On the Global Analogue of the Aharonov–Bohm Effect

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I can't understand it. I can't even understand the people who can understand it.

Queen Juliana of the Netherlands.

Abstract

In this thesis we critically investigate the remarkable claim made by March–Russell, Preskill and Wilczek, that it is possible to have Aharonov–Bohm scattering in a model with a global gauge invariance only. A systematic analysis of the model shows that the arguments in favour of the claim cannot be maintained. We are not able though, to arive at a definite result in the corresponding kinematical regime (small k) but do succeed in calculating a non-trivial cross section in the other (high k) regime. A discussion of and comparison with other results is also presented.

CONTENTS

CHAPTER 1

INTRODUCTION

The Aharonov–Bohm effect is a well-known concept in local gauge theories. It is a purely quantum mechanical effect since its description needs the vector potential or gauge connection, while in classical electrodynamics all observable effects can be described in terms of the field strengths alone.

Since this effect is actually a manifestation of the holonomy of the connection, it was long thought it could only occur in local gauge theories. However this view has been challenged in a recent paper of March–Russell, Preskill and Wilczek where they introduced a Klein–Gordon model, with *only a global* $U(1)$ symmetry which breaks down to its discrete subgroup $\mathbb{Z}_2$ by condensation of a charged scalar field λ. This λ field couples to another scalar field η carrying half the λ charge. In the trivial case this condensation causes a mass splitting between the real and imaginary components of the η field. But in the presence of a vortex configuration these two components will scatter off the global vortex. March–Russell et al. claim that this will yield an Aharonov–Bohm cross section, which would be caused by the so-called "internal frame dragging": in a vortex configuration there is a mixing between the real and imaginary components, which can be removed by redefining the fields; the η field acquires a non single valued phase factor and the internal frame of its two components is dragged along when they circulate the vortex. The objective of this thesis is to have a closer look at the model and to see whether the Aharonov–Bohm effect really does occur in this model.

It is clear that to get a full understanding of the effect, it is necessary to have a good knowledge of the conventional Aharonov–Bohm effect. That is why we will start with a discussion of this effect in Chapter 2. The Aharonov–Bohm effect can be considered as an example of Berry's phase: a very general phenomenon occurring whenever there is a non-trivial connection along a noncontractable loop in space. So in Chapter 3 we discuss as an interesting intermezzo Berry's phase and consider the Aharonov–Bohm effect from that

perspective. In Chapter 4 we will introduce the model of March–Russell et al. and derive the field equations, which correspond to a set of coupled Klein–Gordon equations. As we are interested in the non-relativistic description of the system we derive a Schrödinger system from the field equations. This derivation involves some subtleties which were not appreciated by previous authors, but which turn out to lead to deviations from the calculations of the cross section presented in the existing literature. The obtained Schrödinger equation will be used to calculate the correct cross section up to second order in the relevant parameter related to the energy splitting. This will be done in Chapter 5. We conclude with a discussion of our results in comparison with those of previous papers.

We will use the same conventions as used in the literature: We will keep $\hbar$ and c until the third Chapter and we will use Gaussian units and the metric $\mathrm{Diag}(1, -1, -1, -1)$.

Dankwoord

Na anderhalf jaar met zware tijden en fijne momenten is het dan eindelijk zo ver: de scriptie is af. Maar voordat de jonge onderzoeker door regen en wind op weg zal gaan naar een volgend doel, wil hij eerst nog een paar mensen bedanken. Allereest natuurlijk zijn begeleider Prof. Sander Bais: De vaak lange besprekingen maakten het werk er zeker niet makkelijker maar wel veel beter op, door precies de nog onduidelijke punten naar voren te brengen. Daarnaast wil onze beginnende fysicus zijn medestudenten bedanken en in het bijzonder Erwyn, die altijd een kritisch oog voor de scriptie en een gewillig oor voor discussies had, en Daniel die er was toen het werk het zwaarst en de dagen het donkerst waren. Tot slot nog dank aan alle vrienden die vrienden bleven ook als ik geen tijd voor ze had.

CHAPTER 2

THE AHARONOV–BOHM EFFECT

In this Chapter we discuss the Aharonov–Bohm effect which demonstrates that it is not possible to describe all electromagnetic phenomena in terms of the field strength only. This effect is observed for example in an electron double slit experiment. In the next Chapter where we will discuss Berry's phase we will meet a different form of the same effect.

2.1 A double slit experiment

We consider the double slit experiment sketched in figure 2.1. The magnetic field **B** in the centre is confined to a narrow tube such that the electrons move in a field-free region.

This implies that classically one would not expect to see any effect, since fields interact only locally. It turns out however that there is a quantum mechanical effect. Due to the vector potential **A** the electron interference pattern on the screen on the right shifts over a distance proportional to the magnetic flux.
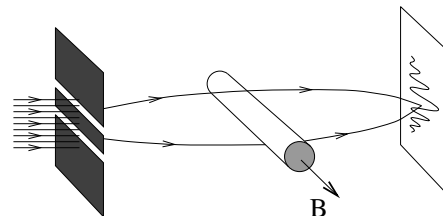
Figure 2.1: *The Aharonov–Bohm effect*

The way to see this is as follows. Free particles in a magnetic field are described by the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\left(\nabla + \frac{\mathrm{i}e}{\hbar c}\mathbf{A}\right)^2 \psi = \mathrm{i}\hbar\frac{\partial}{\partial t}\psi \qquad (2.1)$$

where $-e$ is the electron charge.

This Hamiltonian is obtained from the free Hamiltonian $H = \frac{\mathbf{p}^2}{2m}$ by the minimal substitution rule, which replaces the partial derivative by the covariant

derivative:

$$\partial_\mu \to D_\mu = \partial_\mu - \mathrm{i}\frac{\mathrm{e}}{\hbar c}A_\mu \qquad (2.2)$$

or equivalently — in our case where there is no scalar potential V — $\mathbf{p}$ is replaced by:

$$\mathbf{p} \to \mathbf{p} + \frac{e}{c}\mathbf{A} \qquad (2.3)$$

See appendix A for more details. In regions where the field $\mathbf{B} = \nabla \wedge \mathbf{A} = 0$ we can write $\mathbf{A}$ as the gradient of a function f, so locally we have a pure gauge and we can gauge away the potential:

$$\mathbf{A} \to \mathbf{A}' = \mathbf{A} - \nabla f \qquad (2.4\mathrm{a})$$

$$\psi \to \psi' = \mathrm{e}^{\mathrm{i}(e/\hbar c)f}\psi \qquad (2.4\mathrm{b})$$

There is a problem however: because the region where $\mathbf{A}$ is curlless — $\mathbb{R}^2\backslash\{0\}$ — is non-simply connected, we cannot find a globally acceptable f: take the following $\mathbf{A}$ in cylindrical coordinates:

$$\mathbf{A} = \frac{1}{r}A_\varphi\hat{\varphi} \qquad (2.5)$$

with A_φ a constant equal to the flux Φ divided by 2π. If we want to write this as the gradient of a function f:

$$\nabla f = \mathbf{A} \quad \Rightarrow \quad \frac{\partial f}{\partial \varphi} = A_\varphi \quad \Rightarrow \quad f(\varphi) = \int_0^\varphi A_\varphi \mathrm{d}\varphi' = A_\varphi\varphi \qquad (2.6)$$

For non-zero flux we obtain using Stokes' theorem:

$$f(2\pi) - f(0) = \oint \mathbf{A} \cdot \mathrm{d}\mathbf{r} = \mathbf{B} \neq 0 \qquad (2.7)$$

So $f(\varphi)$ is not single-valued and in general neither will be $\mathrm{e}^{-\mathrm{i}(e/\hbar c)f}$. But that means that we would have to consider the non-single-valued solutions ψ' of the Schrödinger equation, and such solutions are not admissible. To sum up we have two choices: a vector potential in our Hamiltonian or a non-single-valued wavefunction.

We can look at the problem in a semi-classical way however and split the wavefunction ψ into two parts ψ_{upp} and ψ_{low} where ψ_{upp} is the part going on the upper side of the flux tube and ψ_{low} the part going on the lower side. Each part now stays in a simply connected region and in both regions we can

gauge away the vector potential to get a free Hamiltonian. On the screen on the right where they "meet" we have:

$$\psi_{\text{upp}} = e^{i(e/\hbar c)\int_{C_{\text{upp}}} \mathbf{A}\cdot d\mathbf{r}'} \psi_{0,\text{upp}} \tag{2.8a}$$

$$\psi_{\text{low}} = e^{i(e/\hbar c)\int_{C_{\text{low}}} \mathbf{A}\cdot d\mathbf{r}'} \psi_{0,\text{low}} \tag{2.8b}$$

and therefore

$$\begin{aligned} \psi &= \psi_{\text{upp}} + \psi_{\text{low}} \\ &= \left(e^{-i(e/\hbar c)\oint_C \mathbf{A}\cdot d\mathbf{r}'} \psi_{0,\text{upp}} + \psi_{0,\text{low}} \right) e^{i(e/\hbar c)\int_{C_{\text{low}}} \mathbf{A}\cdot d\mathbf{r}'} \end{aligned} \tag{2.9}$$

The interference pattern is produced by $|\psi|^2$, so the only effect of the gauge potential is to change the relative phases of the two parts of the wavefunction and this phase shift depends only on the loop integral of the vector potential $\mathbf{A}$ which is equal to the flux Φ. Notice that this also means that the energy does *not* depend on $\mathbf{A}$ unless it is time dependent.

2.2   The Aharonov–Bohm cross section

This method of splitting the wavefunction in two parts is a semi-classical approximation since we ignore the effects of diffraction. Aharonov and Bohm in their original paper [1] also solve the problem without splitting the wavefunction in two parts. The energy of a plane wave with wavenumber $\mathbf{k}$ is equal to $\frac{k^2}{2m}$ so the wave equation for ψ in the presence of a vector potential is

$$\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\partial}{\partial \varphi} + i\alpha \right)^2 + k^2 \right] \psi = 0 \tag{2.10}$$

where $2\pi\alpha = (e/\hbar c)\Phi$.
If we make a mode expansion like

$$\psi = \sum_{m=-\infty}^{\infty} e^{im\varphi} F_m(r) \tag{2.11}$$

and integrate out φ over $[0, 2\pi]$ using the relation

$$\int_0^{2\pi} e^{i(m-m')\varphi} d\varphi = 2\pi\delta_{mm'} \tag{2.12}$$

we see that $F_m(r)$ satisfies a Bessel equation of order $m + \alpha$:

$$\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} - \frac{(m+\alpha)^2}{r^2} + k^2 \right] F_m(r) = 0 \tag{2.13}$$

For each $(m + \alpha)$ there are two independent solutions: the Bessel functions $J_{m+\alpha}(kr)$ and $J_{-(m+\alpha)}(kr)$. So the general solution of (2.10) is

$$\psi = \sum_{m=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}m\varphi} \left[a_m J_{m+\alpha}(kr) + b_m J_{-(m+\alpha)}(kr) \right] \tag{2.14}$$

where a_m and b_m are arbitrary constants.

Lee Page [2] has solved the problem of a free charged particle moving in a magnetic field and he finds a solution which is finite in the origin. Since we can shrink the size of the core to zero, our solution should also be finite in the origin and therefore negative noninteger order Bessel functions are not allowed since they diverge in the origin (see appendix C). So the general solution reduces to:

$$\psi = \sum_{m=-\infty}^{\infty} a_m J_{|m+\alpha|}(kr)\mathrm{e}^{\mathrm{i}m\varphi} \tag{2.15}$$

To calculate a scattering cross section we only need the large r behaviour of the solution. For general α Aharonov and Bohm find the following expression:

$$\psi = \mathrm{e}^{-\mathrm{i}[\alpha\varphi - \mathbf{r}\cdot\mathbf{k}]} + \frac{\mathrm{e}^{\mathrm{i}rk}}{\sqrt{2\pi rk}} \sin \pi\alpha \frac{\mathrm{e}^{-\mathrm{i}\pi/4}\mathrm{e}^{-\mathrm{i}\varphi/2}}{\cos(\varphi/2)} \tag{2.16}$$

where φ is the azimuthal position coordinate and $\mathbf{k}$ is the wave vector of a wave moving to the left: $\mathbf{k} \cdot \mathbf{r} = -kr \cos\varphi$.

This ψ seems to be non-single-valued but that is due to the fact that it is only valid for $\varphi \neq \pi$. For $\varphi = \pi$ we would need the exact solution. In general this involves unsolvable integrals; they can be evaluated for the simple cases $\alpha = n$ and $\alpha = n + \frac{1}{2}$ and then it turns out that the solution is indeed single-valued.

The first term on the right-hand side of (2.16) represents the incoming wave and this is exactly the wavefunction we got in our semi-classical description where we ignored the effect of diffraction. The second term in (2.16) is the lowest order term in the large r expansion of the scattered wave. From this term the differential scattering cross section can be easily obtained in the following way. If we write ψ as

$$\psi_{\mathrm{tot}} = \psi_{\mathrm{in}} + \mathrm{e}^{\mathrm{i}rk} \frac{f(\varphi)}{\sqrt{r}} \tag{2.17}$$

which defines the scattering amplitude $f(\varphi)$, then the differential cross section is given by (see for example Gasiorowicz [3] Chapter 24)

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(\varphi)|^2 \tag{2.18}$$

So for equation (2.16) we find

$$f(\varphi) = \frac{\sin \pi\alpha}{\sqrt{2\pi k}} \frac{1}{\cos(\varphi/2)} \mathrm{e}^{-\mathrm{i}\pi/4} \mathrm{e}^{-\mathrm{i}\varphi/2} \tag{2.19}$$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\sin^2 \pi\alpha}{2\pi k} \frac{1}{\cos^2(\varphi/2)}$$

$$= \frac{\sin^2 \pi\alpha}{2\pi k} \frac{1}{\sin^2(\theta/2)} \tag{2.20}$$

where θ is the scattering angle. It is measured with respect to the incoming wave vector which makes an angle π with the positive x-axis.

We see that in the cases where α is an integer, i.e. the cases where we don't see a shift in the interference pattern, we have a zero differential scattering cross section. In other cases we have a scattering cross section which is sharply peaked in the forward direction $\theta = 0$.

CHAPTER 3

Berry's Phase

In this Chapter we will discuss the quantum geometric phase, also called Berry's phase [4]. Since the adiabatic theorem is a very important aspect of this phase we will start with a discussion of it, following Messiah [5] Chapter 17. Then in the next paragraph we will explain why there is a geometric phase factor at all and derive an expression for it in terms of the energy eigenstates. In the last paragraph we will discuss two examples: first the prototype of a Berry's phase experiment, a spin in a slowly changing magnetic field, because this is also a good example for the concept of holonomy and finally we will treat the Aharonov–Bohm effect in a Berry context.

3.1   The adiabatic theorem

Consider a system in external field, for example an atom in an magnetic field. We are interested in the resulting change in the system when the external field is slowly changed. Suppose that the changing starts at time t_0 with Hamiltonian H_0 and ends at time t_1 with Hamiltonian H_1. It is then useful to define:

$$T := t_1 - t_0 \qquad \text{and} \qquad s := (t - t_0)/T$$

So that we can parameterize H by s in a T independent way with

$$H(0) = H_0 \qquad \text{and} \qquad H(1) = H_1$$

And we will write the evolution operator $U(t, t_0)$ as

$$U(t, t_0) = U_T(s)$$

Finally we denote the eigenvalues of the Hamiltonian H by ε_n and their corresponding projection operators by P_n. For the Adiabatic Theorem to hold we need a few restrictions.

(*i*) The functions $\varepsilon_n(s)$ and $P_n(s)$ must be continuous functions of s.

(*ii*) The eigenvalues must be "non-crossing", i.e. $\varepsilon_n(s) \neq \varepsilon'_n(s)$ for all s, n, n', and the eigenstates form a complete basis.

(*iii*) The derivatives $\frac{dP_n}{ds}, \frac{d^2 P_n}{ds^2}$ are well-defined and piece-wise continuous for the whole interval $[0, 1]$

Now the Adiabatic Theorem, valid in the limit $T \to \infty$, predicts that if the system is initially in an eigenstate of the Hamiltonian H_0 then at every later time $t = t_0 + sT$ it will be in an eigenstate of the corresponding Hamiltonian $H(s)$. We can write this in a more compact way as:
For all n $U_T(s)$ satisfies the condition:

$$\lim_{T \to \infty} U_T(s) P_n(0) = P_n(s) \lim_{T \to \infty} U_T(s) \tag{3.1}$$

It is easy to see that the two forms are equivalent: Consider an eigenstate $|n(0)\rangle$. This state evolves into $U_T(s)|n(0)\rangle$ at a later time. Since $P_n(s)|n(s)\rangle = |n(s)\rangle$ we have

$$U_T(s)|n(0)\rangle = U_T(s) P_n(0) |n(0)\rangle \tag{3.2}$$

Now if equation (3.1) holds this will be — in the limit $T \to \infty$ — equal to

$$P_n(s) U_T(s) |n(0)\rangle \tag{3.3}$$

But that means that $U_T(s)|n(0)\rangle$ must be an eigenstate of $P_n(s)$ with eigenvalue 1, i.e. an eigenstate of the Hamiltonian $H(s)$. Reversing this argument it follows that if $U_T(s)|n(0)\rangle$ is an eigenstate of the Hamiltonian $H(s)$ equation (3.1) must be fulfilled.

We will not discuss the rather involved proof of the theorem since it does not give much more insight and because we are really only interested in the result itself. See Messiah [5] Chapter 17 for the complete proof.

3.2   Why we need a geometric phase

Suppose we have a Hamiltonian $H(\mathbf{R})$ which depends on an external parameter $\mathbf{R}$, for example a magnetic field, then the eigenstates and therefore the Hilbert space will also depend on $\mathbf{R}$. Suppose for every $\mathbf{R}$ we have a local basis $|n; \mathbf{R}\rangle$ for the Hilbert space. All these bases will be isomorphic but in general not equal. So if $\mathbf{R}$ is not constant in time then a solution to the Schrödinger equation

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = i\frac{d}{dt}|\psi(t)\rangle = H(\mathbf{R}(t))|\psi(t)\rangle \tag{3.4}$$

should be expanded in the basis $|n; \mathbf{R}(t)\rangle$ and not in the basis $|n; \mathbf{R}(0)\rangle$. But this is a difficulty since we do not know how the bases for different $\mathbf{R}$ are connected, that is we seem to be unable to express the state $|\psi(t)\rangle$ in the initial state $|\psi(0)\rangle$. We do know however that if we start in an eigenstate $|n; \mathbf{R}(0)\rangle$ then according to the Adiabatic Theorem the system will — at a later time — be described by a ket $e^{i\alpha} |n; \mathbf{R}(t)\rangle$ where α is an unknown phase factor, which must be included since a quantum mechanical state is only defined up to a phase factor. Of course in the normal quantum mechanical case of a time independent $\mathbf{R}$ we can integrate the Schrödinger equation and find that α is equal to the familiar dynamical phase factor $-E_n/\hbar$. So perhaps in the case of non constant $\mathbf{R}(t)$ we could take

$$\alpha \overset{?}{=} -\frac{1}{\hbar} \int_0^t \mathrm{d}t' \, E_n(\mathbf{R}(t')) \tag{3.5}$$

that is

$$|\psi(t)\rangle \overset{?}{=} e^{-\frac{i}{\hbar} \int_0^t \mathrm{d}t' \, E_n(\mathbf{R}(t'))} |n; \mathbf{R}(t)\rangle \tag{3.6}$$

We will show now that this cannot be true.

At every time $|n; \mathbf{R}(t)\rangle$ is an eigenstate of $H(\mathbf{R}(t))$ with the eigenvalue $E_n(\mathbf{R}(t))$. The ket $|\psi(t)\rangle$ is also an eigenstate of $H(\mathbf{R}(t))$ with eigenvalue $E_n(\mathbf{R}(t))$ but in addition it also satisfies the Schrödinger equation. Therefore we have the following two relations:

$$H(\mathbf{R}(t)) |n; \mathbf{R}(t)\rangle = E_n(\mathbf{R}(t)) |n; \mathbf{R}(t)\rangle \tag{3.7}$$

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t} |\psi(t)\rangle = H(\mathbf{R}(t)) |\psi(t)\rangle = E_n(\mathbf{R}(t)) |\psi(t)\rangle \tag{3.8}$$

Taking the total derivative of (3.6) leads to:

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t} |\psi(t)\rangle = e^{-\frac{i}{\hbar} \int_0^t \mathrm{d}t' \, E_n(\mathbf{R}(t'))} \left[E_n(\mathbf{R}(t)) |n; \mathbf{R}(t)\rangle + i\hbar\frac{\mathrm{d}}{\mathrm{d}t} |n; \mathbf{R}(t)\rangle \right]$$

$$= E_n(\mathbf{R}(t)) |\psi(t)\rangle + i\hbar e^{-\frac{i}{\hbar} \int_0^t \mathrm{d}t' \, E_n(\mathbf{R}(t'))} \frac{\mathrm{d}}{\mathrm{d}t} |n; \mathbf{R}(t)\rangle \tag{3.9}$$

Now using equation (3.8) we get the equality

$$\frac{\mathrm{d}}{\mathrm{d}t} |n; \mathbf{R}(t)\rangle = 0 \tag{3.10}$$

But the eigenstates $|n; \mathbf{R}(t)\rangle$ only depend on t through $\mathbf{R}$, so we get

$$\frac{\mathrm{d}}{\mathrm{d}t} |n; \mathbf{R}(t)\rangle = \dot{\mathbf{R}} \cdot \nabla_\mathbf{R} |n; \mathbf{R}(t)\rangle = 0 \tag{3.11}$$

Since we have not specified the path $\mathbf{R}(t)$ yet, the direction of $\dot{\mathbf{R}}(t)$ is arbitrary and we must conclude that

$$\nabla_{\mathbf{R}} |n; \mathbf{R}(t)\rangle = 0 \tag{3.12}$$

which would imply that $|n; \mathbf{R}(t)\rangle$ does not depend on $\mathbf{R}$, which is obviously incorrect.

So the phase factor cannot be the dynamical phase factor (3.5). It is practical however to extract it by writing α as $\Gamma_n(t) + \gamma_n(t)$ where $\Gamma_n(t)$ is the dynamical phase. Therefore the state $|\psi(t)\rangle$ is equal to:

$$|\psi(t)\rangle = \mathrm{e}^{\mathrm{i}\Gamma_n(t)} \mathrm{e}^{\mathrm{i}\gamma_n(t)} |n; \mathbf{R}(t)\rangle \tag{3.13}$$

Our goal is now to find an expression for this extra phase $\gamma(t)$ and in particular in the case that $\mathbf{R}(t)$ makes a complete loop returning at time T to its initial value $\mathbf{R}(0)$. The accompanying phase change $\gamma_n(T)$ is called Berry's phase. Let us now start by again taking the total time derivative of the ket $|\psi(t)\rangle$

$$
\begin{aligned}
\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi(t)\rangle ={} & \\
={} & \left[\left(E_n(\mathbf{R}(t)) - \hbar \frac{\mathrm{d}}{\mathrm{d}t} \gamma_n(t) \right) |n; \mathbf{R}(t)\rangle + \mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} |n; \mathbf{R}(t)\rangle \right] \mathrm{e}^{\mathrm{i}(\Gamma_n(t)+\gamma_n(t))} \\
={} & E_n(\mathbf{R}(t)) |\psi(t)\rangle - \left[\dot{\gamma}_n(t) |n; \mathbf{R}(t)\rangle - \mathrm{i} \frac{\mathrm{d}}{\mathrm{d}t} |n; \mathbf{R}(t)\rangle \right] \hbar \mathrm{e}^{\mathrm{i}(\Gamma_n(t)+\gamma_n(t))}
\end{aligned}
\tag{3.14}
$$

So after using (3.8) again we get

$$\dot{\gamma}_n(t) |n; \mathbf{R}(t)\rangle = \mathrm{i} \frac{\mathrm{d}}{\mathrm{d}t} |n; \mathbf{R}(t)\rangle \tag{3.15}$$

Taking the inner product with the bra $\langle n; \mathbf{R}(t)|$ on both sides we obtain an expression for $\dot{\gamma}_n(t)$

$$\dot{\gamma}_n(t) = \mathrm{i} \langle n; \mathbf{R}(t)| \frac{\mathrm{d}}{\mathrm{d}t} |n; \mathbf{R}(t)\rangle \tag{3.16}$$

Notice that $\dot{\gamma}_n(t)$ - and therefore $\gamma_n(t)$ - is real:

$$
\begin{aligned}
2\mathrm{Im}\dot{\gamma}_n(t) &= 2\mathrm{Re}\,\langle n; \mathbf{R}(t)|\,\frac{\mathrm{d}}{\mathrm{d}t}\,|n; \mathbf{R}(t)\rangle \\
&= \langle n; \mathbf{R}(t)|\,\frac{\mathrm{d}}{\mathrm{d}t}\,|n; \mathbf{R}(t)\rangle + \langle n; \mathbf{R}(t)|\,\frac{\mathrm{d}}{\mathrm{d}t}\,|n; \mathbf{R}(t)\rangle^* \\
&= \langle n; \mathbf{R}(t)|\,\frac{\mathrm{d}}{\mathrm{d}t}\,|n; \mathbf{R}(t)\rangle + \left(\frac{\mathrm{d}}{\mathrm{d}t}\,\langle n; \mathbf{R}(t)|\right)|n; \mathbf{R}(t)\rangle \\
&= \frac{\mathrm{d}}{\mathrm{d}t}\,\langle n; \mathbf{R}(t)|\, n; \mathbf{R}(t)\rangle = 0
\end{aligned}
\tag{3.17}
$$

so indeed $\gamma_n(t)$ is a good phase factor.
By integrating equation (3.16) we can now write the expression for $\gamma_n(t)$

$$
\begin{aligned}
\gamma_n(t) &= \mathrm{i}\int_0^t \mathrm{d}t'\,\langle n; \mathbf{R}(t')|\,\frac{\mathrm{d}}{\mathrm{d}t'}\,|n; \mathbf{R}(t')\rangle \\
&= \mathrm{i}\int_{\mathbf{R}(0)}^{\mathbf{R}(t)} \mathrm{d}\mathbf{R}\cdot\langle n; \mathbf{R}|\,\nabla_{\mathbf{R}}\,|n; \mathbf{R}\rangle
\end{aligned}
\tag{3.18}
$$

where equation (3.11) was used to obtain the last equality.
Finally by putting $\mathbf{R}(t) = \mathbf{R}(T) = \mathbf{R}(0)$ we obtain Berry's phase:

$$
\gamma_n(C) = \mathrm{i}\oint_C \mathrm{d}\mathbf{R}\cdot\langle n; \mathbf{R}|\,\nabla_{\mathbf{R}}\,|n; \mathbf{R}\rangle
\tag{3.19}
$$

In general this will not be zero since the integrand is not a total derivative.

It will be useful to use Stokes's theorem, combined with the vector identity $\nabla\wedge(f\nabla g) = \nabla f\wedge\nabla g$, to write $\gamma_n(C)$ as a surface integral over the surface S with boundary $\partial S = C$:

$$
\begin{aligned}
\gamma_n(C) &= \mathrm{i}\oint_C \mathrm{d}\mathbf{R}\cdot\langle n; \mathbf{R}|\,\nabla_{\mathbf{R}}\,|n; \mathbf{R}\rangle \\
&= \mathrm{i}\int_S \mathrm{d}\mathbf{S}\cdot(\nabla_{\mathbf{R}}\wedge\langle n; \mathbf{R}|\,\nabla_{\mathbf{R}}\,|n; \mathbf{R}\rangle) \\
&= \mathrm{i}\int_S \mathrm{d}\mathbf{S}\cdot[\,(\nabla_{\mathbf{R}}\,\langle n; \mathbf{R}|)\wedge(\nabla_{\mathbf{R}}\,|n; \mathbf{R}\rangle)\,] \\
&=: -\int_S \mathrm{d}\mathbf{S}\cdot\mathbf{V}_n(\mathbf{R})
\end{aligned}
\tag{3.20}
$$

The fact that a quantum mechanical state is defined upon a phase factor makes it clear that the relevant quantities are the equivalent classes

$$
[|n; \mathbf{R}\rangle] = \{g\,|n; \mathbf{R}\rangle\,|g\in U(1)\}
\tag{3.21}
$$

So our geometry is a $U(1)$ line bundle over the parameter space and fixing the phase of $|n; \mathbf{R}\rangle$ for each point $\mathbf{R}$ amounts to choosing a section. The connection which prescribes how to parallel transport a state through this line bundle is given by the integrand of equation (3.19)[1] and is called Berry's connection (see Barry Simon [6] and Nakahara [7] Chapter 10). Therefore Berry's phase — since it is the integral of a connection — is a holonomy and the two form $\mathbf{V}_n$ is a curvature — Berry's curvature — since it is the exterior derivative of the connection. In the case of the Aharonov–Bohm effect Berry's connection will be (almost) equal to the electromagnetic connection while Berry's curvature or field strength $\mathbf{V}_n$ will be equal to the magnetic field.

3.3   Examples

In this section the two best-known examples of Berry's phase experiments will be discussed: A particle with spin in a slowly changing magnetic field and of course the Aharonov–Bohm effect.

3.3.1   A spin in a magnetic field

Consider a particle with spin in a slowly changing external magnetic field $\mathbf{B}$. The Hamiltonian describing the system is given by the potential energy

$$H = -\mathbf{M} \cdot \mathbf{B} \tag{3.22}$$

where $\mathbf{M}$ is the magnetic moment. For a particle with only spin angular momentum $\mathbf{M}$ is equal to

$$\mathbf{M} = \frac{qg}{2mc}\mathbf{S} \tag{3.23}$$

where g is the gyromagnetic constant (≈ 2 for an electron) and $\mathbf{S}$ is the spin operator with eigenvalues between $-s\hbar$ and $s\hbar$.
So the Hamiltonian can be written as

$$-\frac{qg}{2mc}\mathbf{S} \cdot \mathbf{B} \tag{3.24}$$

Now assume the spin of the particle is initially in the direction of the magnetic field $\mathbf{B}$. Quantum mechanically this means that the ket describing the particle's state is an eigenstate of the spin operator component in that direction and therefore it is an eigenstate of the Hamiltonian (3.24). According to

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[1]Notice that indeed it transforms as a connection: under a gauge transformation $|n; \mathbf{R}\rangle \to \mathrm{e}^{\mathrm{i}\mu(\mathbf{R})} |n; \mathbf{R}\rangle$ it transforms as $\langle n; \mathbf{R}| \nabla_{\mathbf{R}} |n; \mathbf{R}\rangle \to \langle n; \mathbf{R}| \nabla_{\mathbf{R}} |n; \mathbf{R}\rangle + \mathrm{i}\nabla_{\mathbf{R}}\mu(\mathbf{R})$

the Adiabatic Theorem it will stay in an energy eigenstate since the magnetic field and therefore the Hamiltonian are slowly changing. To calculate Berry's phase we need $\mathbf{V}_n(\mathbf{B})$, which boils down to determining how the eigenstates change under a change in $\mathbf{B}$. But for a given d$\mathbf{S}$ the change in $\mathbf{B}$ is small and we can take all $\mathbf{B}$ to be close to a certain basepoint. So we need to know $|n; \mathbf{B}\rangle$. Since the experiment is spherically symmetric we can call the direction of the basepoint $\mathbf{B}_0$ the z-direction and therefore $|n; \mathbf{B}\rangle$ will be close to $|s_z\rangle$. Now we can obtain $|n; \mathbf{B}\rangle$ by starting out with the eigenstate of S_z and then rotating it into the right direction. The spin operator component in the rotated direction and the corresponding eigenstate can be written as

$$|s_z\rangle \rightarrow |n; \mathbf{B}\rangle = U |s_z\rangle \tag{3.25}$$

$$S_z \rightarrow S_{\mathbf{B}} = U S_z U^{-1} \tag{3.26}$$

n denotes the eigenvalues of a spin component in general direction while s_z denotes the eigenvalues of the z-component of the spin. Of course the numerical values of n and s_z are equal.

Equation (3.26) can easily be derived by multiplying the equation

$$S_z |s_z\rangle = s_z |s_z\rangle \tag{3.27}$$

from the left with U and by putting $U^{-1}U$ between S_z and the ket. We see that S transforms in the adjoint representation, which is of course obvious since the spin rotations are generated by the spin operators and the generators of a group always transform in the adjoint representation. We will write the rotation operator $U(\boldsymbol{\alpha})$ as

$$U(\boldsymbol{\alpha}) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\boldsymbol{\alpha}\cdot\mathbf{S}} \tag{3.28}$$

where the rotation is around the axis $\boldsymbol{\alpha}$ over an angle $|\boldsymbol{\alpha}|$.
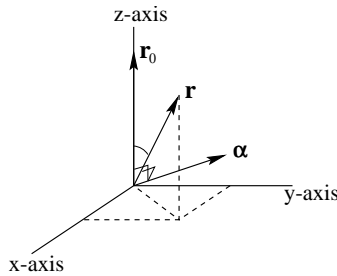
Figure 3.1: *How to rotate a vector*

This definition is in agreement with the commutation relation

$$-\frac{\mathrm{i}}{\hbar}[S_i, S_j] = \varepsilon_{ijk}S_k \tag{3.29}$$

We have seen that we can take all $\mathbf{B}$ close to the z-direction and therefore we can take $|\boldsymbol{\alpha}|$ to be small. Let us now first find an expression for $\boldsymbol{\alpha}$. Suppose we want to rotate a vector $\mathbf{r}_0$ with length r into a vector $\mathbf{r}$. Then the rotation axis $\boldsymbol{\alpha}$ can be found from the relations (see

figure 3.1)

$$\frac{\mathbf{r}_0 \wedge \mathbf{r}}{|\mathbf{r}_0 \wedge \mathbf{r}|} = \frac{\boldsymbol{\alpha}}{|\boldsymbol{\alpha}|} \tag{3.30}$$

$$|\mathbf{r}_0 \wedge \mathbf{r}| = r^2 \sin(|\boldsymbol{\alpha}|) \tag{3.31}$$

and therefore

$$\frac{\mathbf{r}_0 \wedge \mathbf{r}}{r^2 \sin(|\boldsymbol{\alpha}|)} = \frac{\boldsymbol{\alpha}}{|\boldsymbol{\alpha}|} \tag{3.32}$$

Assuming $|\boldsymbol{\alpha}|$ to be small this relation simplifies to

$$\boldsymbol{\alpha} = \frac{\mathbf{r}_0 \wedge \mathbf{r}}{r^2} \tag{3.33}$$

So if we want to express the eigenstates of the spin in the direction of the magnetic field $\mathbf{B}$ in terms of the eigenstates of S_z we find the following expression for $\boldsymbol{\alpha}$:

$$\boldsymbol{\alpha} = \frac{(0,0,B) \wedge \mathbf{B}}{B^2} = \frac{1}{B}(-B_y, B_x, 0) \tag{3.34}$$

It will be easier however to substitute B by B_z which may be done because $|\boldsymbol{\alpha}|$ is small and therefore $B_z = B\cos(|\boldsymbol{\alpha}|) \approx B$. We find $U(\boldsymbol{\alpha})$ and $|n; \mathbf{B}\rangle$ to be:

$$U(\boldsymbol{\alpha}) = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(B_x S_y - B_y S_x)/B_z} \tag{3.35}$$

$$|n; \mathbf{B}\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(B_x S_y - B_y S_x)/B_z} |s_z\rangle \tag{3.36}$$

And we can calculate $\nabla_{\mathbf{B}} |n; \mathbf{B}\rangle$:

$$\nabla_{\mathbf{B}} |n; \mathbf{B}\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(B_x S_y - B_y S_x)/B_z} \frac{-\mathrm{i}}{\hbar B_z^2}(B_z S_y, -B_z S_x, B_x S_y - B_y S_x) |s_z\rangle \tag{3.37}$$

Again using the fact that $|\boldsymbol{\alpha}|$ is small, and therefore $B_z \gg B_x, B_y$, we see that the z-component of (3.37) is much smaller than its x and y-components. By also putting back B instead of B_z equation (3.37) reduces to:

$$\nabla_{\mathbf{B}} |n; \mathbf{B}\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(B_x S_y - B_y S_x)/B_z} \frac{-\mathrm{i}}{\hbar B}(S_y, -S_x, 0) |s_z\rangle \tag{3.38}$$

We are now able to calculate the outer product (3.20)

$$\begin{aligned}
\mathbf{V}_n(\mathbf{B}) &= -\mathrm{i}\left(\nabla_{\mathbf{B}} \langle n; \mathbf{B}|\right) \wedge \left(\nabla_{\mathbf{B}} |n; \mathbf{B}\rangle\right) \\
&= -\frac{\mathrm{i}}{\hbar^2 B^2} \langle s_z| (0, 0, -S_y S_x + S_x S_y) |s_z\rangle \\
&= \frac{1}{\hbar B^2} \langle s_z| \hat{\mathbf{z}} S_z |s_z\rangle \\
&= \frac{s_z}{B^2} \hat{\mathbf{z}}
\end{aligned} \tag{3.39}$$

we have used here the commutation relation for the spin operators:

$$-\frac{\mathrm{i}}{\hbar}[S_x, S_y] = S_z \tag{3.40}$$

Since we look at $\mathbf{B}$ near the z-axis, $\mathrm{d}\mathbf{S}$ is equal to $\hat{\mathbf{z}}\mathrm{d}S$ and we find a total Berry phase equal to

$$\begin{aligned}
\gamma_n(\partial S) = \int_S \mathbf{V}_n \cdot \mathrm{d}\mathbf{S} &= \int_S \frac{n}{B^2}\mathrm{d}S \\
&= \int_S \frac{n}{B^2}B^2\mathrm{d}\Omega \\
&= n\Omega(S)
\end{aligned} \tag{3.41}$$

We see that we have obtained the important result that Berry's phase for a spin in a slowly changing magnetic field is equal to the enclosed solid angle times the spin eigenvalue n of the state. Notice that the phase change depends neither on the total spin s nor on the size of the magnetic field $\mathbf{B}$.

It is instructive to look some more at the special case of $s = \frac{1}{2}$. In that case the Hamiltonian is equal to

$$H = \kappa\boldsymbol{\sigma} \cdot \mathbf{B} = \begin{pmatrix} B_z & B_x - \mathrm{i}B_y \\ B_x + \mathrm{i}B_y & -B_z \end{pmatrix} \tag{3.42}$$

where $\kappa = -\frac{qg\hbar}{4mc}$.

The eigenvalues of this Hamiltonian are $\pm\kappa|\mathbf{B}|$. By introducing spherical coordinates:

$$B_x = B\sin\theta\cos\varphi \tag{3.43a}$$
$$B_y = B\sin\theta\sin\varphi \tag{3.43b}$$
$$B_z = B\cos\theta \tag{3.43c}$$

it can be written as:

$$H = \kappa B \begin{pmatrix} \cos\theta & \mathrm{e}^{-\mathrm{i}\varphi}\sin\theta \\ \mathrm{e}^{\mathrm{i}\varphi}\sin\theta & -\cos\theta \end{pmatrix} \tag{3.44}$$

It is now easy to show that the following ket is an eigenstate with eigenvalue $+\kappa B$:

$$|n; \mathbf{B}\rangle_N = \begin{pmatrix} \cos(\theta/2) \\ \mathrm{e}^{\mathrm{i}\varphi}\sin(\theta/2) \end{pmatrix} \tag{3.45}$$

However for $\theta = 0$ and $\theta = \pi$ the angle φ can have all values between 0 and 2π. The point $\theta = 0$ is no problem since the lower component of the state is

zero. At the point $\theta = \pi$ it is not though and the state is ill defined. But we can find another state:

$$|n; \mathbf{B}\rangle_S = \mathrm{e}^{-\mathrm{i}\varphi} |n; \mathbf{B}\rangle_N = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\varphi} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix} \tag{3.46}$$

This state is multi valued for $\theta = 0$ but single valued for $\theta = \pi$. So for every θ we can find a single valued solution to the Schrödinger equation. Using the expression for the gradient in spherical coordinates:

$$\nabla_{\mathbf{B}} T = \frac{\partial T}{\partial B}\hat{B} + \frac{1}{B}\frac{\partial T}{\partial \theta}\hat{\theta} + \frac{1}{B \sin \theta}\frac{\partial T}{\partial \varphi}\hat{\varphi} \tag{3.47}$$

it is now straightforward to calculate Berry's connection $\langle n; \mathbf{B}| \nabla_{\mathbf{B}} |n; \mathbf{B}\rangle$:

$$\mathbf{A}_N = \frac{1}{2}(1 - \cos\theta)\frac{\hat{\varphi}}{B \sin \theta} \tag{3.48a}$$

$$\mathbf{A}_S = -\frac{1}{2}(1 + \cos\theta)\frac{\hat{\varphi}}{B \sin \theta} \tag{3.48b}$$

which exactly equal to the gauge field for a Dirac magnetic monopole of strength $g = \frac{1}{2}$ except that here B plays the role of the radial coordinate r. See Dirac [8] and Wu & Yang [9]. The reason for this is of course that the magnetic monopole as well as a spin in a changing magnetic field are described by a $U(1)$ line bundle over $\mathbb{R}^3 \backslash \{0\} \cong S^2$. Berry's phase for this experiment is therefore proportional to the holonomy in the monopole field, i.e. to the flux through the enclosed solid angle, just as we found in our general calculation above.

3.3.2 The Aharonov–Bohm effect in a Berry context

Let us consider an electron at a position $\mathbf{r}$ with charge $-e$ confined to a box at a position $\mathbf{R}$. The energy of the electron depends only on the relative position $\mathbf{r} - \mathbf{R}$, i.e. the system is translation invariant. The Hamiltonian H therefore is equal to

$$H = H(\mathbf{p}, \mathbf{r} - \mathbf{R}) \tag{3.49}$$

and the wavefunctions

$$\langle \mathbf{r}| n \rangle = \psi_n(\mathbf{r} - \mathbf{R}) \tag{3.50}$$

If we put the box next to a flux tube we have seen in Chapter 2 that we must replace $\mathbf{p}$ by $\mathbf{p} + \frac{e}{c}\mathbf{A}$. The states now become dependent on $\mathbf{R}$. Locally we can express the inner product $\langle \mathbf{r}| n; \mathbf{R}\rangle$ in terms of the $\psi_n(\mathbf{r} - \mathbf{R})$ in (3.50):

$$\langle \mathbf{r}| n; \mathbf{R}\rangle = \mathrm{e}^{\mathrm{i}(e/\hbar c) \int_{\mathbf{R}}^{\mathbf{r}} \mathrm{d}\mathbf{r}' \cdot \mathbf{A}(\mathbf{r}')} \psi_n(\mathbf{r} - \mathbf{R}) \tag{3.51}$$

These functions are not single-valued but we will only need their derivatives, that is, for a given $\mathbf{R}$ we need to know ψ_n only in a small neighbourhood around this $\mathbf{R}$.

In this case we will not calculate $\mathbf{V}_n$ to determine Berry's phase but use the contour integral form (3.19). So we want to calculate

$$\langle n; \mathbf{R} | \nabla_{\mathbf{R}} | n; \mathbf{R} \rangle$$

The way to do this is to insert the identity

$$\mathbb{1} = \int_{\text{BOX}} \mathrm{d}^3 r \; |\mathbf{r}\rangle \langle \mathbf{r}| \tag{3.52}$$

Since these states $|\mathbf{r}\rangle$ do not depend on $\mathbf{R}$ we can pull $\nabla_{\mathbf{R}}$ through and obtain the following expression

$$\int_{\text{BOX}} \mathrm{d}^3 r \; \langle n; \mathbf{R} | \mathbf{r} \rangle \nabla_{\mathbf{R}} \langle \mathbf{r} | n; \mathbf{R} \rangle \tag{3.53}$$

If we now use equation (3.51) we find

$$\langle n; \mathbf{R} | \nabla_{\mathbf{R}} | n; \mathbf{R} \rangle = \int_{\text{BOX}} \mathrm{d}^3 r \; \psi_n^*(\mathbf{r} - \mathbf{R}) \left[-\frac{iq}{\hbar c} \mathbf{A}(\mathbf{R}) + \nabla_{\mathbf{R}} \right] \psi_n(\mathbf{r} - \mathbf{R})$$

$$= -\frac{iq}{\hbar c} \mathbf{A}(\mathbf{R}) + \int_{\text{BOX}} \mathrm{d}^3 r \; \psi_n^*(\mathbf{r} - \mathbf{R}) \nabla_{\mathbf{R}} \psi_n(\mathbf{r} - \mathbf{R}) \tag{3.54}$$

Berry in his original paper says that the second term vanishes (because of the normalization of the ψ_n) but we find that this is only true after integrating over the closed loop in $\mathbf{R}$. To see this use the normalization of ψ_n:

$$\int_{\text{BOX}} \mathrm{d}^3 r \; \psi_n^*(\mathbf{r} - \mathbf{R}) \psi_n(\mathbf{r} - \mathbf{R}) = \int_{\mathbb{R}^3} \mathrm{d}^3 r \; \psi_n^*(\mathbf{r} - \mathbf{R}) \psi_n(\mathbf{r} - \mathbf{R}) = 1 \tag{3.55}$$

to derive

$$0 = \nabla_{\mathbf{R}} \int \mathrm{d}^3 r \; \psi_n^* \psi_n = \int \mathrm{d}^3 r \; [\psi_n^* \nabla_{\mathbf{R}} \psi_n + (\nabla_{\mathbf{R}} \psi_n^*) \psi_n] \tag{3.56}$$

and therefore

$$\int \mathrm{d}^3 r \; \psi_n^* \nabla_{\mathbf{R}} \psi_n = \frac{1}{2} \int \mathrm{d}^3 r \; [\psi_n^* \nabla_{\mathbf{R}} \psi_n - (\nabla_{\mathbf{R}} \psi_n^*) \psi_n] \tag{3.57}$$

Now take the contour integral:

$$\oint_{\partial S} d\mathbf{R} \cdot \int d^3r \; \psi_n^* \nabla_\mathbf{R} \psi_n = \int_S d\mathbf{S} \cdot \nabla_\mathbf{R} \wedge \int d^3r \; (\psi_n^* \nabla_\mathbf{R} \psi_n)$$

$$= \frac{1}{2} \int_S d\mathbf{S} \cdot \int d^3r \; \nabla_\mathbf{R} \wedge [\psi_n^* \nabla_\mathbf{R} \psi_n - (\nabla_\mathbf{R} \psi_n^*) \, \psi_n] \qquad (3.58)$$

$$= \frac{1}{2} \int_S d\mathbf{S} \cdot \int d^3r \; [(\nabla_\mathbf{R} \psi_n^*) \wedge (\nabla_\mathbf{R} \psi_n) - (\nabla_\mathbf{R} \psi_n^*) \wedge (\nabla_\mathbf{R} \psi_n)] = 0$$

So by integrating equation (3.54) we find the following Berry phase:

$$\gamma_n(C) = i \oint_C d\mathbf{R} \cdot \langle n; \mathbf{R} | \nabla_\mathbf{R} | n; \mathbf{R} \rangle$$

$$= \frac{q}{\hbar c} \oint_C d\mathbf{R} \cdot \mathbf{A}(\mathbf{R}) = \frac{q}{\hbar c} \Phi \qquad (3.59)$$

This is of course again the well-known Aharonov–Bohm phase factor. Note that we do have single-valued wavefunctions since this phase turns up after moving the box around the flux line which must take some time. So in this case the wavefunction can have more than one phase at the same place but not at the same time as well, while globally gauging away the vector potential in the Aharonov–Bohm experiment of Chapter 2 leads to a wavefunction having more than one phase at the same place and time.

Notice also that in the experiment described above we need slow motion around the flux line since otherwise a centrifugal force would appear, although the Aharonov–Bohm effect itself does not depend on the time in which a complete loop is made.

CHAPTER 4

A Global Analogue of the A–B effect

We will now start with the main subject: A Klein–Gordon model with a *only* a global $U(1)$ symmetry group breaking down to a discrete subgroup $\mathbb{Z}_2$. This model was first introduced by March–Russell, Preskill and Wilczek [10] to show that local gauge theories are not the only theories in which Aharonov–Bohm like scattering effects occur. We will start with a discussion of the model. Then we will talk about the non-relativistic interpretation of the complex and the real Klein–Gordon equation since the Aharonov–Bohm effect should appear in the small k limit, i.e. in a non-relativistic limit. We will end this Chapter with a derivation of the Schrödinger equation which follows from this non-relativistic limit. From now on we will take $\hbar = c = 1$.

4.1 The Model

Consider a model with a global $U(1)$ symmetry describing two complex scalar fields η and λ, where the charge of the η field is minus half the charge of the λ field, i.e. symmetry transformations are of the form

$$\lambda \rightarrow \mathrm{e}^{\mathrm{i}\alpha}\lambda \tag{4.1a}$$

$$\eta \rightarrow \mathrm{e}^{-\mathrm{i}\alpha/2}\eta \tag{4.1b}$$

with α a real constant.
Then in general one would expect an interaction term in the invariant Lagrangian density of the form:

$$\Delta\mathcal{L} = -g\lambda\eta^2 + \mathrm{h.c.} \tag{4.2}$$

where g is the (real) coupling constant.

Suppose the λ field has a potential term of a form leading to a non-zero vacuum expectation value:

$$V_\lambda = G\left(|\lambda|^2 - v^2\right)^2 \tag{4.3}$$

where G and v are positive real constants.

The η field has only a mass term and no further self interaction:

$$V_\eta = m^2|\eta|^2 \tag{4.4}$$

The full Lagrangian density will then be

$$\mathcal{L} = \partial_\mu\eta\partial^\mu\eta^* - m^2|\eta|^2 + \partial_\mu\lambda\partial^\mu\lambda^* - G\left(|\lambda|^2 - v^2\right)^2 - g\left(\lambda\eta^2 + \lambda^*\eta^{*2}\right) \tag{4.5}$$

which gives the Euler–Lagrange equations

$$\partial_\mu\partial^\mu\lambda + G\left(|\lambda|^2 - v^2\right)\lambda + g\eta^{*2} = 0 \tag{4.6a}$$

$$\partial_\mu\partial^\mu\eta + m^2\eta + 2g\lambda^*\eta^* = 0 \tag{4.6b}$$

and their complex conjugates.

We are interested in what happens when the λ field condenses. First consider the trivial case where[1] $<\lambda(r,\varphi)> = v$, i.e. the vacuum expectation value is constant in space and time. Equation (4.6a) then gives us $<\eta> = 0$, which shows that in order to study the effective theory for the low lying states, we should make the expansion

$$\lambda = v + \sigma_1 + i\sigma_2 \tag{4.7a}$$
$$\eta = \rho_1 + i\rho_2 \tag{4.7b}$$

where all fields appearing at the right hand side are real.

Since the σ_2 field corresponds to the broken generator this will be a massless Goldstone boson as can also be seen by writing out the V_λ potential in terms of σ_1 and σ_2. The second equation (4.6b) now reduces to the pair

$$\partial_\mu\partial^\mu\rho_1 + (m^2 + \Gamma)\rho_1 = 0 \tag{4.8a}$$
$$\partial_\mu\partial^\mu\rho_2 + (m^2 - \Gamma)\rho_2 = 0 \tag{4.8b}$$

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[1]We will work in cylindrical coordinates with a trivial z dependence, so in fact we consider the theory on the plane $\mathbb{R}^2$

where $\Gamma = 2gv$. We have neglected higher order terms like $\rho_1\sigma_1$ etc.

So we see that the symmetry breaking leads to a mass splitting between the real and imaginary components of the complex scalar field η. We will write the different masses as:

$$\mu_1 = \sqrt{m^2 + \Gamma} \tag{4.9a}$$

$$\mu_2 = \sqrt{m^2 - \Gamma} \tag{4.9b}$$

Now consider the case where the vacuum expectation value of λ is no longer constant in space but corresponds to a vortex configuration:

$$<\lambda(r,\varphi)> \, = v\mathrm{e}^{\mathrm{i}\varphi} \tag{4.10}$$

where φ is the polar angle and $<\lambda(r,\varphi)>$ is single-valued as it should be.

In this case the η Euler–Lagrange equation (4.6b) acquires a φ dependent mixing between the real and imaginary parts of η. We can resolve this point by redefining the η field and absorbing half of the phase factor into it:

$$\eta = \mathrm{e}^{-\mathrm{i}\varphi/2}\tilde{\eta} \tag{4.11}$$

which — by taking the real and imaginary parts of this equation — can also be written as:

$$\begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} = \begin{pmatrix} \cos(\varphi/2) & \sin(\varphi/2) \\ -\sin(\varphi/2) & \cos(\varphi/2) \end{pmatrix} \begin{pmatrix} \tilde{\rho}_1 \\ \tilde{\rho}_2 \end{pmatrix} \tag{4.12}$$

The Euler–Lagrange equation for η in terms of this new $\tilde{\eta}$ now reads:

$$\mathrm{e}^{\mathrm{i}\varphi/2}\Box(\mathrm{e}^{-\mathrm{i}\varphi/2}\tilde{\eta}) + m^2\tilde{\eta} + \Gamma\tilde{\eta}^* = 0 \tag{4.13}$$

So we see the condensation of the λ field again gives rise to a mass splitting between the real and imaginary components of the $\tilde{\eta}$ field, but there are two other important consequences: the $\tilde{\eta}$ field has to be *non* single valued and furthermore we get a change in our terms containing spatial derivatives:

$$\mathrm{e}^{\mathrm{i}\varphi/2}\partial_\varphi\eta = \mathrm{e}^{\mathrm{i}\varphi/2}\partial_\varphi(\mathrm{e}^{-\mathrm{i}\varphi/2}\tilde{\eta}) = (\partial_\varphi - \frac{\mathrm{i}}{2})\tilde{\eta} \tag{4.14}$$

Notice that the expression on the right hand side of this equation just looks as if the field $\tilde{\eta}$ is coupled to a background effective local gauge field $A_\mu = \frac{1}{\mathrm{i}q}(\partial_\mu\Omega)\Omega^{-1}$ (where $\Omega = \mathrm{e}^{-\mathrm{i}\varphi/2}$ and $q = \frac{1}{2}$) equal to the Aharonov–Bohm gauge potential (2.5), in spite of the fact that there is of course no local gauge field present in our theory.

Using the expression for ∇^2 in cylindrical coordinates

$$\frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial z^2} \tag{4.15}$$

we can write out the φ dependence of $\Box\eta = (\partial_t^2 - \nabla^2)\eta$ in terms of $\tilde{\eta}$:

$$\mathrm{e}^{\mathrm{i}\varphi/2}\frac{1}{r^2}\partial_\varphi^2\left(\mathrm{e}^{-\mathrm{i}\varphi/2}\tilde{\eta}\right) = -\frac{1}{4r^2}\tilde{\eta} - \frac{\mathrm{i}}{r^2}\partial_\varphi\tilde{\eta} + \frac{1}{r^2}\partial_\varphi^2\tilde{\eta} \tag{4.16}$$

and therefore we get two extra terms corresponding to $q^2\mathbf{A}^2$ and $2\mathrm{i}q\mathbf{A}\cdot\nabla$ respectively, where $\mathbf{A} = \frac{1}{r}\hat{\varphi}$ and $q = \frac{1}{2}$. In terms of $\tilde{\rho}_1$ and $\tilde{\rho}_2$ we find $\mathbf{A} = \frac{\sigma_2}{r}\hat{\varphi}$, i.e. the second Pauli matrix and therefore these extra terms read:

$$\begin{pmatrix} -\frac{1}{4r^2} & 0 \\ 0 & -\frac{1}{4r^2} \end{pmatrix} + \begin{pmatrix} 0 & \frac{1}{r^2}\partial_\varphi \\ -\frac{1}{r^2}\partial_\varphi & 0 \end{pmatrix}$$

If we now look again at equation (4.6a), the Euler–Lagrange equation for λ, we see that by inserting the vacuum $\lambda = v\mathrm{e}^{\mathrm{i}\varphi}$ we get:

$$-v\nabla^2\mathrm{e}^{\mathrm{i}\varphi} + g\mathrm{e}^{\mathrm{i}\varphi}<\tilde{\eta}^{*2}> = 0 \tag{4.17}$$

and therefore[2]

$$<\tilde{\eta}> = \pm\frac{\mathrm{i}v}{gr^2} \tag{4.18}$$

So actually we should write

$$\tilde{\eta} = \pm\frac{\mathrm{i}v}{gr^2} + \tilde{\rho}_1 + \mathrm{i}\tilde{\rho}_2 \tag{4.19}$$

i.e. we should not expand around 0. Notice however that in the other Euler–Lagrange equation there is no reference to v or g but only to the product $\Gamma = 2gv$. So we can make the quotient v/g arbitrarily small and therefore again expand around 0. In fact this is even necessary since the $\tilde{\eta}$ expectation value is only a solution of the $\tilde{\eta}$ Euler–Lagrange equation if it is zero.

The Euler–Lagrange equation for $\tilde{\rho}_1$ and $\tilde{\rho}_2$ we obtained equals:

$$-\partial_t^2\begin{pmatrix} \tilde{\rho}_1 \\ \tilde{\rho}_2 \end{pmatrix} = \begin{pmatrix} -\nabla^2 + \mu_1^2 + \frac{1}{4r^2} & -\frac{1}{r^2}\partial_\varphi \\ \frac{1}{r^2}\partial_\varphi & -\nabla^2 + \mu_2^2 + \frac{1}{4r^2} \end{pmatrix}\begin{pmatrix} \tilde{\rho}_1 \\ \tilde{\rho}_2 \end{pmatrix} \tag{4.20}$$

So we must solve two coupled Klein–Gordon equations for two real fields. But first let us look at the interpretation.

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[2]Notice that the $\pm$ comes from the unbroken discrete subgroup $\mathbb{Z}_2$

4.2   The interpretation of the non-relativistic Klein–Gordon equation

We started out with a relativistic Lagrange density: A Klein–Gordon Lagrange density with interaction terms. The only context where such a theory can be fully described is Quantum Field Theory. However in a non-relativistic limit we can also give the solutions a one-particle Schrödinger interpretation. In this section we will first discuss how this works for complex solutions and then for real solutions.

4.2.1   The complex Klein–Gordon equation

First consider complex solutions η to the free Klein–Gordon equation:

$$(\Box + m^2)\eta = 0 \tag{4.21}$$

We then have two complex degrees of freedom: η and $\partial_t \eta$. A Schrödinger wavefunction has only one complex degree of freedom so the solution to the Klein–Gordon equation cannot describe one particle, but must describe two particles. If we solve the equation by separation of variables we see that indeed we find two different solutions:

$$\eta_n^\pm(\mathbf{r}, t) = N \mathrm{e}^{\mathrm{i}(\mathbf{k}_n \cdot \mathbf{r} \mp E_n t)} \tag{4.22}$$

where $E_n = \sqrt{m^2 + k_n^2}$. So we have found positive *and* negative energy eigenstates.

Let us now derive the conserved norm. Multiply equation (4.21) from the left by η^* and multiply the complex conjugate equation from the left by η. Taking the difference leads to:

$$0 = \eta^* \Box \eta - \eta \Box \eta^* =: \eta^* \overset{\leftrightarrow}{\Box} \eta \tag{4.23}$$

Integrating this over entire space and using the spatial boundary condition $\eta|_\infty = 0$ we get a conserved norm:

$$\int_{L^3} \mathrm{d}^3 r \; \eta^* \mathrm{i} \frac{\overset{\leftrightarrow}{\partial}}{\partial t} \eta = \text{constant} \tag{4.24}$$

Calculating its value for the two solutions $\eta^\pm$ we find $\pm 2EL^3|N|^2$, i.e. the η^- solution has negative norm. In normal classical quantum mechanics the norm of a wavefunction is a probability density but it is clear that this cannot be true for the Klein–Gordon solutions. It turns out however that

the negative energy states should be interpreted as positive energy anti-particles. The norm therefore — since it is negative for anti-particles and positive for particles — can be interpreted as a charge (not necessarily as an electrical but rather as a "particle number") density and its conservation as charge conservation. So we see that only the total amount of charge is conserved, not the number of particles. A quantum mechanical system with a non constant number of particles however can only be fully described in a second quantized system, i.e. by a quantum field theory. So we cannot expect our first quantized treatment of the Klein–Gordon equation to be completely successful but some important aspects of the full theory can be reliably studied, especially at low energies where no real particle creation can occur and this will also be the domain we are interested in.

A nice example which can be found in Gross [11] Chapter 4 is pair creation described by a Coulomb interaction term

$$\partial_t^2 \rightarrow (\partial_t + \mathrm{i}qV)^2 = \partial_t^2 + 2\mathrm{i}qV\partial_t - q^2V$$

Consider a high Coulomb barrier (i.e. potential energy greater than mass) in the right half of space and no potential in the left part (for simplicity only one dimension is used). One would not expect to see particles propagate in the right half. Anti-particles however do not see a potential barrier but a potential well since they have negative charge. Indeed the solutions show that a particle incoming from the left bounces of the barrier while creating a particle-anti-particle pair, from which the particle travels to the left and the anti-particle travels to the right.

The interpretation of the complex Klein–Gordon field becomes even more clear if we transform the single — second order in time — linear differential equation into two coupled first order linear differential equations, that is if we transform the scalar Klein–Gordon equation into a two component vector Schrödinger equation (see Gross [11] and Feshbach and Villars [12]). As we already mentioned, the solution η and its time derivative $\partial_t\eta$ are independent variables. It is easier however to take two different linear combinations of them. For example:

$$\phi_\pm = \frac{1}{\sqrt{2m}}\left(m \pm \mathrm{i}\partial_t\right)\eta \tag{4.25}$$

And therefore:

$$\eta = \frac{1}{\sqrt{2m}}\left(\phi_+ + \phi_-\right) \tag{4.26a}$$

$$\mathrm{i}\partial_t\eta = \sqrt{\frac{2}{m}}\left(\phi_+ - \phi_-\right) \tag{4.26b}$$

Taking the time derivative of equation (4.25), using the Klein–Gordon equation for the second time-derivative and using the expressions of η and $\partial_t\eta$ we find two coupled first order differential equations for $\phi_\pm$:

$$
\mathrm{i}\partial_t \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix} = \begin{pmatrix} m + \frac{p^2}{2m} & \frac{p^2}{2m} \\ -\frac{p^2}{2m} & -(m + \frac{p^2}{2m}) \end{pmatrix} \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix}
\tag{4.27}
$$

The conserved norm (4.24) now reduces to

$$
\int_{L^3} \mathrm{d}^3 r \ \left(|\phi_+|^2 - |\phi_-|^2 \right) = \text{constant}
\tag{4.28}
$$

If we write $\phi = \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix}$ and introduce $\bar{\phi} = \phi^\dagger \sigma_3$ we can write this as

$$
\int_{L^3} \mathrm{d}^3 r \ \bar{\phi}\phi
\tag{4.29}
$$

which shows a striking resemblance to the Dirac norm (in $d = 2$ we have that γ_0 equals the third Pauli matrix σ_3).

Any other combination $\phi_\pm = \alpha\left[\beta\eta \pm \mathrm{i}\partial_t\eta\right]$ could have been taken as well. We will use this freedom to diagonalize the Hamiltonian. First we will show that we can find a solution by taking $\alpha = 1$ and then we will look what restrictions we should impose on general α by substituting $\phi_\pm \to \alpha\phi_\pm$. First let us write η and $\mathrm{i}\partial_t\eta$ in terms of $\phi_\pm$:

$$
\eta = \frac{1}{2}\beta^{-1}(\phi_+ + \phi_-)
\tag{4.30a}
$$

$$
\mathrm{i}\partial_t\eta = \frac{1}{2}(\phi_+ - \phi_-)
\tag{4.30b}
$$

Now differentiating $\phi_\pm$ and using the Klein–Gordon equation we find:

$$
\begin{aligned}
\mathrm{i}\partial_t\phi_\pm &= \beta\mathrm{i}\partial_t\eta \pm (-\partial_t^2\eta) \\
&= \frac{1}{2}\left[\beta(\phi_+ - \phi_-) \pm (-\nabla^2 + m^2)\beta^{-1}(\phi_+ + \phi_-)\right] \\
&= \frac{1}{2}\left[\beta \pm (-\nabla^2 + m^2)\beta^{-1}\right]\phi_+ \\
&\quad \frac{1}{2}\left[-\beta \pm (-\nabla^2 + m^2)\beta^{-1}\right]\phi_-
\end{aligned}
\tag{4.31}
$$

So the Hamiltonian will be diagonal if and only if

$$
\beta = (-\nabla^2 + m^2)\beta^{-1}
\tag{4.32}
$$

that is if

$$\beta^2 = -\nabla^2 + m^2 \tag{4.33}$$

Equation (4.31) now reduces to the Schrödinger equation $i\partial_t\phi_\pm = \pm\beta\phi_\pm$ so if we want the ϕ_+ to describe positive energy states we see that we should take

$$\beta = +\sqrt{-\nabla^2 + m^2} \tag{4.34}$$

and we find:

$$i\partial_t \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix} = \begin{pmatrix} \sqrt{-\nabla^2 + m^2} & 0 \\ 0 & -\sqrt{-\nabla^2 + m^2} \end{pmatrix} \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix} =: H \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix} \tag{4.35}$$

while

$$\phi_\pm = \sqrt{-\nabla^2 + m^2}\,\eta \pm i\partial_t\eta \tag{4.36}$$

Notice that the conserved norm is of the form $\int d^3r \; (|\phi_+|^2 - |\phi_-|^2) = \int d^3r \; \phi^\dagger\sigma_3\phi$ if and only if $\sigma_3 H$ is hermitian:

$$i\partial_t \int d^3r \; \phi^\dagger\sigma_3\phi = \int d^3r \; \phi^\dagger\sigma_3 i\partial_t\phi - (i\partial_t\phi)^\dagger\sigma_3\phi$$

$$= \int d^3r \; \phi^\dagger\sigma_3 H\phi - (H\phi)^\dagger\sigma_3\phi$$

$$= \int d^3r \; \phi^\dagger[\sigma_3 H - H^\dagger\sigma_3]\phi$$

$$= \int d^3r \; \phi^\dagger[\sigma_3 H - (\sigma_3 H)^\dagger]\phi \tag{4.37}$$

Of course this is the case for the ϕ in relation (4.36), but what if we make the substitution $\tilde{\phi}_\pm = \alpha\phi_\pm$:

$$i\partial_t\alpha^{-1}\tilde{\phi}_\pm = H\alpha^{-1}\tilde{\phi}_\pm \tag{4.38}$$

and therefore

$$i\partial_t\tilde{\phi}_\pm = \alpha H\alpha^{-1}\tilde{\phi}_\pm =: \tilde{H}\tilde{\phi}_\pm \tag{4.39}$$

If $\sigma_3\tilde{H}$ must be hermitian we find:

$$\sigma_3\alpha H\alpha^{-1} = \alpha\sigma_3 H\alpha^{-1} = (\alpha\sigma_3 H\alpha^{-1})^\dagger$$

$$= \underbrace{(\alpha^{-1})^\dagger}_{(\alpha^\dagger)^{-1}} \sigma_3 H\alpha^\dagger \tag{4.40}$$

and therefore:

$$\sigma_3 H \alpha^\dagger \alpha = \alpha^\dagger \alpha \sigma_3 H \tag{4.41}$$

So we see $\alpha \phi_\pm$ is also a good solution if $\sigma_3 H$ and therefore also H itself commutes with $\alpha^\dagger \alpha$.

In a nonrelativistic limit the particles should decouple since we do not expect to see any signs of pair creation/annihilation in a low energy limit. We can find the nonrelativistic limit by assuming that the quantities $|\mathbf{p}|$ and $T := E - m$ are much smaller than the mass m. Now look for a solution of the form

$$\phi = \begin{pmatrix} \chi_1(\mathbf{r}) \\ \chi_2(\mathbf{r}) \end{pmatrix} \mathrm{e}^{-\mathrm{i}Et} \tag{4.42}$$

That is look for the influence of anti-particles on a particle. By using the two-component Schrödinger equation we find

$$T\chi_1 = \frac{p^2}{2m}\chi_1 + \frac{p^2}{2m}\chi_2 \tag{4.43a}$$

$$(2m + T)\chi_2 = -\frac{p^2}{2m}\chi_1 - \frac{p^2}{2m}\chi_2 \tag{4.43b}$$

and therefore

$$\left(1 + \frac{T}{2m} + \frac{p^2}{4m^2}\right)\chi_2 = -\frac{p^2}{4m^2}\chi_1 \tag{4.44}$$

So we see that χ_2 is of order $1/m^2$ times χ_1. The first equation (4.43a) now reduces to

$$T\chi_1 = \left(\frac{p^2}{2m} - \frac{p^4}{8m^3}\right)\chi_1 \tag{4.45}$$

That is we are left with an ordinary Schrödinger equation for the χ_1 field and we have even found the lowest order correction term to it. The χ_2 field which describes anti-particles is indeed much smaller and has only influence on the correction terms. If we would have taken $\mathrm{e}^{+\mathrm{i}Et}$ as time dependence for the fields we had found exactly the same equations. Only the roles of χ_1 and χ_2 would have been interchanged.

Finally we can look at Coulomb scattering from a central potential $V = \frac{Q}{r}$ in the two-component description in second order perturbation theory (see Gross [11] Chapter 4). The first order term matrix element gives us the familiar Coulomb differential cross section

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{2QE}{4k^2 \sin(\varphi/2)}\right)^2 \tag{4.46}$$
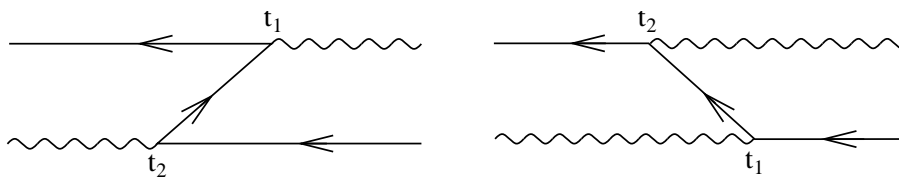
Figure 4.1: *The two second order Coulomb scattering Feynman diagrams*

The second order element gives us scattering with intermediate propagating states: one diagram with a positive energy state and one with a negative energy state as propagator. It can be shown that mathematically we can turn around the direction of motion of the negative energy state and therefore that we can also look at a diagram where the negative energy propagator is travelling backwards in time. If we interpret it as a positive energy antiparticle travelling forward in time however we see that at time t_1 a particle-antiparticle pair is created from which the particle will be the outgoing state while at the later time t_2 the antiparticle annihilates the incoming particle. This is of course the Feynman prescription: negative energy states travelling backwards in time are positive energy antiparticles travelling forwards in time. The two diagrams with — respectively — a particle and an antiparticle propagator are drawn in figure 4.1.

4.2.2   The real Klein–Gordon equation

We will now look for real solutions ρ of the free Klein–Gordon equation. Since we have a differential equation which is second order in time we have two real degrees of freedom. So a real Klein–Gordon field can be transformed into *one* Schrödinger field. For example take

$$\psi = \alpha \left[\beta \rho + \mathrm{i}\partial_t \rho \right] \tag{4.47}$$

with β real. We can again solve this by first taking $\alpha = 1$ and then look for restrictions to be imposed on general α. First write ρ and $\mathrm{i}\partial_t\rho$ in terms of ψ and ψ^*:

$$\rho = \frac{1}{2}\beta^{-1}\left(\psi + \psi^*\right) \tag{4.48a}$$

$$\mathrm{i}\partial_t\rho = \frac{1}{2}\left(\psi - \psi^*\right) \tag{4.48b}$$

Notice that these equations look exactly the same as the complex Klein–Gordon expressions if we make the following substitutions:

$$\psi \leftrightarrow \phi_+ \tag{4.49a}$$

$$\psi^* \leftrightarrow \phi_- \tag{4.49b}$$

$$\eta \leftrightarrow \rho \tag{4.49c}$$

Therefore we can immediately write down the Schrödinger equation:

$$
\begin{aligned}
\mathrm{i}\partial_t\psi &= \frac{1}{2}\left[\beta + \left(-\nabla^2 + m^2\right)\beta^{-1}\right]\psi \\
&\quad \frac{1}{2}\left[-\beta + \left(-\nabla^2 + m^2\right)\beta^{-1}\right]\psi^*
\end{aligned}
\tag{4.50}
$$

We do not want mixing between the wavefunction and its complex conjugate since this leads to decaying and growing states. So we again find:

$$\beta^2 = -\nabla^2 + m^2 \tag{4.51}$$

and we find *two* possible Schrödinger equations:

$$\mathrm{i}\partial_t\psi = \pm\sqrt{-\nabla^2 + m^2}\,\psi \tag{4.52}$$

for $\psi = \pm\sqrt{-\nabla^2 + m^2}\,\rho + \mathrm{i}\partial_t\rho$ respectively.

We see that we have to choose between only positive energy solutions or only negative energy solutions, but the two choices are equivalent. This is a consequence of the fact that a real Klein–Gordon equation describes particles which are their own anti-particles. So we can describe them as particles — i.e. as positive energy solutions — and as anti-particles — i.e. as negative energy solutions.

In this case H is hermitian itself (i.e. without a σ_3) and we get the usual Schrödinger conserved norm $\int \mathrm{d}^3r\ |\psi|^2$. H must stay hermitian if we substitute $\tilde{\psi} = \alpha\psi$. Of course this again leads to the restriction that $\alpha^\dagger\alpha$ must commute with $H = \pm\sqrt{-\nabla^2 + m^2}$.

Notice that it is not possible to derive a conserved norm for real Klein–Gordon fields like we did for complex Klein–Gordon fields. This is a direct result of the fact that the real Klein–Gordon Lagrangian only has a discrete symmetry and not the continuous $U(1)$ symmetry. However we have seen that we can reduce the Klein–Gordon equation to a Schrödinger equation with a hermitian Hamiltonian and therefore with a Schrödinger conserved norm $\int \mathrm{d}^3r\ |\psi|^2$.

4.3 The frame-dragging Hamiltonian

Let us now return to our original problem of the coupled Klein–Gordon equations (4.20):

$$-\partial_t^2 \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} = \begin{pmatrix} -\nabla^2 + \mu_1^2 + \frac{1}{4r^2} & -\frac{1}{r^2}\partial_\varphi \\ \frac{1}{r^2}\partial_\varphi & -\nabla^2 + \mu_2^2 + \frac{1}{4r^2} \end{pmatrix} \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} \qquad (4.53)$$

where we have dropped the tildes on ρ_1 and ρ_2.

We will use the results of the previous section to obtain a non-relativistic Schrödinger equation. Of course now two coupled Schrödinger wavefunctions are needed. Before we proceed we will first prove an important lemma:

Lemma 4.1 We cannot take the Schrödinger solution ψ_1 as a linear combination of the Klein–Gordon solution ρ_1 and $i\partial_t\rho_1$ alone and likewise for ψ_2, but we need combinations of ρ_1 and ρ_2 to form ψ_1 and ψ_2 if we do not want terms involving the complex conjugate solutions $\psi_{1,2}^*$.

Proof: The most general linear combination ψ_1 of ρ_1 and $i\partial_t\rho_1$ can be written as:

$$\psi_1 = \alpha_1 \left[\beta_1\rho_1 + i\partial_t\rho_1\right] \qquad (4.54)$$

where α_1 and β_1 are some (complex) operators. We will write similar expression for ψ_2 with operators α_2 and β_2.

ρ_1 and $i\partial_t\rho_1$ can now be expressed in terms of ψ_1:

$$\rho_1 = [\beta_1 + \beta_1^*]^{-1} \left[\alpha_1^{-1}\psi_1 + (\alpha_1^{-1})^*\psi_1^*\right] \qquad (4.55a)$$

$$i\partial_t\rho_1 = \left[\beta_1^{-1} + (\beta_1^{-1})^*\right]^{-1} \left[\beta_1^{-1}\alpha_1^{-1}\psi_1 - (\beta_1^{-1})^*(\alpha_1^{-1})^*\psi_1^*\right] \qquad (4.55b)$$

and likewise for ρ_2 and $i\partial_t\rho_2$.

If we now differentiate ψ_1 to t we find only one term containing ψ_2^* coming from $\partial_t^2\rho_1$:

$$i\partial_t\psi_1 = \cdots - \frac{\alpha_1}{r^2}\partial_\varphi \left[(\beta_2 + \beta_2^*)^{-1} (\alpha_2^{-1})^*\psi_2^*\right] \qquad (4.56)$$

So we see we cannot get the complex conjugate fields disappear from the Schrödinger equation if we take combinations of the form (4.54) which proves the lemma.

Having terms involving $\psi_{1,2}^*$ would result in a Hamiltonian which is no longer hermitian and all kinds of decaying and growing states would have to be considered. So in the expressions for $\psi_{1,2}$ we need terms connecting the two Klein–Gordon fields. Writing out the equations like we did before

will give a lot of difficult equations involving many unknown parameters and therefore we will follow a different approach.

We can always write the Klein–Gordon equation as:

$$-\partial_t^2 \eta = K\eta \qquad (4.57)$$

where η can be a vector or a scalar, real or complex and therefore K can be a matrix or a scalar operator. The free scalar Klein–Gordon K will be $-\nabla^2 + m^2$ but a more general K like the matrix on the right-hand side of equation (4.53) is also possible. Now notice that the squares of all the effective Hamiltonians we have found so far are equal to their corresponding K. Further notice that every time we wanted the Schrödinger equation diagonal, that is without mixing between ϕ_+ and ϕ_- or between ψ and ψ^*, we could find a splitting of the form

$$\psi = H\rho + \mathrm{i}\partial_t \rho \qquad (4.58)$$

So define a vector ψ with components ψ_1 and ψ_2 and a vector ρ with components ρ_1 and ρ_2. We can then indeed show that this ψ satisfies a Schrödinger equation of the form:

$$\mathrm{i}\partial_t \psi = H\psi \qquad (4.59)$$

if only $H^2 = K$ and $\partial_t H = 0$. To prove this differentiate (4.58):

$$\begin{aligned}
\mathrm{i}\partial_t \psi &= H\mathrm{i}\partial_t \rho + (-\partial_t^2 \rho) \\
&= H\mathrm{i}\partial_t \rho + K\rho \\
&= H\mathrm{i}\partial_t \rho + H^2 \rho \\
&= H\left[\mathrm{i}\partial_t \rho + H\rho\right] \\
&= H\psi \qquad (4.60)
\end{aligned}$$

So we can always find a Schrödinger equation by only looking for a time independent root of the Klein–Gordon operator K. Of course it is not always possible to find a hermitian root. For example in the case of a complex Klein–Gordon field we cannot take the simple hermitian root

$$\begin{pmatrix} \sqrt{-\nabla^2 + m^2} & 0 \\ 0 & \sqrt{-\nabla^2 + m^2} \end{pmatrix}$$

since this would make the two fields $\phi_\pm$ equal. In the case of two coupled real Klein–Gordon fields we do not have this problem of making the fields equal.

Notice that if we can find a hermitian root or a root which forms a hermitian matrix after multiplying with some other matrix (like the third Pauli matrix) we also have a conserved norm, since every solution to a Schrödinger equation with such a Hamiltonian, has a conserved norm. So our task now is to find a *hermitian* root of the matrix on the right-hand side of equation (4.53):

$$\begin{pmatrix} -\nabla^2 + \mu_1^2 + \frac{1}{4r^2} & -\frac{1}{r^2}\partial_\varphi \\ \frac{1}{r^2}\partial_\varphi & -\nabla^2 + \mu_2^2 + \frac{1}{4r^2} \end{pmatrix}$$

Since the two fields have different masses a linear combination of them cannot have a definite mass. But we are using a first quantized i.e. a non relativistic theory and in the limit where the mass splitting and all other energies are much smaller than the mass m it will turn out that it is no real problem if the two masses are not equal in the original Klein–Gordon equation.

One root of a matrix can be found by inserting the matrix in the standard Taylor expansion $\sqrt{1+x} \approx 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \mathcal{O}(x^3)$. Writing our matrix in the following way:

$$m^2\left\{ \mathbb{1} + \frac{1}{m^2}\begin{pmatrix} -\nabla^2 + \Gamma + \frac{1}{4r^2} & -\frac{1}{r^2}\partial_\varphi \\ \frac{1}{r^2}\partial_\varphi & -\nabla^2 - \Gamma + \frac{1}{4r^2} \end{pmatrix} \right\}$$

we find the following root:

$$H \approx m\mathbb{1} + \frac{1}{2m}\begin{pmatrix} -\nabla^2 + \Gamma + \frac{1}{4r^2} & -\frac{1}{r^2}\partial_\varphi \\ \frac{1}{r^2}\partial_\varphi & -\nabla^2 - \Gamma + \frac{1}{4r^2} \end{pmatrix} + \mathcal{O}(m^{-3}) \qquad (4.61)$$

Notice that the order $\mathcal{O}(m^{-2})$ terms are zero.
We see that we have found a hermitian (approximate) root of the Klein–Gordon operator K. Since

$$\frac{1}{\mu_{1,2}} = \frac{1}{m\sqrt{1 \pm \frac{\Gamma}{m^2}}} \approx \frac{1}{m}\frac{1}{1 \pm \frac{\Gamma}{2m^2}} \approx \frac{1}{m}(1 \mp \frac{\Gamma}{2m^2}) = \frac{1}{m} \mp \frac{\Gamma}{2m^3} \qquad (4.62)$$

we could also write the Hamiltonian in the following non-hermitian form:

$$H \approx \begin{pmatrix} \mu_1 + \frac{1}{2\mu_1}\left[-\nabla^2 + \frac{1}{4r^2}\right] & -\frac{1}{2\mu_1 r^2}\partial_\varphi \\ \frac{1}{2\mu_2 r^2}\partial_\varphi & \mu_2 + \frac{1}{2\mu_2}\left[-\nabla^2 + \frac{1}{4r^2}\right] \end{pmatrix} + \mathcal{O}(m^{-3}) \qquad (4.63)$$

which is the form March–Russell et al. [10] find, but according to them ρ_1 and ρ_2 satisfy the obtained Schrödinger equation instead of their linear combinations ψ_1 and ψ_2.

Let us conclude this Chapter with the main results: We have found a non relativistic Schrödinger equation which describes the two particles upto order $1/m^3$, while the wavefunctions of the particles can be derived from the Klein–Gordon solutions using the relation:

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = (H + \mathrm{i}\partial_t) \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} \tag{4.64}$$

where H is the Hamiltonian of the system given by equation (4.61).

CHAPTER 5

CALCULATION OF THE CROSS SECTION

In this Chapter we will calculate the differential scattering cross section for the "internal frame dragging" Hamiltonian, which we derived in Chapter 4. We will first look at the solutions for $\Gamma = 0$, before calculating the cross section up to second order using a perturbative method.

5.1 The basic equations

Notice that every wavefunction which satisfies the Schrödinger equation also satisfies the corresponding Klein–Gordon equation since the Hamiltonian is time independent and therefore:

$$-\partial_t^2 \psi = \mathrm{i}\partial_t \mathrm{i}\partial_t \psi = \mathrm{i}\partial_t(H\psi) = H\mathrm{i}\partial_t \psi = H^2 \psi = K\psi \tag{5.1}$$

Further note that by taking $H = +m(\mathbb{1} + \frac{1}{2}K)$ in equation (4.61) we have taken a positive root of K so that we should consider only positive energy solutions. This eliminates half of the solutions to the complex Klein–Gordon equation and we see that instead of looking for *all* solutions to the Schrödinger equation we could equally well look for *all* complex solutions to the corresponding Klein–Gordon equation with the condition that their time dependence is of the form $\mathrm{e}^{-\mathrm{i}\omega t}$. Therefore we will look for solutions of the original coupled pair Klein–Gordon equations with such a time dependence. Notice that the solutions we then find are *not* the the fields $\rho_{1,2}$ but $\psi_{1,2}$, linear combinations of them. It will be practical to define the operator L as

$$L = -\nabla^2 + \frac{1}{4r^2} + m^2 = -(\partial_r^2 + \frac{1}{r}\partial_r + \frac{1}{r^2}\partial_\varphi^2) + \frac{1}{4r^2} + m^2 \tag{5.2}$$

Together with the condition that the time dependence of the two fields is of the form $e^{-i\omega t}$ we get the following equations to solve:

$$\omega^2 \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} L + \Gamma & -\frac{1}{r^2}\partial_\varphi \\ \frac{1}{r^2}\partial_\varphi & L - \Gamma \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = 0 \tag{5.3}$$

The case of Γ equals zero can be solved exactly and therefore we will start with that.

5.2   The spectrum for $\Gamma = 0$

We can find the solutions by performing a mode expansion:

$$\psi_{1,2} = \sum_{n=-\infty}^{\infty} e^{i(n+\frac{1}{2})\varphi} R_{1,2}^{(n)}(r) \tag{5.4}$$

The factor $\exp(i\varphi/2)$ is necessary to account for the boundary condition: ψ_1 and ψ_2 are both equal to this factor times a single valued function. By putting these solutions into equation (5.3) with $\Gamma = 0$ and integrating out the φ dependence we get

$$r^2(\omega^2 - \tilde{L})R_1^{(n)}(r) = -i(n + \frac{1}{2})R_2^{(n)}(r) \tag{5.5a}$$

$$r^2(\omega^2 - \tilde{L})R_2^{(n)}(r) = i(n + \frac{1}{2})R_1^{(n)}(r) \tag{5.5b}$$

where $\tilde{L}$ is equal to L with ∂_φ^2 replaced by $-(n + \frac{1}{2})^2$:

$$r^2(\omega^2 - \tilde{L}) = r^2\partial_r^2 + r\partial_r + r^2 \underbrace{(\omega^2 - m^2)}_{=:k^2} - \left[(n + \frac{1}{2})^2 + \frac{1}{4}\right] \tag{5.6}$$

Inserting the first equation into the second one we find an equation in $R_2^{(n)}$ only:

$$\left[r^2(\omega^2 - \tilde{L})\right]^2 R_2^{(n)} = (n + \frac{1}{2})^2 R_2^{(n)} \tag{5.7}$$

This single fourth order differential equation can of course be reduced to two second order differential equations by taking the square root of the operators on both sides:

$$r^2(\omega^2 - \tilde{L})R_2^{(n)} = \pm(n + \frac{1}{2})R_2^{(n)} \tag{5.8}$$

and therefore

$$(r^2\partial_r^2 + r\partial_r + r^2k^2 - \nu_n^2)R_2^{(n)} = 0 \tag{5.9}$$

This is a Bessel equation[1] for $R_2^{(n)}$ of order ν_n which is equal to $(n+1)$ for the positive root and equal to n for the negative root. For a Bessel equation of integer order the two independent solutions are the Bessel functions of the first and second kind $J_{|n|}(kr)$ and $Y_{|n|}(kr)$. The Bessel functions of the second kind are not finite near the origin and so only the $J_{|n|}(kr)$ and $J_{|n+1|}(kr)$ solutions remain. If we now combine the equations (5.5b) and (5.8) we see that the most general form for $R_{1,2}^{(n)}$ equals:

$$\begin{pmatrix} R_1^{(n)} \\ R_2^{(n)} \end{pmatrix} = \frac{A_n}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} J_{|n+1|}(kr) + \frac{B_n}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} J_{|n|}(kr) \tag{5.10}$$

where the factors $\sqrt{2}$ are included just for practical purposes and where A_n and B_n are unknown complex coefficients depending only on n.

We will now show that there is indeed no scattering in the $\Gamma = 0$ case. Since we know the wave function solutions we can determine the differential scattering cross section by taking an incident plane wave and using the well-known relation

$$\psi_{\text{tot}} = \psi_{\text{in}} + \frac{f(\varphi)}{\sqrt{r}}\psi_{\text{scat}} \tag{5.11}$$

where ψ_{in} is the incident plane wave, while ψ_{scat} is the scattered (radial) outgoing wave, proportional to $\exp(ikr)$.

The most general incoming plane wave can be written as:

$$\psi_{in} = e^{i(\mathbf{k}\cdot\mathbf{r}+\varphi/2)} \begin{pmatrix} C \\ D \end{pmatrix} \tag{5.12}$$

where the factor $\exp(i\varphi/2)$ is necessary to account for the multi-valuedness of the solution and where $\mathbf{k}$ is parallel to the negative x-axis as usual.

We can now determine the unknown coefficients A_n and B_n by matching the incoming parts — the terms with r dependence $\exp(-ikr)$ — onto each other. Using the large r behaviour of the Bessel functions

$$J_n(kr) \approx \sqrt{\frac{2}{\pi kr}} \cos\left[kr - \frac{\pi}{2}(n+\frac{1}{2})\right] \tag{5.13}$$

---

[1]See appendix C

and the usual expansion

$$\exp(-\mathrm{i}kr\cos\varphi) = \sum_{n=-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\frac{\pi}{2}|n|}\mathrm{e}^{\mathrm{i}n\varphi}J_{|n|}(kr) \tag{5.14}$$

the incoming parts now become

$$\mathrm{e}^{-\mathrm{i}\frac{\pi}{2}|n|}\mathrm{e}^{\mathrm{i}\frac{\pi}{2}(|n|+\frac{1}{2})}\begin{pmatrix}C\\D\end{pmatrix} = \frac{A_n}{\sqrt{2}}\mathrm{e}^{\mathrm{i}\frac{\pi}{2}(|n+1|+\frac{1}{2})}\begin{pmatrix}1\\\mathrm{i}\end{pmatrix} + \frac{B_n}{\sqrt{2}}\mathrm{e}^{\mathrm{i}\frac{\pi}{2}(|n|+\frac{1}{2})}\begin{pmatrix}1\\-\mathrm{i}\end{pmatrix} \tag{5.15}$$

where we have divided out the obvious common factors, and integrated out the φ dependence which removes the summation.
We have found the two equations:

$$\sqrt{2}C = A_n\mathrm{e}^{\mathrm{i}\frac{\pi}{2}|n+1|} + B_n\mathrm{e}^{\mathrm{i}\frac{\pi}{2}|n|} \tag{5.16a}$$

$$-\mathrm{i}\sqrt{2}D = A_n\mathrm{e}^{\mathrm{i}\frac{\pi}{2}|n+1|} - B_n\mathrm{e}^{\mathrm{i}\frac{\pi}{2}|n|} \tag{5.16b}$$

By taking the sum and the difference of these two equations it is clear that A_n and B_n must be of the form:

$$A_n = A\mathrm{e}^{-\mathrm{i}\frac{\pi}{2}|n+1|} \tag{5.17a}$$

$$B_n = B\mathrm{e}^{-\mathrm{i}\frac{\pi}{2}|n|} \tag{5.17b}$$

where A and B are some constants.
The outgoing parts are now equal to

$$f(\varphi)\begin{pmatrix}E\\F\end{pmatrix} + \frac{1}{\sqrt{2\pi k}}\sum_{n=-\infty}^{\infty}(-1)^n\mathrm{e}^{\mathrm{i}n\varphi}\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}\begin{pmatrix}C\\D\end{pmatrix} =$$

$$\frac{1}{\sqrt{2\pi k}}\sum_{n=-\infty}^{\infty}(-1)^n\mathrm{e}^{\mathrm{i}n\varphi}\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}\left[-\frac{A}{\sqrt{2}}\begin{pmatrix}1\\\mathrm{i}\end{pmatrix} + \frac{B}{\sqrt{2}}\begin{pmatrix}1\\-\mathrm{i}\end{pmatrix}\right] \tag{5.18}$$

where we divided out the common factor $\exp(\mathrm{i}kr)/\sqrt{r}$.
So $f(\varphi)$ is proportional to:

$$f(\varphi) \sim \sum_{n=-\infty}^{\infty}(-1)^n\mathrm{e}^{\mathrm{i}n\varphi} \tag{5.19}$$

$$= \frac{1}{\mathrm{e}^{-\mathrm{i}\varphi}+1}\sum_{n=-\infty}^{\infty}(-1)^n\left(\mathrm{e}^{\mathrm{i}n\varphi} + \mathrm{e}^{\mathrm{i}(n-1)\varphi}\right) \tag{5.20}$$

$$= 0 \quad \text{if and only if} \quad \varphi \neq \pi \tag{5.21}$$

To see that the expression between parentheses is zero write the lower and upper limits as $-N$ and M. The only terms that remain are of the form $\exp(\mathrm{i}M\varphi)$ and $\exp(-\mathrm{i}(N+1)\varphi)$. Furthermore note that the differential cross section actually is a mean over a small interval $[\varphi - \epsilon/2, \varphi + \epsilon/2]$ around a certain φ. But since the exponentials are oscillating very fast, the mean is zero. A more rigorous proof can be given by first integrating φ over the afore mentioned interval, then taking the limits M and N to infinity, and finally dividing by ϵ and taking the limit of ϵ to zero. The integration gives a factor of $1/M$ or $1/N$ and therefore the expression is zero in the limit of M and N to infinity.

We will now look some more at solutions which match onto incoming plane waves. We have seen that the most general solution can be written as:

$$
\begin{aligned}
\psi &= \frac{\mathrm{i}A}{\sqrt{2}} \mathrm{e}^{-\mathrm{i}\varphi/2} \begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix} \sum_{n=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}(n+1)\varphi} \mathrm{e}^{-\mathrm{i}|n+1|} J_{|n+1|} + \\
&\quad \frac{-\mathrm{i}B}{\sqrt{2}} \mathrm{e}^{\mathrm{i}\varphi/2} \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix} \sum_{n=-\infty}^{\infty} \mathrm{e}^{\mathrm{i}n\varphi} \mathrm{e}^{-\mathrm{i}|n|} J_{|n|} \\
&= A\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \mathrm{e}^{\mathrm{i}(\pi-\varphi)/2} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \mathrm{i} \end{pmatrix} + B\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \mathrm{e}^{-\mathrm{i}(\pi-\varphi)/2} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix} \\
&=: A\psi_{\mathbf{k}}^{+} + B\psi_{\mathbf{k}}^{-}
\end{aligned}
\tag{5.22}
$$

where we have redefined A and B by extracting factors $\pm\mathrm{i}$ just to make the expression simpler for general wave vectors where $\mathbf{k}$ does not point in the negative x-direction. We will show that these $\psi_{\pm}$ form a complete and orthogonal set of solutions, i.e. a basis of eigenfunctions of the free Hamiltonian.

For all $\mathbf{k}$ and $\mathbf{k}'$ $\psi_{\mathbf{k}}^{+}$ and $\psi_{\mathbf{k}'}^{-}$ are orthogonal since the inner-product $\begin{pmatrix} 1 \\ \pm\mathrm{i} \end{pmatrix}^{\dagger} \cdot \begin{pmatrix} 1 \\ \mp\mathrm{i} \end{pmatrix}$ vanishes. Furthermore the $\psi_{\mathbf{k}}^{\pm}$ and $\psi_{\mathbf{k}'}^{\pm}$ are orthonormal with respect to a Dirac normalization:

$$
\begin{aligned}
\int \frac{\mathrm{d}^2 r}{(2\pi)^2} (\psi_{\mathbf{k}}^{\pm})^{\dagger} \psi_{\mathbf{k}'}^{\pm} &= \int \frac{\mathrm{d}^2 r}{(2\pi)^2} \left[\mathrm{e}^{\pm\mathrm{i}(\theta-\varphi)/2} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm\mathrm{i} \end{pmatrix} \right]^{\dagger} \\
&\qquad \cdot \mathrm{e}^{\pm\mathrm{i}(\theta'-\varphi)/2} \mathrm{e}^{\mathrm{i}\mathbf{k}'\cdot\mathbf{r}} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm\mathrm{i} \end{pmatrix} \\
&= \mathrm{e}^{\pm\mathrm{i}(\theta'-\theta)/2} \int \frac{\mathrm{d}^2 r}{(2\pi)^2} \mathrm{e}^{\mathrm{i}(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}} \\
&= \delta^{(2)}(\mathbf{k}-\mathbf{k}')
\end{aligned}
\tag{5.23}
$$

where θ and θ' are the angles $\mathbf{k}$ and $\mathbf{k}'$ make with the x-axis.

To show that the solutions form a complete set, notice that $\begin{pmatrix} 1 \\ \pm\mathrm{i} \end{pmatrix}$ form a

orthogonal basis for two component vectors while plane waves form a basis of eigenfunctions of the free Schrödinger equation. So together they will form a basis for the solutions to a two component Schrödinger equation. This is shown directly by the fact that we can form the 2×2 identity operator with them:

$$\int \frac{\mathrm{d}^2 k}{(2\pi)^2} \, \psi_{\mathbf{k}}^+(\mathbf{r}') \left[\psi_{\mathbf{k}}^+(\mathbf{r})\right]^\dagger + \psi_{\mathbf{k}}^-(\mathbf{r}') \left[\psi_{\mathbf{k}}^-(\mathbf{r})\right]^\dagger$$

$$= \int \frac{\mathrm{d}^2 k}{(2\pi)^2} \, \mathrm{e}^{-\mathrm{i}(\varphi'-\varphi)/2} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})} \frac{1}{2} \begin{pmatrix} 1 & -\mathrm{i} \\ \mathrm{i} & 1 \end{pmatrix} + $$

$$\mathrm{e}^{+\mathrm{i}(\varphi'-\varphi)/2} \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot(\mathbf{r}'-\mathbf{r})} \frac{1}{2} \begin{pmatrix} 1 & \mathrm{i} \\ -\mathrm{i} & 1 \end{pmatrix}$$

$$= \mathbb{1}\, \delta^{(2)}(\mathbf{r}' - \mathbf{r}) \tag{5.24}$$

We end this section about the $\Gamma = 0$ case with an overview of the results:

- For each value of $\mathbf{k}$ the Schrödinger equation has two independent solutions.

- For neither of these solutions scattering occurs.

- The solutions that can be matched on an incoming plane wave form a complete and orthonormal set, i.e. a basis for all solutions to the two component Schrödinger equation.

5.3   The general case $\Gamma \neq 0$, a perturbation approach

We will now determine the differential scattering cross section in second order perturbation theory using the S-matrix formalism as described in appendix B. We will use the $\Gamma = 0$ Hamiltonian as the unperturbed Hamiltonian. So we will split the Hamiltonian (4.61):

$$H = H_0 + H_I \tag{5.25}$$

where

$$H_0 = \begin{pmatrix} m + \frac{1}{2m}\left[-\nabla^2 + \frac{1}{4r^2}\right] & -\frac{1}{2mr^2}\partial_\varphi \\ \frac{1}{2mr^2}\partial_\varphi & m + \frac{1}{2m}\left[-\nabla^2 + \frac{1}{4r^2}\right] \end{pmatrix}$$

$$= \mathbb{1}\left[m + \frac{1}{2m}\left(-\nabla^2 + \frac{1}{4r^2}\right)\right] - \sigma_2 \frac{1}{2mr^2}\mathrm{i}\partial_\varphi \tag{5.26a}$$

and

$$H_I = \frac{\Gamma}{2m} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_3 \frac{\Gamma}{2m} \tag{5.26b}$$

The solutions to the unperturbed Hamiltonian are the $\psi_{\mathbf{k}}^{\pm}$ of section 5.2. Since we have shown that these solutions form a complete set, every solution can be written as a linear combination of them and so they are the only solutions we have to look at. The results however will be valid only for $k^2 > \Gamma$ since $H_0 \psi_{\mathbf{k}}^{\pm} = (m + \frac{k^2}{2m})\psi_{\mathbf{k}}^{\pm}$ and as mentioned in appendix B any constant multiple of the identity is irrelevant so it is clear we should compare $\frac{k^2}{2m}$ with $\frac{\Gamma}{2m}$.

We will calculate the matrix elements t_{fi} for scattering from an initial state $|i\rangle$ into a final state $|f\rangle$ in second order. From equation (B.21) it follows that we will need the matrix elements

$$\langle f| H_I(t) |i\rangle \qquad \text{and} \qquad \langle f| H_I(t') H_I(t'') |i\rangle$$

Notice that H_I transforms $\left(\begin{smallmatrix} 1 \\ i \end{smallmatrix}\right)$ into $\left(\begin{smallmatrix} 1 \\ -i \end{smallmatrix}\right)$ and vice versa. We can therefore immediately see that the matrix elements $\langle +| H_I |+\rangle$ and $\langle -| H_I |-\rangle$ vanish. So only the cross terms $\langle \pm| H_I(t) |\mp\rangle$ remain in the first order. The scattering cross section for both possibilities will of course be equal since it depends only on the absolute square of this matrix element. In second order the only terms which will remain are those involving $\langle \pm| H_I(t') H_I(t'') |\pm\rangle$ since $H_I(t') H_I(t'')$ will leave the two orthogonal vectors $\left(\begin{smallmatrix} 1 \\ \pm i \end{smallmatrix}\right)$ invariant. So for scattering from $\pm$ states into a state of the same type we only need the second order while for scattering into a state of the other type we only need the first order.

5.3.1   The first order matrix element

We will now start with the first order term in t_{fi} for scattering from an initial state $|i, -\rangle$ into a final state $|f, +\rangle$. According to equation (B.21) the first order term is equal to

$$-2\pi i \delta(E_i - E_f) t_{fi}^{(1)} = -i \int_{-\infty}^{\infty} dt' \ \langle f, +| H_I(t') |i, -\rangle \tag{5.27}$$

which we can write out using the explicit form of the $\psi_{\mathbf{k}}^{\pm}$:

$$
-2\pi i\delta(E_i - E_f)t_{fi}^{(1)} = -i \int_{-\infty}^{\infty} \mathrm{d}t' \int \mathrm{d}^2r \left[e^{+i\mathbf{k}_f \cdot \mathbf{r}} e^{i(\theta_f - \varphi)/2} \frac{1}{\sqrt{2V}} \begin{pmatrix} 1 \\ i \end{pmatrix} \right]^{\dagger}
$$

$$
\cdot\, e^{iH_0 t'} \frac{\Gamma}{2m} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} e^{-iH_0 t'}
$$

$$
\cdot\, e^{i\mathbf{k}_i \cdot \mathbf{r}} e^{-i(\theta_i - \varphi)/2} \frac{1}{\sqrt{2V}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \tag{5.28}
$$

$$
= -i \frac{\Gamma}{2m} e^{-i(\theta_f + \theta_i)/2} \int_{-\infty}^{\infty} \mathrm{d}t'\, e^{i(E_f - E_i)t'} \int \frac{\mathrm{d}^2r}{V}\, e^{i(\mathbf{k}_i - \mathbf{k}_f)\cdot \mathbf{r}} e^{i\varphi}
$$

where a factor $1/\sqrt{V}$ is included since the wavefunctions should be normalized to 1 particle in the whole space. The t integral gives an energy δ-function and we find

$$
-2\pi i\delta(E_i - E_f)t_{fi}^{(1)} = -i2\pi\delta(E_i - E_f)\frac{\Gamma}{2m} e^{-i(\theta_f + \theta_i)/2} \int \frac{\mathrm{d}^2r}{V}\, e^{i(\mathbf{k}_i - \mathbf{k}_f)\cdot \mathbf{r}} e^{i\varphi} \tag{5.29}
$$

By choosing $\mathbf{k}_i$ parallel to the negative x-axis ($\theta_i = \pi$) and using the fact that since $E = \frac{k^2}{2m}$ the delta function ensures that $k_f = k_i$ we find the following expression:

$$
t_{fi}^{(1)} = -\frac{\Gamma}{2m} e^{-i\theta/2} \int \frac{\mathrm{d}^2r}{V}\, e^{ikr[\cos(\theta - \varphi) - \cos(\varphi)]} e^{i\varphi} \tag{5.30}
$$

where we have introduced the scattering angle $\theta := \theta_f - \theta_i = \theta_f - \pi$.
The expression between square brackets can be written as $K(\theta)\sin(\varphi - \alpha(\theta))$ where $\alpha(\theta)$ can be found by substituting $\varphi = \alpha(\theta)$, while $K(\theta)$ can be found by substituting $\varphi = \alpha(\theta) + \pi/2$. We then find:

$$
\cos(\theta - \varphi) - \cos(\varphi) = 2\sin\frac{\theta}{2}\sin(\varphi - \theta/2) \tag{5.31}
$$

We can now use the standard integral representation for the Bessel functions (see appendix C)

$$
J_n(z) = \frac{1}{2\pi} \int_{\alpha}^{2\pi + \alpha} \mathrm{d}\varphi\, e^{i(n\varphi - z\sin\varphi)} \tag{5.32}
$$

and find the following expression for $t_{fi}^{(1)}$:

$$
t_{fi}^{(1)} = \frac{\Gamma}{2m} e^{-i\theta/2} \int_0^{\infty} \frac{r\mathrm{d}r}{V}\, 2\pi J_1(2kr\sin\frac{\theta}{2}) \tag{5.33}
$$

where we have used $J_1(-z) = -J_1(z)$.

As long as $\sin\frac{\theta}{2} \neq 0$ we can rewrite the integral as:

$$\frac{\Gamma}{2m}\frac{1}{V}\frac{2\pi e^{-i\theta/2}}{(2k\sin\frac{\theta}{2})^2}\int_0^\infty r \mathrm{d}r\; J_1(r) \tag{5.34}$$

(notice that $\sin\frac{\theta}{2} \geq 0$ since $0 \leq \theta/2 \leq \pi$).

This remaining integral can be evaluated by inserting an extra factor $e^{-\epsilon r}$ and by taking the limit $\epsilon \downarrow 0$ after the calculation. According to appendix C we get

$$\int_0^\infty r \mathrm{d}r\; e^{-\epsilon r} J_1(r) = \frac{1}{(\epsilon^2+1)^{3/2}} \tag{5.35}$$

So we have found

$$t_{fi}^{(1)} = \frac{\Gamma}{2m}\frac{1}{V}\frac{2\pi e^{-i\theta/2}}{(2k\sin\frac{\theta}{2})^2} \tag{5.36}$$

Using

$$\delta(E_f - E_i) = \frac{\delta(k_f - k_i)}{\left|\frac{\mathrm{d}E}{\mathrm{d}k}\right|_{k=k_f}} = \frac{m}{k_f}\delta(k_f - k_i) \tag{5.37}$$

we can (for $k^2 > \Gamma$) calculate the differential scattering cross section (B.20)

$$\begin{aligned}
\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} &= \frac{1}{v}\int_0^\infty \frac{k_f \mathrm{d}k_f}{(2\pi)^2}\, 2\pi\delta(E_f - E_i)\left|V\frac{\Gamma}{2m}\frac{1}{V}\frac{-2\pi e^{-i\theta/2}}{(2k_f\sin\frac{\theta}{2})^2}\right|^2 \\
&= \frac{2\pi}{v}\left(\frac{\Gamma}{2m}\right)^2\int_0^\infty \mathrm{d}k_f\, \frac{m}{k_f}\delta(k_f - k_i)\frac{k_f}{(2k_f\sin\frac{\theta}{2})^4} \\
&= \frac{2\pi m^2}{k}\left(\frac{\Gamma}{2m}\right)^2\frac{1}{(2k\sin\frac{\theta}{2})^4} \tag{5.38}
\end{aligned}$$

It is clear that this is not the Aharonov–Bohm cross section. In fact it looks more like the Rutherford cross section for the three dimensional Coulomb scattering. In Chapter 6 we will give an extensive discussion of this result.

5.3.2   The second order matrix element

We will now determine the second order matrix element, that is we will determine the cross section for scattering where the initial and final states are both $\psi_{\mathbf{k}}^+$ or both $\psi_{\mathbf{k}}^-$ states.

The second order matrix element for scattering from a $\pm$ state into a $\pm$ state is equal to:

$$-2\pi\mathrm{i}\delta(E_i - E_f)t_{fi}^{(2)} = -\frac{1}{2}\int_{-\infty}^{\infty}\mathrm{d}t_1\mathrm{d}t_2\ \langle f,\pm|\,T(H_I(t_2)H_I(t_1))\,|i,\pm\rangle$$

$$= -\int_{-\infty}^{\infty}\mathrm{d}t_1\mathrm{d}t_2\ \theta(t_2 - t_1)\,\langle f,\pm|\,H_I(t_2)H_I(t_1)\,|i,\pm\rangle$$

(5.39)

where $\theta(t)$ is the Heaviside step function.

We will again take the incident wave vector parallel to the x-axis while the outgoing wave vector will make an angle θ with the x-axis. The complete expression will therefore look like:

$$\mathcal{T}_{fi}^{(2)} = -\int_{-\infty}^{\infty}\mathrm{d}t_1\mathrm{d}t_2\ \theta(t_2-t_1)\int\mathrm{d}^2r\ \left[\mathrm{e}^{\mathrm{i}\mathbf{k}_f\cdot\mathbf{r}}\mathrm{e}^{\pm\mathrm{i}(\theta-\varphi)/2}\frac{1}{\sqrt{2V}}\begin{pmatrix}1\\\pm\mathrm{i}\end{pmatrix}\right]^{\dagger}$$

$$\cdot\,\mathrm{e}^{\mathrm{i}H_0t_2}\frac{\Gamma}{2m}\sigma_3\mathrm{e}^{-\mathrm{i}H_0t_2}\mathrm{e}^{\mathrm{i}H_0t_1}\frac{\Gamma}{2m}\sigma_3\mathrm{e}^{-\mathrm{i}H_0t_1}\mathrm{e}^{\mathrm{i}\mathbf{k}_i\cdot\mathbf{r}}\mathrm{e}^{\mp\mathrm{i}\varphi/2}\frac{1}{\sqrt{2V}}\begin{pmatrix}1\\\pm\mathrm{i}\end{pmatrix}$$

$$= -\int_{-\infty}^{\infty}\mathrm{d}t_1\mathrm{d}t_2\ \theta(t_2-t_1)\mathrm{e}^{\mathrm{i}(E_ft_2-E_it_1)}\left(\frac{\Gamma}{2m}\right)^2\int\frac{\mathrm{d}^2r}{V}\ \mathrm{e}^{-\mathrm{i}\mathbf{k}_f\cdot\mathbf{r}}\mathrm{e}^{\mp\mathrm{i}(\theta-\varphi)/2}$$

$$\cdot\,\frac{1}{\sqrt{2}}\begin{pmatrix}1&\mp\mathrm{i}\end{pmatrix}\sigma_3\mathrm{e}^{-\mathrm{i}H_0(t_2-t_1)}\sigma_3\mathrm{e}^{\mathrm{i}\mathbf{k}_i\cdot\mathbf{r}}\mathrm{e}^{\mp\mathrm{i}\varphi/2}\frac{1}{\sqrt{2}}\begin{pmatrix}1\\\pm\mathrm{i}\end{pmatrix}$$

(5.40)

It is clear that we need expressions of the following form:

$$\sigma_3(H_0)^n\sigma_3 = \sigma_3\big(L\mathbb{1} - \frac{1}{2mr^2}\mathrm{i}\sigma_2\partial_{\varphi}\big)^n\sigma_3 = \Big[\sigma_3\big(L\mathbb{1} - \frac{1}{2mr^2}\mathrm{i}\sigma_2\partial_{\varphi}\big)\sigma_3\Big]^n$$

where we have introduced $L := m + \frac{1}{2m}(-\nabla^2 + \frac{1}{4r^2})$ and used the fact $\sigma_3^2 = \mathbb{1}$. It is easy to show that

$$\sigma_3\big(L\mathbb{1} - \frac{1}{2mr^2}\mathrm{i}\sigma_2\partial_{\varphi}\big)\sigma_3 = L\mathbb{1} + \frac{1}{2mr^2}\mathrm{i}\sigma_2\partial_{\varphi}$$

$$= H_0 + \frac{1}{mr^2}\mathrm{i}\sigma_2\partial_{\varphi}$$

(5.41)

We now need the action of this operator on $\psi_{\mathbf{k}_i}^{\pm}$:

$$\mathrm{i}\sigma_2\partial_{\varphi}\psi_{\mathbf{k}_i}^{\pm} = \begin{pmatrix}0&-\mathrm{i}\\\mathrm{i}&0\end{pmatrix}\mathrm{i}\partial_{\varphi}\left[\mathrm{e}^{-\mathrm{i}[k_ir\cos\varphi\pm\varphi/2]}\frac{1}{\sqrt{2V}}\begin{pmatrix}1\\\pm\mathrm{i}\end{pmatrix}\right]$$

$$= \pm[-k_ir\sin\varphi\pm\frac{1}{2}]\,\mathrm{e}^{-\mathrm{i}[k_ir\cos\varphi\pm\varphi/2]}\frac{1}{\sqrt{2V}}\begin{pmatrix}1\\\pm\mathrm{i}\end{pmatrix}$$

$$= -[\pm k_ir\sin\varphi - \frac{1}{2}]\psi_{\mathbf{k}_i}^{\pm}$$

(5.42)

So we have found:

$$\sigma_3 e^{-iH_0(t_2-t_1)}\sigma_3\psi_{\mathbf{k}_i}^{\pm} = e^{-i\left[E_i - \frac{\pm k_i r \sin\varphi - \frac{1}{2}}{mr^2}\right](t_2-t_1)}\psi_{\mathbf{k}_i}^{\pm} \tag{5.43}$$

and therefore

$$\mathcal{T}_{fi}^{(2)} = -\left(\frac{\Gamma}{2m}\right)^2 e^{\mp i\theta/2}\int_{-\infty}^{\infty} dt_1 dt_2 \; \theta(t_2-t_1)e^{i(E_f t_2 - E_i t_1)}e^{-iE_i(t_2-t_1)}$$

$$\cdot \int \frac{d^2 r}{V} \; e^{i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{r}}e^{i\left[\frac{\pm k_i r \sin\varphi - \frac{1}{2}}{mr^2}\right](t_2-t_1)}$$

$$= -\left(\frac{\Gamma}{2m}\right)^2 e^{\mp i\theta/2}\int_{-\infty}^{\infty} dt_2 \; e^{i(E_f-E_i)t_2}\int \frac{d^2 r}{V}\; e^{i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{r}}$$

$$\cdot \int_{-\infty}^{\infty} dt\; \theta(t)e^{i\left[\frac{\pm k_i r \sin\varphi - \frac{1}{2}}{mr^2}\right]t} \tag{5.44}$$

where we have substituted $t_2 - t_1$ by t.

We see that the integral over t_2 gives the factor $2\pi\delta(E_f - E_i)$ and thus we have found the following expression for the reduced matrix element $t_{fi}^{(2)}$:

$$t_{fi}^{(2)} = -i\left(\frac{\Gamma}{2m}\right)^2 e^{-i\theta/2}\int \frac{d^2 r}{V}\; e^{i(\mathbf{k}_i-\mathbf{k}_f)\cdot\mathbf{r}}\int_{-\infty}^{\infty} dt\; \theta(t)e^{i\left[\frac{\pm 2k_i r \sin\varphi - 1}{2mr^2}\right]t} \tag{5.45}$$

As mentioned in section B we should include a factor $\exp(-\epsilon t)$ in $H_I(t)$ and take ϵ to zero after the calculation. We then get:

$$\int_{-\infty}^{\infty} dt\; \theta(t)e^{i\frac{\pm 2kr \sin\varphi - 1}{2mr^2}t}e^{-\epsilon t} = \frac{1}{i\frac{\pm 2kr \sin\varphi - 1}{2mr^2} - \epsilon}\left[e^{i\frac{\pm 2kr \sin\varphi - 1}{2mr^2}t}e^{-\epsilon t}\right]_0^{\infty}$$

$$= \frac{i2mr^2}{\pm 2kr \sin\varphi - 1 + i\tilde{\epsilon}} \tag{5.46}$$

In the rest of the calculation we will assume that we can take the limit $\tilde{\epsilon} := 2mr^2\epsilon$ to zero, that is that we can take ϵ to go to zero faster than r goes to infinity. We will drop the tilde from now on. Using equation (5.31) again we can now write $t_{fi}^{(2)}$ as:

$$2m\left(\frac{\Gamma}{2m}\right)^2 e^{\mp i\theta/2}\int_{r=0}^{\infty}\int_{\varphi=0}^{2\pi} \frac{rdrd\varphi}{V}\; \frac{r^2 e^{i2kr \sin\frac{\theta}{2}\sin(\varphi-\theta/2)}}{\pm 2kr \sin\varphi - 1 + i\epsilon} \tag{5.47}$$

As long as $k \neq 0$ we can rewrite this double integral as

$$\frac{1}{(2k)^4}\int_{R=0}^{\infty}\int_{\varphi=0}^{2\pi} \frac{RdRd\varphi}{V}\; \frac{R^2 e^{i[(\sin\frac{\theta}{2}\cos\frac{\theta}{2})R\sin\varphi - (\sin^2\frac{\theta}{2})R\cos\varphi]}}{\pm R \sin\varphi - 1 + i\epsilon} \tag{5.48}$$

If we now return to Cartesian coordinates $x = R\cos\varphi$ and $y = R\sin\varphi$ we have to solve the integral:

$$
\int_{-\infty}^{\infty} \mathrm{d}x\mathrm{d}y \, \frac{(x^2 + y^2)\mathrm{e}^{-\mathrm{i}(ax-by)}}{\pm y - 1 + \mathrm{i}\epsilon} = \int_{-\infty}^{\infty} \mathrm{d}x\mathrm{d}y \, \frac{x^2 + 1 + y^2 - 1}{\pm y - 1 + \mathrm{i}\epsilon}\mathrm{e}^{-\mathrm{i}(ax-by)}
$$

$$
= \int_{-\infty}^{\infty} \mathrm{d}x \, (x^2 + 1)\mathrm{e}^{-\mathrm{i}ax} \int_{-\infty}^{\infty} \mathrm{d}y \, \frac{\mathrm{e}^{\mathrm{i}by}}{\pm y - 1 + \mathrm{i}\epsilon} +
$$

$$
\int_{-\infty}^{\infty} \mathrm{d}x \, \mathrm{e}^{-\mathrm{i}ax} \int_{-\infty}^{\infty} \mathrm{d}y \, (1 \pm y)\mathrm{e}^{\mathrm{i}by} \tag{5.49}
$$

where we have introduced the symbols $a = \sin^2\frac{\theta}{2}$ and $b = \sin\frac{\theta}{2}\cos\frac{\theta}{2}$ and already taken the limit of $\epsilon \downarrow 0$ in the second term.
The x-integrals are equal to respectively

$$
-\frac{\mathrm{d}^2\delta(a)}{\mathrm{d}a^2} + \delta(a) = 0 \qquad \text{and} \qquad \delta(a) = 0 \tag{5.50}
$$

provided that a is not zero.
The second y-integral is equal to

$$
-\mathrm{i}\frac{\mathrm{d}\delta(b)}{\mathrm{d}b} \pm \delta(b) = 0 \tag{5.51}
$$

provided that b is not zero.
To evaluate the first y-integral we can close the contour in the upper half plane if b is positive and in the lower half plane if b is negative. We have a simple pole at $y = \pm(1 - \mathrm{i}\epsilon)$ and therefore we find this integral to be

$$
\int_{-\infty}^{\infty} \mathrm{d}y \, \frac{\mathrm{e}^{\mathrm{i}by}}{y - 1 + \mathrm{i}\epsilon} = \begin{cases} 0 & \text{for } b \text{ positive} \\ 2\pi\mathrm{i}\mathrm{e}^{\mathrm{i}b(1-\mathrm{i}\epsilon)} & \text{for } b \text{ negative} \end{cases} \tag{5.52}
$$

for the $+$ scattering case and

$$
\int_{-\infty}^{\infty} \mathrm{d}y \, \frac{\mathrm{e}^{\mathrm{i}by}}{-y - 1 + \mathrm{i}\epsilon} = \begin{cases} 2\pi\mathrm{i}\mathrm{e}^{-\mathrm{i}b(1-\mathrm{i}\epsilon)} & \text{for } b \text{ positive} \\ 0 & \text{for } b \text{ negative} \end{cases} \tag{5.53}
$$

for the $-$ scattering case.
Taking the limit of ϵ to zero we see that these expressions do not diverge as long as $b \neq 0$. To conclude: we have seen that $t_{fi}^{(2)}$ is equal to zero, provided $\sin^2\frac{\theta}{2} \neq 0$ and $\sin\frac{\theta}{2}\cos\frac{\theta}{2} \neq 0$. So for all θ not equal to a multiple of π we have found that scattering from a $\psi_{\mathbf{k}}^+$ into a $\psi_{\mathbf{k}'}^+$ and scattering from a $\psi_{\mathbf{k}}^-$ into a $\psi_{\mathbf{k}'}^-$ results in a differential cross section which is zero upto second

order. Since the zeroth order of S vanishes too if $\mathbf{k}_f$ is not parallel to $\mathbf{k}_i$, we suspect that all even orders may be zero (as long as the scattering angle differs from some finite number of angles). We are not able to prove this in general however and we will not go into it any further.

In the next Chapter we will discuss the obtained results. We will also discuss other previous papers written about this subject.

CHAPTER **6**

DISCUSSION AND COMPARISON OF THE RESULTS

In this Chapter we will start with a discussion of our own results of Chapter 5 followed by a comparison with the results obtained in previous papers written about this subject.

6.1 The results

Looking at the cross section formula (5.38) it is clear that we do not find the Aharonov–Bohm cross section but instead find one with exactly the same θ dependence a three dimensional Coulomb potential would give. To examine where this result comes from, we will start with a discussion of the important ingredients of the model and their effects on the cross section.

Let use first mention however that the result we found is only valid for the energy region where $k^2 > \Gamma$ since the interaction Hamiltonian H_I should be smaller than H_0. Unfortunately this is *not* the region on which all previous papers where focusing: they focused on the adiabatic limit in which $k \to 0$. There are some previous results about this "upper energy" region however and we will discuss them in the next section.

The model has three important ingredients: the half integer phase factor $\mathrm{e}^{\mathrm{i}\varphi/2}$ and the vector potential $A_\varphi = \frac{\sigma_2}{r}\tilde{\varphi}$ both coming from the redefinition of the fields and the additional potential $\frac{\Gamma}{2m}\sigma_3$. The effects of the first two ingredients can be seen most clearly when we neglect the Γ potential. As we have already seen, no scattering occurs in that case. But if we look at the effect of *only the phase factor*, so temporarily neglect the whole potential, we see that the two coupled equations (5.5) reduce to two independent Bessel equations for $\psi_{1,2}$ of order $n + \frac{1}{2}$ (the $\frac{1}{4}$ disappears as well as the right hand sides of the coupled equations). The most general solution in the case of *only*

a double valued phase factor can therefore be written as

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \sum_n \begin{pmatrix} a_n \\ b_n \end{pmatrix} J_{|n+\frac{1}{2}|}(kr)\mathrm{e}^{\mathrm{i}(n+\frac{1}{2})\varphi} \tag{6.1}$$

If we compare this with the most general solution for the maximal Aharonov–Bohm effect

$$\psi = \sum_n a_n J_{|n+\frac{1}{2}|}(kr)\mathrm{e}^{\mathrm{i}n\varphi} \tag{6.2}$$

we see that the Bessel functions are of the same order. The only difference is the phase factor. However in *these* expressions the phase factor is irrelevant since if we would have solved the maximal Aharonov–Bohm problem using a multi-valued wavefunction instead of a vector potential we would have found the same solution (6.2), but with the extra phase factor present. It is therefore clear that the effect of a multi-valued phase factor is to shift the order of the Bessel functions with a half and thus to result in a maximal Aharonov–Bohm effect.

If we now look for *single valued solutions* of our problem but *with the vector potential* we see that the coupled equations (5.5) remain two coupled equations, only all factors $n + \frac{1}{2}$ are replaced by n. We therefore get two different possible orders of the Bessel equation:

$$\sqrt{n^2 + \frac{1}{4} \pm n} = |n \pm \frac{1}{2}|$$

So in this case of only the vector potential, the most general solutions can be written as:

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}^+ = \sum_n a_n \begin{pmatrix} 1 \\ +\mathrm{i} \end{pmatrix} J_{|n+\frac{1}{2}|}(kr)\mathrm{e}^{\mathrm{i}n\varphi} \tag{6.3a}$$

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}^- = \sum_n a_n \begin{pmatrix} 1 \\ -\mathrm{i} \end{pmatrix} J_{|n-\frac{1}{2}|}(kr)\mathrm{e}^{\mathrm{i}n\varphi} \tag{6.3b}$$

We see that the result of including *only* the vector potential, is the maximal Aharonov–Bohm effect as well, but it also gives rise to a doubling of the number of possible solutions; this is caused by the off-diagonal terms. Notice that both the diagonal *and* the off-diagonal parts of the vector potential contribute to the maximal Aharonov–Bohm effect. By neglecting only the off-diagonal part we therefore get an approximate Aharonov–Bohm effect. When we combine the vector potential *with* the multi-valued phase factor

but still neglect the Γ potential we see that the Aharonov–Bohm scattering disappears since the orders of both the Bessel functions are shifted twice over one half[1]. There remain two solutions however, which we have already used in section 5.2 as a starting point for our perturbative calculation.

We will now check that instead of redefining the fields — as we did in section 4.1 — we could equally well have used the original fields η, which satisfy the equation

$$-\partial_t^2 \eta = (-\nabla^2 + m^2)\eta + \Gamma e^{i\varphi} \eta^* \tag{6.4}$$

or in terms of $\rho_{1,2}$

$$-\partial_t^2 \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} = \left[(-\nabla^2 + m^2)\mathbb{1} + \Gamma \begin{pmatrix} \cos\varphi & \sin\varphi \\ \sin\varphi & -\cos\varphi \end{pmatrix} \right] \begin{pmatrix} \rho_1 \\ \rho_2 \end{pmatrix} \tag{6.5}$$

This leads again to a non-relativistic Schrödinger equation and again we can use the two vectors $\begin{pmatrix} 1 \\ \pm i \end{pmatrix}$ as a basis for the vectorial parts of the free solutions. Notice that again one of the effects of the Γ potential H_I is to transform a $\begin{pmatrix} 1 \\ \pm i \end{pmatrix}$ into a $\begin{pmatrix} 1 \\ \mp i \end{pmatrix}$:

$$\begin{pmatrix} \cos\varphi & \sin\varphi \\ \sin\varphi & -\cos\varphi \end{pmatrix} \begin{pmatrix} 1 \\ \pm i \end{pmatrix} = \begin{pmatrix} \cos\varphi \pm i\sin\varphi \\ \mp i(\cos\varphi \pm i\sin\varphi) \end{pmatrix} = e^{\pm i\varphi} \begin{pmatrix} 1 \\ \mp i \end{pmatrix} \tag{6.6}$$

So we see that we find exactly the same form for $\langle f| H_I |i\rangle$ as we derived in our previous calculation using the redefined fields $\tilde{\eta}$. Only this time the phase factor in the matrix element comes directly from the Γ potential and not from the states.

Using the original fields instead of the redefined ones makes it easier to see what changes in the cross section if we consider a vortex of the more general form $<\lambda(r,\varphi)> = ve^{i\alpha\varphi}$, where α is some general real constant: in equation (5.30) the phase factor $\exp(i\varphi)$ changes into $\exp(i\alpha\varphi)$. The phase factor in front of the integral vanishes if we use the original fields so no changes occur in this factor. According to appendix C the integral is equal to a Bessel function for integer values of α. For non-integer values it diverges[2]. Non-integer values are also forbidden for the simple reason that the λ vacuum must be single valued. So for integer values $\alpha = a$ we find that the effect is to change the first order Bessel function in an ath order Bessel function:

$$t_{fi}^{(1)} = -\frac{\Gamma}{2m} \frac{1}{V} \frac{2\pi}{(2k\sin\frac{\theta}{2})^2} \underbrace{\lim_{\epsilon\downarrow 0} \int_0^\infty r\,\mathrm{d}r \; J_a(r)e^{-\epsilon r}}_{=a} \tag{6.7}$$

---

[1]We get orders 0 and 1 which result in a vanishing cross section.
[2]We did not prove this in appendix C.

and therefore the effect of a vortex of the form $v \exp(\mathrm{i}a\varphi)$ is a factor a^2 in the cross section. We now immediately find that the cross section vanishes for the trivial configuration $<\lambda> = v = v\exp(\mathrm{i}0\varphi)$ as expected: the scattering is an effect of the vortex.

It is also interesting to look at the more general case where we imagine that the Γ potential has an r dependence of the form r^m. We see that in that case the integral in expression (5.33) becomes:

$$\int_0^\infty \mathrm{d}r \; r^{1+m} J_1(2kr\sin\frac{\theta}{2}) = \frac{1}{(2k\sin\frac{\theta}{2})^{m+2}} \int_0^\infty \mathrm{d}r \; r^{1+m} J_1(r)$$

Since the integral is equal to a finite constant (if $m \geq -1$) only depending on m, the cross section will be equal to

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \sim \frac{1}{(2k\sin\frac{\theta}{2})^{2m+4}} \tag{6.8}$$

The fourth power in the cross section is therefore an immediate result of the constant Γ potential. The second power occuring in the Aharonov–Bohm cross section would be obtained by a factor $1/r$ in the potential. Let us check that the Aharonov–Bohm Hamiltonian indeed satisfies this condition although this perturbative approach will not be very useful because it will turn out that the higher order terms diverge. According to equation (2.10) the Aharonov–Bohm Hamiltonian is equal to

$$H_0 + H_I = -\frac{\nabla^2}{2m} - \frac{-\mathrm{i}2\alpha\partial_\varphi + \alpha^2}{2mr^2} \tag{6.9}$$

Since the free solutions are equal to $\mathrm{e}^{-\mathrm{i}(\omega t - kr\cos\varphi)}$ we see that $\mathrm{i}\partial_\varphi \to kr\sin\varphi$. The first term of the interaction Hamiltonian therefore reduces to $\frac{\alpha k \sin\varphi}{mr}$. The second term is proportional to $1/r^2$, but it is actually a higher order term since it comes from $\mathbf{A}^2$. To lowest order the reduced scattering matrix element can now be calculated by

$$t_{fi}^{(1)} = -\int \frac{r\mathrm{d}r\mathrm{d}\varphi}{V} \mathrm{e}^{\mathrm{i}kr(\cos(\varphi-\theta)-\cos\varphi)}\frac{\alpha k\sin\varphi}{mr} = -\mathrm{i}\frac{2\pi\alpha}{2mV\tan\theta/2} \tag{6.10}$$

which yields a lowest order cross section equal to

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\pi^2\alpha^2}{2\pi k\tan^2\theta/2} \tag{6.11}$$

We see that for small angles and small α this looks just like the Aharonov–Bohm cross section but the typical Aharonov–Bohm α dependence is not

visible: we cannot see that for $\alpha = n + \frac{1}{2}$ the cross section is maximal. This is caused by the perturbation theory approach, in which α is assumed to be small. Much more important however is that the second order diverges: the full Aharonov–Bohm cross section with the important $\sin^2 \pi \alpha$ cannot be calculated in perturbation theory. This is a possible risk for all potentials with a $1/r^m$ dependence. Interesting is that the factor a in our vortex $<\lambda(r, \varphi)> = v e^{i a \varphi}$ plays the same role as α in the Aharonov–Bohm effect, which one would perhaps expect from the fact that both cross sections can be calculated using a multi valued phase factor $\exp(i a \varphi / 2)$. However if the extra factor $1/r$ would have been present in the interaction Hamiltonian resulting in the Aharonov–Bohm $\sin^2 \theta / 2$ in the denominator, the a^2 would disappear from the cross section.

Now let us look at the connection with the Coulomb potential. As we have seen, the $\sin \theta / 2$ dependence comes solely from the power of r and since for a three dimensional Coulomb potential we have one factor of r more in the Jacobian: $r^2 \sin \varphi \, \mathrm{d}r \mathrm{d}\varphi$ versus $r \mathrm{d}r \mathrm{d}\varphi$ but also one factor of r more in the denominator of the potential, we see that we will find the same power of $\sin \theta / 2$. The physical origin however is totally different. It is interesting to notice that if we would take the three dimensional Coulomb potential in *two* dimensions, that is if we would take a $1/r$ potential in two dimensions we find the Aharonov–Bohm cross section. Normally one thinks of a logarithmic potential when talking about a Coulomb potential for two dimensions since the field strength should have a $1/r$ dependence to satisfy Gauss' law. We can however also think of a three dimensional problem where all particles are confined to a plane like for example the Aharonov–Bohm effect or the Quantum Hall effect. In fact for such a system the cross section is calculated by Law et al. [13] and indeed it yields the Aharonov–Bohm cross section (plus some extra terms).

6.2   Previous literature

We will start this discussion with the first paper written about the subject, i.e. that of March–Russell et al. [10]. They found an approximate maximal Aharonov–Bohm scattering cross section:

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{1}{2\pi k} \frac{1}{\sin^2 \theta / 2} [1 + C(\theta)] \tag{6.12}$$

where $C(\theta)$ is a small correction depending only on θ (i.e. not on $\mathbf{k}$). We have calculated $C(\theta)$ numerically and plotted it in figure 6.1. This result was obtained by ignoring the off-diagonal terms of the Hamiltonian (4.63).

According to March–Russell et al. a calculation in which they are included in second order perturbation theory would show that they can be ignored for small incoming momenta: $(2k\sin\theta/2)^2 < \Gamma$.
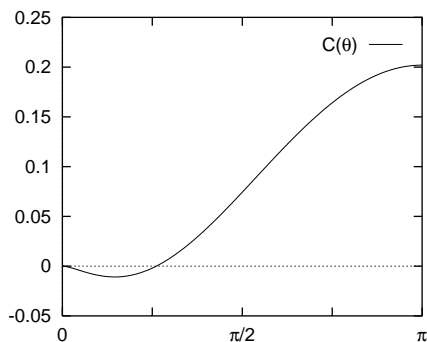

Figure 6.1: *The correction $C(\theta)$*

One of the main arguments for ignoring them is that the masses of the two particles are different. This is however only the case for $\rho_{1,2}$ in the original Klein–Gordon equation, but as we have seen, to derive the non-relativistic Schrödinger equation it was necessary to take linear combinations of them, resulting in two particles with effectively the same mass. This can also be seen directly from the fact that we can equally well use the hermitian Hamiltonian (4.61) in which the two masses are equal.

The fact that the off-diagonal terms cannot be taken into account perturbatively can also be seen from the first order term of the S-matrix: $\langle f| H_I(t) |i\rangle$. The wavefunction contains a factor $\mathrm{e}^{\mathrm{i}(\varphi/2 - kr\cos\varphi)}$. The derivative of this term to φ gives us

$$-\frac{\mathrm{i}\partial_\varphi}{2mr^2}\,|i\rangle = \left[\frac{1}{2}\frac{k\sin\varphi}{mr} + \frac{1}{4}\frac{1}{mr^2}\right]|i\rangle \qquad (6.13)$$

Notice that these two terms are almost equal to the two terms we found in our naive perturbative calculation of the Aharonov–Bohm effect: again the first term can be calculated but the second term diverges. The reason we find almost the same two terms as in the Aharonov–Bohm case is that the off-diagonal terms play an important role in the cancellation of the Aharonov–Bohm cross section as we have shown in section 6.1. The second (divergent) term equals twice the second term in the Aharonov–Bohm case, but combined with the diagonal potential $1/(4r^2)$ they become equal, except for an overall minus sign. So by neglecting the off-diagonal terms we neglect a part of the vector potential which is essential for the cancellation of the $\sin^{-2}\theta/2$ cross section. Taking these terms into account perturbatively therefore means taking into account the Aharonov–Bohm effect perturbatively which is bound to fail. This argument is of course only qualitative since we ignored the effects of Γ, but still, it makes visible the main problem - the $1/r^2$ term.

We now turn to an other paper, written by Robert Navin [14]. He has made a very extensive calculation which I will briefly recapitulate. He looks

for complex solutions with time dependence $\mathrm{e}^{-\mathrm{i}\omega t}$ of the Klein–Gordon and tries to solve it without ignoring the off-diagonal terms by making a mode expansion and looking at the large r behaviour. The first step is to make the assumption that both ψ_1 and ψ_2 have the asymptotic form

$$r^{\gamma}(\alpha_1 \mathrm{e}^{\mathrm{i}k_{1,2}r} + \alpha_2 \mathrm{e}^{-\mathrm{i}k_{1,2}r})$$

By substituting these into the coupled differential equations and retaining only the highest powers in the large r expansion we find the most general solution

$$\psi = \sum_n \mathrm{e}^{\mathrm{i}(n+\frac{1}{2})\varphi} \begin{pmatrix} \frac{2\Gamma}{\mathrm{i}(n+\frac{1}{2})} \frac{\beta_1 \mathrm{e}^{\mathrm{i}k_1 r} + \beta_2 \mathrm{e}^{-\mathrm{i}k_1 r}}{r^{1/2}} + \frac{\mathrm{i}(n+\frac{1}{2})}{2\Gamma} \frac{\alpha_1 \mathrm{e}^{\mathrm{i}k_2 r} + \alpha_2 \mathrm{e}^{-\mathrm{i}k_2 r}}{r^{5/2}} \\ \frac{\alpha_1 \mathrm{e}^{\mathrm{i}k_2 r} + \alpha_2 \mathrm{e}^{-\mathrm{i}k_2 r}}{r^{1/2}} + \frac{\beta_1 \mathrm{e}^{\mathrm{i}k_1 r} + \beta_2 \mathrm{e}^{-\mathrm{i}k_1 r}}{r^{5/2}} \end{pmatrix} \tag{6.14}$$

where $\omega^2 = k_1^2 + m^2 + \Gamma = k_2^2 + m^2 - \Gamma$.

There are four complex parameters left. Notice however that since k_1 is imaginary for energies $m^2 - \Gamma < \omega^2 < m^2 + \Gamma$, there are two energy regimes to look at. Navin tries to find the unknown coefficients by taking the limit of $\Gamma \to 0$ in the upper energy regime since we know we should find Bessel functions then. He claims to find pure transmission for the upper regime and the exact maximal Aharonov–Bohm cross section for the intermediate regime. However the aforementioned limit is ill defined since we see that the second term of ψ_1 blows up unless $\alpha_{1,2}$ are of the order of Γ, but then only the $r^{-5/2}$ terms remain and those functions cannot be matched onto Bessel functions which is necessary to finally calculate the cross section. There is another more transparent argument to see why this matching cannot be done: If we match in the upper regime and want to know the solution in the intermediate regime we should assume that the coefficients have the same form. But if they do, the coefficient of $\mathrm{e}^{k_1 r}$ will be nonzero which means that the solution is not bounded for large r. The conclusion must be that we cannot determine the unknown coefficients and therefore cannot make any further calculation of the cross section.

The article we will discuss next is that of C. R. Hagen [15]. He makes roughly speaking two remarks. First of all he points out that the gradient energy of the λ field diverges logarithmically since the energy density

$$|\nabla \lambda|^2 = |\nabla(v\mathrm{e}^{\mathrm{i}\varphi})|^2 = \frac{v^2}{r^2} \tag{6.15}$$

cannot be integrated over the whole space. Notice that this problem is linked to the fact that we have only a global gauge symmetry: a local gauge symmetry makes it possible to gauge away the nasty gradient term at infinity,

i.e. the gauge field must approach a pure gauge for $r \to \infty$. For an excellent discussion of local vortices - the so called Nielsen-Olesen vortices - see J. Preskill [16]. For the present global vortex we can overcome the problem by cutting off the large r behaviour. In fact in calculating the cross section we already used an extra factor $\exp(-\epsilon r)$ which essentially does this. Hagen worries about the fact that a cut-off would obscure the $\sin^{-2}\theta/2$ cross section, since the large r behaviour corresponds to small k, which is the momentum regime where March–Russell et al. in their original paper were looking at. As mentioned before our calculation focuses on larger k, since only then a perturbative approach can be successful as the Aharonov–Bohm example has shown to us. Further notice that that v must be much smaller than g according to the remark in section 4.1 below equation (4.19). This means that the energy of the λ field is much smaller than other energies: we can take all limits in such a way that there is no problem with a divergent gradient energy. The second remark Hagen makes is about the fact that we can find an Aharonov–Bohm cross section by taking a $1/r$ potential, i.e. when $<\lambda> \sim \text{const}/r$ for large r (see also the article of Law et al. [13]). We have discussed this already in section 6.1.

We now turn to the review article of A. C. Davis and A. P. Martin [17]. They use the same method as March–Russell et al. in neglecting the off-diagonal terms since these would connect terms with different masses. They also claim to make a relativistic calculation but they only use the Klein–Gordon equation in the way we mentioned in section 5.1: looking for all solutions to the Schrödinger equation is equivalent to looking for all complex solutions with time dependence $\mathrm{e}^{-\mathrm{i}\omega t}$ to the Klein–Gordon equation. Indeed they also use equations (2.17)–(2.18) which are only applicable for non-relativistic situations to calculate the differential cross section. Very interesting however is their discussion of the article of Khazan [18], which is about certain line defects in liquid ^{3}He in the A phase. To be more precise it is about the dynamics of the so called collective clapping mode near a vortex with half integer quanta. The equation of motion of this clapping mode is a Schrödinger equation with a vector potential $\mathbf{A} = \frac{1}{2r}\hat{\varphi}$ and a scalar potential $U = \frac{1}{4r^2}$. The vector potential is exactly of the Aharonov–Bohm form leading to half integer Bessel functions. The effect of the diagonal scalar potential is just as in the paper of March–Russell et al. to shift this order:

$$\sqrt{(n+\tfrac{1}{2})^2} \quad \to \quad \sqrt{(n+\tfrac{1}{2})^2 + \tfrac{1}{4}}$$

They (M.–R.) obtained this result by neglecting the off diagonal terms which leaves them with only the multi-valued phase factor and this scalar potential,

while Khazan has a single valued function with an Aharonov–Bohm vector potential and this scalar potential, without ignoring any terms (Khazan actually has missed the scalar potential and therefore finds the exact Aharonov–Bohm cross section as Davis and Martin point out). The result of Khazan is due to an actual Aharonov–Bohm vector potential while March–Russell et al.'s vector potential is an artifact of the "gauge" transformation. In the latter experiment all real effects come from Γ. So in spite of the fact that the two cases look very alike they are completely different. For the ^{3}He case the vector potential really is of the form March–Russell et al. claim it to be, i.e. without the off-diagonal part. Therefore the cross section for this experiment is equal to equation (6.12) with $C(\theta)$ given by figure 6.1.

So we observe that our results do not agree with most of the work discussed in this section; the ^{3}He problem however is of a different type and does deserve further study.

CHAPTER 7

CONCLUSIONS AND OUTLOOK

In contrast with the results presented in all of the previous literature we have found very strong indications that the so-called frame-dragging model does not lead to an Aharonov–Bohm cross section. Instead we obtained that to lowest order in the level splitting parameter $\frac{\Gamma}{2m}$ it leads to the cross section

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{2\pi m^2}{k}\left(\frac{\Gamma}{2m}\right)^2 \frac{1}{(2k\sin\theta/2)^4}$$

which has the same θ dependence as Coulomb scattering in three dimensions, but we have seen that this is merely a coincidence. An Aharonov–Bohm cross section would have been obtained if the the vacuum expectation value of the Higgs field λ had a factor $1/r$ in it.

Because of the perturbative approach our result is only valid for the energy regime $k^2 > \Gamma$, while all previous literature focused on the adiabatic limit where k is small. The odd orders contribute to the cross section only for scattering from a $\psi^\pm$ to a $\psi^\mp$, while the even orders contribute only for situations where the initial and final state are of the same kind. However the second order contribution vanishes completely as long as the scattering angle is not equal to an integer multiple of π.

A more general vacuum expectation value of the form $\mathrm{e}^{\mathrm{i}a\varphi}$ would lead to a factor a^2 in the cross section from which it is clear that the effect we have found really is linked to the vortex configuration, since $a = 0$ results in a vanishing cross section.

One of the main difficulties is the off-diagonal part of the Hamiltonian which connects the two different particles. In the previous literature it was claimed that these two have different masses, but as we have shown this claim is mistaken. This is one of the main reasons why our result differs from previous ones: the off-diagonal parts are not suppressed for small momenta which was a key assumption used before. Maybe a fully relativistic

calculation would prevent some of these difficulties. Further research on this model will be interesting, especially in the adiabatic limit since there are still no good results for this regime, while it is clear that although not of an Aharonov–Bohm form the vortex still does induce scattering.

So our result does not support the expectation that the Aharonov–Bohm effect could be obtained in a theory with global gauge invariance only. Surprisingly enough there is a physical system different from the one we have studied, where this effect is claimed to occur nevertheless. This is the case of liquid ^{3}He which is indeed very different from this "frame dragging" model since it has approximately the Aharonov–Bohm potential without the multi-valued phase factor to cancel it off. Therefore an Aharonov–Bohm cross section *can* be found in it.

Let me conclude by saying that so far we have only looked at this problem from a theoretical perspective, but that in the end experimental evidence in support of these ideas would be as desirable as exciting.

APPENDIX A

<div align="right">

THE COVARIANT DERIVATIVE

</div>

In this appendix we will describe how one can obtain the correct signs for the covariant derivative using the metric and the Lorentz force law. Throughout this thesis we will use the metric $\text{Diag}(1, -1, -1, -1)$ and therefore $\partial_\mu \partial^\mu = \Box = \partial_t^2 - \nabla^2$.

A.1 The covariant derivative

Since in Gaussian units $\mathbf{E}$ is equal to $-\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} - \nabla V$ and $\mathbf{B}$ is equal to $\nabla \wedge \mathbf{A}$ the Lorentz force looks like

$$F_{\text{Lor}} = q \left[-\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} - \nabla V + \frac{\mathbf{v}}{c} \wedge (\nabla \wedge \mathbf{A}) \right] \tag{A.1}$$

Now we want to know the value of the unknown constant α in

$$H = \frac{(\mathbf{p} + \alpha q\mathbf{A})^2}{2m} + qV \tag{A.2}$$

Using the Hamilton equations

$$\dot{\mathbf{r}} = \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \nabla_{\mathbf{p}} H \tag{A.3a}$$

$$\dot{\mathbf{p}} = \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\nabla_{\mathbf{r}} H \tag{A.3b}$$

combined with $\mathbf{A} = \mathbf{A}(\mathbf{r}, t)$ we get

$$\dot{\mathbf{r}} = \frac{\mathbf{p} + \alpha q\mathbf{A}}{m} \tag{A.4a}$$

$$\dot{\mathbf{p}} = -\left[\nabla (\mathbf{p} + \alpha q\mathbf{A}) \right] \cdot \frac{\mathbf{p} + \alpha q\mathbf{A}}{m} - q\nabla V$$

$$= -\alpha q (\nabla \mathbf{A}) \cdot \frac{\mathbf{p} + \alpha q\mathbf{A}}{m} - q\nabla V \tag{A.4b}$$

So combining these two we get

$$\mathbf{v} = \dot{\mathbf{r}} = \frac{\mathbf{p} + \alpha q \mathbf{A}}{m} \tag{A.5a}$$

$$\dot{\mathbf{p}} = -\alpha q \left(\nabla \mathbf{A} \right) \cdot \mathbf{v} - q \nabla V \tag{A.5b}$$

Now use these expressions in the Newtonian equation of motion

$$F_{\text{Lor}} = m\ddot{\mathbf{r}} \tag{A.6}$$

to get

$$F_{\text{Lor}} = m\ddot{\mathbf{r}} = m\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{v} = \dot{\mathbf{p}} + \alpha q \frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t} \tag{A.7}$$

Again using $\mathbf{A} = \mathbf{A}(\mathbf{r}, t)$ we get

$$\frac{\mathrm{d}\mathbf{A}}{\mathrm{d}t} = \frac{\partial \mathbf{A}}{\partial t} + \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} \cdot \nabla \mathbf{A} = \frac{\partial \mathbf{A}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{A} \tag{A.8}$$

and therefore the Lorentz force is equal to

$$\begin{aligned} F_{\text{Lor}} &= \dot{\mathbf{p}} + \alpha q \left(\frac{\partial \mathbf{A}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{A} \right) \\ &= -\alpha q \left(\nabla \mathbf{A} \right) \cdot \mathbf{v} - q \nabla V + \alpha q \left(\frac{\partial \mathbf{A}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{A} \right) \\ &= q \left[\alpha \frac{\partial \mathbf{A}}{\partial t} - \nabla V - \alpha \left[(\nabla \mathbf{A}) \cdot \mathbf{v} - \mathbf{v} \cdot (\nabla \mathbf{A}) \right] \right] \end{aligned} \tag{A.9}$$

Since we can write out $\mathbf{v} \wedge (\nabla \wedge \mathbf{A})$ as

$$\mathbf{v} \wedge (\nabla \wedge \mathbf{A}) = (\nabla \mathbf{A}) \cdot \mathbf{v} - \mathbf{v} \cdot (\nabla \mathbf{A}) \tag{A.10}$$

we can simplify equation (A.9) to

$$F_{\text{Lor}} = q \left[\alpha \frac{\partial \mathbf{A}}{\partial t} - \nabla V - \alpha \mathbf{v} \wedge (\nabla \wedge \mathbf{A}) \right] \tag{A.11}$$

Using the expressions for $\mathbf{E}$ and $\mathbf{B}$ we conclude that α must be equal to $-1/c$ and we get for the Hamiltonian H

$$H = \frac{(\mathbf{p} + \alpha q \mathbf{A})^2}{2m} + qV = \frac{(\mathbf{p} - \frac{q}{c}\mathbf{A})^2}{2m} + qV \tag{A.12}$$

We are now able to generalize this to a relativistic expression. We have seen that the momentum $\mathbf{p}$ must be replaced by $\mathbf{p} - \frac{q}{c}\mathbf{A}$ so the four-momentum p_μ

will be replaced by $p_\mu - \frac{q}{c}A_\mu$. We want $\mathbf{p}$ and $\mathbf{A}$ to be the spatial coordinates of the contravariant four vectors p_μ and A_μ, i.e. $p_\mu = (E/c, \mathbf{p})$ and $A_\mu = (V, \mathbf{A})$. The correct factor c can be found by a simple dimension analysis. Furthermore we have that $\partial_\mu = (\frac{1}{c}\partial_t, \nabla)$ and therefore $\partial^\mu = (\frac{1}{c}\partial_t, -\nabla)$. Since $\mathbf{p} = \frac{\hbar}{i}\nabla$ we must conclude that $p_\mu = -\frac{\hbar}{i}\partial^\mu = i\hbar\partial^\mu$. This is indeed in agreement with the fact that $E = H = i\hbar\partial_t$. So since we have established that p_μ becomes $p_\mu - \frac{q}{c}A_\mu$ we see that we must substitute ∂_μ by $\partial_\mu + i\frac{q}{\hbar c}A_\mu$ where $A_\mu = (V, -\mathbf{A})$. So to sum up we have found the following relations:

$$p^\mu \to p^\mu - \frac{q}{c}A^\mu \tag{A.13}$$

$$\mathbf{p} \to \mathbf{p} - \frac{q}{c}\mathbf{A} \tag{A.14}$$

$$\partial_\mu \to \partial_\mu + i\frac{q}{\hbar c}A_\mu = D_\mu \tag{A.15}$$

$$\nabla \to \nabla - i\frac{q}{\hbar c}\mathbf{A} \tag{A.16}$$

Now we finally need to know the signs and factors in a gauge transformation. We want to know the transformation behaviour of A_μ when ψ transform as

$$\psi \to \psi' = e^{i\lambda}\psi \tag{A.17}$$

where λ is a function of t and $\mathbf{r}$.

The gauge field A_μ must behave in such a way that the covariant derivative of a field or wavefunction transforms as a covariant vector, i.e. the following holds

$$D_\mu\psi \to D'_\mu\psi' = e^{i\lambda}D_\mu\psi \tag{A.18}$$

Writing this out leads to

$$\begin{aligned} D'_\mu\psi' &= \left(\partial_\mu + i\frac{q}{\hbar c}A'_\mu\right)e^{i\lambda}\psi \\ &= e^{i\lambda}\left(\partial_\mu + i\partial_\mu\lambda + i\frac{q}{\hbar c}A'_\mu\right)\psi \\ &= e^{i\lambda}\left(\partial_\mu + i\frac{q}{\hbar c}A_\mu\right)\psi \end{aligned} \tag{A.19}$$

where we have used equation (A.18) in the last step.

Since this must hold for all ψ we see that A'_μ must satisfy

$$A'_\mu = A_\mu - \frac{\hbar c}{q}\partial_\mu\lambda \tag{A.20}$$

It is customary however to absorb the pre-factor in λ and we get the following two relations for a general gauge transformation:

$$\psi \to \psi' = \mathrm{e}^{\mathrm{i}(q/\hbar c)\lambda}\psi \tag{A.21a}$$

$$A_\mu \to A'_\mu = A_\mu - \partial_\mu\lambda \tag{A.21b}$$

In terms of the vector potential $\mathbf{A}$ this reads

$$\mathbf{A} \to \mathbf{A}' = \mathbf{A} + \nabla\lambda \tag{A.22}$$

APPENDIX B

In this appendix an expression for the differential scattering cross section is derived using the S-matrix formalism. We will do this following Sitenko [19] Chapter 2 and Gross [11] Chapter 4.

B.1 Introduction

The S-matrix formalism is used when the total Hamiltonian can be split into two parts: the free Hamiltonian H_0 and the interaction Hamiltonian H_I, where H_I is assumed to be much smaller than H_0, so that its effects will be small perturbations around the free solutions. Furthermore for the calculation of the S-matrix it is convenient to use the interaction picture instead of the Heisenberg or Schrödinger picture. In the interaction picture the time dependence corresponding to the free Hamiltonian is in the operators while the time dependence of the interaction Hamiltonian is in the states. So the interaction Hamiltonian will be equal to:

$$H_I(t) = U_0^{-1}(t) H_I(0) U_0(t) \tag{B.1}$$

where $U_0(t) = \mathrm{e}^{-\mathrm{i}H_0 t}$ is the free evolution operator while H_0 and $H_I(0)$ are the operators as used in the Schrödinger picture. Notice that H_0 looks the same in both pictures.

B.2 The S-matrix

In scattering experiments it is assumed that at $t = -\infty$ the particles are free, then they approach and interact with each other, while at $t = \infty$ they are free again. Calling the initial state $\psi(-\infty)$ and the final state $\psi(\infty)$ the

scattering operator S is defined by

$$\psi(\infty) = S\psi(-\infty) \tag{B.2}$$

It is clear from the normalization of ψ that S is unitary. Furthermore if the final and the initial state are the same no scattering has occurred. Scattering is therefore characterized by the difference of the initial and final state:

$$\mathcal{T}\psi(-\infty) := S\psi(-\infty) - \psi(-\infty) \tag{B.3}$$

Notice that this is the same reasoning as used in the previous section where the scattering amplitude was defined by the difference between the total wave function and the incoming plane wave.

Since the initial and final states are assumed to be free they can be expanded in the complete orthogonal set of solutions to the free Hamiltonian:

$$\psi(-\infty) = \sum_n c_n \psi_n \tag{B.4a}$$

$$\psi(\infty) = \sum_n d_n \psi_n \tag{B.4b}$$

where the sum is to be read as an integral over $\mathbf{k}$ and a sum over the $+$ and $-$ states. Substituting these into definition (B.2) and using the orthogonality of the ψ_n we obtain:

$$d_n = \sum_m c_m \langle n| \, S \, |m\rangle =: \sum_m c_m S_{nm} \tag{B.5}$$

and therefore if we assume the initial state is a certain eigenstate such that only one $c_n \neq 0$ we see that the S-matrix elements are equal to the expansion coefficients d_n of the final state. The probability of finding the system in the final state ψ_n if it was initially in the state ψ_m is therefore equal to $|S_{nm}|^2$. From the unitarity of S it immediately follows:

$$\sum_n |S_{nm}|^2 = \sum_n S_{nm}^* S_{nm} = \sum_n (S^\dagger)_{mn} S_{nm} = (S^\dagger S)_{mm} = 1 \tag{B.6}$$

So indeed the total probability is unity.

The total transition probability as a result of scattering is equal to

$$W_{m\to n} = |\mathcal{T}_{nm}|^2 \tag{B.7}$$

where $\mathcal{T}_{nm}$ is the matrix element of $\mathcal{T}$ between the states ψ_n and ψ_m. The total transition probability per unit time $w_{m\to n}$ can be found by dividing

$W_{m\to n}$ by the time T in which the transition takes place. To find an expression for this $w_{m\to n}$ we write $\mathcal{T}_{nm}$ in terms of a new quantity t_{nm}, the reduced transition matrix element:

$$\mathcal{T}_{nm} = -2\pi \mathrm{i} t_{nm} \delta(E_m - E_n) \tag{B.8}$$

With this definition we find

$$
\begin{aligned}
w_{m\to n} &= 2\pi\delta(E_m - E_n)|t_{nm}|^2 \lim_{T\to\infty} \frac{2\pi\delta(E_m - E_n)}{T} \\
&= 2\pi\delta(E_m - E_n)|t_{nm}|^2 \lim_{T\to\infty} \frac{\int_{-T/2}^{T/2} \mathrm{d}t\; \mathrm{e}^{\mathrm{i}(E_m - E_n)t}}{T} \\
&= 2\pi\delta(E_m - E_n)|t_{nm}|^2
\end{aligned} \tag{B.9}
$$

Our next task is to find an expression for S_{nm} in terms of the interaction Hamiltonian H_I. For this purpose we introduce the time evolution operator $U(t, t_0)$:

$$\psi(t) = U(t, t_0)\psi(t_0) \tag{B.10}$$

In the interaction picture the time dependence of the wave functions is solely due to the interaction Hamiltonian:

$$\mathrm{i}\partial_t \psi(t) = H_I(t)\psi(t) \tag{B.11}$$

and therefore

$$\mathrm{i}\partial_t U(t, t_0) = H_I(t)U(t, t_0) \tag{B.12}$$

which is valid since equation (B.11) applies for arbitrary $\psi(t)$.

It is clear that the evolution operator should also satisfy the boundary condition $U(t_0, t_0) = 1$. We can now write down an integral equation

$$U(t, t_0) = 1 - \mathrm{i}\int_{t_0}^t \mathrm{d}t'\; H_I(t')U(t, t') \tag{B.13}$$

which can be iterated to yield

$$1 - \mathrm{i}\int_{t_0}^t \mathrm{d}t'\; H_I(t') + (-\mathrm{i})^2 \int_{t_0}^t \mathrm{d}t' \int_{t_0}^{t'} \mathrm{d}t''\; H_I(t')H_I(t'') + \cdots \tag{B.14}$$

It can be shown that this can also be written as

$$
\begin{aligned}
U(t, t_0) &= \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \int_{t_0}^t \mathrm{d}t_1 \int_{t_0}^t \mathrm{d}t_2 \cdots \int_{t_0}^t \mathrm{d}t_n\; T\big(H_I(t_1)H_I(t_2)\cdots H_I(t_n)\big) \\
&= T\mathrm{e}^{-\mathrm{i}\int_{t_0}^t \mathrm{d}t'\; H_I(t')}
\end{aligned} \tag{B.15}
$$

where we have introduced the time ordering operator T which orders its argument chronologically:

$$T\big(H_I(t_1)H_I(t_2)\big) = \begin{cases} H_I(t_1)H_I(t_2) & t_1 > t_2 \\ H_I(t_2)H_I(t_1) & t_2 > t_1 \end{cases} \tag{B.16}$$

and similarly for more than two arguments.

By comparing definitions (B.2) and (B.10) we see that we can define the S-matrix by

$$S = \lim_{\substack{t_0 \to -\infty \\ t \to \infty}} U(t, t_0) = T\mathrm{e}^{-\mathrm{i}\int_{-\infty}^{\infty} \mathrm{d}t'\, H_I(t')} \tag{B.17}$$

A few remarks about the derivation of this expression should be made. In the first place the interaction Hamiltonian $H_I(t) = \mathrm{e}^{\mathrm{i}H_0 t} H_I(0) \mathrm{e}^{-\mathrm{i}H_0 t}$ generally does not vanish for $t = \pm\infty$ which is needed because the initial and final states should be free states. We can however insert a factor $\exp(-\epsilon|t|)$ and after the calculation take $\epsilon \to 0$.

Secondly the result is independent from any constant multiple of the identity in H_0 since this part commutes with everything and therefore vanishes from $H_I(t)$.

B.3   The scattering cross section

We can now derive an expression for the differential scattering cross section in terms of the reduced transition matrix elements. The differential scattering cross section is defined by

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\#\text{ particles scattered into d}\Omega\text{ per sec.}}{\#\text{ particles incident per sec. } \cdot \#\text{ scatterers per area}} \tag{B.18}$$

where:

- The number of particles scattered into dΩ per second is equal to the sum of $w_{m \to n}$ over all final states $|n\rangle$ which have their momentum vector in the solid angle dΩ. In the continuum limit this sum goes to an integral as follows:

$$\sum_{\mathbf{n}\text{ in d}\Omega} \Delta\mathbf{n}\, w_{m \to n} \to V \int_{\mathbf{k}\text{ in d}\Omega} \frac{\mathrm{d}^3 k}{(2\pi)^3}\, w_{m \to n} \tag{B.19}$$

  where V is the total space which is infinite, but we will see that in the final result all factors V will cancel.

- The number of incoming particles per second is equal to the volume swept out per second Av times the density of the beam which is equal to $1/V$ since we consider one incoming particle in the whole space.

- The number of scatterers is also assumed to be one and therefore the number of scatterers per area is equal to $1/A$.

In two dimensions areas should be substituted by line elements, total volumes by total areas and solid angles by angles.

We can now write down the differential scattering cross section:

$$
\begin{aligned}
\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} &= \frac{1}{v} \int_{\mathrm{d}\Omega} \frac{\mathrm{d}^2 k}{(2\pi)^2} \, V^2 w_{m\to n} \\
&= \frac{1}{v} \int_{\mathrm{d}\Omega} \frac{\mathrm{d}^2 k}{(2\pi)^2} \, 2\pi\delta(E_m - E_n)|V t_{nm}|^2
\end{aligned}
\tag{B.20}
$$

where the reduced transition matrix t_{nm} was defined in equation (B.8):

$$
-2\pi \mathrm{i}\delta(E_m - E_n)t_{nm} = \mathcal{T}_{nm} = \langle n| \, T\mathrm{e}^{-\mathrm{i}\int_{-\infty}^{\infty} \mathrm{d}t' \, H_I(t')} - 1 \, |m\rangle
\tag{B.21}
$$

Notice that the effect of using $\mathcal{T}$ instead of S is to remove the zeroth order.

APPENDIX C

In this appendix some important properties of Bessel functions are stated together with the proofs of used relations involving Bessel functions. We use the convention that Roman indices are integer while Greek indices are real. All citations are taken from Watson [20]; we will indicate the appropriate Chapters between square brackets.

C.1 Basic relations involving Bessel functions

Bessel functions are solutions to the Bessel equation:

$$z^2 \frac{\mathrm{d}^2 J_\nu(z)}{\mathrm{d}z^2} + z \frac{\mathrm{d}J_\nu(z)}{\mathrm{d}z} + (z^2 - \nu^2)J_\nu(z) = 0 \qquad \text{(C.1)}$$

The constant ν is called the order. For non-integer order all solutions can be written as a linear sum of J_ν and $J_{-\nu}$ while for integer order all solutions can be written as a linear sum of J_n and Y_n, the Bessel functions of the first and second kind respectively.

Bessel used as definition of J_n [§2.2]:

$$J_n(z) = \int_0^{2\pi} \mathrm{d}\varphi \; \cos(n\varphi - z\sin\varphi) \qquad \text{(C.2)}$$

which Hankel has generalized to

$$J_n(z) = \int_\alpha^{2\pi+\alpha} \mathrm{d}\varphi \; \mathrm{e}^{\mathrm{i}(n\varphi - z\sin\varphi)} \qquad \text{(C.3)}$$

For general order the Bessel functions of the first kind can be defined by a series solution:

$$J_\nu(z) = \sum_{m=0}^\infty \frac{(-1)^m \left(\tfrac{1}{2}z\right)^{\nu+2m}}{m! \, \Gamma(\nu + m + 1)} \qquad \text{(C.4)}$$

These are the Bessel functions of the first kind. The Bessel functions of the second kind of integer order are all defined from the zeroth order Bessel function of the second kind Y_0 [§3.57]:

$$\frac{\pi}{2}Y_0(z) := Y^{(0)}(z) + (\gamma - \log 2)J_0(z) \tag{C.5}$$

where γ is Euler's constant, and $Y^{(0)}$ is Neumann's function of the second kind defined by

$$Y^{(0)}(z) := J_0(z)\log z - 2\sum_{n=1}^{\infty}\frac{(-1)^n J_{2n}(z)}{n} \tag{C.6}$$

The higher order Bessel functions can be found using the recurrence relations

$$J_{\nu-1}(z) + J_{\nu+1}(z) = \frac{2\nu}{z}J_\nu(z) \tag{C.7a}$$

$$J_{\nu-1}(z) - J_{\nu+1}(z) = 2J_\nu'(z) \tag{C.7b}$$

$$Y_{\nu-1}(z) + Y_{\nu+1}(z) = \frac{2\nu}{z}Y_\nu(z) \tag{C.7c}$$

$$Y_{\nu-1}(z) - Y_{\nu+1}(z) = 2Y_\nu'(z) \tag{C.7d}$$

The small z behaviour of $J_\nu(z)$ follows immediately from equation (C.4):

$$J_\nu(z) \approx \frac{(\frac{1}{2}z)^\nu}{\Gamma(\nu+1)} + \mathcal{O}(z^{\nu+2}) \tag{C.8}$$

and we therefore see that the negative order Bessel functions of non-integer order all diverge near the origin while the positive order Bessel functions all go to zero. The negative integer order Bessel functions are finite near the origin which follows from the original definition (C.2) given by Bessel. It is also clear from the fact that they are linearly dependent on the positive integer order Bessel functions:

$$J_n(-z) = (-1)^n J_n(z) \tag{C.9a}$$
$$J_{-n}(z) = (-1)^n J_n(z) \tag{C.9b}$$
$$Y_n(-z) = (-1)^n Y_n(z) \tag{C.9c}$$
$$Y_{-n}(z) = (-1)^n Y_n(z) \tag{C.9d}$$

These relations follow immediately from the relations in [§3.61] and [§3.62]. The Bessel functions of the second kind Y_ν all diverge near zero. For non-integer values of ν this follows from the relation connecting Y_ν with $J_{\pm\nu}$ [§3.61]:

$$Y_\nu(z) = \frac{J_\nu(z)\cos\nu\pi - J_{-\nu}(z)}{\sin\nu\pi} \tag{C.10}$$

For integer order we will determine the leading behaviour near zero in section C.2.

The large z asymptotic expansion of $J_\nu(z)$ [§7.21] is

$$
J_\nu(z) \approx \sqrt{\frac{2}{\pi z}} \left[\cos\left[z - \frac{\pi}{2}\left(\nu + \frac{1}{2}\right)\right] \sum_{m=0}^{\infty} \frac{(-1)^m \cdot (\nu, 2m)}{(2z)^{2m}} \right.
$$
$$
\left. - \sin\left[z - \frac{\pi}{2}\left(\nu + \frac{1}{2}\right)\right] \sum_{m=0}^{\infty} \frac{(-1)^m \cdot (\nu, 2m+1)}{(2z)^{2m+1}} \right] \qquad \text{(C.11)}
$$

where (ν, m) is defined using the Gamma function:

$$
(\nu, m) = \frac{\Gamma(\nu + m + \frac{1}{2})}{m! \, \Gamma(\nu - m + \frac{1}{2})}
$$

We end this section with the expansion of $\exp(-iz \cos\varphi)$ in terms of Bessel functions. According to Watson [§2.22]:

$$
e^{-iz \cos\varphi} = J_0(z) + \sum_{n=1}^{\infty} \left[e^{in(\frac{\pi}{2} - \varphi)}(-1)^n + e^{-in(\frac{\pi}{2} - \varphi)} \right] J_n(z)
$$
$$
= J_0(z) + \sum_{n=1}^{\infty} \left[e^{-in\frac{\pi}{2}} e^{-in\varphi} + e^{-in\frac{\pi}{2}} e^{in\varphi} \right] J_n(z)
$$
$$
= \sum_{n=-\infty}^{\infty} e^{-i\frac{\pi}{2}|n|} e^{in\varphi} J_{|n|}(z) \qquad \text{(C.12)}
$$

C.2   Some proofs

First we will prove that the Bessel functions of the second kind $Y_n(z)$ behave like

$$
Y_n(z) \approx \begin{cases} \frac{2}{\pi} \log z & \text{for } n = 0 \\ -\frac{2^n (n-1)!}{\pi z^n} & \text{for } n > 0 \end{cases} \qquad \text{(C.13)}
$$

For $n = 0$ we can use definitions (C.5) and (C.6) combined with the series expansion (C.4) from which it follows that $J_0(z) \log z \approx \log z$ is the only term in $Y_0(z)$ which diverges near zero. So the small z behaviour of Y_0 is determined by the first term in the Neumann function. The higher order behaviour can be found by adding the recursion relations (C.7c) and (C.7d):

$$
Y_{n+1}(z) = \frac{n}{z} Y_n(z) - Y_n' \qquad \text{(C.14)}
$$

For $n = 0$ we find

$$Y_1(z) = -Y_0'(z) \approx \left(-\frac{2}{\pi} \log z\right)' = -\frac{2}{\pi z} \tag{C.15}$$

which satisfies (C.13).

By induction it is now easy to prove the general formula.

We continue with the proof of relation (5.35). Instead of proving the relation directly we shall prove a much more general relation from which many similar relations can be derived:

$$\int_0^\infty \mathrm{d}z\, J_\nu(z)\mathrm{e}^{-\epsilon z} = \frac{1}{\sqrt{\epsilon^2 + 1}\left(\epsilon + \sqrt{\epsilon^2 + 1}\,\right)^\nu} \tag{C.16}$$

which is valid for if $\epsilon > 0$ and if $\mathrm{Re}(\nu) > -1$ or $\nu \in \mathbb{Z}$.

We shall prove it only for the special case $\nu \in \mathbb{Z}$. See also [§13.2] and reference [21]. Notice that this integral is *not* equal to

$$\int_0^\infty \mathrm{d}z\, \mathrm{e}^{-\epsilon z} \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\varphi\, \mathrm{e}^{\mathrm{i}(\nu\varphi - z\sin\varphi)} \tag{C.17}$$

since equation (C.3) is valid only for integer order.

The only integral we really need is the above integral for $n = 0$, which we will evaluate using Bessel's original definition (C.2)

$$J_0(z) = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\varphi\, \cos(z\sin\varphi) = \frac{1}{2\pi}\mathrm{Re}\int_0^{2\pi} \mathrm{d}\varphi\, \mathrm{e}^{-\mathrm{i}z\sin\varphi} \tag{C.18}$$

We see we have to calculate

$$\mathrm{Re}\left(\frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\varphi \int_0^\infty \mathrm{d}z\, \mathrm{e}^{-z(\epsilon + \mathrm{i}\sin\varphi)}\right) \tag{C.19}$$

The z-integral is easy to evaluate since its integrand is analytical:

$$\int_0^\infty \mathrm{d}z\, \mathrm{e}^{-z(\epsilon + \mathrm{i}\sin\varphi)} = -\left[\frac{\mathrm{e}^{-z(\epsilon + \mathrm{i}\sin\varphi)}}{\epsilon + \mathrm{i}\sin\varphi}\right]_0^\infty = \frac{1}{\epsilon + \mathrm{i}\sin\varphi} \tag{C.20}$$

where the factor $\exp(-\epsilon z)$ ensures the vanishing at the upper boundary.

We have therefore found

$$\int_0^\infty \mathrm{d}z\, J_0(z)\mathrm{e}^{-\epsilon z} = \mathrm{Re}\left(\frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\varphi\, \frac{1}{\epsilon + \mathrm{i}\sin\varphi}\right)$$

$$= \frac{\epsilon}{2\pi} \int_0^{2\pi} \mathrm{d}\varphi\, \frac{1}{\epsilon^2 + \sin^2\varphi} \tag{C.21}$$

Since the integrand is symmetrical under the substitution $\varphi \to \varphi + \pi$ we can also take the boundaries from 0 to π:

$$\frac{2\epsilon}{2\pi} \int_0^\pi \mathrm{d}\varphi \, \frac{1}{\epsilon^2 + \sin^2\varphi} = \frac{\epsilon}{\pi} \int_{-\pi/2}^{\pi/2} \mathrm{d}\varphi \, \frac{1}{\epsilon^2 + \cos^2\varphi} \tag{C.22}$$

By dividing the numerator and the denominator by $\cos^2\varphi$ we find:

$$\frac{\epsilon}{\pi} \int_{\varphi=-\pi/2}^{\pi/2} \frac{\mathrm{d}\tan\varphi}{\epsilon^2(1 + \tan^2\varphi) + 1} = \frac{1}{\pi} \frac{1}{\sqrt{\epsilon^2 + 1}} \int_{-\infty}^{\infty} \frac{\mathrm{d}u}{u^2 + 1}$$

$$= \frac{1}{\sqrt{\epsilon^2 + 1}} \left[\frac{\operatorname{atan} u}{\pi} \right]_{-\infty}^{\infty} = \frac{1}{\sqrt{\epsilon^2 + 1}} \tag{C.23}$$

where we have made the substitution $u = \frac{\epsilon}{\sqrt{\epsilon^2+1}} \tan\varphi$ in the first step.

To prove the general relation (C.16) (for integers) it will be convenient to introduce the notation

$$G_n(\epsilon) := \int_0^\infty \mathrm{d}z \, J_n(z)\mathrm{e}^{-\epsilon z} \tag{C.24}$$

Using the recursion relation (C.7b) we find

$$\frac{1}{2}\left[G_{n+1}(\epsilon) - G_{n-1}(\epsilon)\right] = -\int_0^\infty \mathrm{d}z \, J_n'(z)\mathrm{e}^{-\epsilon z}$$

$$= \underbrace{-\left[J_n(z)\mathrm{e}^{-\epsilon z}\right]_0^\infty}_{\delta_{0n}} - \epsilon \int_0^\infty \mathrm{d}z \, J_n(z)\mathrm{e}^{-\epsilon z}$$

$$= \delta_{0n} - \epsilon G_n(\epsilon) \tag{C.25}$$

It is clear from the definition of $G_n(\epsilon)$ that $G_{-n}(z) = (-1)^n G_n(z)$ and therefore

$$G_1(z) = G_1(z) - G_{-1}(z) = 1 - \epsilon G_0(z) =$$

$$1 - \frac{\epsilon}{\sqrt{\epsilon^2 + 1}} = \frac{\sqrt{\epsilon^2 + 1} - \epsilon}{\sqrt{\epsilon^2 + 1}} = \frac{1}{\sqrt{\epsilon^2 + 1}\left(\epsilon + \sqrt{\epsilon^2 + 1}\right)} \tag{C.26}$$

For general integer ν formula (C.16) can now be proven using induction from the recursion relation (C.25) combined with the expressions for $G_0(\epsilon)$ and $G_1(\epsilon)$.

Using this general formula (C.16) it is easy to derive a general expression for the important set of integrals

$$\int_0^\infty \mathrm{d}z \, z J_\nu(z)\mathrm{e}^{-\epsilon z} \tag{C.27}$$

by differentiating $G_\nu(\epsilon)$:

$$\int_0^\infty \mathrm{d}z \, z J_\nu(z) \mathrm{e}^{-\epsilon z} = -\frac{\mathrm{d}}{\mathrm{d}\epsilon} G_\nu(\epsilon) = \frac{1}{(\epsilon^2+1)^{3/2}} \frac{\epsilon + \nu\sqrt{\epsilon^2+1}}{\left(\epsilon + \sqrt{\epsilon^2+1}\right)^\nu} \tag{C.28}$$

It is clear that for $\nu = 1$ we find equation (5.35). Taking the limit of $\epsilon \downarrow 0$, we find the important relation

$$\lim_{\epsilon\downarrow 0} \int_0^\infty \mathrm{d}z \, z J_\nu(z) \mathrm{e}^{-\epsilon z} = \nu \tag{C.29}$$

By using the recursion relation (C.7a) we can also find expressions for another important set of integrals

$$\begin{aligned}
\int_0^\infty \mathrm{d}z \, \frac{J_\nu(z)}{z} \mathrm{e}^{-\epsilon z} &= \frac{1}{2\nu} \int_0^\infty \mathrm{d}z \, \left(J_{\nu-1}(z) + J_{\nu+1}(z) \right) \\
&= \frac{1}{2\nu} \left(G_{\nu-1}(\epsilon) + G_{\nu+1}(\epsilon) \right) \\
&= \frac{1}{2\nu} \frac{1}{\sqrt{\epsilon^2+1}\left(\epsilon + \sqrt{\epsilon^2+1}\right)^{\nu+1}} \underbrace{\left[\left(\epsilon + \sqrt{\epsilon^2+1}\right)^2 + 1 \right]}_{2\left[\sqrt{\epsilon^2+1}+\epsilon\right]\sqrt{\epsilon^2+1}} \\
&= \frac{1}{\nu} \frac{1}{\left(\epsilon + \sqrt{\epsilon^2+1}\right)^\nu} \tag{C.30}
\end{aligned}$$

It is clear that this integral diverges if $\nu = 0$.

We end this section with a derivation of a recursion relation for the most general form of all these integral expressions:

$$F_\nu^m := \lim_{\epsilon\downarrow 0} \int_0^\infty \mathrm{d}z \, J_\nu(z) \mathrm{e}^{-\epsilon z} z^m \tag{C.31}$$

Together with the previous results (C.16) and (C.27)

$$F_\nu^0 = 1 \tag{C.32a}$$
$$F_\nu^1 = \nu \tag{C.32b}$$

we can then find expressions for all ν and m. Since $J_\nu(z) \sim z^\nu$ for $\nu \notin \mathbb{Z}$ and $J_n(z) \sim z^{|n|}$ for $n \in \mathbb{Z}$ it is clear that we have the restrictions $\nu + m > -1$ $|n| + m > -1$. From the recursion relation (C.7a) it follows

$$\frac{1}{2}(F_{\nu-1}^m + F_{\nu+1}^m) = \nu F_\nu^{m-1} \tag{C.33}$$

and from relation (C.7b)

$$\frac{1}{2}(F_{\nu-1}^m - F_{\nu+1}^m) = \lim_{\epsilon \downarrow 0} \int_0^\infty \mathrm{d}z \; J_\nu'(z)\mathrm{e}^{-\epsilon z} z^m$$

$$= \lim_{\epsilon \downarrow 0} \left[J_\nu(z)\mathrm{e}^{-\epsilon z} z^m \Big|_0^\infty + \right.$$

$$\lim_{\epsilon \downarrow 0} \int_0^\infty \mathrm{d}z \; (\epsilon - \frac{m}{z}) J_\nu(z)\mathrm{e}^{-\epsilon z}$$

$$= -m F_\nu^{m-1} \qquad\qquad\qquad\qquad (C.34)$$

where the vanishing of the boundary term follows from the fact that we have
already taken $|\nu| > -m$. We have furthermore assumed that F_ν^m is finite so
that the first term - involving ϵ - in the remaining integral vanishes.
By adding and subtracting these two relations we find

$$F_{\nu-1}^m = (\nu - m)F_\nu^{m-1} \quad \Rightarrow \quad F_\nu^{m+1} = (\nu - m)F_{\nu+1}^m \qquad (C.35a)$$
$$F_{\nu+1}^m = (\nu + m)F_\nu^{m-1} \qquad\qquad\qquad\qquad\qquad\qquad (C.35b)$$

By combining these two relations we find

$$F_\nu^{m+1} = (\nu^2 - m^2)F_\nu^{m-1} \qquad\qquad\qquad (C.36)$$

which is valid as long as $|\nu| \geq -m$.

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