S18: Advanced Quantum Mechanics
HT 2021

Professor John Wheater*

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This is a short introductory course on two slightly more advanced topics in Quantum Mechanics. It covers non-relativistic scattering theory, and gives an introduction to relativistic quantum mechanics. I assume that you have done a basic quantum mechanics course, and have met the Schrodinger equation for simple systems, Dirac notation, the conservation of angular momentum in central potentials, and perturbation theory. The recommended books for the course are

1. *Quantum Mechanics* by Schiff, which is available as a pdf from https://archive.org, contains a very thorough exposition of scattering theory.

2. *Modern Quantum Mechanics* by Sakurai, which is available on line from within the OU library system or as a paperback, has a very good chapter on relativistic QM.

As this is a Short Option course there are no problem sets, but there are Homeworks scattered through the course which you are encouraged to do. Problems at the level of the course can be found in past exam papers.

1 Scattering: an introduction

1.1 Overview

Scattering Theory is important because it provides the mechanism for relating the results of many experiments to the underlying theory that we believe describes them. A large part of experimental physics – from the interaction of light with atoms to the collision of very high energy protons at the Large Hadron Collider – involves scattering one particle off another. In these experiments we typically know what the state of the system is at the beginning and at the end. We set up an initial state with a known target and fire in a particle of known momentum or wavelength. We do not see directly what happens in the interaction region – but just the particles or waves which emerge and trigger our observational apparatus. On the other hand our theories are precisely supposed to provide a mathematical description of what *does* happen in the interaction region. It is scattering theory that enables us to connect the two.

These lectures introduce the basic ideas of non-relativistic scattering theory, focussing on elastic scattering. Inelastic scattering is of course just as important – it is the way we usually discover new particles, or store quantum information in an ion for example – but adds new layers of complexity.

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1.2 Currents

The current associated with a wavefunction is a crucial ingredient in developing scattering theory so here is a quick reminder. The wave function satisfies the Schrödinger equation

$$i\hbar\frac{\partial\psi(\mathbf{x},t)}{\partial t} = H\psi(\mathbf{x},t) \tag{1}$$

and we will consider systems with Hamiltonian of the form

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}), \tag{2}$$

where $V(\mathbf{x})$ is a real function. It follows from the Schrödinger equation that

$$\begin{aligned}
\frac{\partial\psi^*\psi}{\partial t} &= \psi^*\frac{1}{i\hbar}\left(\frac{-\hbar^2}{2m}\boldsymbol{\nabla}^2\psi + V\psi\right) + \frac{-1}{i\hbar}\left(\frac{-\hbar^2}{2m}\boldsymbol{\nabla}^2\psi^* + V\psi^*\right)\psi && (3)\\
&= \frac{i\hbar}{2m}\left(\psi^*\boldsymbol{\nabla}^2\psi - \boldsymbol{\nabla}^2(\psi^*)\psi\right) && (4)\\
&= \boldsymbol{\nabla}.\frac{i\hbar}{2m}\left(\psi^*\boldsymbol{\nabla}\psi - \boldsymbol{\nabla}(\psi^*)\psi\right). && (5)
\end{aligned}$$

So there is a probability current

$$\mathbf{j} = -\frac{i\hbar}{2m}\left(\psi^*\boldsymbol{\nabla}\psi - \boldsymbol{\nabla}(\psi^*)\psi\right) \tag{6}$$

associated with the probability density $\rho = \psi^*\psi$ and a current conservation law

$$\frac{\partial\rho}{\partial t} = -\boldsymbol{\nabla}.\mathbf{j}\,. \tag{7}$$

For a plane wave

$$\psi = Ae^{-i(Et-\mathbf{p}.\mathbf{x})/\hbar}, \tag{8}$$

the current is

$$\mathbf{j} = |A|^2\,\frac{\mathbf{p}}{m}, \tag{9}$$

so it is proportional to the velocity.

1.3 Scattering in one dimension

You are probably familiar with the one-dimensional potential barrier problem in quantum mechanics. It can be viewed as the simplest scattering problem of all, and it has some, though not all, of the features of scattering in higher dimensions. In this section we'll remind ourselves of the essential features, and use the opportunity to interpret what we find in scattering language.

Consider the square potential barrier of height V_0 and width a located at the origin, and a wave/particle of momentum $\mathbf{p} = \hbar\mathbf{k}$ and energy $E = \hbar\omega = \frac{\mathbf{p}^2}{2m}$ incident from $x = -\infty$ as shown in Fig. 1. Classically we expect

1. If $E < V_0$ there is total reflection;
2. If $E > V_0$ there is total transmission. Note that this is true even when $V < 0$; a classical particle will travel over the potential dip undeflected.

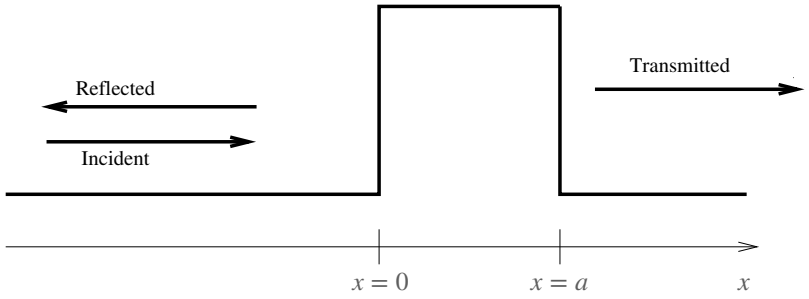


Figure 1: The one-dimensional potential barrier.

Quantum mechanically we have to allow for the possibility that the particle can be present in all three domains:

1. $x < 0$ there is the incident wave, but also a reflected wave so

$$\psi = e^{-i(\omega t - kx)} + \rho e^{-i(\omega t + kx)}, \tag{10}$$

where we have normalised the incident amplitude to 1 and called the reflected amplitude ρ; remember that ρ is a *complex* number.

2. $0 < x < a$ to satisfy the Schrödinger equation the wavenumber must change to k' where

$$\frac{\hbar^2 k'^2}{2m} + V_0 = E = \frac{\hbar^2 k^2}{2m}. \tag{11}$$

We choose k' to be the positive square root,

$$k' = +\sqrt{\frac{2m}{\hbar^2}(E - V_0)}. \tag{12}$$

so the wavefunction takes the form

$$\psi = Ae^{-i(\omega t - k'x)} + Be^{-i(\omega t + k'x)}. \tag{13}$$

3. $x > a$ there is just a transmitted wave, and the wavenumber is back to its initial value because $V = 0$ so

$$\psi = \tau e^{-i(\omega t - kx)}. \tag{14}$$

The boundary conditions are that ψ and $\frac{\partial \psi}{\partial x}$ are continuous which leads to the constraints

$$\begin{aligned} 1 + \rho &= A + B, & (15)\\ ik(1 - \rho) &= ik'(A - B), & (16)\\ \tau e^{-ika} &= Ae^{ik'a} + Be^{-ik'a}, & (17)\\ ik\tau e^{-ika} &= ik'(Ae^{ik'a} - Be^{-ik'a}). & (18) \end{aligned}$$

These equations are a little tedious to solve. We are interested in ρ and τ as they tell us about the asymptotic states; they can be written

$$\begin{aligned} \rho &= \frac{(1 - e^{2ik'a})(1 - r^2)}{(1 + r)^2 - e^{2ik'a}(1 - r)^2}, & (19)\\ \tau &= \frac{4re^{ik'a}e^{-ika}}{(1 + r)^2 - e^{2ik'a}(1 - r)^2}, & (20) \end{aligned}$$

where $r = \frac{k'}{k}$.

Homework 1.1: Check that these are indeed the solutions for ρ and τ.

To find out what these results mean physically we must calculate the currents which, using (6) are

$$j_x = \frac{\hbar k}{m}(1 - |\rho|^2), \quad x < 0 \tag{21}$$

$$= \frac{\hbar k}{m}|\tau|^2, \quad x > a \tag{22}$$

We see that there is a reflected current and a transmitted current in addition to the incident current. The reflection and transmission coefficients are

$$R = \frac{j_{reflected}}{j_{incident}} = |\rho|^2, \tag{23}$$

$$T = \frac{j_{transmitted}}{j_{incident}} = |\tau|^2. \tag{24}$$

R and T relate to the physical properties of the barrier – they are not dependent on the normalization of the incoming wave, which cancels out, and in an experiment they are not dependent on how intense the initial beam is. All the useful quantities that we look at in scattering theory have these properties.

Homework 1.2: Show that $|\rho|^2 + |\tau|^2 = 1$. Be careful, there are different regimes depending upon whether k' is real or imaginary, and you may find it easier to analyze them separately

It is instructive to explore how R and T behave as E varies; we will assume that $E > V_0$ so that k' is real in which case $r = \sqrt{1 - \frac{V_0}{E}}$.

1. If $k'a = n\pi, n = 1, 2, 3 \ldots$ then

$$\rho = 0, \tag{25}$$

$$\tau = e^{i(n\pi - ka)}, \tag{26}$$

   so there is no back-scattering (reflection) but the phase of the transmitted wave is *shifted* relative to the incident wave; this is our first example of a 'phase-shift' in scattering theory.

2. Note that T can be manipulated into the form

$$T = \frac{4}{4 + (r - r^{-1})^2 \sin^2 k'a}. \tag{27}$$

   Homework 1.3: Check this.

   So as E increases and r gets closer to 1 we see that T gets closer to 1 but with ripples because of the sine term in the denominator. When $E \gg V_0$ there is almost total transmission and the behaviour is very close to classical. Note that this behaviour is insensitive to whether V_0 is positive ($r < 1$) or negative ($r > 1$).

3. If $V_0 < 0$ and E is very small (and still positive) we see that $r \gg 1$. Equation (27) then shows us that T will be very small unless $k'a$ is very close to $n\pi$. So there is almost total reflection which is completely different from the classical case where there would be total transmission.

Some of these characteristics of one-dimensional scattering will be shared by higher dimensional systems, but clearly the characterisation by two numbers, R and T will not. Our calculations also depended on exact solution which relies on the potential being square; clearly the real world is not often so accommodating and we need better methods which we will develop over the next few sections. However our first task is to understand how to characterise the outcome of a scattering experiment in higher dimensions.

2 Scattering: moving up to three dimensions

2.1 Defining the problem

In three dimensions the scattered particles can come off the target in any direction and the simple characterisation by reflection and transmission does not make sense any more – the scattered particles fly out in all directions.

To make this quantitative consider a system in which a very massive target sits at the origin. A particle beam with flux (or current) f particles per second per unit area moving in the z direction is directed at it from $z = -\infty$. The direction of motion of a scattered particle can be described by the polar angle θ and the azimuthal angle ϕ. Suppose that δn particles per second are detected by an idealised detector that subtends solid angle $\delta\Omega$ at the target, see Fig. 2. Then

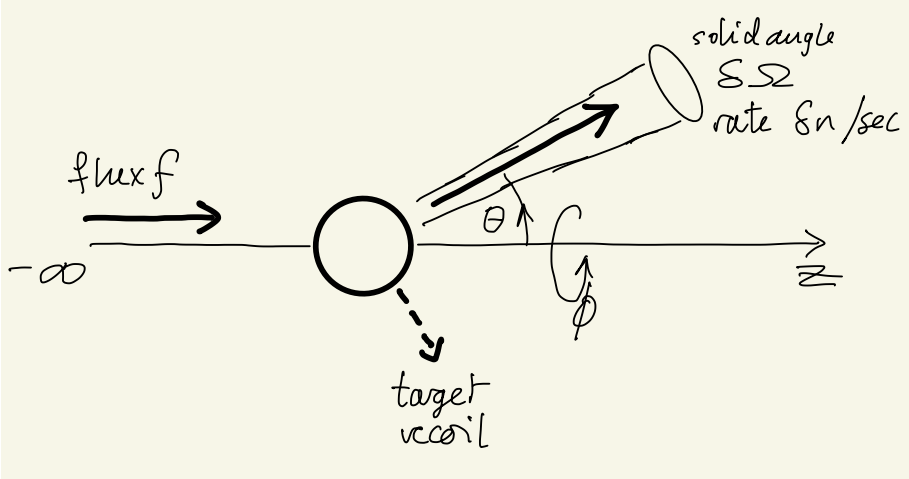


Figure 2: The basic set-up for three-dimensional scattering in the lab frame with an initially stationary target.

$$\delta n = f \frac{d\sigma(\theta,\phi)}{d\Omega}\delta\Omega \tag{28}$$

where we have introduced the *differential cross-section* $\frac{d\sigma(\theta,\phi)}{d\Omega}$. Note that if we double f we expect δn to double but the differential cross-section which reflects the underlying physics of the scattering processes is unaffected. Clearly δn is (a slightly idealised) measurable, f is a tunable parameter of the experiment and $\delta\Omega$ is determined by the architecture of the detector so $\frac{\delta n}{f\delta\Omega}$ is an experimentally measurable quantity. On the other hand it also equals the differential cross-section which we will show can be calculated from quantum mechanics and knowledge of the potential. It is good to realise two things about this construction:

1. Usually what we are trying to do in real life is deduce the potential from the differential cross-section which is rather harder than just calculating for a known potential;

2. Real detectors are inefficient - they don't detect all the particles going past and they don't have uniform sensitivity over the solid angle.

A target of finite mass recoils in a collision so we have to consider the wavefunction for two particles $\Psi(\mathbf{x}_1, \mathbf{x}_2)$. However we expect the interaction potential to depend only on the relative separation $\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2$ so the Schrödinger equation takes the form

$$\left(-\frac{\hbar^2}{2m_1}\boldsymbol{\nabla}^2_{\mathbf{x}_1} - \frac{\hbar^2}{2m_2}\boldsymbol{\nabla}^2_{\mathbf{x}_2} + V(\mathbf{x})\right)\Psi = i\hbar\frac{\partial\Psi}{\partial t}. \tag{29}$$

This can be rewritten in terms of $\mathbf{x}$ and the centre of mass coordinate

$$\mathbf{X} = \frac{m_1\mathbf{x}_1 + m_2\mathbf{x}_2}{M}, \quad M = m_1 + m_2, \tag{30}$$

as

$$\left(-\frac{\hbar^2}{2M}\boldsymbol{\nabla}^2_{\mathbf{X}} - \frac{\hbar^2}{2\mu}\boldsymbol{\nabla}^2_{\mathbf{x}} + V(\mathbf{x})\right)\Psi = i\hbar\frac{\partial\Psi}{\partial t}, \tag{31}$$

where μ is the reduced mass given by $\mu^{-1} = m_1^{-1} + m_2^{-1}$.
Homework 2.1: Derive (31).
This equation is separable so we write

$$\Psi(\mathbf{X}, \mathbf{x}, t) = e^{-i(E_{CM}+E_{int})/\hbar}e^{i\mathbf{P}.\mathbf{X}/\hbar}\psi(\mathbf{x}), \tag{32}$$

where $E_{CM} = \frac{\mathbf{P}^2}{2M}$ is the energy associated with the motion of the centre of mass motion with momentum $\mathbf{P}$. Substituting this into the Schrödinger equation we find

$$\left(-\frac{\hbar^2}{2\mu}\boldsymbol{\nabla}^2_{\mathbf{x}} + V(\mathbf{x})\right)\psi = E_{int}\psi, \tag{33}$$

so E_{int} is the energy associated with the internal (or relative) motion of the two particles. This calculation shows that we can always deal with the recoil by working in the centre of mass frame where the Schrödinger equation we have to solve takes exactly the same form of a particle moving in a fixed potential as it would if we had an infinite mass target – the only difference is that we replace the beam particle mass with the reduced mass. From now on we will drop the label and just call the internal energy E. There are two regimes in which we can look for solutions to (33):

1. If $E < 0$ then the wavefunction will describe a *bound state*. Generally the absolute value of the wavefunction will decay exponentially at large distances, and the allowed E values will form a discrete spectrum – think of the hydrogen atom for example.

2. If $E > 0$ then the wavefunction at infinity remains finite, and the allowed E values form a continuum – corresponding to the fact that in an experiment we can dial the kinetic energy of the beam particle to anything positive we like. It is convenient to rewrite the equation by defining $E = \frac{\hbar^2k^2}{2\mu}$ and $U(\mathbf{x}) = \frac{2\mu}{\hbar^2}V(\mathbf{x})$ so that

$$(\boldsymbol{\nabla}^2 + k^2)\psi - U(\mathbf{x})\psi = 0 \tag{34}$$

which we call the scattering equation.

The next step is to understand what is the appropriate generalization of the form of the wavefunction from the 1D case (10),(14) to 3D. We do this by looking at the asymptotic behaviour a long way from the target.

1. We want an incident plane wave of energy $E = \frac{\hbar^2k^2}{2\mu}$ propagating from $z = -\infty$; this must take the form

$$\psi_{inc} = 1\, e^{ikz}, \tag{35}$$

where we have emphasized that the normalization is chosen so that the coefficient is 1. Note that ψ_{inc} satisfies the scattering equation in the region where $U(\mathbf{x}) = 0$,

$$(\boldsymbol{\nabla}^2 + k^2)\psi_{inc} = 0. \tag{36}$$

2. Long after interacting with the target the scattered particles can come out in any direction and the wave function describing them must take the form of a spherical wave modulated by the angular distribution and again satisfying the scattering equation

$$0 = (\boldsymbol{\nabla}^2 + k^2)\psi = \left(\frac{1}{r}\frac{\partial^2(r\psi)}{\partial r^2} + k^2\psi\right) + \frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial\psi}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right). \tag{37}$$

You can check that

$$\psi_{scatt} = \frac{e^{ikr}}{r} f_k(\theta,\phi)\left(1 + O(r^{-1})\right) \tag{38}$$

satisfies (37) to leading order in r^{-1}.
Homework 2.2: Do this!
The, as yet unknown, function $f_k(\theta,\phi)$ is called the *scattering amplitude*.

We conclude that at large distances from the target, where $U(\mathbf{x}) = 0$, the wavefunction takes the form

$$\psi = e^{ikz} + \frac{e^{ikr}}{r} f_k(\theta,\phi)\left(1 + O(r^{-1})\right). \tag{39}$$

The scattering amplitude is computed by requiring in addition that this asymptotic wavefunction is consistent with the properties of the exact wavefunction in the region where $U(\mathbf{x}) \neq 0$. The current associated with ψ is

$$\mathbf{j} = \hat{\mathbf{z}}\frac{\hbar k}{\mu} + \frac{\hat{\mathbf{r}}}{r^2}\frac{\hbar k}{\mu}|f_k(\theta,\phi)|^2 + O(r^{-3}) + \text{interference terms}. \tag{40}$$

Homework 2.3: Calculate $\mathbf{j}$ starting from the expression (39) for ψ.
The terms that are $O(r^{-3})$ do not contribute to the flux at large r, but what about the interference terms? Treating the incident particle as a plane wave is an idealization. In reality the state of the initial particle will be collimated in some kind of beam with finite transverse extent – so it would better be described by a wavepacket. In turn this makes the calculations that we have to do very much more complicated (they can be done of course); but for scattering angle $\theta \neq 0, \pi$ and at very large r the interference terms will not be present for a finite width beam. In that case the only currents we see are the incident current which is the $\hat{\mathbf{z}}$ component of $\mathbf{j}$ and the scattered current which is the $\hat{\mathbf{r}}$ component. Using these currents in (28) gives

$$\begin{aligned}\frac{d\sigma(\theta,\phi)}{d\Omega} &= f^{-1}\frac{\delta n}{\delta\Omega} \\ &= \left(\frac{\hbar k}{\mu}\right)^{-1}\frac{r^2\delta\Omega\frac{\hbar k}{\mu}|f_k(\theta,\phi)|^2}{\delta\Omega} \\ &= |f_k(\theta,\phi)|^2.\end{aligned} \tag{41}$$

If we can compute the scattering amplitude we know the differential cross-section; this is the essential connection between theory and experiment that we have been aiming for. Lastly it is worth remembering that in some cases it is possible to set up experiments where the detector is not really at asymptotically large r in which case the interference terms cannot be ignored; this has some similarity to the near-field effects around a radiating antenna for example.

2.2 The Dirac delta function

Most of you will have come across the Dirac delta function before but here is a summary of what we need. The first thing to realise is that it is not actually a function in the usual sense at all. It is an example of what mathematicians call a *distribution*. You can think of $\delta(x)$ as an object that takes the value zero everywhere except at $x = 0$ where its value is (positive) infinite; it has the properties

$$\begin{aligned} \int_{-\infty}^{\infty} \delta(x)\, dx &= 1 \\ \int_{-\infty}^{\infty} \delta(x)\, g(x)\, dx &= g(0) \end{aligned} \tag{42}$$

provided that $g(x)$ is continuous at $x = 0$. There are various ways of thinking of the delta function as the limit of some smooth function that becomes more and more spiked at the origin as the limit is taken. These can be useful but underestimate the power of the true delta function as they always imply extra conditions on the function $g(x)$ in the property (42). The second useful property is that

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx}\, dk \tag{43}$$

ie it is the Fourier transform of 1. The three dimensional delta function is simply the product of three delta functions - one for each coordinate so

$$\delta^3(\mathbf{x}) = \delta(x)\delta(y)\delta(z). \tag{44}$$

Homework 2.4: Show that

$$\int_{-\infty}^{\infty} \delta(f(x))\, g(x) dx = \sum_n \frac{g(x_n)}{f'(x_n)}, \tag{45}$$

where the x_n are the zeroes of $f(x)$.

2.3 Green's functions

We define a Green's function $G(\mathbf{x})$ of the operator $\boldsymbol{\nabla}^2 + k^2$ to be a solution of the equation

$$\left(\boldsymbol{\nabla}^2 + k^2\right) G(\mathbf{x}) = \delta^3(\mathbf{x}). \tag{46}$$

This is useful because we can then write the formal solution of the scattering equation in the form

$$\psi(\mathbf{x}) = \psi_0(\mathbf{x}) + \int d^3\mathbf{x}' G(\mathbf{x} - \mathbf{x}') U(\mathbf{x}') \psi(\mathbf{x}'), \tag{47}$$

where $\psi_0(\mathbf{x})$ is a solution of the homogeneous equation

$$\left(\boldsymbol{\nabla}^2 + k^2\right) \psi_0(\mathbf{x}) = 0. \tag{48}$$

This is easy to check by operating with $\boldsymbol{\nabla}^2 + k^2$ on (47) to get

$$\begin{aligned} \left(\boldsymbol{\nabla}^2 + k^2\right) \psi(\mathbf{x}) &= \int d^3\mathbf{x}' (\boldsymbol{\nabla}^2_{\mathbf{x}} + k^2) G(\mathbf{x} - \mathbf{x}') U(\mathbf{x}') \psi(\mathbf{x}') \\ &= \int d^3\mathbf{x}' \delta^3(\mathbf{x} - \mathbf{x}') U(\mathbf{x}') \psi(\mathbf{x}') \\ &= U(\mathbf{x}) \psi(\mathbf{x}). \end{aligned} \tag{49}$$

It is not enough to know that we have a solution to the scattering equation – it must have the right asymptotic large distance behaviour (39). So we choose

$$\psi_0(\mathbf{x}) = e^{ikz}, \tag{50}$$

which describes the incoming plane wave. The right choice for the Green's function turns out to be

$$G(\mathbf{x}) = -\frac{e^{ik|\mathbf{x}|}}{4\pi|\mathbf{x}|}, \tag{51}$$

which, as we will see, describes the outgoing spherical wave. First though we need to check that this form of $G(\mathbf{x})$ really is a Green's function. Setting $|\mathbf{x}| = r$ we have, provided $r \neq 0$, that

$$(\boldsymbol{\nabla}^2 + k^2)G(r) \quad = \quad \frac{1}{r}\frac{\partial^2(rG)}{\partial r^2} + k^2 G(r) = 0. \tag{52}$$

So the only question is what happens at $\mathbf{r} = 0$ where the derivatives are ill-defined? Using

$$\boldsymbol{\nabla} G(r) = \hat{\mathbf{r}}\frac{\partial G}{\partial r} \quad = \quad \frac{\hat{\mathbf{r}}}{4\pi}\left(\frac{1}{r^2} - \frac{ik}{r}\right) e^{ikr} \tag{53}$$

and integrating over the surface of a sphere of radius ϵ centred on $\mathbf{x} = 0$ we find that

$$\int dA\, \hat{\mathbf{r}}.\boldsymbol{\nabla} G(r) = 4\pi\epsilon^2 \times \frac{1}{4\pi}\left(\frac{1}{\epsilon^2} - \frac{ik}{\epsilon}\right) e^{ik\epsilon}, \tag{54}$$

which converges to 1 as $\epsilon \to 0$. Applying the divergence theorem we get

$$\int dV\, \boldsymbol{\nabla}^2 G(r) = 1. \tag{55}$$

This is the analogue of Gauss's Law in electrostatics – the net outward flux is $+1$ from which we deduce that the charge at $\mathbf{x} = 0$ must be $+1$, so the charge density must be $\delta(\mathbf{x})$ and we conclude that $G(\mathbf{x})$ satisfies (46). If you find this justification for the form of $G(\mathbf{x})$ slightly unsatisfactory, we will calculate it in a more sophisticated way in Sections 2.5 and 2.6.

2.4 The Born Approximation

The solution (47) really only replaces a differential equation for ψ, so what do we do with it? The trick is to *iterate* it by substituting the expression for ψ into the right hand side; doing this once we get

$$\psi(\mathbf{x}) = \psi_0(\mathbf{x}) + \int d^3\mathbf{x}'\, G(\mathbf{x}-\mathbf{x}')U(\mathbf{x}')\left(\psi_0(\mathbf{x}') + \int d^3\mathbf{x}''\, G(\mathbf{x}'-\mathbf{x}'')U(\mathbf{x}'')\psi(\mathbf{x}'')\right); \tag{56}$$

repeating gives

$$\begin{aligned}\psi(\mathbf{x}) \quad &= \quad \psi_0(\mathbf{x}) + \int d^3\mathbf{x}'\, G(\mathbf{x}-\mathbf{x}')U(\mathbf{x}')\psi_0(\mathbf{x}') \\ &\quad + \int d^3\mathbf{x}'\, G(\mathbf{x}-\mathbf{x}')U(\mathbf{x}')\int d^3\mathbf{x}''\, G(\mathbf{x}'-\mathbf{x}'')U(\mathbf{x}'')\psi_0(\mathbf{x}'') + O(U^3).\end{aligned} \tag{57}$$

The expressions rapidly become unwieldy but you can see what is happening; each successive term contains an extra power of U so essentially we are generating a perturbation expansion in the potential. This is called the *Born Expansion* and it is the scattering theory equivalent of

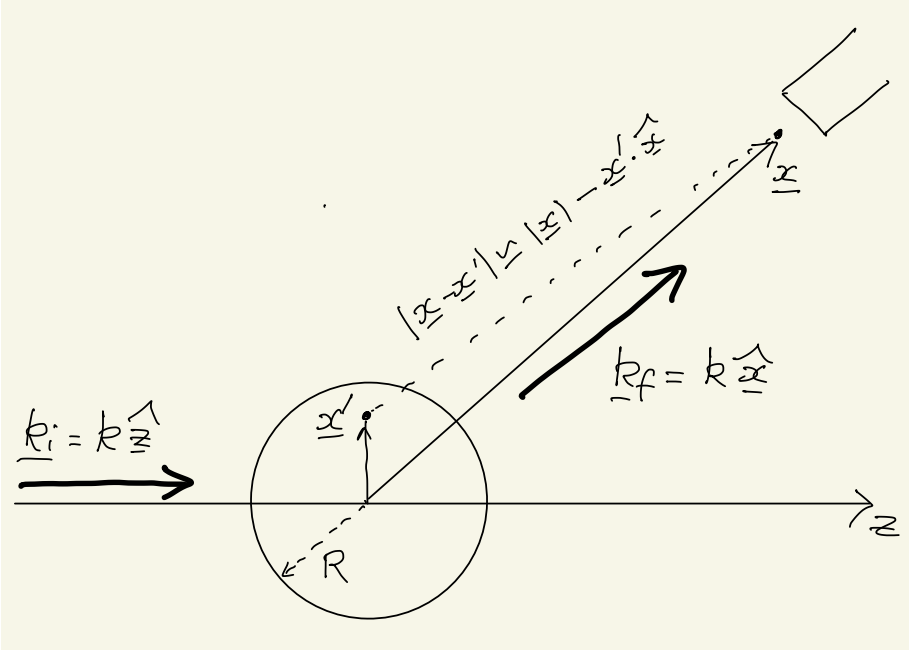


Figure 3: Configuration for scattering by a finite range potential.

the method of time independent perturbation theory that you have already learned about for bound states. It is useful because ψ_0 is known; term by term all that is left to do is an integral of an (increasingly complicated) known function. The *first Born approximation* simply takes the first tem of the expansion which gives

$$\psi^{(1)}_{scatt}(\mathbf{x}) = -\int d^3\mathbf{x}'\,\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}\,U(\mathbf{x}')\,e^{ikz'}. \tag{58}$$

The second Born approximation takes the first two terms so

$$\psi^{(2)}_{scatt}(\mathbf{x}) = \psi^{(1)}_{scatt}(\mathbf{x}) + \int d^3\mathbf{x}'\,\frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|}\,U(\mathbf{x}')\int d^3\mathbf{x}''\,\frac{e^{ik|\mathbf{x}'-\mathbf{x}''|}}{4\pi|\mathbf{x}'-\mathbf{x}''|}U(\mathbf{x}'')e^{ikz''}. \tag{59}$$

Let's examine the first Born approximation expression. If $U(\mathbf{x})$ is non-zero only for $|\mathbf{x}| < R$, then we can simplify this expression further because then the integral actually only runs over $|\mathbf{x}'| < R$, see Fig. 3, so

$$\begin{aligned} |\mathbf{x}-\mathbf{x}'| &= \sqrt{(\mathbf{x}-\mathbf{x}').(\mathbf{x}-\mathbf{x}')} \\ &= \sqrt{|\mathbf{x}|^2 - 2\mathbf{x}.\mathbf{x}' + |\mathbf{x}'|^2} \\ &= |\mathbf{x}| - \hat{\mathbf{x}}.\mathbf{x}' + O\left(\frac{|\mathbf{x}'|}{|\mathbf{x}|^2}\right). \end{aligned} \tag{60}$$

Using this in (58) and dropping $O(|\mathbf{x}|^{-2})$ terms gives

$$\begin{aligned} \psi^{(1)}_{scatt}(\mathbf{x}) &= -\frac{e^{ik|\mathbf{x}|}}{4\pi|\mathbf{x}|}\int d^3\mathbf{x}'\,e^{ikz'-ik\hat{\mathbf{x}}.\mathbf{x}'}U(\mathbf{x}'), \\ &= -\frac{e^{ik|\mathbf{x}|}}{4\pi|\mathbf{x}|}\int d^3\mathbf{x}'\,e^{ik\hat{\mathbf{z}}.\mathbf{x}'-ik\hat{\mathbf{x}}.\mathbf{x}'}U(\mathbf{x}'), \\ &= -\frac{e^{ik|\mathbf{x}|}}{4\pi|\mathbf{x}|}\int d^3\mathbf{x}'\,e^{i(\mathbf{k}_i-\mathbf{k}_f).\mathbf{x}'}U(\mathbf{x}'), \end{aligned} \tag{61}$$

where $\mathbf{k}_i, \mathbf{k}_f$ are the wavevectors of the incident and scattered particle respectively. This is exactly of the expected asymptotic form (39) with the scattering amplitude given by

$$\begin{aligned} f_k(\theta,\phi) &= -\frac{1}{4\pi}\int d^3\mathbf{x}' e^{i(\mathbf{k}_i-\mathbf{k}_f).\mathbf{x}'}U(\mathbf{x}'), \\ &= -\frac{\mu}{2\pi\hbar^2}\int d^3\mathbf{x}' e^{i(\mathbf{k}_i-\mathbf{k}_f).\mathbf{x}'}V(\mathbf{x}'). \end{aligned} \tag{62}$$

We see that $f_k(\theta,\phi) = f(\mathbf{k}_f, \mathbf{k}_i)$ is essentially the Fourier transform of the scattering potential. A simple example is the spherical well potential

$$\begin{aligned} U(\mathbf{x}) &= U_0, \quad |\mathbf{x}| \le R \\ &= 0, \quad |\mathbf{x}| > R. \end{aligned} \tag{63}$$

Using spherical polar coordinates with polar axis along $\mathbf{K} = \mathbf{k}' - \mathbf{k}$ we get

$$\begin{aligned} f_k(\theta,\phi) &= -\frac{U_0}{4\pi}\int_0^R r'^2 dr' \int_0^{2\pi} d\phi' \int_{-1}^{+1} d(\cos\theta') e^{-iKr'\cos\theta'} \\ &= \frac{U_0}{2iK}\int_0^R r'(e^{-iKr'} - e^{iKr'})dr' \\ &= -\frac{U_0}{K}\int_0^R r' \sin Kr'\, dr' \\ &= \frac{U_0}{K^3}(KR\cos KR - \sin KR). \end{aligned} \tag{64}$$

It's easy to show that $K = |\mathbf{K}| = 2k\sin\frac{1}{2}\theta$, so we have found the scattering amplitude as a function of scattering angle θ – note that it is independent of the azimuthal angle ϕ.
Homework 2.5: Show that $K = 2k\sin\frac{1}{2}\theta$.

We can see that the behaviour of f_k is quite different for different kinematical regimes. If $kR \ll 1$ the wavelength of the beam particles is much greater than the extent of the potential and we find that

$$f_k(\theta,\phi) = -\frac{U_0}{3}R^3\left(1 - \frac{1}{5}(kR)^2(1-\cos\theta) + O((kR)^4)\right), \tag{65}$$

and the amplitude has a large component independent of θ with a small piece proportional to $\cos\theta$ superimposed. If $kR \gg 1$ the wavelength of the beam particles is much smaller than the extent of the potential and the amplitude has many zeroes; for example Fig.4 shows f_k for $kR = 4\pi$. The presence of the zeroes shows that we are able to resolve much more detail about the nature of the potential because of the small wavelength.
Homework 2.6: The numerator of f_k always has a zero at $\theta = 0$. Show that a second zero emerges when $kR > \frac{1}{2}\pi$, and find the criterion for f_k to have n zeroes.

It is of course more complicated to calculate the second Born approximation and we won't do that here. However to be sure that the first approximation is a reliable description of the physics we do need the 2nd order correction to be small which means that the potential U_0 must be small enough.

2.5 The Lippmann-Schwinger equation

The Lippmann-Schwinger equation is a more formal way of looking at the Green's function calculations we have just done. Consider a Hamiltonian which is made up of a free part H_0

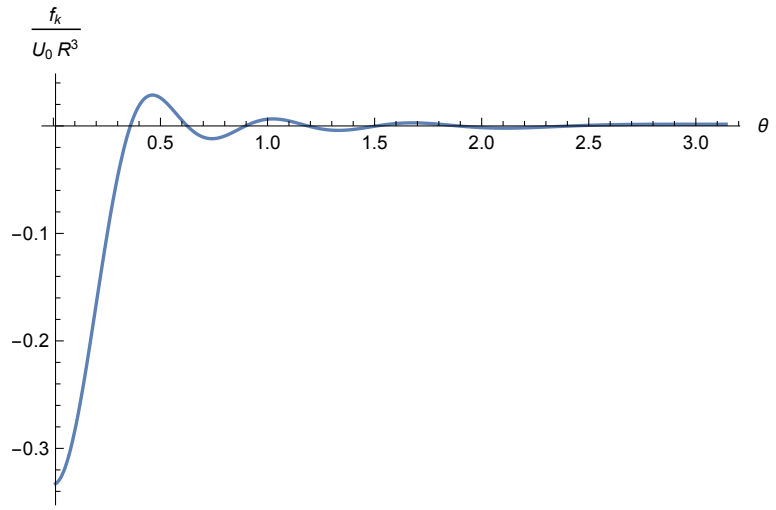


Figure 4: The scattering amplitude for a spherical well potential with $kR = 4\pi$.

and a potential part V (remember that any interesting potential is a function of $\mathbf{x}$ which is an operator so V is an operator),

$$H = H_0 + V. \tag{66}$$

Denote by $|\phi\rangle$ an eigenstate of H_0 with energy E,

$$H_0|\phi\rangle = E|\phi\rangle, \tag{67}$$

and by $|\psi\rangle$ an eigenstate of the full Hamiltonian with the *same* energy,

$$(H_0 + V)|\psi\rangle = E|\psi\rangle. \tag{68}$$

Of course this only works when $E > 0$ so that there is a continuum of states – precisely the situation in a scattering problem. We want to find the relationship, called the Lippmann-Schwinger equation, between ψ and ϕ.

Before we solve the problem we need to recall a few facts and establish some conventions about position and momentum eigenstates. The eigenstates of the momentum and position operators satisfy (we have temporarily put hats on operators),

$$\begin{aligned} \hat{\mathbf{x}}|\mathbf{x}\rangle &= \mathbf{x}|\mathbf{x}\rangle, \\ \hat{\mathbf{p}}|\mathbf{p}\rangle &= \mathbf{p}|\mathbf{p}\rangle. \end{aligned} \tag{69}$$

These eigenstates are normalised as

$$\begin{aligned} \langle\mathbf{x}|\mathbf{x}'\rangle &= \delta^3(\mathbf{x} - \mathbf{x}'), \\ \langle\mathbf{p}|\mathbf{p}'\rangle &= \delta^3(\mathbf{p} - \mathbf{p}'), \end{aligned} \tag{70}$$

and the identity operator can be written

$$1 = \int d^3\mathbf{x}\, |\mathbf{x}\rangle\langle\mathbf{x}| = \int d^3\mathbf{p}\, |\mathbf{p}\rangle\langle\mathbf{p}|. \tag{71}$$

The wavefunction $\psi(\mathbf{x})$ is given by

$$\langle\mathbf{x}|\psi\rangle = \psi(\mathbf{x}), \tag{72}$$

and the plane wave by

$$\langle \mathbf{x}|\mathbf{p}\rangle = \frac{e^{i\frac{\mathbf{p}\cdot\mathbf{x}}{\hbar}}}{(2\pi\hbar)^{\frac{3}{2}}}. \tag{73}$$

Homework 2.7: Using this expression for $\langle \mathbf{x}|\mathbf{p}\rangle$ show that

$$\int d^3\mathbf{p}\, \langle \mathbf{x}'|\mathbf{p}\rangle\langle \mathbf{p}|\mathbf{x}\rangle = \delta^3(\mathbf{x}-\mathbf{x}') \tag{74}$$

Now, suppose that Q is a hermitian operator with a complete set of eigenstates $|n\rangle$ and corresponding eigenvalues q_n so

$$Q|n\rangle = q_n|n\rangle. \tag{75}$$

Then Q has the representation

$$Q = \sum_n |n\rangle q_n \langle n|, \tag{76}$$

as you can easily check by applying the r.h.s. to an arbitrary state.
Homework 2.8: Check this statement by considering the operation of Q on the state $|\chi\rangle = \sum_\ell a_\ell|\ell\rangle$
If Q has an inverse (which requires $q_n \neq 0\,\forall n$) then we also have

$$Q^{-1} = \sum_n |n\rangle q_n^{-1}\langle n|. \tag{77}$$

If some of the eigenvalues are zero then of course this doesn't work but we can still consider

$$(Q \pm i\epsilon)^{-1} = \sum_n |n\rangle (q_n \pm i\epsilon)^{-1}\langle n|, \tag{78}$$

where ϵ is small, real and positive. This inverse is well defined because all the eigenvalues of a hermitian operator are real and so the denominator cannot vanish. Finally note that if the eigenvalues form a continuum then the sum is replaced by an integral – we will see an example of this below.

Now we can return to the Lippmann-Schwinger problem. Consider the states $|\psi_\pm\rangle$ defined implicitly by

$$|\psi_\pm\rangle = |\phi\rangle + (E - H_0 \pm i\epsilon)^{-1} V|\psi_\pm\rangle. \tag{79}$$

Note that because $E > 0$ and H_0 has a continuous positive spectrum the $i\epsilon$ is definitely needed here to make the inverse well defined. Then

$$\begin{aligned}(H_0 - E)|\psi_\pm\rangle &= (H_0 - E)|\phi\rangle + (H_0 - E)(E - H_0 \pm i\epsilon)^{-1} V|\psi_\pm\rangle \\ &= 0 - V|\psi_\pm\rangle,\end{aligned} \tag{80}$$

so $|\psi_\pm\rangle$ are eigenstates of the full Hamiltonian, provided that we can take $\epsilon \to 0$ at the end of the calculation. The expression (79) looks reminiscent of the formal solution of the scattering equation (47); it is called the Lippmann-Schwinger equation. By taking matrix elements and introducing the operator 1 in a convenient place we can show that they are in fact the same,

$$\begin{aligned}\langle \mathbf{x}|\psi_\pm\rangle &= \langle \mathbf{x}|\phi\rangle + \langle \mathbf{x}|(E - H_0 \pm i\epsilon)^{-1} \int d^3\mathbf{x}'|\mathbf{x}'\rangle\langle \mathbf{x}'|V|\psi_\pm\rangle \\ &= \langle \mathbf{x}|\phi\rangle + \int d^3\mathbf{x}'\langle \mathbf{x}|(E - H_0 \pm i\epsilon)^{-1}|\mathbf{x}'\rangle V(\mathbf{x}')\langle \mathbf{x}'|\psi_\pm\rangle.\end{aligned} \tag{81}$$

Note that we have used the fact that V is a function of the $\mathbf{x}$-operator. We conclude that the Green's functions are

$$G_{\pm}(\mathbf{x}-\mathbf{x}') = \frac{\hbar^2}{2\mu}\langle \mathbf{x}|(E-H_0 \pm i\epsilon)^{-1}|\mathbf{x}'\rangle. \tag{82}$$

It turns out that '+' is the same function as $G(\mathbf{x})$ and is the correct solution – it has an outgoing spherical wave whereas the '−' solution has an ingoing spherical wave; we will calculate $G_{\pm}(\mathbf{x})$ in the next section. Now define the T operator (or T matrix which strictly speaking refers to its matrix elements) by

$$V|\psi_+\rangle = T|\phi\rangle. \tag{83}$$

On the left hand side of this expression we are using the basis of exact eigenstates, and on the right hand side the basis of asymptotic states, which we have so far chosen to be momentum eigenstates of course. We then have using (79) that

$$\begin{aligned} T|\phi\rangle &= V|\psi_+\rangle, \\ &= V|\phi\rangle + V(E-H_0+i\epsilon)^{-1}V|\psi_+\rangle, \\ &= V|\phi\rangle + V(E-H_0+i\epsilon)^{-1}T|\phi\rangle, \end{aligned} \tag{84}$$

from which, using the fact that $|\phi\rangle$ is arbitrary state, we deduce

$$T = V + V(E-H_0+i\epsilon)^{-1}T. \tag{85}$$

Iterating this equation we find

$$T = V + V(E-H_0+i\epsilon)^{-1}V + V(E-H_0+i\epsilon)^{-1}V(E-H_0+i\epsilon)^{-1}V + \ldots, \tag{86}$$

which is precisely the Born expansion. The matrix element $\langle \mathbf{p}_f|T|\mathbf{p}_i\rangle$ is, up to a factor, the scattering amplitude; for example in first Born approximation we have (setting $|\phi\rangle = |\mathbf{p}_i\rangle$ an incoming momentum eigenstate)

$$\begin{aligned} \langle \mathbf{p}_f|T|\mathbf{p}_i\rangle &= \langle \mathbf{p}_f| \int d^3\mathbf{x}\, |\mathbf{x}\rangle\langle \mathbf{x}|V|\mathbf{p}_i\rangle, \\ &= \int d^3\mathbf{x}\, \langle \mathbf{p}_f|\mathbf{x}\rangle V(\mathbf{x})\langle \mathbf{x}|\mathbf{p}_i\rangle, \\ &= \frac{1}{(2\pi\hbar)^3}\int d^3\mathbf{x}\; e^{i\frac{(\mathbf{p}_i-\mathbf{p}_f)\cdot\mathbf{x}}{\hbar}}\, V(\mathbf{x}), \\ &= -\frac{1}{4\pi^2\hbar\mu} f(\mathbf{k}_f,\mathbf{k}_i). \end{aligned} \tag{87}$$

It is instructive to compare the scattered rate into a solid angle $\delta\Omega$ with Fermi's second Golden Rule. In doing so it is important to remember that in this section the plane wave is normalized as in (73) which affects the flux. We have

$$\begin{aligned} \text{Rate} &= (\text{Incident flux})|f(\mathbf{k}_f,\mathbf{k}_i)|^2\delta\Omega, \\ &= \left(\frac{p_i}{\mu}\frac{1}{(2\pi\hbar)^3}\right)(4\pi^2\hbar\mu)^2|\langle \mathbf{p}_f|T|\mathbf{p}_i\rangle|^2\delta\Omega, \\ &= \frac{2\pi}{\hbar}|\langle \mathbf{p}_f|T|\mathbf{p}_i\rangle|^2\; p_i\mu\,\delta\Omega, \\ &= \frac{2\pi}{\hbar}|\langle \mathbf{p}_f|T|\mathbf{p}_i\rangle|^2\left(p_i^2\frac{dp_i}{dE_i}\delta\Omega\right), \end{aligned} \tag{88}$$

which is Fermi's Golden Rule, as we recognise the term in brackets as the density of states. The T matrix itself will reappear in Section 2.9.

2.6 Computing $G_\pm(\mathbf{x}-\mathbf{x}')$

This calculation requires the contour integration method. Many of you will have met this in S1 'Functions of a Complex Variable'. If you haven't done S1 and are planning to carry on in theoretical physics then I strongly recommend that you take it this summer term.

We have

$$G_\pm(\mathbf{x}-\mathbf{x}') = \frac{\hbar^2}{2\mu}\langle\mathbf{x}|(E-H_0\pm i\epsilon)^{-1}|\mathbf{x}'\rangle. \tag{89}$$

Since $H_0 = \frac{\mathbf{p}^2}{2\mu}$ the operator to be inverted is diagonal in the momentum, so introducing a complete set of momentum eigenstates gives

$$\begin{aligned} G_\pm(\mathbf{x}-\mathbf{x}') &= \frac{\hbar^2}{2\mu}\int d^3\mathbf{p}'\,\langle\mathbf{x}|(E-H_0\pm i\epsilon)^{-1}|\mathbf{p}'\rangle\langle\mathbf{p}'|\mathbf{x}'\rangle \\ &= \frac{\hbar^2}{2\mu}\int d^3\mathbf{p}'\langle\mathbf{x}|\mathbf{p}'\rangle(E-\frac{\mathbf{p}'^2}{2\mu}\pm i\epsilon)^{-1}\langle\mathbf{p}'|\mathbf{x}'\rangle \\ &= \frac{\hbar^2}{2\mu}\frac{1}{(2\pi\hbar)^3}\int d^3\mathbf{p}'\,e^{i\frac{\mathbf{p}'.(\mathbf{x}-\mathbf{x}')}{\hbar}}(E-\frac{\mathbf{p}'^2}{2\mu}\pm i\epsilon)^{-1}. \end{aligned} \tag{90}$$

It's convenient to introduce $\mathbf{p}'=\hbar\mathbf{k}'$ and $E=\frac{\hbar^2\mathbf{k}^2}{2\mu}$ to get

$$G_\pm(\mathbf{x}-\mathbf{x}') = \int\frac{d^3\mathbf{k}'}{(2\pi)^3}\frac{e^{i\mathbf{k}'.(\mathbf{x}-\mathbf{x}')}}{k^2-k'^2\pm i\epsilon}. \tag{91}$$

As usual, introduce polar coordinates with the polar axis along $\mathbf{x}'-\mathbf{x}$ and do the angle integrals to get

$$G_\pm(\mathbf{x}-\mathbf{x}') = \frac{-i}{(2\pi)^2}\frac{1}{2|\mathbf{x}-\mathbf{x}'|}\int_{-\infty}^{\infty}\frac{k'dk'}{k'^2-k^2\mp i\epsilon}\left(e^{-ik'|\mathbf{x}-\mathbf{x}'|}-e^{ik'|\mathbf{x}-\mathbf{x}'|}\right), \tag{92}$$

where we also used the fact that the integrand is even to extend the integration range from the positive real axis to the whole real axis.

Homework 2.9: Do the angle integrals to get (92) from (91)

The idea is now to extend the integral along the real k' axis to an integral around a closed contour Γ in the complex plane

$$\int_{-\infty}^{\infty}dk'\ldots\to\int_\Gamma dk'\ldots \tag{93}$$

in such a way that the integrand vanishes on the added part of the contour, see Fig.5. So for example $e^{-ik'|\mathbf{x}-\mathbf{x}'|}$ vanishes along the circular part of Γ_- because it gives $e^{-\infty}$ (of course $|\mathbf{x}-\mathbf{x}'|>0$ by definition). We can therefore re-write (92) as

$$G_\pm(\mathbf{x}-\mathbf{x}') = \frac{-i}{(2\pi)^2}\frac{1}{2|\mathbf{x}-\mathbf{x}'|}\left(\int_{\Gamma_-}\frac{k'dk'}{k'^2-k^2\mp i\epsilon)}e^{-ik'|\mathbf{x}-\mathbf{x}'|}-\int_{\Gamma_+}\frac{k'dk'}{k'^2-k^2\mp i\epsilon)}e^{ik'|\mathbf{x}-\mathbf{x}'|}\right), \tag{94}$$

and use Cauchy's Residue Theorem to calculate the integrals. For G_+ the integrand has poles at $k'=\pm\sqrt{k^2+i\epsilon}$ which gives

$$\begin{aligned} G_+(\mathbf{x}-\mathbf{x}') &= \frac{-i}{(2\pi)^2}\frac{1}{2|\mathbf{x}-\mathbf{x}'|}2\pi i\left((-1)\frac{1}{2}e^{(-i)(-k)|\mathbf{x}-\mathbf{x}'|}-\frac{1}{2}e^{ik|\mathbf{x}-\mathbf{x}'|}\right) \\ &= -\frac{1}{4\pi|\mathbf{x}-\mathbf{x}'|}e^{ik|\mathbf{x}-\mathbf{x}'|}, \end{aligned} \tag{95}$$

which, as promised, is exactly the Green's function $G(\mathbf{x})$. (Note that once the $i\epsilon$ terms have told us where the poles are we can set $\epsilon=0$.)

Homework 2.10: Find $G_-(\mathbf{x}-\mathbf{x}')$.

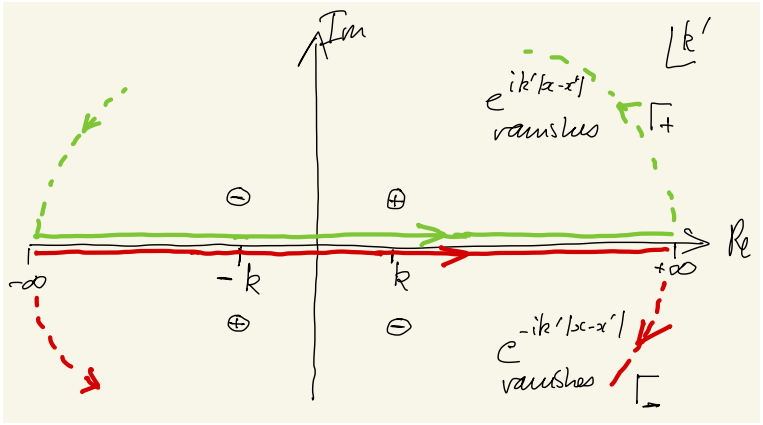


Figure 5: The integration contours closed in upper half plane, Γ_+ (green) and the lower half plane Γ_- (red). The poles in the integrand are marked by $\oplus$ for G_+ and $\ominus$ for G_-.

2.7 The Partial Wave expansion

The methods we have discussed so far work for any potential whose range is short enough, regardless of its other properties. However when the potential has spherical symmetry the angular momentum operators commute with the Hamiltonian which gives us and extra powerful tool. In spherical polar coordinates the Schrödinger equation is

$$-\frac{\hbar^2}{2\mu}\left(\frac{1}{r}\frac{\partial^2(r\psi)}{\partial r^2}+\frac{1}{r^2}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial\psi}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right)\right)+V(r)\psi=E\psi. \tag{96}$$

It can be solved by separation of variables

$$\psi = R_{E,\ell}(r)Y_{\ell,m}(\theta,\phi), \tag{97}$$

where the spherical harmonic functions have the familiar properties

$$\begin{aligned}\mathbf{L}^2Y_{\ell,m} &= \hbar^2\ell(\ell+1)Y_{\ell,m}, \quad \ell\in(0,1,2,3\ldots)\\ L_zY_{\ell,m} &= \hbar mY_{\ell,m}, \quad m\in(-\ell,-\ell+1,\ldots\ell).\end{aligned} \tag{98}$$

Using (97) and (98) shows that $R_{E,\ell}(r)$ satisfies the radial wave equation

$$-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{d^2(rR)}{dr^2}+\frac{\hbar^2}{2\mu r^2}\ell(\ell+1)R+V(r)R=ER. \tag{99}$$

The solutions of this equation are known for many standard potentials. They fall into two classes

1. For $E<0$ the spectrum is discrete and $R(r)$ falls off exponentially at large r (think, for example, of the Coulomb potential)

2. For $E>0$ the spectrum is continuous and at large r where the potential is (assumed to be) negligible $R(r)$ describes a propagating wave.

As we have argued before scattering is really about asymptotic states so we should examine the form of the solutions when $V(r)$ can be ignored. Setting $E=\frac{\hbar^2k^2}{2\mu}$ and $\rho=kr$ the radial wave equation becomes

$$-\frac{1}{\rho}\frac{d^2(\rho R(\rho))}{d\rho^2}+\left(\frac{1}{\rho^2}\ell(\ell+1)-1\right)R(\rho)=0, \tag{100}$$

which is the Spherical Bessel Equation (a somewhat unfortunate name as it rather implies that Bessel was spherical!). It is a second order linear o.d.e. so has two independent solutions which are denoted $j_\ell(\rho)$ and $y_\ell(\rho)$; these spherical Bessel functions are tabulated in many places. Here are some examples and basic properties:

$$\begin{aligned}
& & j_0(\rho) &= \frac{\sin\rho}{\rho}, & y_0(\rho) &= -\frac{\cos\rho}{\rho}, \\
& & j_1(\rho) &= \frac{\sin\rho}{\rho^2} - \frac{\cos\rho}{\rho}, & y_1(\rho) &= -\frac{\cos\rho}{\rho^2} - \frac{\sin\rho}{\rho}. \\
\rho \to 0: & & j_\ell(\rho) &\approx \frac{\rho^\ell}{(2\ell+1)(2\ell-1)\dots 1}, & y_\ell(\rho) &\approx \frac{(2\ell-1)\dots 1}{\rho^{\ell+1}} \\
\rho \to \infty: & & j_\ell(\rho) &\approx \frac{1}{\rho}\cos\left(\rho - (\ell+1)\frac{\pi}{2}\right), & j_\ell(\rho) &\approx \frac{1}{\rho}\sin\left(\rho - (\ell+1)\frac{\pi}{2}\right).
\end{aligned} \tag{101}$$

The functions $y_\ell(kr)$ are not allowed in the wavefunction for the neighbourhood of the origin because $\boldsymbol{\nabla}^2 y_0$ gives a delta function and $\boldsymbol{\nabla}^2 y_{\ell>0}$ is not defined at all at $r=0$; so these functions cannot be a solution of the Schrödinger equation in the neighbourhood of the origin. Of course in a region that does not include the neighbourhood of the origin $y_\ell(kr)$ are allowed. On the other hand the $j_\ell(kr)$ are all regular at $r=0$ and the functions

$$\phi_{k,\ell,m}(\mathbf{x}) = \sqrt{\frac{2k^2}{\pi}} j_\ell(kr) Y_{\ell,m}(\theta,\phi) \tag{102}$$

are an ortho-normalized complete set in the sense

$$\int d^3\mathbf{x}\, \phi_{k,\ell,m}(\mathbf{x})^* \phi_{k',\ell',m'}(\mathbf{x}) = \delta(k-k')\delta_{\ell'\ell}\delta_{mm'}. \tag{103}$$

In the ϕ basis the plane wave is given by

$$e^{ikz} = \sum_{\ell=0}^{\infty} e^{i\frac{\pi}{2}\ell}\sqrt{4\pi(2\ell+1)}\, j_\ell(kr) Y_{\ell,0}(\theta,\phi), \tag{104}$$

which at large r takes the asymptotic form

$$e^{ikz} = \sum_{\ell=0}^{\infty} e^{i\frac{\pi}{2}\ell}\sqrt{4\pi(2\ell+1)}\, Y_{\ell,0}(\theta,\phi)\frac{1}{2kr}\left(e^{ikr - i(\ell+1)\frac{\pi}{2}} + e^{-ikr + i(\ell+1)\frac{\pi}{2}}\right). \tag{105}$$

You can see that this form is a superposition of an ingoing and an outgoing spherical wave. If $V \neq 0$ but still short range then it must still be the case that the asymptotic behaviour is a superposition of ingoing and outgoing waves, but there should be some tell-tale that there is a potential in the neighbourhood of the origin. Considering the time-dependent wavefunction, the ingoing waves have not yet reached the potential so cannot be affected by it; on the other hand the outgoing waves have already interacted with the potential and their amplitude been changed by the interaction. We must also conserve the currents which restricts the change in the amplitude induced by the potential to a *phase* so the full wave function must take the asymptotic form

$$\psi = \sum_{\ell=0}^{\infty} e^{i\frac{\pi}{2}\ell}\sqrt{4\pi(2\ell+1)}\, Y_{\ell,0}(\theta,\phi)\frac{1}{2kr}\left(e^{ikr - i(\ell+1)\frac{\pi}{2}} e^{i2\delta_\ell} + e^{-ikr + i(\ell+1)\frac{\pi}{2}}\right). \tag{106}$$

The phase angle δ_ℓ is called the *phase shift*; note that there is an independent phase shift for each ℓ because $[\mathbf{L}^2, H] = 0$. We can find the scattering amplitude implied by this wave function

by computing

$$\begin{aligned}\psi - e^{ikz} &= \sum_{\ell=0}^{\infty} e^{i\frac{\pi}{2}\ell}\sqrt{4\pi(2\ell+1)}\,Y_{\ell,0}(\theta,\phi)\frac{1}{2kr}e^{ikr-i(\ell+1)\frac{\pi}{2}}(e^{i2\delta_\ell}-1) \\ &= \frac{e^{ikr}}{r}\sum_{\ell=0}^{\infty}\frac{1}{k}e^{i\delta_\ell}\sin(\delta_\ell)\,\sqrt{4\pi(2\ell+1)}\,Y_{\ell,0}(\theta,\phi). \end{aligned} \tag{107}$$

Te scattering amplitude is then

$$f_k(\theta,\phi) = \sum_{\ell=0}^{\infty}\frac{1}{k}e^{i\delta_\ell}\sin(\delta_\ell)\,\sqrt{4\pi(2\ell+1)}\,Y_{\ell,0}(\theta,\phi), \tag{108}$$

which can also be written conveniently as

$$f_k(\theta,\phi) = \sum_{\ell=0}^{\infty}\frac{2\ell+1}{k}e^{i\delta_\ell}\sin(\delta_\ell)\,P_\ell(\cos\theta). \tag{109}$$

Now let's look at the total cross-section which is given by

$$\sigma_{total} = \int \frac{d\sigma}{d\Omega}\,d\Omega = \int |f_k(\theta,\phi)|^2 d\Omega. \tag{110}$$

Using the orthonormality of the Spherical Harmonics gives

$$\sigma_{total} = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell. \tag{111}$$

This is already interesting: the total cross-section is the sum of independent terms in each angular momentum channel, and has a very simple dependence on the phase shift. But there is more; because $P_\ell(1) = 1$, we also have from (109) that

$$f_k(0,\phi) = \sum_{\ell=0}^{\infty}\frac{2\ell+1}{k}e^{i\delta_\ell}\sin(\delta_\ell), \tag{112}$$

from which

$$\mathrm{Im} f_k(0,\phi) = \sum_{\ell=0}^{\infty}\frac{2\ell+1}{k}\sin^2(\delta_\ell) \tag{113}$$

so that

$$\sigma_{total} = \frac{4\pi}{k}\mathrm{Im} f_k(0,\phi). \tag{114}$$

ie the total cross-section is given by a simple kinematical factor multiplied by the imaginary part of the forward (zero scattering angle) scattering amplitude. This remarkable result is called the *Optical Theorem*. You might object that it looks like a slightly flakey algebraic coincidence, but the partial wave expansion is completely general for a rotation invariant potential which makes that unlikely. In fact the Optical theorem is even more general than that, and follows from unitarity considerations – we'll come back to this in Section (2.9).

2.8 Computing phase shifts

The bad news is that this is often not very easy – after all, the phase shift is an exact quantity and will typically get a contribution at all orders in the Born expansion. A simple case that can be done is the spherical well potential (63) when $E > V_0$. The wavefunction takes a different form depending on whether $r < R$ or vice versa:

1. For $r < R$ the solution is a free spherical wave of wavenumber

$$k'^2 = k^2 - U_0, \tag{115}$$

and can only contain j_ℓ functions so

$$\psi_< = \sum_{\ell=0}^{\infty} e^{i\frac{\pi}{2}\ell}\sqrt{4\pi(2\ell+1)}\, a_\ell j_\ell(k'r)Y_{\ell,0}(\theta,\phi). \tag{116}$$

2. For $r > R$ the solution is a free spherical wave of wavenumber k but can contain both j_ℓ and y_ℓ functions so

$$\psi_> = \sum_{\ell=0}^{\infty} e^{i\frac{\pi}{2}\ell}\sqrt{4\pi(2\ell+1)}\, (b_\ell j_\ell(kr) + c_\ell y_\ell(kr))Y_{\ell,0}(\theta,\phi). \tag{117}$$

At $r = R$ the wavefunction must be continuous and differentiable in the r direction (the angular conditions are then satisfied automatically Homework 2.11: Explain why) so

$$\begin{aligned} a_\ell j_\ell(k'R) &= b_\ell j_\ell(kR) + c_\ell y_\ell(kR) \\ a_\ell k' j'_\ell(k'R) &= b_\ell k j'_\ell(kR) + c_\ell k y'_\ell(kR). \end{aligned} \tag{118}$$

which can be solved for the ratio $\alpha_\ell = \frac{c_\ell}{b_\ell}$,

$$\alpha_\ell = -\frac{\frac{k'}{k} j'_\ell(k'R)j_\ell(kR) - j_\ell(k'R)j'_\ell(kR)}{\frac{k'}{k} j'_\ell(k'R)y_\ell(kR) - j_\ell(k'R)y'_\ell(kR)}. \tag{119}$$

Using (117) we can relate α_ℓ to the phase shift. $\psi_>$ can be rewritten for $r \gg R$ as

$$\psi_> = \sum_{\ell=0}^{\infty} e^{i\frac{\pi}{2}\ell}\sqrt{4\pi(2\ell+1)}\, \frac{1}{2kr}\left((b_\ell - ic_\ell)e^{ikr - i(\ell+1)\frac{\pi}{2}} + (b_\ell + ic_\ell)e^{-ikr + i(\ell+1)\frac{\pi}{2}}\right) Y_{\ell,0}(\theta,\phi), \tag{120}$$

from which we read off that

$$e^{2i\delta_\ell} = \frac{1 - i\alpha_\ell}{1 + i\alpha_\ell}, \tag{121}$$

which in turn can written in terms of spherical Bessel functions using the solution to (118). Homework 2.12: Use these results to find the $\ell = 0$ partial amplitude for small U_0 and compare the result with our earlier calculation in Section 2.4.

2.9 Unitarity

The S-matrix relates initial states, at a time long before the influence of the potential is felt, to final states at a time when the influence of the potential is long in the past. So given two eigenstates of the free Hamiltonian, ϕ and ϕ', the amplitude for ending up in ϕ' at time $t = +\infty$ having stated in ϕ at $t = -\infty$ is

$$\langle\phi'|S|\phi\rangle. \tag{122}$$

For example, these states could be eigenstates of momentum in which case we have the amplitude for starting with momentum $\mathbf{p}_i$ and scattering to a state with momentum $\mathbf{p}_f$ for which the amplitude is

$$\langle \mathbf{p}_f | S | \mathbf{p}_i \rangle. \tag{123}$$

Of course S is really an operator and the S-matrix is its matrix representation in a particular basis – here the momentum basis. The eigenstates of the free Hamiltonian form a complete basis and by unitarity the probability of ending up in any state must be 1 so

$$\begin{aligned} 1 &= \sum_{\phi'} |\langle \phi' | S | \phi \rangle|^2 \\ &= \sum_{\phi'} \langle \phi | S^\dagger | \phi' \rangle \langle \phi' | S | \phi \rangle \\ &= \langle \phi | S^\dagger S | \phi \rangle, \end{aligned} \tag{124}$$

from which we deduce that $S^\dagger S = 1$, in other words that the S-matrix is unitary. Formally we can introduce an operator $\overline{T}$ related to S by

$$S = 1 - i\overline{T}. \tag{125}$$

The unitarity condition on S then implies

$$\overline{T}^\dagger \, \overline{T} = i(\overline{T}^\dagger - \overline{T}), \tag{126}$$

which is actually the Optical Theorem in disguise as we'll now show.

We know from Lippmann-Schwinger (79)(83) that the state including the effect of the potential is

$$|\psi_+\rangle = |\phi\rangle + (E - H_0 + i\epsilon)^{-1} T |\phi\rangle. \tag{127}$$

It follows that in the momentum basis

$$S \, |\mathbf{p}_i\rangle \;=\; \left(1 + (E_{\mathbf{p}_i} - H_0 + i\epsilon)^{-1} T\right) |\mathbf{p}_i\rangle, \tag{128}$$

and

$$\langle \mathbf{p}_f | S \, | \mathbf{p}_i \rangle = \langle \mathbf{p}_f | \left(1 + (E_{\mathbf{p}_i} - E_{\mathbf{p}_f} + i\epsilon)^{-1} T\right) | \mathbf{p}_i \rangle. \tag{129}$$

Together with the unitarity condition this implies

$$\begin{aligned} \langle \mathbf{p}_j | \mathbf{p}_i \rangle &= \int d^3\mathbf{p}_f \, \langle \mathbf{p}_j | S^\dagger \, | \mathbf{p}_f \rangle \langle \mathbf{p}_f | S \, | \mathbf{p}_i \rangle \\ &= \int d^3\mathbf{p}_f \, \langle \mathbf{p}_j | \left(1 + (E_{\mathbf{p}_j} - E_{\mathbf{p}_f} - i\epsilon)^{-1} T^\dagger\right) | \mathbf{p}_f \rangle \langle \mathbf{p}_f | \left(1 + (E_{\mathbf{p}_i} - E_{\mathbf{p}_f} + i\epsilon)^{-1} T\right) | \mathbf{p}_i \rangle \\ &= \langle \mathbf{p}_j | \mathbf{p}_i \rangle + (E_{\mathbf{p}_i} - E_{\mathbf{p}_j} + i\epsilon)^{-1} \left(\langle \mathbf{p}_j | T | \mathbf{p}_i \rangle - \langle \mathbf{p}_j | T^\dagger | \mathbf{p}_i \rangle \right) \\ &\quad + \int d^3\mathbf{p}_f \, (E_{\mathbf{p}_j} - E_{\mathbf{p}_f} - i\epsilon)^{-1} (E_{\mathbf{p}_i} - E_{\mathbf{p}_f} + i\epsilon)^{-1} \langle \mathbf{p}_j | T^\dagger | \mathbf{p}_f \rangle \langle \mathbf{p}_f | T | \mathbf{p}_i \rangle. \end{aligned} \tag{130}$$

Now we cancel the $\langle \mathbf{p}_j | \mathbf{p}_i \rangle$ term, set $\mathbf{p}_i = \mathbf{p}_j$, and rearrange to get

$$\int d^3\mathbf{p}_f \, \frac{\epsilon}{(E_{\mathbf{p}_i} - E_{\mathbf{p}_f})^2 + \epsilon^2} \, \langle \mathbf{p}_i | T^\dagger | \mathbf{p}_f \rangle \langle \mathbf{p}_f | T | \mathbf{p}_i \rangle = -i \left(\langle \mathbf{p}_i | T^\dagger | \mathbf{p}_i \rangle - \langle \mathbf{p}_i | T | \mathbf{p}_i \rangle \right), \tag{131}$$

which is essentially (126) in the momentum eigenstate basis. Remember that ϵ has to be taken to zero in this expression so we need to know that the ϵ dependent factor is actually a representation of the Dirac delta function,

$$\lim_{\epsilon\to 0}\int \frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2}\,f(x)dx = \int \delta(x)f(x)dx = f(0). \tag{132}$$

Using this result we get

$$\begin{aligned}
-2\,\mathrm{Im}\,\langle \mathbf{p}_i|T|\mathbf{p}_i\rangle &= \pi\int d^3\mathbf{p}_f\,\delta(E_{\mathbf{p}_i}-E_{\mathbf{p}_f})\,|\langle \mathbf{p}_f|T|\mathbf{p}_i\rangle|^2 \\
&= \pi\int d\Omega\, p_f^2 dp_f\,\delta(E_{\mathbf{p}_i}-E_{\mathbf{p}_f})\,|\langle \mathbf{p}_f|T|\mathbf{p}_i\rangle|^2 \\
&= \pi\int d\Omega\, p_f^2\frac{dp_f}{dE_f}dE_f\,\delta(E_{\mathbf{p}_i}-E_f)\,|\langle \mathbf{p}_f|T|\mathbf{p}_i\rangle|^2 \\
&= \pi\int d\Omega\,\left(p_f^2\frac{dp_f}{dE_f}\right)_{E_f=E_{\mathbf{p}_i}}|\langle \mathbf{p}_f|T|\mathbf{p}_i\rangle|^2.
\end{aligned} \tag{133}$$

Finally, combining this with (41) and (87) gives

$$\begin{aligned}
\sigma_{total} &= \int d\Omega\,|f(\mathbf{k}_f,\mathbf{k}_i)|^2 \\
&= (4\pi^2\hbar\mu)^2\int d\Omega\,|\langle \mathbf{p}_f|T|\mathbf{p}_i\rangle|^2 \\
&= \frac{4\pi^2\hbar\mu}{2\pi\hbar k_i\mu}\times 2\,\mathrm{Im}\,f(\mathbf{k}_i,\mathbf{k}_i) \\
&= \frac{4\pi}{k_i}\,\mathrm{Im}\,f(\mathbf{k}_i,\mathbf{k}_i),
\end{aligned} \tag{134}$$

which we recognise as the Optical Theorem again, but this time applying to a more general scattering potential, not just a spherically symmetric one.

Homework 2.13: In the partial wave formalism the S-matrix is diagonal in the angular momentum representation ie $S_{\ell\ell'} = S_\ell\delta_{\ell\ell'}$. What is S_ℓ in terms of the phase shift? Find the matrix element $\langle \ell'|T|\ell\rangle$ and the scattering amplitude.

3 Relativistic QM: The Klein-Gordon Equation

3.1 A relativistic wave equation

The Schrödinger Equation for a free particle is based on the Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} \tag{135}$$

which is non-relativistic so the resulting wave equation is not Lorentz covariant. To make a covariant wave equation we must use the relativistic energy-momentum relationship

$$E^2 = \mathbf{p}^2 + m^2, \qquad (c=1) \tag{136}$$

or, maybe,

$$E = \sqrt{\mathbf{p}^2+m^2}. \tag{137}$$

If we use (137) then we get an evil-looking wave equation

$$i\hbar\frac{\partial\psi}{\partial t} = \left(\sqrt{-\hbar^2\boldsymbol{\nabla}^2 + m^2}\right)\,\psi. \tag{138}$$

It is not at all clear how the square root of a differential operator should be treated, so instead Schrodinger considered the second order wave equation built on (136)

$$-\hbar^2\frac{\partial^2\psi}{\partial t^2} = (-\hbar^2\boldsymbol{\nabla}^2 + m^2)\psi \tag{139}$$

which is properly called the relativistic Schrodinger equation. However Schrödinger did not like the consequences and quietly dropped it; Klein and Gordon rehabilitated the equation and usually it is called the Klein-Gordon (or KG) equation. So what are the consequences that made Schrödinger uneasy?

The KG equation has plane wave solutions of the usual form

$$\psi(\mathbf{x},t) = e^{-i(Et-\mathbf{p}.\mathbf{x})/\hbar}\,\psi_0, \tag{140}$$

where ψ_0 is a constant. Substituting this form into the KG differential equation we do indeed find that

$$E^2 = \mathbf{p}^2 + m^2, \qquad (c=1). \tag{141}$$

Now there are two square roots, plus and minus, so the general solution for a state of momentum $\mathbf{p}$ is

$$\psi(\mathbf{x},t) = a_{\mathbf{p}}e^{-i(E_{\mathbf{p}t}-\mathbf{p}.\mathbf{x})/\hbar} + b_{\mathbf{p}}e^{-i(-E_{\mathbf{p}t}-\mathbf{p}.\mathbf{x})/\hbar} \tag{142}$$

where $E_{\mathbf{p}=} + \sqrt{\mathbf{p}^2+m^2}$, and $a_{\mathbf{p}}, b_{\mathbf{p}}$ are constants. We can have positive and negative energy states in contrast to the Schrödinger equation where states have $E = \frac{\mathbf{p}^2}{2m} > 0$. In fact it appears that we can have states of arbitrarily negative energy which raises the issue of existence of a ground (lowest energy) state. For example a charged KG particle would be able to emit photons and transition to a lower energy state *ad infinitum*. Also the KG equation does not *require* that ψ is complex as the Schrodinger equation does, so it is not clear that ψ is really a quantum mechanical wavefunction. It is instructive to calculate the conserved charge and current; we have

$$\psi^*(-\hbar^2\frac{\partial^2\psi}{\partial t^2}) - (-\hbar^2\frac{\partial^2\psi^*}{\partial t^2})\psi = \psi^*(-\hbar^2\boldsymbol{\nabla}^2\psi + m^2\psi) - (-\hbar^2\boldsymbol{\nabla}^2\psi^* + m^2\psi^*)\psi \tag{143}$$

so

$$-\hbar^2\frac{\partial}{\partial t}\left(\psi^*\frac{\partial\psi}{\partial t} - \frac{\partial\psi^*}{\partial t}\psi)\right) = -\hbar^2\boldsymbol{\nabla}.\left(\psi^*\boldsymbol{\nabla}\psi - (\boldsymbol{\nabla}\psi^*)\psi\right). \tag{144}$$

It follows that there is a density ρ and a current $\mathbf{j}$ satisfying the conservation law

$$\frac{\partial\rho}{\partial t} + \boldsymbol{\nabla}.\mathbf{j} = 0, \tag{145}$$

and given by

$$\begin{aligned}\rho &= \frac{i\hbar}{2m}\left(\psi^*\frac{\partial\psi}{\partial t} - \frac{\partial\psi^*}{\partial t}\psi)\right),\\ \mathbf{j} &= -\frac{i\hbar}{2m}\left(\psi^*\boldsymbol{\nabla}\psi - (\boldsymbol{\nabla}\psi^*)\psi\right).\end{aligned} \tag{146}$$

We have chosen the prefactor so that both quantities are real and the current is the same as the Schrodinger current in the non-relativistic limit. The charge and current are real but, because of the time derivative in its definition, our new ρ is not positive definite. Therefore the quantity $\int d^3\mathbf{x}\,\rho$ cannot be a probability; on the other hand $\psi^*\psi$, which could be a probability density as it is positive definite, is not conserved! We conclude that there are some problems with interpreting the KG equation as a quantum mechanical wave equation with the usual postulates of quantum mechanics.

3.2 Covariant form of the KG equation

Although the KG equation is certainly relativistic we haven't written it in a form which makes the Lorentz transformation properties manifest. It's very convenient to have a Lorentz covariant formulation both for the KG and for the Dirac equation. We define the metric and various four vectors as follows[1]

$$\begin{aligned} g_{\mu\nu} &= \mathrm{diag}(1,-1,-1,-1) && (147)\\ x^\mu &= (t,\mathbf{x}) && (148)\\ x_\mu &= x^\nu g_{\mu\nu} = (t,-\mathbf{x}) && (149)\\ \partial^\mu &= \frac{\partial}{\partial x_\mu} = (\frac{\partial}{\partial t},-\boldsymbol{\nabla}) && (150)\\ \partial_\mu &= \frac{\partial}{\partial x^\mu} = (\frac{\partial}{\partial t},\boldsymbol{\nabla}) && (151)\\ p^\mu &= i\hbar\partial^\mu = (i\hbar\frac{\partial}{\partial t},-i\hbar\boldsymbol{\nabla}) = (E,\mathbf{p}) && (152) \end{aligned}$$

By convention repeated indices – one upper and one lower are summed over – this process is called *contraction* of indices. We see that, for example, $x^\mu x_\mu = t^2 - \mathbf{x}.\mathbf{x}$ and $\partial^\mu\partial_\mu = \frac{\partial^2}{\partial t^2} - \boldsymbol{\nabla}^2$. These quantities are Lorentz scalars because they have no uncontracted indices.
Homework 3.1: Compute $\partial^\nu x_\nu$, $\partial^\nu(x^\mu a_\mu)$ (here a_μ is independent of x_μ) and $x^\nu\partial_\nu(x^\mu x_\mu)$. Be sure to express your results in covariant notation.

In covariant form the KG equation in units with $\hbar = 1$, which we will use from now on, is

$$\left(\partial^\mu\partial_\mu + m^2\right)\psi = 0. \tag{153}$$

As the KG operator is Lorentz-invariant (ie takes the same form in different inertial frames), the wavefunction ψ is a Lorentz scalar.
Homework 3.2: Prove that $\partial^\mu\partial_\mu \to \partial'^\mu\partial'_\mu$ under a Lorentz boost along the z-axis.
The conserved four-current is

$$j^\mu = (\rho,\mathbf{j}) = \frac{i}{2m}\left(\psi^*\partial^\mu\psi - (\partial^\mu\psi^*)\psi\right) \tag{154}$$

and satisfies the conservation equation $\partial_\mu j^\mu = 0$.
Homework 3.3: Check that these expressions for the current reproduce (145) and (146). Compute $\partial_\mu j^\mu = 0$ explicitly in covariant notation and use the KG equation to show that it vanishes.

3.3 KG equation in an electromagnetic field

The KG equation is coupled to an electromagnetic field by using the minimal coupling prescription

$$\partial_\mu \to \partial_\mu + ieA_\mu, \tag{155}$$

[1] We use the same conventions as *An Introduction to Quantum Field Theory* by Peskin and Schroeder.

where $A_\mu = (V, \mathbf{A})$ is the four-potential and e the charge. The KG equation becomes

$$\left((\partial^\mu + ieA^\mu)(\partial_\mu + ieA_\mu) + m^2\right)\psi = 0. \tag{156}$$

Note that this equation is *gauge invariant* under the local transformation

$$\begin{aligned} \psi(x) &\rightarrow e^{ie\alpha(x)}\psi(x) \\ A_\mu(x) &\rightarrow A_\mu(x) - \partial_\mu\alpha(x) \end{aligned} \tag{157}$$

where $\alpha(x)$ is any real differentiable function. The law for A_μ is exactly the gauge transformation law for classical electromagnetism. It is useful to define the *covariant derivative* $D_\mu = \partial_\mu + ieA_\mu$ in terms of which the KG equation is

$$(D^\mu D_\mu + m^2)\psi = 0. \tag{158}$$

We can get a little more insight by considering the KG equation in a region of constant but non-zero scalar potential V

$$-\left(\frac{\partial}{\partial t} + ieV\right)^2 \psi = \left(-\frac{\partial^2}{\partial x^2} + m^2\right)\psi. \tag{159}$$

Substituting in the plane wave solution

$$\psi(\mathbf{x}, t) = e^{-i(Et - \mathbf{p}.\mathbf{x})}\,\psi_0 \tag{160}$$

we get

$$(E - eV)^2 = \mathbf{p}^2 + m^2. \tag{161}$$

So

$$E = eV \pm E_\mathbf{p} \tag{162}$$

where, as before,

$$E_{\mathbf{p}_=} + \sqrt{\mathbf{p}^2 + m^2}. \tag{163}$$

We can interpret this as follows

1. The '+ve' energy solution with $E = eV + E_\mathbf{p}$ describes a particle of momentum $\mathbf{p}$, kinetic energy $E_\mathbf{p}$ and electric charge e in an electric potential V.

2. We note that for the '-ve' energy solution we have

$$-E = -eV + E_\mathbf{p} \tag{164}$$

and interpret it as a particle of momentum $\mathbf{p}$, kinetic energy $E_\mathbf{p}$ and electric charge $-e$. That is to say, we interpret it as an *anti-particle*; looking closely at the time dependence of the wave equation we can see that the anti-particle moves *backwards* in time.

If this is right then the wave function when $V = 0$,

$$\psi(\mathbf{x}, t) = a_\mathbf{p} e^{-i(E_{\mathbf{p}_t} - \mathbf{p}.\mathbf{x})/\hbar} + b_\mathbf{p} e^{-i(-E_{\mathbf{p}_t} - \mathbf{p}.\mathbf{x})/\hbar} \tag{165}$$

ought to be a mixture of particle and anti-particle! Let's compute ρ to check this out.

$$\begin{aligned}\rho &= \frac{1}{2m}\left(\psi^*(i\partial_t)\psi - (i\partial_t\psi^*)\psi\right) && (166)\\ &= \frac{1}{2m}\Big((a^*e^{iE_{\mathbf{p}t}} + b^*e^{-iE_{\mathbf{p}t}})E_{\mathbf{p}(}ae^{-iE_{\mathbf{p}t}} - be^{iE_{\mathbf{p}t}}) && (167)\\ &\quad -E_{\mathbf{p}(} - a^*e^{iE_{\mathbf{p}t}} + b^*e^{-iE_{\mathbf{p}t}})(ae^{-iE_{\mathbf{p}t}} + be^{iE_{\mathbf{p}t}})\Big) && (168)\\ &= \frac{E_{\mathbf{p}}}{m}(a^*a - b^*b) && (169)\end{aligned}$$

which is exactly what we would expect if ρ is actually the *charge density*!

Note that this is a purely heuristic discussion – we have not really solved the underlying problem, which is the existence or otherwise of a ground state. We'll come back to that when we've learnt about the Dirac equation.

3.4 KG Equation: angular momentum

The KG equation in a spherically symmetric potential is, from (159)

$$\left(i\frac{\partial}{\partial t} - eV(r)\right)^2\psi = \left(-\boldsymbol{\nabla}^2 + m^2\right)\psi. \tag{170}$$

The $\boldsymbol{\nabla}^2$ operator can be re-written in terms of the radial derivative and the orbital angular momentum $\mathbf{L} = \mathbf{x}\times\mathbf{p}$,

$$\boldsymbol{\nabla}^2 = \frac{1}{r^2}\frac{\partial^2}{\partial r^2}r^2 - \frac{1}{r^2}\mathbf{L}^2 \tag{171}$$

so we get

$$\left(i\frac{\partial}{\partial t} - eV(r)\right)^2\psi = -\frac{1}{r^2}\frac{\partial^2}{\partial r^2}(r^2\psi) + \frac{1}{r^2}\mathbf{L}^2\psi + m^2\psi. \tag{172}$$

from which we see that a stationary state takes the form[2]

$$\psi = e^{-iEt}Y_{\ell,m}(\theta,\phi)R(r). \tag{174}$$

This shows that the KG equation describes a particle which can have orbital angular momentum but does not have spin.

4 Relativistic QM: The Dirac Equation

4.1 A first order wave equation

Historically the Dirac equation was introduced in an attempt to rectify the defects of the KG equation, in particular the absence of a current with positive definite density, and the presence of negative energy modes. To obtain a density with no derivatives in it (which as we have seen leads to it not being positive definite) Dirac required that the wave equation should be first order

[2] $Y_{\ell,m}(\theta,\phi)$ are the spherical harmonics. They satisfy

$$\mathbf{L}^2Y_{\ell,m} = \ell(\ell+1)Y_{\ell,m}, \quad L_zY_{\ell,m} = mY_{\ell,m}, \quad -\ell\le m\le\ell, \quad \ell = 0,1,2,3,\ldots \tag{173}$$

in the time derivative, while respecting the usual relativistic energy momentum relationship for a free particle (keeping c explicit just for now)

$$E^2 = c^2\mathbf{p}^2 + m^2c^4. \tag{175}$$

But if the wave equation is first order in time it must be first order in spatial derivatives too, otherwise it could not be Lorentz covariant (as Lorentz transformations mix space and time coordinates). Dirac proposed that

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi = (c\,\boldsymbol{\alpha}.\hat{\mathbf{p}} + mc^2\beta)\psi \tag{176}$$

where we have temporarily put hats on operators and next need to establish what $\boldsymbol{\alpha}, \beta$ are. Now for a free particle of energy E and momentum $\mathbf{p}$ we must have a plane wave solution

$$\psi \;=\; e^{-\frac{i}{\hbar}(Et-\mathbf{p}.\mathbf{x})}\psi_0 \tag{177}$$

(but be aware we don't yet know what sort of quantity ψ_0 is except that it is space-time independent). Substituting in (176) gives

$$E\psi_0 = \hat{H}\psi_0 = (c\,\boldsymbol{\alpha}.\hat{\mathbf{p}} + mc^2\beta)\psi_0 \tag{178}$$

from which we get

$$E^2\psi_0 \;=\; \hat{H}^2\psi = (c^2(\mathbf{p}.\boldsymbol{\alpha})^2 + mc^3(\mathbf{p}.\boldsymbol{\alpha}\beta + \beta\mathbf{p}.\boldsymbol{\alpha}) + m^2c^4\beta^2)\psi_0. \tag{179}$$

This equation can only reproduce the relativistic energy-momentum relation (175) if

$$\begin{aligned} \alpha_i\alpha_j + \alpha_j\alpha_i &= 2\delta_{ij}, \\ \alpha_i\beta + \beta\alpha_i &= 0, \\ \beta^2 &= 1, \end{aligned} \tag{180}$$

where $i, j = 1, 2, 3$. Clearly these are not commuting objects so they must be matrices (and therefore the right hand sides of these three equations all multiply an identity matrix). It is easy to show that one choice of matrices satisfying these requirements is

$$\beta = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad \alpha_i = \begin{pmatrix} -\sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix}, \tag{181}$$

where σ_i are the Pauli sigma matrices[3] and I is the 2×2 identity matrix. There are in fact many choices, and we will return to this question later, but note now that there are no sets of matrices *smaller* than 4×4 that will satisfy the requirements; the Pauli matrices satisfy very similar anti-commutation rules but there are only three of them, and it is impossible to construct a fourth 2×2 matrix that anti-commutes with all the Pauli matrices.

[3]The Pauli sigma matrices are

$$\sigma_1 \;=\; \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{182}$$

They satisfy the relationships

$$\sigma_i\sigma_j + \sigma_j\sigma_i \;=\; 2\delta_{ij}, \quad \sigma_i\sigma_j = \delta_{ij} + i\epsilon_{ijk}\sigma_k, \quad [\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k \tag{183}$$

where repeated indices are summed over; and $\delta_{ij} = 1$ if $i = j$, zero otherwise; and $\epsilon_{ijk} = 1$ if ijk is an even permutation of 123 and $\epsilon_{ijk} = -1$ if ijk is an odd permutation of 123.

Homework 4.1: Check that α_i and β do indeed satisfy (180). Prove that there is no 2×2 matrix that anticommutes with all the Pauli matrices. Prove that there are no 3×3 matrices satisfying (180).

The equation (176) together with the relationships (180) essentially defines a unique relativistic wave equation that is first order in time derivatives. In fact they show that there is a way of taking the square root in (138) but at the price of working in a space of 4×4 hermitian matrices rather than real numbers. We see that ψ_0 must actually be a four component constant object satisfying the equation (from now on we will revert to $c = 1$ units)

$$(\mathbf{p}.\boldsymbol{\alpha} + m\beta)\psi_0 = E\psi_0. \tag{184}$$

That is to say ψ_0 is the eigenvector of the matrix $\mathbf{p}.\boldsymbol{\alpha} + m\beta$ with eigenvalue E; ψ_0 is called a *spinor* (NB although it has four components it is *not* a four-vector), and, in the context of the Dirac equation, often a *Dirac spinor*. It is easy to check that the eigenvalue condition is $(E^2 - (\mathbf{p}^2 + m^2))^2 = 0$ so there are two eigenstates of positive $E = +\sqrt{\mathbf{p}^2 + m^2}$ and two of negative $E = -\sqrt{\mathbf{p}^2 + m^2}$. Despite the Dirac equation being first order in the time derivative, there are still negative energy solutions; as for the KG equation these negative energy solutions turn out to describe antiparticles, we will return to this in a while.

Homework 4.2: Show by explicit calculation of the determinant that

$$\mathrm{Det}(\mathbf{p}.\boldsymbol{\alpha} + m\beta - E) = (E^2 - (\mathbf{p}^2 + m^2))^2. \tag{185}$$

We can find the conserved charge and current by starting with

$$i\hbar\frac{\partial\psi}{\partial t} = (-i\hbar\boldsymbol{\nabla}.\boldsymbol{\alpha} + m\beta)\psi \tag{186}$$

and then taking the hermitian conjugate (note that α, β are hermitian matrices)

$$-i\hbar\frac{\partial\psi^\dagger}{\partial t} = (i\hbar(\boldsymbol{\nabla}\psi^\dagger).\boldsymbol{\alpha} + m\psi^\dagger\beta. \tag{187}$$

Multiplying the first by $\psi^\dagger$ on the left and the second by ψ on the right and subtracting gives

$$i\left(\psi^\dagger\frac{\partial\psi}{\partial t} + \frac{\partial\psi^\dagger}{\partial t}\psi\right) = -i\left(\psi^\dagger\boldsymbol{\nabla}.\boldsymbol{\alpha}\psi + (\boldsymbol{\nabla}\psi^\dagger).\boldsymbol{\alpha}\psi\right) \tag{188}$$

so $\rho = \psi^\dagger\psi$ and $\mathbf{j} = \psi^\dagger\boldsymbol{\alpha}\psi$ satisfy the conservation equation.

4.2 Angular momentum and spin

To understand the solutions of the Dirac equation we need to know what quantities are conserved so we need to find operators that commute with the free particle Hamiltonian

$$H = \boldsymbol{\alpha}.\mathbf{p} + m\beta. \tag{189}$$

In these calculations we have to keep track of two sets of non-commuting quantities. As well as the matrix relations (180), we have the usual quantum commutation rule $[p_i, x_j] = -i\hbar\delta_{ij}$; but crucially x_i and p_i commute with β and α_i.

Of course linear momentum is conserved

$$[H, p_i] = [\alpha_k p_k + m\beta, p_i] = \alpha_k[p_k, p_i] = 0. \tag{190}$$

The orbital angular momentum operator is as usual

$$\begin{aligned} \mathbf{L} &= \mathbf{x} \times \mathbf{p} \\ L_i &= \epsilon_{ijk} x_j p_k, \end{aligned} \tag{191}$$

and then

$$\begin{aligned} [L_i, H] &= \alpha_l [\epsilon_{ijk} x_j p_k, p_l] \\ &= \alpha_l \epsilon_{ijk} [x_j, p_l], p_k \\ &= i\hbar \epsilon_{ijk} \alpha_j p_k \neq 0 \end{aligned} \tag{192}$$

so $\mathbf{L}$ is not conserved; we have to add something to it to get a conserved quantity. Consider

$$\mathbf{S} = \frac{\hbar}{2} \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} \tag{193}$$

which by construction commutes with β but not $\boldsymbol{\alpha}$ so

$$\begin{aligned} [S_i, H] &= \frac{\hbar}{2} [\begin{pmatrix} \sigma_i & 0 \\ 0 & \sigma_i \end{pmatrix}, \begin{pmatrix} -\sigma_k p_k & 0 \\ 0 & \sigma_k p_k \end{pmatrix}] \\ &= \frac{\hbar}{2} \begin{pmatrix} -[\sigma_i, \sigma_k] p_k & 0 \\ 0 & [\sigma_i, \sigma_k] p_k \end{pmatrix} \\ &= \frac{\hbar}{2} \begin{pmatrix} -2i\epsilon_{ikj} \sigma_j p_k & 0 \\ 0 & 2i\epsilon_{ikj} \sigma_j p_k \end{pmatrix} \\ &= i\hbar \epsilon_{ikj} \alpha_k p_j. \end{aligned} \tag{194}$$

Therefore

$$[L_i + S_i, H] = 0 \tag{195}$$

$$\tag{196}$$

and it is the *total angular momentum operator* $\mathbf{J} = \mathbf{L} + \mathbf{S}$ that commutes with H. Note that $\mathbf{S}$ by itself satisfies the usual commutation algebra for spin-$\frac{1}{2}$; so particles at rest (for which $\mathbf{L}$ must be zero) simply have spin-$\frac{1}{2}$. This explains why there are two solutions of positive energy, and two solutions of negative energy; each has two spin states – in the rest frame simply spin-up and spin-down. A stationary ($\mathbf{p} = 0$) state therefore has four independent solutions, ψ^{s}_E, labelled by the sign of the energy E and the spin component S,

$$\begin{aligned} H\psi^{\pm}_{+} &= +m\psi^{\pm}_{+}, \quad S_z \psi^{\pm}_{+} = \pm \frac{\hbar}{2} \psi^{\pm}_{+}; \\ H\psi^{\pm}_{-} &= -m\psi^{\pm}_{-}, \quad S_z \psi^{\pm}_{-} = \pm \frac{\hbar}{2} \psi^{\pm}_{-}. \end{aligned} \tag{197}$$

Homework 4.3: Show that $\mathbf{S}$ satisfies the usual angular momentum rules for spin quantum number $S = \frac{1}{2}$ ie the eigenvalues of $\mathbf{S}^2$ and S_z are $\frac{1}{2}(\frac{1}{2}+1)\hbar^2$ and $\pm\frac{1}{2}\hbar$ respectively.

4.3 Covariant form of the Dirac equation

The formulation of the Dirac equation that we have been looking at does not look covariant; space derivatives are multiplied by αs but time derivatives are not, and the mass appears multiplied by β. Actually the Dirac equation *is* covariant; but it doesn't look it and it is very often convenient

to write it in a more covariant form. Multiplying (176) through by β (and from now on taking $\hbar = 1$) we get

$$\begin{aligned} 0 &= \left(-i\beta\frac{\partial}{\partial t} - i\beta\boldsymbol{\alpha}.\boldsymbol{\nabla} + m\right)\psi \\ &= \left(-i\gamma^\mu\partial_\mu + m\right)\psi \end{aligned} \tag{198}$$

where

$$\gamma^\mu = (\beta, \beta\boldsymbol{\alpha}) \tag{199}$$

are called the gamma-matrices. It is straightforward to show, using the definition of the γs and the anticommutation properties of $(\boldsymbol{\alpha}, \beta)$, that

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}. \tag{200}$$

Homework 4.4: Show directly from the anticommutation properties (180) that the gamma-matrices do indeed satisfy (200).

In the representation (181) the γs are given by

$$\text{Rep 1}: \quad \gamma^0 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad \gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} \tag{201}$$

There is an infinite number of representations of the gamma-matrices and it turns out that particular forms are more or less convenient for different applications. Another representation that is very convenient is

$$\text{Rep 2}: \quad \gamma^0 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \quad \gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}. \tag{202}$$

Most of the time, and especially in quantum field theory, (198) is the form in which the Dirac equation is written. Sets of matrices satisfying the relationships (200) are called Clifford Algebras and are an important topic in mathematical physics.

Homework 4.5: Show that the current conservation equation (188) can be written as $\partial_\mu j^\mu = 0$ with $j^\mu = \psi^\dagger\gamma^0\gamma^\mu\psi$.

4.4 Plane wave spinor solutions

We are now in a position to find the constant spinor solution for an eigenstate of 4-momentum

$$\psi = c^{-ip_\mu x^\mu}\psi_0(\mathbf{p}) \tag{203}$$

– note that it will turn out to depend on $\mathbf{p}$ which we have emphasized by making the moment an argument. Substituting into the Dirac Equation we get

$$(-p_\mu\gamma^\mu + m)\psi_0(\mathbf{p}) = 0. \tag{204}$$

It's convenient to define $\not{p} = p_\mu\gamma^\mu$ so we can also write this as

$$(-\not{p} + m)\psi_0(\mathbf{p}) = 0. \tag{205}$$

To proceed we need to choose a representation of the gamma matrices; it turns out that to analyse the spin in the rest frame it is best to use Rep 2 (202) which gives

$$0 = \begin{pmatrix} -E + m & \mathbf{p}.\boldsymbol{\sigma} \\ -\mathbf{p}.\boldsymbol{\sigma} & E + m \end{pmatrix}\psi_0(\mathbf{p}). \tag{206}$$

Clearly we can write the four-component spinor in the form

$$\psi_0(\mathbf{p}) = \begin{pmatrix} u_A \\ u_B \end{pmatrix} \tag{207}$$

where $u_{A,B}$ are two component objects. Then

$$\begin{aligned} 0 &= (-E+m)u_A + \mathbf{p}.\boldsymbol{\sigma} u_B & (208)\\ 0 &= -\mathbf{p}.\boldsymbol{\sigma} u_A + (E+m)u_B. & (209) \end{aligned}$$

Homework 4.6: Show that (208) and (209) are equivalent provided $E = \pm E_{\mathbf{p}}$.
Looking at positive energy solutions, ie $E = +E_{\mathbf{p}}$, and using (209) we have

$$\psi^s_+(\mathbf{p}) = u^s(\mathbf{p}) = const \begin{pmatrix} \xi^s \\ \frac{\mathbf{p}.\boldsymbol{\sigma}}{E_{\mathbf{p}_+} m}\xi^s \end{pmatrix}, \tag{210}$$

where ξ^s is a normalized two-component spinor. If $E = -E_{\mathbf{p}}$ similar reasoning leads to

$$\psi^s_-(\mathbf{p}) = v^s(\mathbf{p}) = const \begin{pmatrix} -\frac{\mathbf{p}.\boldsymbol{\sigma}}{E_{\mathbf{p}_+} m}\xi^s \\ \xi^s \end{pmatrix}. \tag{211}$$

For a particle at rest, $\mathbf{p} = 0$, the lower half of the spinors $u^{\pm}(\mathbf{p})$ vanishes. It is useful to choose ξ^s to be an eigenstate of σ_z ie

$$\sigma_z \xi^+ = \xi^+, \quad \sigma_z \xi^- = -\xi^-. \tag{212}$$

Then $u^{\pm}(\mathbf{p})$ are eigenstates of S_z with eigenvalues $\pm\frac{\hbar}{2}$; they represent spin-half particles with spin up and down in the rest-frame respectively. Similarly the upper half of $v^{\pm}(\mathbf{p})$ vanishes and they represent spin-half anti-particles with spin up and down in the rest-frame respectively.
Homework 4.7: Show that the four spinors $u^{\pm}(\mathbf{p}), v^{\pm}(\mathbf{p})$ are mutually orthogonal.

We showed earlier that $\psi^\dagger\psi$ is a density and thus the zero-th component of a four-vector. It is therefore conventional to normalise Dirac spinors so that

$$u^{s\dagger}(\mathbf{p})u^s(\mathbf{p}) = v^{s\dagger}(\mathbf{p})v^s(\mathbf{p}) = 2E_{\mathbf{p}} \tag{213}$$

The $E_{\mathbf{p}}$ is exactly the 0-component of a 4-vector, the 2 is purely convention. We get finally[4]

$$\begin{aligned} u^s(\mathbf{p}) &= \sqrt{E_{\mathbf{p}_+} m} \begin{pmatrix} \xi^s \\ \frac{\mathbf{p}.\boldsymbol{\sigma}}{E_{\mathbf{p}_+} m}\xi^s \end{pmatrix} \\ v^s(\mathbf{p}) &= \sqrt{E_{\mathbf{p}_+} m} \begin{pmatrix} -\frac{\mathbf{p}.\boldsymbol{\sigma}}{E_{\mathbf{p}_+} m}\xi^s \\ \xi^s \end{pmatrix}. & (214) \end{aligned}$$

When $\mathbf{p} \neq 0$, it is $J_z = L_z + S_z$ that commutes with H so of course $u^{\pm}(\mathbf{p}), v^{\pm}(\mathbf{p})$ are no longer eigenstates of S_z. However we observe that since $\mathbf{p}$ and $\mathbf{J}$ commute with H so does $\mathbf{p}.\mathbf{J}$; but $\mathbf{p}.\mathbf{L} = 0$ so this implies that the spin projection operator $\mathbf{p}.\mathbf{S}$, ie the component of spin along $\mathbf{p}$, commutes with H. Therefore it is often convenient to choose the two-component spinors to be eigenstates of $\mathbf{p}.\mathbf{S}$ rather than S_z and we define $\xi^{\pm}(\mathbf{p})$ with the properties

$$\begin{aligned} \boldsymbol{\sigma}.\mathbf{p}\,\xi^{\pm}(\mathbf{p}) &= \pm|\mathbf{p}|\,\xi^{\pm}(\mathbf{p}) \\ \xi^{\pm}(\mathbf{p})^\dagger \xi^{\pm}(\mathbf{p}) &= 1. & (215) \end{aligned}$$

[4]NB In quantum field theory it is conventional to call the anti-particle spinor defined here $v^{\pm}(-\mathbf{p})$.

Homework 4.8: Find explicit expressions for $\xi^{\pm}(\mathbf{p})$ in terms of the components (p_x, p_y, p_z). Note that by changing $\mathbf{p} \to -\mathbf{p}$ you can see from (215) that $\xi^{\pm}(-\mathbf{p}) = \xi^{\mp}(\mathbf{p})$; check that your expressions have this property.

Clearly if particles are massless we cannot study them in the rest-frame. It's helpful to use Rep 1 (201) which gives

$$0 = \begin{pmatrix} 0 & -(E - \mathbf{p}.\boldsymbol{\sigma}) \\ -(E + \mathbf{p}.\boldsymbol{\sigma}) & 0 \end{pmatrix} \psi_0(\mathbf{p}) \tag{216}$$

We see that the upper and lower components of the Dirac spinor are not mixed and that solutions take the form

$$\psi_0(\mathbf{p}) = \begin{pmatrix} \xi^s(\mathbf{p}) \\ 0 \end{pmatrix}, \text{or } \psi_0(\mathbf{p}) = \begin{pmatrix} 0 \\ \xi^s(\mathbf{p}) \end{pmatrix} \tag{217}$$

so really they are two-component spinors. The origin of this is that if $m = 0$ we do not need the β matrix, just the α_i and since there are only three of them we can choose $\alpha_i = \sigma_i$. The resulting two-component spinors are called *Weyl spinors*; the eigenvalue of $\hat{\mathbf{p}}.\boldsymbol{\sigma}$ is usually called the *helicity* of the state.

We can also find Dirac spinors in Rep 1 (201) by repeating the steps above. Substituting a plane wave state into the Dirac Equation we get

$$0 = \begin{pmatrix} m & -(E - \mathbf{p}.\boldsymbol{\sigma}) \\ -(E + \mathbf{p}.\boldsymbol{\sigma}) & m \end{pmatrix} \psi^s_E(\mathbf{p}) \tag{218}$$

where as usual $E = \pm E_{\mathbf{p}}$. We then decompose the four-component spinor into spin projection two-component spinors (215)

$$\psi^s_E(\mathbf{p}) = \begin{pmatrix} A\,\xi^s(\mathbf{p}) \\ B\,\xi^s(\mathbf{p}) \end{pmatrix} \tag{219}$$

and substituting into (218) gives

$$\begin{aligned} 0 &= mA - (E - s|\mathbf{p}|)B \\ 0 &= -(E + s|\mathbf{p}|)A + mB. \end{aligned} \tag{220}$$

Again these equations are equivalent to each other. Normalizing to $2E_{\mathbf{p}}$ we finally obtain

1. the positive energy spinors

$$u^{\pm}(\mathbf{p}) = \begin{pmatrix} \sqrt{E_{\mathbf{p}_\mp}|\mathbf{p}|}\,\xi^{\pm}(\mathbf{p}) \\ \sqrt{E_{\mathbf{p}_\pm}|\mathbf{p}|}\,\xi^{\pm}(\mathbf{p}) \end{pmatrix} \tag{221}$$

2. and the negative energy spinors (see footnote 4)

$$v^{\pm}(-\mathbf{p}) = \begin{pmatrix} \sqrt{E_{\mathbf{p}_\pm}|\mathbf{p}|}\,\xi^{\pm}(\mathbf{p}) \\ -\sqrt{E_{\mathbf{p}_\mp}|\mathbf{p}|}\,\xi^{\pm}(\mathbf{p}) \end{pmatrix} \tag{222}$$

4.5 Properties under Lorentz transformations

We have seen that $\psi^\dagger\psi$ is not a Lorentz scalar. So what combination *is* a scalar? The answer is $\psi^\dagger\gamma^0\psi$. Computing explicitly in Rep 1 (201) (221) (222) for the positive energy spinors we get

$$u^{\pm}(\mathbf{p})^\dagger \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} u^{\pm}(\mathbf{p}) = 2\sqrt{E_{\mathbf{p}_\mp}|\mathbf{p}|}\sqrt{E_{\mathbf{p}_\pm}|\mathbf{p}|} \tag{223}$$

$$= 2m \tag{224}$$

Similarly we find that

$$v^{\pm}(\mathbf{p})^{\dagger}\begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix} v^{\pm}(\mathbf{p}) = -2\sqrt{E_{\mathbf{p}_{\mp}}|\mathbf{p}|}\sqrt{E_{\mathbf{p}_{\pm}}|\mathbf{p}|} \quad (225)$$

$$= -2m \quad (226)$$

Of course the result is explicitly a Lorentz scalar. The combination $\psi^{\dagger}\gamma_0$ is ubiquitous and usually called $\bar{\psi}$.

Homework 4.9: Check these relationships in Rep 2.

4.6 Dirac Equation in an external E.M. field I

As for the KG equation, the Dirac spin-half particle is coupled to an electromagnetic field by using the minimal coupling prescription

$$\partial_\mu \to D_\mu = \partial_\mu + ieA_\mu \quad (227)$$

where $A_\mu = (V, \mathbf{A})$ is the vector potential and e the charge. The Dirac equation becomes

$$(-i\not{D} + m)\psi = 0 \quad (228)$$

Again this equation is *gauge invariant* under the local transformation

$$\begin{aligned} \psi(x) &\to e^{ie\alpha(x)}\psi(x) \\ A_\mu(x) &\to A_\mu(x) - \partial_\mu\alpha(x). \end{aligned} \quad (229)$$

We first look at scattering from a potential step $A_\mu = (V, 0)$ for $z > 0$, and $A_\mu = 0$ for $z < 0$.

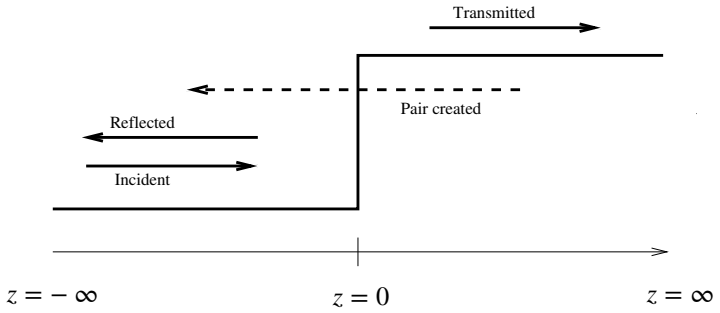


Figure 6: The potential step. The labelled arrowed lines show the particle *currents* discussed on page 33.

Consider a Dirac particle of momentum $\mathbf{p} = (0, 0, p_z)$, energy $E = E_{\mathbf{p}}$ and $S_z = +\frac{1}{2}$ incident from $z = -\infty$, Fig 6. Note that $\mathbf{S}$ commutes with γ_0 so the spin will be conserved in this process and we only have to consider spin $+\frac{1}{2}$ states throughout; we set $\xi_s = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ everywhere. Considering the usual plane wave solutions we have energy conservation at the barrier and the energy-momentum relations are

$$\begin{aligned} E^2 &= p_z^2 + m^2, \quad z < 0 \\ (E - eV)^2 &= {p'_z}^2 + m^2, \quad z \geq 0. \end{aligned} \quad (230)$$

The boundary conditions are simply continuity of the wave-function at the interface; there is no condition on the derivative because the Hamiltonian is first order in $\mathbf{p}$. Otherwise the calculation is very similar to the non-relativistic case; equating ingoing plus reflected to transmitted waves at $z = 0$,

$$e^{ip_z z}\begin{pmatrix} 1 \\ 0 \\ \frac{p_z}{E+m} \\ 0 \end{pmatrix} + re^{-ip_z z}\begin{pmatrix} 1 \\ 0 \\ \frac{-p_z}{E+m} \\ 0 \end{pmatrix}\Bigg|_{z=0} = Ae^{ip'_z z}\begin{pmatrix} 1 \\ 0 \\ \frac{p'_z}{E+m-V} \\ 0 \end{pmatrix}\Bigg|_{z=0} \tag{231}$$

which gives two equations to determine r and A. As usual the physical information is in the current j_3 which is given by

$$j_3 = \psi^\dagger \alpha_3 \psi = \psi^\dagger \begin{pmatrix} 0 & \sigma_3 \\ \sigma_3 & 0 \end{pmatrix} \psi \tag{232}$$

For $z < 0$ this gives

$$j_3 = \frac{2p_z}{E+m}(1 - r^* r) \tag{233}$$

and for $z > 0$

$$j_3 = \frac{2p'_z}{E - eV + m} A^* A \tag{234}$$

if p'_z is real and $j_3 = 0$ if p'_z is imaginary.

Eliminating A from the boundary conditions (231) gives

$$\frac{1-r}{1+r} = \frac{p'_z(E+m)}{p_z(E-eV+m)} = \kappa \tag{235}$$

so

$$r = \frac{1-\kappa}{1+\kappa}. \tag{236}$$

There are three regimes (see Fig 6)

1. If $E > eV + m$ then the particle has sufficient kinetic energy $E_K = E - m > eV$ to overcome the barrier; p'_z is real and $1 > \kappa > 0$. The reflection and transmission coefficients are given by

$$R = \frac{j_{reflected}}{j_{incident}} = \left(\frac{1-\kappa}{1+\kappa}\right)^2, \qquad T = \frac{j_{transmitted}}{j_{incident}} = \frac{4\kappa}{(1+\kappa)^2} \tag{237}$$

   so $R < 1$ and $T > 0$ which is again what we would expect as now the particle has enough kinetic energy to get over the barrier. It is easy to check that $R + T = 1$.

2. If $eV - m < E < eV + m$ then the particle has insufficient kinetic energy $E_K = E - m < eV$ to overcome the barrier; then p'_z is imaginary, as is κ, therefore $|r|^2 = 1$ and there is total reflection, $R = 1$. The particle does not have enough kinetic energy $E_K = E - m$ to overcome the barrier height eV. This is as we would expect.

3. But if $m < E < eV - m$ (which can only happen if the barrier is high enough $eV > 2m$) then p'_z is again real and, assuming $p'_z > 0$, $\kappa < 0$; so (237) tells us that and $R > 1, T < 0$ – but still $R + T = 1$. This can only be understood if we assume that there must be pair creation of particles and anti-particles at the boundary. Particles of energy E can only inhabit the $z < 0$ region; however anti-particles see a potential *drop* of V from $z < 0$ to $z > 0$ because they have the opposite charge to particles. So if pairs are created at the boundary the particles must have momentum $-\mathbf{p}$ and move to the left while the antiparticles must have momentum $+\mathbf{p}$ and move to the right. The left moving particles augment the totally reflected incident particles so $R > 1$. The stream of right moving antiparticles constitutes a current which is equivalent to a stream of left moving particles ie $j_{transmitted} < 0$ so $T < 0$. Of course this explanation is not totally convincing; we have forced changing particle number on a formalism that requires fixed particle number.

Homework 4.10: What is the significance of the fact that regime (3) above only occurs when $eV > 2m$?

Homework 4.11: Compute the scattering of a KG particle off the potential step in Fig 6. Remember that because the KG equation is second order in spatial derivatives, the first derivative of the wave function must be continuous at the step.

5 Dirac Equation in an external E.M. field II

In this section we'll look at some of the other consequences of the Dirac equation for a particle in an E.M. field. Starting from the Dirac equation

$$(-i\not{D} + m)\psi = 0 \tag{238}$$

and acting on the left with $(i\not{D} + m)$ we find

$$\left(\gamma^\mu\gamma^\nu D_\mu D_\nu + m^2\right)\psi = 0. \tag{239}$$

Now

$$\begin{aligned} \gamma^\mu\gamma^\nu &= \frac{1}{2}(\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu) + \frac{1}{2}[\gamma^\mu, \gamma^\nu] \\ &= g^{\mu\nu} + \Sigma^{\mu\nu} \end{aligned} \tag{240}$$

where we have introduced $\Sigma^{\mu\nu} = \frac{1}{2}[\gamma^\mu, \gamma^\nu]$; so (239) can be written

$$(D^\mu D_\mu + m^2)\psi + \Sigma^{\mu\nu} D_\mu D_\nu \psi = 0. \tag{241}$$

The first term is the Klein Gordon operator in the presence of an E.M. field – it is the same as for spinless particles. The second term is the modification for spin-$\frac{1}{2}$ particles. Note that $\Sigma_{\mu\nu}$ is antisymmetric on its two indices but that $D_\mu D_\nu \psi$ is *not* symmetric because the derivatives ∂_μ act on A_μ as well as on ψ; we can write this as

$$\begin{aligned} 0 &= (D^\mu D_\mu + m^2)\psi + \frac{1}{2}\Sigma^{\mu\nu}[D_\mu, D_\nu]\psi \\ &= (D^\mu D_\mu + m^2)\psi + ie\frac{1}{2}\Sigma^{\mu\nu}(\partial_\mu A_\nu - \partial_\nu A_\mu)\psi \\ &= (D^\mu D_\mu + m^2)\psi + ie\frac{1}{2}\Sigma^{\mu\nu} F_{\mu\nu}\psi \end{aligned} \tag{242}$$

where $F_{\mu\nu}$ is the electromagnetic field strength tensor. Note that the new term only depends on the physical field $F_{\mu\nu}$ which is gauge invariant, and not on the vector potential which is not.

To see the implications of the new term let's look at the situation with a static uniform $\mathbf{B}$ field. First choose $\mathbf{A} = (-By, 0, 0)$ so $\mathbf{B} = \text{curl}\mathbf{A} = (0, 0, B)$. Then $A_\mu = (0, -By, 0, 0)$ and

$$F_{12} = -F_{21} = \partial_1 A_2 - \partial_2 A_1 = \partial_x 0 - \partial_y(By) = B. \tag{243}$$

Using

$$\Sigma^{12} = -\Sigma^{21} = \frac{1}{2}(\gamma^1\gamma^2 - \gamma^2\gamma^1) = 2iS_3 \tag{244}$$

we get

$$0 = (D^\mu D_\mu + m^2)\psi - 2eBS_3\psi. \tag{245}$$

Homework 5.1: Check (244).

By translation and rotation invariance of the spatial coordinates the result for general $\mathbf{B}$ must be

$$0 = (D^\mu D_\mu + m^2)\psi - 2e\mathbf{B}.\mathbf{S}\psi. \tag{246}$$

so this looks like a magnetic dipole interaction but to read off the magnetic dipole moment we need to look at the system in the non-relativistic limit. In this limit $E = m + \epsilon$ with $\frac{\epsilon}{m} \ll 1$ and we set

$$\psi = e^{-it(m+\epsilon)}\phi(\mathbf{x}) \tag{247}$$

which gives

$$0 = (-(m+\epsilon)^2 - (\boldsymbol{\nabla} + ie\mathbf{A})^2 + m^2)\phi(\mathbf{x}) - 2e\mathbf{B}.\mathbf{S}\phi(\mathbf{x}) \tag{248}$$

or, neglecting terms of order $\frac{\epsilon^2}{m}$,

$$\epsilon\phi(\mathbf{x}) = -\frac{1}{2m}(\boldsymbol{\nabla} + ie\mathbf{A})^2\phi(\mathbf{x}) - \frac{e}{m}\mathbf{B}.\mathbf{S}\phi(\mathbf{x}). \tag{249}$$

So we see that the particle has a magnetic dipole moment $\boldsymbol{\mu} = \frac{e}{m}\mathbf{S} = 2\mu_B\mathbf{S}$ where we have introduced the Bohr magneton $\mu_B = \frac{e}{2m}$. The magnetic dipole moment arising from orbital motion is $\boldsymbol{\mu} = \mu_B\mathbf{L}$; the extra factor 2, usually called the g-factor, arising in the spin case is one of the original triumphs of the Dirac equation – experimentally this number is extremely close to 2 for the electron and the discrepancy is explained by Quantum Electrodynamics.

Homework 5.2: Restore the $\hbar$ factors in (249).

Homework 5.3: Show that the term linear in $\mathbf{A}$ in (249) leads to an interaction term $-\frac{e}{2m}\mathbf{B}.\mathbf{L}\phi(\mathbf{x})$ and thus confirm that the g-factor associated with orbital motion is indeed 1. Hint: use (and first check!) the fact that for a constant magnetic field $\mathbf{B}$ the vector potential is given by $\mathbf{A} = \frac{1}{2}\mathbf{x} \times \mathbf{B}$, and then make some vector operator manipulations.

Using the vector potential $\mathbf{A} = (-By, 0, 0)$ in (249) we can solve the eigenvalue problem for ϵ. Setting

$$\phi(\mathbf{x}) = e^{i(p_x x + p_z z)}\phi_S(y) \tag{250}$$

where $S_z\phi_S(y) = S\phi_S(y)$ we get

$$\epsilon\phi_S(y) = \frac{1}{2m}\left((p_x - eBy)^2 - \frac{d^2}{dy^2} + p_z^2\right)\phi_S(y) - \frac{e}{m}BS\phi_S(y) \tag{251}$$

Now choose $y = y' + p_x/(eB)$ to get

$$\epsilon\phi_S(y') = \left(-\frac{1}{2m}\frac{d^2}{dy'^2} + \frac{(eB)^2}{2m}y'^2 + \frac{p_z^2}{2m} - \frac{e}{m}BS\right)\phi_S(y') \tag{252}$$

which shows that this is just a shifted SHO problem with frequency $\omega = \frac{eB}{m}$. We see that

$$\epsilon = \frac{p_z^2}{2m} + (n + \frac{1}{2} - S_z)\omega, \quad n = 0, 1, 2, \ldots; S = \pm\frac{1}{2} \tag{253}$$

Homework 5.4: The $S\omega$ contribution in (253) is exactly the interaction energy of a magnetic dipole $2S\mu_B$ lying parallel to a magnetic field B. Because of the way we've done the calculation it's not so clear whether our result is really dependent only on physical fields and not directly on the vector potential. To check this, repeat the calculation with $\mathbf{A} = (-\frac{1}{2}By, \frac{1}{2}Bx, 0)$. Discuss the gauge dependence of ϵ and of ϕ_S.

6 Relativistic Quantum Mechanics in the Round

Relativistic Quantum Mechanics is a necessary step but it cannot be the end of the story. There are some successes:

1. It is Lorentz covariant. (We haven't explored this in much depth here; see André Lukas's lectures in the MMathPhys for a thorough treatment of the Lorentz transformation properties of spinors.)

2. It naturally contains anti-particles with the opposite charge to the particles but the same mass.

3. It explains why the spin of electrons couples to an external magnetic field with twice the strength of the orbital angular momentum coupling.

4. It explains why the spin-orbit coupling Hamiltonian in a single electron atom or ion takes the form it does (we haven't looked at this at all but it is straightforward to derive).

But also there are some failings that are inherent in the approach:

1. The negative energy states remain a problem; despite reinterpreting them as something to do with anti-particles we do not have a way of calculating a total energy for the system which is really bounded below. – something that is certainly required by experiment.

2. Particles and antiparticles can annihilate (experimental fact) so the number of particles is not conserved. The formalism of a wave function with the Born interpretation necessarily describes a fixed number of particles so Relativistic QM is bound to fail in circumstances where pair creation can occur.

The next step is to develop Quantum Field Theory which is able to describe varying particle number, describes particles and anti-particles, and has a true ground state. It's worth noting that real relativistic systems are not the only variable-particle-number systems. We now understand that many quasi-particle descriptions of condensed matter systems are also like this and can also be described by quantum field theories (which are typically not Lorentz invariant but Galilean invariant).