phi_2)$$
$$\times (\sin\alpha)^{\ell_2}(\cos\alpha)^{\ell_1} {}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2\alpha\right)$$
$$\times \int_S dw du_1 du_2 dv_1 dv_2 \; \gamma(u_1,u_2,v_1,v_2,w) \sin u_1 Y_{\ell_1}^{*m_1}(u_1,v_1) \sin u_2 Y_{\ell_2}^{*m_2}(v_2,v_2)$$
$$\times (\sin w)^{\ell_2+2}(\cos w)^{\ell_1+2} {}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2 w\right) \psi(r_0,w,u_1,u_2,v_1,v_2) \quad (4.92)$$

where the $r_<$ and $r_>$ symbols now means

$$r_< = \min(r, r_0)$$
$$r_> = \max(r, r_0)$$

Once again, if we know the value of integral in the last equation, we know everything about the wave function. But in order to do this calculation, we should need to know what the γ function is. As an elementary example, let us consider the simplest case – $\gamma = const.$

The case $\gamma = \gamma_0$:

We label this integral as $a(r_0)$:

$$a(r_0) = \int_S dw du_1 du_2 dv_1 dv_2 \sin u_1 Y_{\ell_1}^{*m_1}(u_1,v_1) \sin u_2 Y_{\ell_2}^{*m_2}(v_2,v_2)$$
$$\times (\sin w)^{\ell_2+2}(\cos w)^{\ell_1+2} {}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2 w\right) \psi(r_0,w,u_1,u_2,v_1,v_2) \quad (4.93)$$

Upon doing so, we note that equation (4.92) becomes

$$\psi(\mathbf{r}) = \varphi(\mathbf{r}) + \frac{i\pi A r_0^5 \gamma_0}{2} \sum_q \left[\frac{\Gamma(n+\ell_2+3/2)(\ell_1+\ell_2+2n+2)(\ell_1+\ell_2+n+1)!}{n![\Gamma(\ell_2+3/2)]^2\Gamma(\ell_1+n+3/2)} \right] a(r_0)$$
$$\times \frac{J_{\ell_1+\ell_2+2n+2}(kr_<)}{r_<^2} \frac{H^{(1)}_{\ell_1+\ell_2+2n+2}(kr_>)}{r_>^2} Y_{\ell_1}^{m_1}(\theta_1,\phi_1) Y_{\ell_2}^{m_2}(\theta_2,\phi_2)$$
$$\times (\sin\alpha)^{\ell_2}(\cos\alpha)^{\ell_1} {}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2\alpha\right). \quad (4.94)$$

Now is possible to use the orthogonality properties of both spherical harmonics and the hypergeometric function to calculate the coefficients. Multiplying both sides of equation (4.94) by

$$\sin u_1 Y^{*m_1'}_{\ell_1'}(u_1,v_1)\sin u_2 Y^{*m_2'}_{\ell_2'}(v_2,v_2) \times (\sin w)^{\ell_2'}(\cos w)^{\ell_1'}{}_2F_1\left(-n,n+\ell_1'+\ell_2'+2;\ell_2'+\frac{3}{2};\sin^2 w\right) \tag{4.95}$$

remembering that $\varphi(\mathbf{r})$ is a plane-wave and integrating on the surface of the 5-sphere, we get

$$\begin{aligned} a(r) &= c(r) + \frac{i\pi A r_0^5\gamma_0}{4}\sum_q a(r_0)\frac{J_{\ell_1+\ell_2+2n+2}(kr_<)}{r_<^2}\frac{H^{(1)}_{\ell_1+\ell_2+2n+2}(kr_>)}{r_>^2}\delta_{\ell_1,\ell_1'}\delta_{\ell_2,\ell_2'}\delta_{m_1,m_1'}\delta_{m_2,m_2'} \\ &= c(r) + \frac{i\pi A r_0^5\gamma_0}{4}a(r_0)\frac{J_{\ell_1+\ell_2+2n+2}(kr_<)}{r_<^2}\frac{H^{(1)}_{\ell_1+\ell_2+2n+2}(kr_>)}{r_>^2}. \end{aligned} \tag{4.96}$$

Evaluating in $r=r_0$, we can isolate $a(r_0)$ to get

$$a(r_0) = \frac{c(r_0)}{1-\frac{i\pi A r_0\gamma_0}{4}J_{\ell_1+\ell_2+2n+2}(kr_0)H^{(1)}_{\ell_1+\ell_2+2n+2}(kr_0)} \tag{4.97}$$

Since $\varphi(\mathbf{r})$ is a plane-wave, we must find its eigenfunction expansion. To do so, we set $\mathcal{N}=6$ in equation (3.144), attaining

$$G\left(\mathbf{r}|\mathbf{r}'\right) = \frac{i}{4}\left(\frac{k}{2\pi|\mathbf{r}-\mathbf{r}'|}\right)^{6/2-1} H^{(1)}_{\frac{6}{2}-1}(k|\mathbf{r}-\mathbf{r}'|) = \frac{ik^2}{16\pi^2}\frac{H^{(1)}_2(k|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|^2} \tag{4.98}$$

The asymptotic behavior of the Hankel function (4.12) gives rise to

$$\begin{aligned} H^{(1)}_2(k|\mathbf{r}-\mathbf{r}'|) &= \sqrt{\frac{2}{\pi k|\mathbf{r}-\mathbf{r}'|}}\exp\left\{i\left[k|\mathbf{r}-\mathbf{r}'|-\left(\frac{5}{2}\right)\frac{\pi}{2}\right]\right\} \\ &= \sqrt{\frac{2}{\pi k|\mathbf{r}-\mathbf{r}'|}}e^{ik|\mathbf{r}-\mathbf{r}'|}\left(\frac{-1}{\sqrt{2}}+\frac{i}{\sqrt{2}}\right) \\ &= \frac{(-1+i)}{\sqrt{\pi}}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{\sqrt{k|\mathbf{r}-\mathbf{r}'|}}. \end{aligned} \tag{4.99}$$

If $\mathbf{r}'\to\infty$, $|\mathbf{r}-\mathbf{r}'|\approx r'-\hat{\mathbf{n}}\cdot\mathbf{r}$. Moreover, in the denominators, $r'-\hat{\mathbf{n}}\cdot\mathbf{r}\approx r'$, so

$$H^{(1)}_2(k|\mathbf{r}-\mathbf{r}'|) \approx \frac{(-1+i)}{\sqrt{\pi}}\frac{e^{ikr'}e^{-ik\hat{\mathbf{n}}\cdot\mathbf{r}}}{\sqrt{kr'}} = \frac{(-1+i)}{\sqrt{\pi}}\frac{e^{ikr'}e^{-i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{kr'}} \tag{4.100}$$

and consequently,

$$G\left(\mathbf{r}|\mathbf{r}'\right) = \frac{ik^2}{16\pi^2}\frac{H_2^{(1)}(k|\mathbf{r}-\mathbf{r}'|)}{|\mathbf{r}-\mathbf{r}'|^2} \approx \frac{ik^2}{16\pi^2}\frac{(-1+i)}{\sqrt{\pi}}\frac{e^{ikr'}e^{-i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{kr'}}\frac{1}{r'^2} \tag{4.101}$$

On the other hand, the same considerations for the Hankel function in the eigenfunction expansion (4.87) produces

$$\begin{aligned} G^{(6)}(\mathbf{r}|\mathbf{r}') = \frac{i\pi}{2}\sum_q \Bigg[& \frac{\Gamma(n+\ell_2+3/2)(\ell_1+\ell_2+2n+2)(\ell_1+\ell_2+n+1)!}{n![\Gamma(\ell_2+3/2)]^2\Gamma(\ell_1+n+3/2)}\frac{J_{\ell_1+\ell_2+2n+2}(kr)}{r^2} \\ & \times \frac{(-1+i)}{\sqrt{\pi}}\frac{e^{ikr'}}{\sqrt{kr'}}\frac{(-i)^{\ell_1+\ell_2+2n}}{r'^2} Y_{\ell_1}^{m_1}(\theta_1,\phi_1)Y_{\ell_1}^{*m_1}(\theta_1',\phi_1')Y_{\ell_2}^{m_2}(\theta_2,\phi_2)Y_{\ell_2}^{*m_2}(\theta_2',\phi_2') \\ & \times (\sin\alpha)^{\ell_2}(\cos\alpha)^{\ell_1}{}_2F_1\left(-n,n+\ell_1+\ell_2+2;\ell_2+\frac{3}{2};\sin^2\alpha\right) \\ & \times (\sin\alpha')^{\ell_2}(\cos\alpha')^{\ell_1}{}_2F_1\left(-n,n+\ell_1+\ell_2+2;\ell_2+\frac{3}{2};\sin^2\alpha'\right)\Bigg] \end{aligned} \tag{4.102}$$

Comparison between (4.101) and (4.102) generates

$$\begin{aligned} \frac{ik^2}{16\pi^2}\frac{(-1+i)}{\sqrt{\pi}}\frac{e^{ikr'}e^{-i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{kr'}}\frac{1}{r'^2} = \frac{i\pi}{2}\sum_q \Bigg[& \frac{\Gamma(n+\ell_2+3/2)(\ell_1+\ell_2+2n+2)(\ell_1+\ell_2+n+1)!}{n![\Gamma(\ell_2+3/2)]^2\Gamma(\ell_1+n+3/2)} \\ & \times \frac{J_{\ell_1+\ell_2+2n+2}(kr_<)}{r_<^2}\frac{(-1+i)}{\sqrt{\pi}}\frac{e^{ikr'}}{\sqrt{kr'}}\frac{(-i)^{\ell_1+\ell_2+2n}}{r'^2} \\ & \times Y_{\ell_1}^{m_1}(\theta_1,\phi_1)Y_{\ell_1}^{*m_1}(\theta_1',\phi_1')Y_{\ell_2}^{m_2}(\theta_2,\phi_2)Y_{\ell_2}^{*m_2}(\theta_2',\phi_2') \\ & \times (\sin\alpha)^{\ell_2}(\cos\alpha)^{\ell_1}{}_2F_1\left(-n,n+\ell_1+\ell_2+2;\ell_2+\frac{3}{2};\sin^2\alpha\right) \\ & \times (\sin\alpha')^{\ell_2}(\cos\alpha')^{\ell_1}{}_2F_1\left(-n,n+\ell_1+\ell_2+2;\ell_2+\frac{3}{2};\sin^2\alpha'\right)\Bigg] \end{aligned} \tag{4.103}$$

and we can simplify terms, to get

$$\begin{aligned} e^{-i\mathbf{k}\cdot\mathbf{r}} = \frac{8\pi^3}{k^2}\sum_q \Bigg[& \frac{\Gamma(n+\ell_2+3/2)(\ell_1+\ell_2+2n+2)(\ell_1+\ell_2+n+1)!}{n![\Gamma(\ell_2+3/2)]^2\Gamma(\ell_1+n+3/2)}(-i)^{\ell_1+\ell_2+2n} \\ & \times \frac{J_{\ell_1+\ell_2+2n+2}(kr)}{r^2} Y_{\ell_1}^{m_1}(\theta_1,\phi_1)Y_{\ell_1}^{*m_1}(\theta_1',\phi_1')Y_{\ell_2}^{m_2}(\theta_2,\phi_2)Y_{\ell_2}^{*m_2}(\theta_2',\phi_2') \\ & \times (\sin\alpha)^{\ell_2}(\cos\alpha)^{\ell_1}{}_2F_1\left(-n,n+\ell_1+\ell_2+2;\ell_2+\frac{3}{2};\sin^2\alpha\right) \\ & \times (\sin\alpha')^{\ell_2}(\cos\alpha')^{\ell_1}{}_2F_1\left(-n,n+\ell_1+\ell_2+2;\ell_2+\frac{3}{2};\sin^2\alpha'\right)\Bigg] \end{aligned} \tag{4.104}$$

Additionally, we take the complex conjugate of the last equation, to breed

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{8\pi^3}{k^2}\sum_q \Bigg[\frac{\Gamma(n+\ell_2+3/2)(\ell_1+\ell_2+2n+2)(\ell_1+\ell_2+n+1)!}{n![\Gamma(\ell_2+3/2)]^2\Gamma(\ell_1+n+3/2)}(i)^{\ell_1+\ell_2+2n} \times \frac{J_{\ell_1+\ell_2+2n+2}(kr)}{r^2} Y^{*m_1}_{\ell_1}(\theta_1,\phi_1)Y^{m_1}_{\ell_1}(\theta'_1,\phi'_1)Y^{*m_2}_{\ell_2}(\theta_2,\phi_2)Y^{m_2}_{\ell_2}(\theta'_2,\phi'_2) \times (\sin\alpha)^{\ell_2}(\cos\alpha)^{\ell_1}{}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2\alpha\right) \times (\sin\alpha')^{\ell_2}(\cos\alpha')^{\ell_1}{}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2\alpha'\right)\Bigg] \tag{4.105}$$

which is the plane-wave expansion in 6 dimensions. Therefore, the calculation of the function $c(r_0)$ is easy to do. We set $r = r_0$ in the last expression, multiply it by the weight function (4.95) and integrate on the surface of the 6-dimensional hypersphere, bringing forth

$$c(r_0) = \frac{4\pi^3}{k^2}(i)^{\ell_1+\ell_2+2n}\frac{J_{\ell_1+\ell_2+2n+2}(kr_0)}{r_0^2}Y^{m_1}_{\ell_1}(\theta'_1,\phi'_1)Y^{m_2}_{\ell_2}(\theta'_2,\phi'_2) \times (\sin\alpha')^{\ell_2}(\cos\alpha')^{\ell_1}{}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2\alpha'\right) \tag{4.106}$$

Thus, the coefficients become

$$a(r_0) = \frac{4\pi^3}{k^2}(i)^{\ell_1+\ell_2+2n}\frac{J_{\ell_1+\ell_2+2n+2}(kr_0)}{r_0^2}Y^{m_1}_{\ell_1}(\theta'_1,\phi'_1)Y^{m_2}_{\ell_2}(\theta'_2,\phi'_2) \times (\sin\alpha')^{\ell_2}(\cos\alpha')^{\ell_1}{}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2\alpha'\right) \times \left[1 - \frac{i\pi A r_0\gamma_0}{4}J_{\ell_1+\ell_2+2n+2}(kr_0)H^{(1)}_{\ell_1+\ell_2+2n+2}(kr_0)\right]^{-1} \tag{4.107}$$

and the wave function shall be [46]

$$
\begin{aligned}
\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{i\pi A r_0^5 \gamma_0}{2} \sum_q & \left[\frac{\Gamma(n+\ell_2+3/2)(\ell_1+\ell_2+2n+2)(\ell_1+\ell_2+n+1)!}{n![\Gamma(\ell_2+3/2)]^2\Gamma(\ell_1+n+3/2)} \right] \\
& \times \frac{4\pi^3}{k^2}(i)^{\ell_1+\ell_2+2n} \frac{J_{\ell_1+\ell_2+2n+2}(kr_0)}{r_0^2} Y_{\ell_1}^{m_1}(\theta_1', \phi_1') Y_{\ell_2}^{m_2}(\theta_2', \phi_2') \\
& \times (\sin\alpha')^{\ell_2}(\cos\alpha')^{\ell_1} {}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2\alpha'\right) \\
& \times \left[1 - \frac{i\pi A r_0 \gamma_0}{4} J_{\ell_1+\ell_2+2n+2}(kr_0) H^{(1)}_{\ell_1+\ell_2+2n+2}(kr_0)\right]^{-1} \\
& \times \frac{J_{\ell_1+\ell_2+2n+2}(kr_<)}{r_<^2} \frac{H^{(1)}_{\ell_1+\ell_2+2n+2}(kr_>)}{r_>^2} Y_{\ell_1}^{m_1}(\theta_1, \phi_1) Y_{\ell_2}^{m_2}(\theta_2, \phi_2) \\
& \times (\sin\alpha)^{\ell_2}(\cos\alpha)^{\ell_1} {}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2\alpha\right). \quad (4.108)
\end{aligned}
$$

In section 4.1.2 we calculated the scattering amplitude and total cross section for one-particle scattering in four dimensions. Similar reasoning shows that

$$
\lim_{kr\to\infty} \psi(r, \alpha, \theta_1, \phi_1, \theta_2, \phi_2) = e^{ikr} + f_6(\alpha, \theta_1, \phi_1, \theta_2, \phi_2)\frac{e^{ikr}}{r^{5/2}}. \quad (4.109)
$$

Setting

$$
N^2_{n,\ell_1,\ell_2} = \frac{\Gamma(n+\ell_2+3/2)(\ell_1+\ell_2+2n+2)(\ell_1+\ell_2+n+1)!}{n![\Gamma(\ell_2+3/2)]^2\Gamma(\ell_1+n+3/2)},
$$

we can see that the scattering amplitude is

$$
\begin{aligned}
f_6(\alpha, \theta_1, \phi_1, \theta_2, \phi_2) = -iAR^{7/2}\gamma_0 e^{-i\pi/4} \sum_q e^{-i\pi(\ell_1+\ell_2+2n)/2} N^2_{n,\ell_1,\ell_2} a^{m_1,m_2}_{n,\ell_1,\ell_2}(R)\ j_{\ell_1+\ell_2+2n+3/2}(kR) \\
\times Y_{\ell_1}^{m_1}(\theta_1,\phi_1) Y_{\ell_2}^{m_2}(\theta_2,\phi_2)(\sin\alpha)^{\ell_2}(\cos\alpha)^{\ell_1} {}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2\alpha\right) \quad (4.110)
\end{aligned}
$$

and consequently the total cross-section is

$$
\sigma_6 = \frac{A^2R^7\gamma_0^2}{2} \sum_{n,\ell_1,\ell_2,m_1,m_2} N^2_{n,\ell_1,\ell_2} |a^{m_1,m_2}_{n,\ell_1,\ell_2}(R)|^2\ j^2_{\ell_1+\ell_2+2n+3/2}(kR). \quad (4.111)
$$

Finally, we show the quantum refraction index (2.101):

$$
\begin{aligned}
n = 1 - \frac{2\pi\gamma_0^2}{k^2} iAR^{7/2} e^{-i\pi/4} \sum_q e^{-i\pi(\ell_1+\ell_2+2n)/2} N^2_{n,\ell_1,\ell_2} a^{m_1,m_2}_{n,\ell_1,\ell_2}(R)\ j_{\ell_1+\ell_2+2n+3/2}(kR) \\
\times \sqrt{\frac{(2\ell_1+1)}{4\pi}\frac{(2\ell_2+1)}{4\pi}} (\sin\alpha)^{\ell_2}(\cos\alpha)^{\ell_1} {}_2F_1\left(-n, n+\ell_1+\ell_2+2; \ell_2+\frac{3}{2}; \sin^2\alpha\right). \quad (4.112)
\end{aligned}
$$

In Figure 4.10 we plot the above total cross-section as a function of γ_0 considering the wavenumber to be equal to the first four zeros of the spherical Bessel functions $j_{1/2}$ and $j_{5/2}$. We also choose $\tilde{\theta}_1 = 0$ and $\tilde{\theta}_2 = \pi$ in order to simulate a head-on collision between particles. Notice that certain combinations of incident wave number and coupling constant produce sharp peaks in the total cross-section.

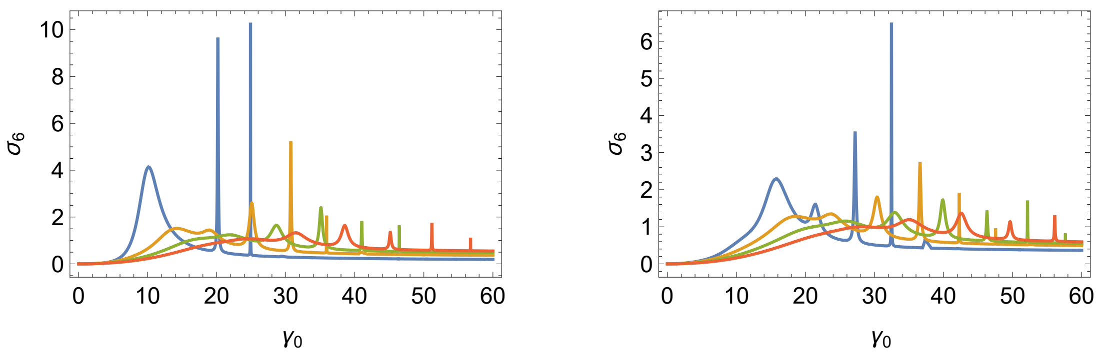
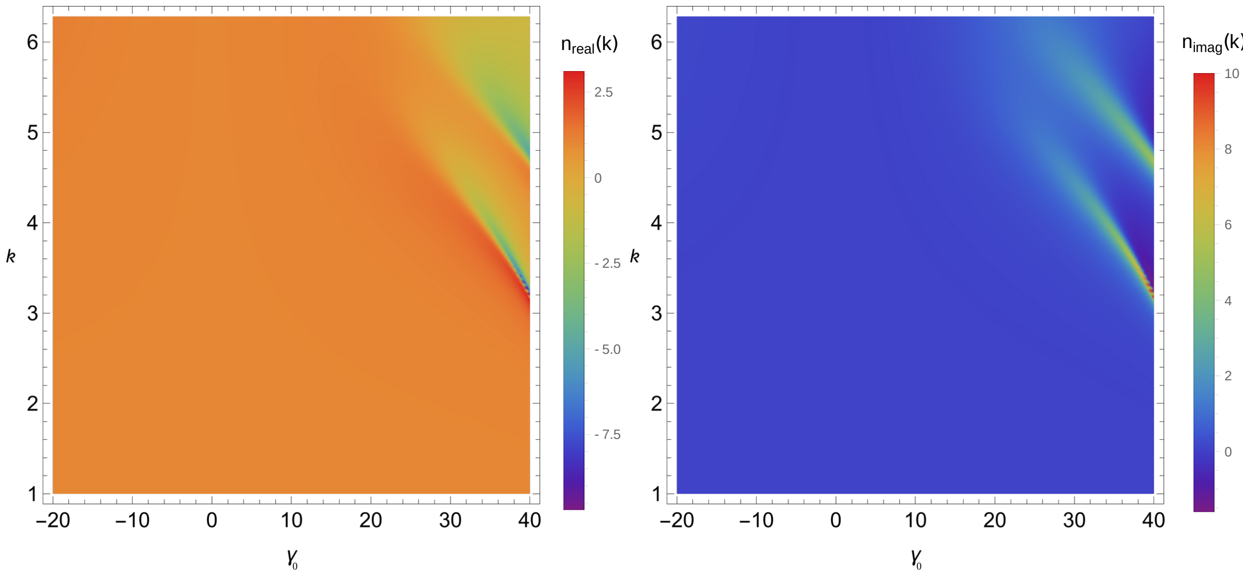


Figure 4.10: Plot of total cross-section σ_6 for the scattering of a plane wave by a five-dimensional Dirac hyper-spherical shell, incident at the direction $\tilde{\theta}_1 = 0, \tilde{\theta}_2 = \pi, \tilde{\phi}_1 = \tilde{\phi}_2 = \tilde{\alpha} = 0$. In the left figure we plot four curves $\sigma_6 = \sigma_6(\gamma_0)$ taking the wave number to be a zero of the spherical Bessel function $j_{1/2}(kR)$, namely, $k = \pi, 2\pi, 3\pi$ and 4π (blue, yellow, green and red, respectively). Observe that there are certain values of γ_0 which produce a sharp peak. In the right box we also plot four curves $\sigma_6 = \sigma_6(\gamma_0)$ now taking the wave number to be a zero of $j_{5/2}(kR)$, namely, $5.763; 9.095; 12.323; 15.514$ (blue, yellow, green and red, respectively). We take $R = 1$, truncate the series at $n = 8$ and we use atomic units where $\hbar = 2m^* = 1/2$.

In Figure 4.11 we plot the quantum refraction index as a function of γ and k. We set $\theta_1 = 0$, $\theta_2 = 0$, $\phi_1 = 0$ and $\phi_2 = 0$ in order to account for the forward scattering amplitude. Again, we use spherical symmetry to expedite our calculations. Notice that certain combinations of incident wave number and coupling constant makes the real part of the quantum refractive index to be *negative*.



(a) Re(n)

(b) Im(n)

Figure 4.11: Real and imaginary parts of the quantum refraction index, taking $\alpha = \pi/4$ for simplicity. Additionally, all other angles are zero, such that the solid angle of observation is zero (forward scattering amplitude).

Chapter 5

Conclusions

In this thesis we have presented a concise approach to quantum scattering theory, using both wavefunction formalism and the operator formalism, otherwise known as the formal theory of quantum scattering, in chapter 2. After articulating the necessary concepts for the understanding of the equations in chapter 4, that is, the asymptotic behavior of the wavefunction (2.4), the scattering amplitude (2.25), the differential cross-section (2.12) and the Lippmann–Schwinger equation (2.21), we presented the formal scattering theory. In the formal scattering theory, we introduced Møller operators (2.36) and the S-operator (2.43), which is of great significance in physics, for it led us to the development of the S-matrix theory and string theory. After exploring the principal results of the formal scattering theory, we have once again a formula for the scattering amplitude (2.51), the differential cross-section (2.66), and the optical theorem (2.72), which links the imaginary part of the scattering amplitude with a physical observable, the cross-section. Additionally, we revealed a less-known result of quantum scattering theory, which is called the *quantum refraction index* (2.99). This number is meant to be an analogous to the electromagnetic refraction index, and it is dependent on the scatterers' density in a medium, as well as the momentum of the incident wave or wave-packet.

In chapter 3, we disclosed an extensive analysis on how separate Helmholtz equation in a $\mathcal{N}$-dimensional rotational coordinate system (3.24) and how to construct the associated free Green's function (3.41). We introduced the Robertson condition (3.18), which was paramount for our goal. Having separated Helmholtz equation, we showed one method for how to get a closed-form solution for the Green's function (3.144). Upon obtaining the closed-form solution, we investigated two ways of calculating the eigenfunction expansion of Green's function: the first method we called *the* *construction method*, exposed in chapter 3, at subsection 3.3.1, and the second method, which for lack of creativity was labeled *the differential equation method*, revealed in chapter 3, subsection 3.3.2. This result is notable for the fact that it reduces to the well-known Green's function expansion in three dimensions, as in Jackson [52]. Upon a simple comparison between the results, i.e., equations (3.144) and (3.119), we arrived at a well-known relation, a Gegenbauer expansion of Hankel's function (3.145).

Possessing the Green's function, we were able to solve Lippmann–Schwinger equation in four and six dimensions, presented in chapter 4. We investigated two different systems in four dimensions: the first was the scattering of a scalar particle by a potential boundary-wall, i.e., a hyperspherical shell, defined by (4.18), and the second one was the scattering of a scalar particle by a potential *region*, called *Dirac's medium*, or *Dirac's sphere*, for it is a spherical region where there exists a radially uniform distribution of delta functions, as defined in (4.34). In the case of the hyperspherical shell, we were able to analytically calculate the wavefunction (4.29), giving it an exact eigenfunction expansion. As a consequence, we calculated the scattering amplitude (4.31) and the total cross-section, in (4.32). In possession of the scattering amplitude, and knowing that the scatterers' density (the coupling function) $\gamma(\Omega)$ was a constant, we calculated the quantum refraction index (4.33). This calculation was indeed made easy because of spherical symmetry, which allowed us to drop the calculation of average in equation (2.101). In the case of Dirac's sphere, we calculated an exact solution for Lippmann–Schwinger equation, both at the interior domain, i.e., inside Dirac's sphere, and at the exterior domain, i.e., outside Dirac's sphere thus obtaining two eigenfunction expansion of the wavefunction, in (4.47) and (4.37). These solutions include the reflection and transmission coefficients, which tells us how much of the wavefunction is reflected or transmitted through the interface between Dirac's sphere and the vacuum. From there, the asymptotic behavior of the exterior solution revealed the scattering amplitude (4.58), and the total cross-section (4.59). Once the scattering amplitude is known, it is easy to once again calculate the quantum refraction index (4.60).

In the second geometry, we calculated the scattering of two non-interacting particles by a three-dimensional spherical boundary-wall, manifested again as a potential (4.89). Because there were two particles, the whole system had six dimensions, and therefore we calculated the Green's function (4.87) and the wavefunction (4.108), as a solution for Lippmann–Schwinger equation, in six dimensions. Once again, we calculated the scattering amplitude (4.110) and total cross-section (4.111). Finally, we showed the quantum refractive index (4.112), taking advantage of spherical symmetry.

The methodology we developed in our work can be applied to several systems, in Euclidean spaces, changing the potential definitions: such as polar curves — which could be used to model rough or imperfect particles —, spheroidal surfaces, as well as the challenging toroidal surface. We could also apply the same technique to scattering problems formulated in non-Euclidean spaces such as Poincaré disk, Poincaré upper half-plane [23] and other more sophisticated generalizations of geometries where the fifth Euclides' postulate does not hold.[1]

In order to avoid the difficulties presented by the plane-waves Kouri and Hoffmann [53] reformulated the Lippmann–Schwinger so as to consider the scattering of a wave-packet by a given potential. They split the problem into three domains: (i) close to the potential; (ii) far from it; and (iii) intermediary region. In the first two the Lippmann–Schwinger equation which governs the wave-packet dynamics seems amenable to exact solution while the same equation written in the intermediary region would be more challenging. In the near future we propose to tackle the scattering problem formulated in terms of wave-packets. Another interest is to apply the machine learning technique to these scattering problems [54] in order to adjust coupling constant to produce a given, predefined, total cross-section. In other words, we propose to implement machine learning techniques to solve the *inverse quantum scattering problem.* Additionally, we will continue to investigate more numerical and exact results on the quantum refraction index.

Finally, we look forward to bring our methodology to try to solve two more challenging problems: (i) the relativistic Lippmann–Schwinger equation as formulated by Landau [55]; and (ii) the Faddeev equation [56, 57].

[1] Euclides' fifth postulate states: "... if a straight line falling on two straight lines makes the interior angles on the same side less than two right angles, the two straight lines, if produced indefinitely, meet on that side on which are the angles less than the two right angles".

Bibliography

[1] J. W. Strutt, *LVIII. On the scattering of light by small particles*, The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science **41**, 447 (1871).

[2] M. I. Mishchenko, *Electromagnetic scattering by particles and particle groups: an introduction*, Cambridge University Press (2014).

[3] D. Belkić, *Principles of Quantum Scattering Theory*, Institute of Physics (2004).

[4] K. A. Khan, R. Penrose, Nature **229**, 185 (1971).

[5] V. Ferrari, M. Germano, Proc. Math. Phys. Eng. Sci. **444**, 389 (1994).

[6] L. Annulli, L. Bernard, D. Blas, V. Cardoso, Phys. Rev. D **98**, 084001 (2018).

[7] S. R. Dolan, T. Stratton, Phys. Rev. D **95**, 124055 (2017).

[8] R. Takahashi, T. Suyama, S. Michikoshi, A&A **438**, L5 (2005).

[9] P. B. Dev, M. Lindner, S. Ohmer, Phys. Lett. B **773**, 219 (2017).

[10] B. P. Abbott et al., Phys. Rev. Lett. **116**, 061102, (2016).

[11] J. R. Taylor, *Scattering Theory*, John Wiley (1972).

[12] A. Gonis, W. H. Butler, *Multiple Scattering in Solids*, Springer (2000).

[13] R. P. Feynman, Rev. Mod. Phys. **20**, 267 (1948).

[14] B. A. Lippmann, J. Schwinger, Phys. Rev. **79**, 469 (1950).

[15] F. W. Byron, R. W. Fuller, *Mathematics of Classical and Quantum Physics*, Dover Publications (1992).

[16] R. G. Newton, *Scattering Theory of Waves and Particles*, Springer-Verlag (1982).

[17] A. C. Maioli, A. G. M. Schmidt, J. Math. Phys. **59**, 122102 (2018).

[18] M. G. E. da Luz, A. S. Lupu-Sax, E. J. Heller, Phys. Rev. E **56**, 2496 (1997).

[19] G. B. Folland, *Fourier Analysis and its Applications*, Brooks/Cole Publishing Company (1992).

[20] A. C. Maioli, A. G. M. Schmidt, Physica E **111**, 51 (2019).

[21] P. C. Azado, A. C. Maioli, A. G. M. Schmidt, Phys. Scr. **96**, 085205 (2021).

[22] A. G. M. Schmidt, A. C. Maioli, P. C. Azado, J. Quant. Spectrosc. Radiat. Transfer **253**, 107154 (2020).

[23] A. L. de Jesus, A. C. Maioli, A. G. M. Schmidt, Phys. Scr. **96**, 125264 (2021).

[24] A. C. Maioli, A. G. M. Schmidt, Phys. Scr. **95**, 035227 (2020).

[25] N. Bohr, R. Peierls, G. Placzek, Nature **144**, 200 (1939).

[26] P. Moon, D. E. Spencer, J. Franklin Institute **253**, 585 (1952).

[27] P. Moon, D. E. Spencer, J. Franklin Institute **254**, 227 (1952).

[28] P. Moon, D. Spencer, *Field Theory Handbook: Including Coordinate Systems, Differential Equations and Their Solutions*, Springer Berlin Heidelberg (2012).

[29] G. N. Watson, *A Treatise on the Theory of Bessel Functions*, Cambridge Univ. Press (1995).

[30] F. W. J. Olver, D. W. Lozier, R. F. Boisvert, C. W. Clark, *NIST Handbook of Mathematical Functions*, Cambridge Univ. Press (2010).

[31] E. Merzbacher, *Quantum Mechanics*, Wiley (1998).

[32] J. J. Sakurai, J. Napolitano, *Modern Quantum Mechanics*, Pearson (2013).

[33] L. L. Foldy, Phys. Rev. **67**, 107 (1945).

[34] M. Lax, Rev. Mod. Phys. **23**, 287 (1951).

[35] M. Goldberger, K. Watson, *Collision Theory*, Dover Publications (2004).

[36] T. Hammond, M. Chapman, A. Lenef, J. Schmiedmayer, E. Smith, R. Rubenstein, D. Kokorowski, D. Pritchard, Braz. J. Phys. **27**, 193 (1997).

[37] J. Schmiedmayer, M. S. Chapman, C. R. Ekstrom, T. D. Hammond, S. Wehinger, D. E. Pritchard, Phys. Rev. Lett. **74**, 1043 (1995).

[38] J. Vigué, Phys. Rev. A **52**, 3973 (1995).

[39] C. Champenois, M. Jacquey, S. Lepoutre, M. Büchner, G. Trénec, J. Vigué, Phys. Rev. A **77** (2008).

[40] E. Butkov, *Física Matemática*, LTC (1988).

[41] P. Morse, H. Feshbach, *Methods of Theoretical Physics*, McGraw-Hill (1953).

[42] M. Viola, "Fundamental solution for helmholtz equation in higher dimensions." Mathematics Stack Exchange, "https://math.stackexchange.com/q/2255877". (version: 2017-04-30).

[43] J. E. Avery, J. S. Avery, *Hyperspherical harmonics and their physical applications.* World Scientific (2017).

[44] A. Sommerfeld, *Partial Differential Equations in Physics.* Lectures on theoretical physics, Academic Press (1964).

[45] G. Arfken, H. Weber, *Mathematical Methods For Physicists International Student Edition.* Elsevier Science, 6th ed. (2005).

[46] M. E. Pereira and A. G. M. Schmidt, Few-Body Syst. **63**, 25 (2022).

[47] A. Meremianin, J. Math. Phys. **50**, 013526 (2009).

[48] I. S. Gradshteyn, I. M. Ryzhik, *Table of integrals, series, and products.* Elsevier/Academic Press, Amsterdam, 7th ed. (2007).

[49] D. Kouri, A. Vijay, Phys. Rev. E **67**, 046614 (2003).

[50] D. J. Kouri, A. Vijay, D. K. Hoffman, J. Phys. Chem. A **107**, 7230 (2003).

[51] P. Polyanin, A. Manzhirov, *Handbook of Integral Equations: Second Edition.* Handbooks of mathematical equations, CRC Press (2008).

[52] J. D. Jackson, *Classical Electrodynamics*, John Wiley & Sons (1999).

[53] D. Kouri, D. Hoffmann, Few-Body Syst. **18**, 203 (1995).

[54] A. C. Maioli, "https://arxiv.org/abs/2009.09944". (2020).

[55] R. Landau, *Quantum Mechanics II: A Second Course in Quantum Theory*, Wiley, 2008.

[56] L. Faddeev, Sov. Phys. JETP **12**, 1014 (1961).

[57] L. D. Faddeev, S. P. Merkuriev, *Quantum Scattering Theory for Several Particle Systems*, Springer (1993).