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1.1   Time evolution in Quantum mechanics

Time evolution in quantum mechanics is given by the Schrödinger equation

$$\hat{H}|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle. \tag{1}$$

The way we are used to solve this is to find a basis of eigenstates of the Hamiltonian, i.e. to solve the equation

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle. \tag{2}$$

Each of these states evolve very simply with time since

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle = E_n|\psi_n\rangle, \tag{3}$$

so that

$$|\psi_n(t)\rangle = e^{-\frac{i}{\hbar}E_n t}|\psi_n\rangle. \tag{4}$$

Since $|\psi_n\rangle$ is a complete basis, we can express any wave function as a linear combination of the $|\psi_n\rangle$ states

$$|\psi\rangle = \sum_n c_n|\psi_n\rangle, \tag{5}$$

and since we know how each of the basis states evolve in time, we know the full time evolution

$$|\psi(t)\rangle = \sum_n c_n e^{-\frac{i}{\hbar}E_n t}|\psi_n\rangle. \tag{6}$$

This method is not always possible to use however. For instance, if the Hamiltonian itself $\hat{H}(t)$ depends on time we cannot solve equation (2) and we will have to find a different method. It is also possible that this method does not give the simplest description of time evolution. For instance if the initial wave function is very different from the base states.

Let us now look for a more general solution to (1). Infinitesimally we may write it as

$$\hat{H}(t)|\psi(t)\rangle = i\hbar\frac{|\psi(t + \Delta t)\rangle - |\psi(t)\rangle}{\Delta t}. \tag{7}$$

Or, turning it around

$$|\psi(t + \Delta t)\rangle = |\psi(t)\rangle - \frac{i}{\hbar}\hat{H}(t)\Delta t|\psi(t)\rangle = \left(1 - \frac{i}{\hbar}\hat{H}(t)\Delta t\right)|\psi(t)\rangle. \tag{8}$$

We see that we may define an operator

$$\hat{U}(t + \Delta t, t) = 1 - \frac{i}{\hbar}\hat{H}(t)\Delta t, \tag{9}$$

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which evolves arbitrary wave functions from time t to time $t+\Delta t$. Notice that the only approximation we made was to assume that the time increment was infinitesimal. In particular, the Hamiltonian was arbitrary. We can observe that

$$\lim_{\Delta t \to 0} \hat{U}(t + \Delta t, t) = 1, \tag{10}$$

so that the time evolution is continuous. We also see that $\hat{U}$ is a unitary operator. That is, $\hat{U}^\dagger \hat{U} = \hat{U}\hat{U}^\dagger = 1$ (to lowest order in Δt). This has to be since we do not want that probability density is lost in the time evolution (that is, independently of what the physical situation is and what the particle does, the probability of finding it anywhere in space should always be one). Mathematically we write this as

$$1 = \langle \psi(\mathrm{t} + \Delta \mathrm{t}) | \psi(\mathrm{t} + \Delta \mathrm{t}) \rangle = \langle \psi(\mathrm{t}) | \hat{U}^\dagger U | \psi(\mathrm{t}) \rangle. \tag{11}$$

We can rewrite $\hat{U}$ in such a way that the unitarity becomes manifest. Namely, for the infinitesimal time evolution we have

$$\hat{U}(t + \Delta t, t) = 1 - \frac{i}{\hbar}\hat{H}(t)\Delta t \approx e^{-\frac{i}{\hbar}\hat{H}(t)\Delta t}. \tag{12}$$

This is manifestly unitary since $\hat{H}$ is hermitian. This we will take as the definition of the infinitesimal time evolution operator. To be able to handle arbitrary time evolutions we will use that any arbitrary time interval can be divided into infinitesimal pieces. We therefore define the arbitrary time evolution operator $\hat{U}(t', t)$ by dividing the time interval $t' - t$ into N pieces. Letting N go to infinity makes the intervals arbitrarily small so in each interval the time evolution operator can be taken in its infinitesimal form. Thus we get:

$$\begin{aligned}
\hat{U}(t', t) &= \lim_{N \to \infty} \hat{U}(t', t_{N-1})\hat{U}(t_{N-1}, t_{N-2}) \ldots \hat{U}(t_2, t_1)\hat{U}(t_1, t), \tag{13} \\
t_i &= t + \frac{t' - t}{N}i,
\end{aligned}$$

and this is the most general definition of the time evolution operator. It works for arbitrary Hamiltonians and in the following we will evaluate it in various special cases where it simplifies.

The problem of taking the product in (13) is the fact that the $\hat{H}$ operator appearing in each $\hat{U}$ is taken at a different time. If the Hamiltonians at

different times do not commute we cannot perform the product of the $\hat{U}$ operators in a simple form. A good exercise to see why this is so is to try to derive the Baker-Campbell-Hausdorff formula for two operators $\hat{A}$ and $\hat{B}$

$$e^{\hat{A}}e^{\hat{B}} = e^{\hat{A}+\hat{B}+\frac{1}{2}[\hat{A},\hat{B}]+\frac{1}{12}[\hat{A},[\hat{A},\hat{B}]]+\frac{1}{12}[[\hat{A},\hat{B}]\hat{B}]+\cdots}. \tag{14}$$

Only in the special case where the Hamiltonians at different times commute with themselves can we simplify the expression (13) for $\hat{U}$ as follows

$$
\begin{aligned}
\hat{U}(t',t) &= \lim_{N\to\infty} e^{-\frac{i}{\hbar}\hat{H}(t_{N-1})\Delta t - \frac{i}{\hbar}\hat{H}(t_{N-2})\Delta t - \ldots - \frac{i}{\hbar}\hat{H}(t_1)\Delta t - \frac{i}{\hbar}\hat{H}(t)\Delta t} \\
&= e^{-\frac{i}{\hbar}\int_t^{t'} ds\, \hat{H}(s)}.
\end{aligned}
\tag{15}
$$

This is such a nice and compact form that one would like to use it for the general case. This we can do if we define a new operator T called the *time ordering operator*. T acting on a product of operators always reorders them so that operators evaluated at earlier times stands to the right of operators evaluated at later times. Using T we can write the general expression for $\hat{U}$ as

$$\hat{U}(t',t) = T\left[e^{-\frac{i}{\hbar}\int_t^{t'} ds\, \hat{H}(s)}\right]. \tag{16}$$

The appearance of $T[\star]$ in this expression tells us that we have to write $\hat{U}$ in such a way that all operators taken at earlier times are written to the right of operators at later times, just as is manifestly done in the original definition (13).

1.2   The propagator

Now let us try to use the time evolution operator in some specific cases. The wave function at arbitrary time t is given by

$$|\psi(\mathrm{t})\rangle = \hat{U}(t,t')|\psi(\mathrm{t}')\rangle \tag{17}$$

In coordinate representation this looks like

$$
\begin{aligned}
\psi(\mathbf{x},t) &= \langle\mathbf{x}|\psi(\mathrm{t})\rangle = \langle\mathbf{x}|\hat{U}(t,t')|\psi(\mathrm{t}')\rangle \\
&= \int d^3\mathbf{x}'\, \langle\mathbf{x}|\hat{U}(t,t')|\mathbf{x}'\rangle\, \langle\mathbf{x}'|\psi(\mathrm{t}')\rangle \\
&= \int d^3\mathbf{x}'\, K(\mathbf{x},t;\mathbf{x}',t')\, \psi(\mathbf{x}',t'),
\end{aligned}
\tag{18}
$$

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where we have inserted 1 in the form $\int d^3\mathbf{x}'|\mathbf{x}'\rangle\langle\mathbf{x}'|$ and defined the configuration space *propagator*

$$K(\mathbf{x}, t; \mathbf{x}', t') = \langle\mathbf{x}|\hat{U}(t, t')|\mathbf{x}'\rangle. \tag{19}$$

The name propagator is chosen because $K(\mathbf{x}, t; \mathbf{x}', t')$ takes the wave function at time t' and *propagates* it to time t and space point $\mathbf{x}$. It works very much like in electrodynamics where we can use the knowledge of the potential (and its normal derivative) on the border of a region to find the potential everywhere in this region with the help of a Green function. In our case the border is the space time surface at t', the potential is the wave function and the Green function is the propagator. We shall see later that this is no coincidence, K is indeed the Green function for the Schrödinger operator.

In the special case where the initial wave function is completely localized at a point, $\psi(\mathbf{x}', t') = \delta^{(3)}(\mathbf{x}' - \mathbf{x}_0)$ we have

$$\psi(\mathbf{x}, t) = \int d^3\mathbf{x}' \; K(\mathbf{x}, t; \mathbf{x}', t') \; \delta^{(3)}(\mathbf{x}' - \mathbf{x}_0) = K(\mathbf{x}, t; \mathbf{x}_0, t'), \tag{20}$$

so we see that a direct physical interpretation of the propagator is that it is the wave function of a particle which was completely localized at the initial time.

Since the propagator has the interpretation as a wave function, it has to fulfill the Schrödinger equation. This we now prove in the special case that the Hamiltonian has the form

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}}) \tag{21}$$

First we notice that for infinitesimal Δt

$$K(\mathbf{x}, t + \Delta t; \mathbf{x}', t') = \langle\mathbf{x}|\hat{U}(t + \Delta t, t')|\mathbf{x}'\rangle = \langle\mathbf{x}|\hat{U}(t + \Delta t, t)\hat{U}(t, t')|\mathbf{x}'\rangle. \tag{22}$$

Since the leftmost time evolution operator is infinitesimal, we know how to evaluate it

$$\hat{U}(t + \Delta t, t) = 1 - \frac{i}{\hbar}\hat{H}(t)\Delta t. \tag{23}$$

Inserting the identity operator we have

$$\begin{aligned}
K(\mathbf{x}, t + \Delta t; \mathbf{x}', t') &= \int d^3\mathbf{y} \; \langle\mathbf{x}|1 - \frac{i}{\hbar}\hat{H}(t)\Delta t|\mathbf{y}\rangle \; \langle\mathbf{y}|\hat{U}(t, t')|\mathbf{x}'\rangle \\
&= \int d^3\mathbf{y} \; \langle\mathbf{x}|1 - \frac{i}{\hbar}\hat{H}(t)\Delta t|\mathbf{y}\rangle \; K(\mathbf{y}, t; \mathbf{x}', t'). \tag{24}
\end{aligned}$$

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Using the explicit form of the Hamiltonian we can compute

$$\langle \mathbf{x}|\hat{H}|\mathbf{y}\rangle = -\frac{\hbar^2}{2m}(\nabla_y)^2 \delta^{(3)}(\mathbf{x}-\mathbf{y}) + V(\mathbf{y})\delta^{(3)}(\mathbf{x}-\mathbf{y}), \qquad (25)$$

where we have use the fact that

$$\begin{aligned}
\langle \mathbf{x}|\hat{\mathbf{x}}|\mathbf{y}\rangle &= \mathbf{x}\delta^{(3)}(\mathbf{x}-\mathbf{y}) = \mathbf{y}\delta^{(3)}(\mathbf{x}-\mathbf{y}), \\
\langle \mathbf{x}|\hat{\mathbf{p}}|\mathbf{y}\rangle &= -i\hbar\nabla_x \delta^{(3)}(\mathbf{x}-\mathbf{y}) = i\hbar\nabla_y \delta^{(3)}(\mathbf{x}-\mathbf{y}).
\end{aligned} \qquad (26)$$

Inserting this we get

$$K(\mathbf{x},t+\Delta t;\mathbf{x}',t') = \int d^3\mathbf{y}\, \delta^{(3)}(\mathbf{x}-\mathbf{y})\, K(\mathbf{y},t;\mathbf{x}',t')$$

$$-\frac{i}{\hbar}\Delta t \int d^3\mathbf{y}\left(-\frac{\hbar^2}{2m}(\nabla_y)^2 \delta^{(3)}(\mathbf{x}-\mathbf{y}) + V(\mathbf{y})\delta^{(3)}(\mathbf{x}-\mathbf{y})\right)\, K(\mathbf{y},t;\mathbf{x}',t'). \,(27)$$

After integrating by parts we can use the delta functions to perform the integral

$$\begin{aligned}
K(\mathbf{x},t+\Delta t;\mathbf{x}',t') &= K(\mathbf{x},t;\mathbf{x}',t') \\
&\quad - \frac{i}{\hbar}\Delta t\left(-\frac{\hbar^2}{2m}(\nabla_x)^2 + V(\mathbf{x})\right) K(\mathbf{x},t;\mathbf{x}',t'), \quad (28)
\end{aligned}$$

or, reshuffling the terms a little bit

$$\frac{i\hbar}{\Delta t}\left(K(\mathbf{x},t+\Delta t;\mathbf{x}',t') - K(\mathbf{x},t;\mathbf{x}',t')\right) = \left(-\frac{\hbar^2}{2m}(\nabla_x)^2 + V(\mathbf{x})\right) K(\mathbf{x},t;\mathbf{x}',t'),(29)$$

which for infinitesimal Δt is the same as

$$i\hbar\frac{\partial}{\partial t}K(\mathbf{x},t;\mathbf{x}',t') = \left(-\frac{\hbar^2}{2m}(\nabla_x)^2 + V(\mathbf{x})\right) K(\mathbf{x},t;\mathbf{x}',t'), \qquad (30)$$

in which we recognize the Schrödinger equation as we set out to show above. We therefore see that $K(\mathbf{x},t;\mathbf{x}',t')$ is a solution to the Schrödinger equation with boundary conditions

$$\lim_{t\to t'} K(\mathbf{x},t;\mathbf{x}',t') = \delta^{(3)}(\mathbf{x}-\mathbf{x}'). \qquad (31)$$

If we require that the propagator should be zero if $t < t'$ (there is no evolution *backwards* in time) we can define it as

$$\tilde{K}(\mathbf{x},t;\mathbf{x}',t') = K(\mathbf{x},t;\mathbf{x}',t')\Theta(t-t'), \qquad (32)$$

where Θ is a step function. This new $\tilde{K}$ satisfies the equation

$$
\begin{aligned}
\left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)\tilde{K}(\mathbf{x},t;\mathbf{x}',t') &= \left[\left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)K(\mathbf{x},t;\mathbf{x}',t')\right]\Theta(t-t') \\
&+ K(\mathbf{x},t;\mathbf{x}',t')\, i\hbar\frac{\partial}{\partial t}\Theta(t-t') \\
&= i\hbar K(\mathbf{x},t;\mathbf{x}',t')\delta(t-t') \\
&= i\hbar\delta^{(3)}(\mathbf{x}-\mathbf{x}')\delta(t-t'),
\end{aligned}
\tag{33}
$$

where we used that fact that the derivative of the step function is a delta function and that K evaluated at zero time-step is a delta function in space. This shows that $\tilde{K}$ is indeed a Green function of the Schrödinger differential operator $i\hbar\frac{\partial}{\partial t} - \hat{H}$.

As an illustration, let us evaluate the propagator for the one dimensional free particle. From the definition we have

$$
K(x,t;x',t') = \langle \mathrm{x}|T\left[e^{-\frac{i}{\hbar}\int_{t'}^{t} ds\hat{H}(s)}\right]|\mathrm{x}'\rangle,
\tag{34}
$$

where now $\hat{H}$ is the Hamiltonian for a free particle $\hat{H} = \frac{\hat{p}^2}{2m}$. Since this Hamiltonian does not depend on time it commutes with itself for all times. That means that the T operator acts trivially and that the integral in the exponential can be written $\int_{t'}^{t} ds\hat{H}(s) = (t-t')\hat{H}$. Since the Hamiltonian contains $\hat{p}$ it is useful to insert a complete set of momentum eigenstates

$$
\begin{aligned}
K(x,t;x',t') &= \int_{-\infty}^{\infty} dp\, \langle \mathrm{x}|e^{-\frac{i}{\hbar}\hat{H}(t-t')}|\mathrm{p}\rangle\, \langle \mathrm{p}|\mathrm{x}'\rangle \\
&= \int_{-\infty}^{\infty} dp\, e^{-\frac{i}{\hbar}(t-t')\frac{p^2}{2m}}\, \langle \mathrm{x}|\mathrm{p}\rangle\, \langle \mathrm{p}|\mathrm{x}'\rangle,
\end{aligned}
\tag{35}
$$

and using the explicit form of the wave function $\langle \mathrm{x}|\mathrm{p}\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}px}$ we get

$$
K(x,t;x',t') = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar}\, e^{-\frac{i}{\hbar}(t-t')\frac{p^2}{2m}+\frac{i}{\hbar}p(x-x')}.
\tag{36}
$$

The integral over p is not really well defined since the integrand does not fall off for large p. It is possible to define it correctly mathematically in various ways. For instance, we can make the integral convergent by defining

$$
K_{\mathrm{new}}(x,t;x',t') = \lim_{\epsilon\to 0} K_{\mathrm{old}}(x,t-i\epsilon;x',t').
\tag{37}
$$

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For each non-zero ϵ the integrand falls off like a Gaussian so the integral is convergent and gives us

$$K(x, t - i\epsilon; x', t') = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \ e^{-\frac{\epsilon}{2m\hbar}p^2 - \frac{i}{\hbar}(t-t')\frac{p^2}{2m} + \frac{i}{\hbar}p(x-x')}$$

$$= e^{-\frac{m(x-x')^2}{2\hbar(i(t-t')+2m\epsilon)}} \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} \ e^{-\frac{i(t-t')+2m\epsilon}{2m\hbar}\left(p - i\frac{m(x-x')}{i(t-t')+2m\epsilon}\right)^2}. \quad (38)$$

Shifting the integration variable p gives a Gaussian integral of the type

$$\int_{-\infty}^{\infty} dx e^{-ax^2} = \sqrt{\frac{\pi}{a}}, \quad (39)$$

and using this we finally have

$$K(x, t - i\epsilon; x', t') = \sqrt{\frac{m}{2\pi\hbar(i(t - t') + 2m\epsilon)}} e^{-\frac{m(x-x')^2}{2\hbar(i(t-t')+2m\epsilon)}}. \quad (40)$$

In this expression we can without worries take the limit $\epsilon \to 0$ to get the configuration space propagator for the one dimensional free particle

$$K(x, t; x', t') = \sqrt{\frac{m}{2\pi i\hbar(t - t')}} e^{\frac{im(x-x')^2}{2\hbar(t-t')}}. \quad (41)$$

It is interesting to try to interpret this propagator physically since we know that $K(x, t, ; 0, 0)$ should be the wave function for a particle which at $t = 0$ was completely localized at $x = 0$. Since $|K(x, t; 0, 0)|^2$ is the same everywhere in space it means that at any instant after $t = 0$ the probability to find the particle anywhere in space is the same!! This can be understood since in non-relativistic physics there is no maximum velocity. When we try to localize a particle we need to use waves of all possible momenta, even infinitely high. These wave will of course propagate arbitrarily far in infinitesimal time giving us the above result. In relativistic quantum mechanics the propagator is modified in such a way that nothing can propagate faster than light so that the probability density is always zero outside the light cone.

1.3 The propagator as a Green function

Well, if the propagator is a Green function we must be able to calculate it using standard methods. We now illustrate this on exactly the same problem

as in the previous section, namely the configuration space propagator for the one dimensional free particle. The general equation for the Green function of an operator gives

$$\left(i\hbar\frac{\partial}{\partial t} - \hat{H}\right)K(x,t;0,0) = i\hbar\delta(x)\delta(t), \tag{42}$$

where we have put x' and t' to zero without loss of generality. In our case we have to choose the Hamiltonian $\hat{H} = -\frac{\hbar^2\partial_x^2}{2m}$ so we have

$$\left(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2\partial_x^2}{2m}\right)K(x,t;0,0) = i\hbar\delta(x)\delta(t). \tag{43}$$

Such equations are very nicely solved using Fourier transforms. Namely, write the Fourier transform of $K(x,t)$ as $L(k,\omega)$ such that

$$K(x,t) = \int \frac{dk\,d\omega}{(2\pi)^2}L(k,\omega)e^{ikx-i\omega t}, \tag{44}$$

we can write the left hand side of (43) as

$$\left(i\hbar\frac{\partial}{\partial t} + \frac{\hbar^2\partial_x^2}{2m}\right)\int \frac{dk\,d\omega}{(2\pi)^2}L(k,\omega)\,e^{ikx-i\omega t} \tag{45}$$

$$= \int \frac{dk\,d\omega}{(2\pi)^2}\left(\hbar\omega - \frac{\hbar^2k^2}{2m}\right)L(k,\omega)\,e^{ikx-i\omega t}. \tag{46}$$

Using that we know how the Fourier transform of a delta function looks like $(\delta(t) = \int \frac{d\omega}{2\pi}e^{-i\omega t})$ we can then write the right hand side of (43) as

$$i\hbar\int \frac{dk\,d\omega}{(2\pi)^2}e^{ikx-i\omega t}. \tag{47}$$

We see that the two sides are equal if and only if

$$\left(\hbar\omega - \frac{\hbar^2k^2}{2m}\right)L(k,\omega) = i\hbar, \tag{48}$$

or, if you wish

$$L(k,\omega) = \frac{i\hbar}{\hbar\omega - \frac{\hbar^2k^2}{2m}}. \tag{49}$$

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Well, now we have $L(k, \omega)$ but since it is just the Fourier transform of $K(x, t)$ we just need to transform back to get $K(x, t)$. That should be a piece of cake! Let us try. Using (44) we can write

$$K(x, t) = \int \frac{dk \, d\omega}{(2\pi)^2} \frac{i\hbar}{\hbar\omega - \frac{\hbar^2 k^2}{2m}} e^{ikx - i\omega t}$$
$$= \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \left(\int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{-1}{\omega - \frac{\hbar k^2}{2m}} e^{-i\omega t} \right). \tag{50}$$

We will do the integral over ω using contour methods.

In order to be able to write the integral as a sum over residues, using the Cauchy theorem, we need to have a closed contour. This we get by closing the contour either with a half circle in the upper half plane or with a half circle in the lower half plane as shown in picture 1 We can then write the

Figure 1: The possible contours

closed contour I as the sum of the integral in which we are interested I_1 and the integral over the half circle I_2 (or I_2'). Since I is given by the integral around a closed contour it can be calculated simply as the sum over the residues of the poles enclosed by the contour. Then we have $I_1 = I - I_2$ and since we will now show that $I_2 = 0$ we in fact have that $I_1 = I$.

To show that $I_2 = 0$ we need to estimate the integral. The contour is over values of ω with $|\omega|$ constant and large (going to infinity even). $\arg(\omega)$ varies between 0 and π for I_2 and 0 and $-\pi$ for I_2'. To make the estimate for

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this contour we write

$$
\begin{aligned}
\left| \frac{1}{\omega - \frac{\hbar k^2}{2m}} \right| &\approx \frac{1}{|\omega|} + \mathcal{O}\left(\frac{1}{|\omega|^2} \right), \\
\left| e^{-i\omega t} \right| &= \left| e^{-i|\omega|(\cos\theta + i\sin\theta)t} \right| = \left| e^{|\omega| t \sin\theta} \right|, \\
d\omega &= \omega i \, d\theta,
\end{aligned}
\tag{51}
$$

which means that we can estimate the integral as

$$
\int_{C_2} \frac{d\omega}{2\pi i} \frac{1}{\omega - \frac{\hbar k^2}{2m}} e^{-i\omega t} \leq \int \frac{d\theta}{2\pi i} \frac{|\omega|}{|\omega|} e^{|\omega| t \sin\theta}.
\tag{52}
$$

Notice that $|\omega|$ is really a constant all through the calculation. Furthermore, this constant we will take to infinity (corresponding to an infinitely large half circle). The integrand is therefore very much suppressed if we choose θ so that $|\omega| t \sin(\theta) < 0$. In other words, for $t > 0$ we have to choose $-\pi \leq \theta \leq 0$ corresponding to I_2' and for $t < 0$ we have to choose $0 \leq \theta \leq \pi$ corresponding to I_2.

There is one more problem with the integral I_1 which we skipped over in the previous discussion. Namely, there is a pole (singularity) of the integrand for $\omega = \frac{\hbar k^2}{2m}$. The usual way to avoid this problem is to let the integration contour pass the singularity in a small circle. But there are two ways we can do this. Either above or below. Which is the correct way? Physics will have to tell us. Namely, from the four possible contours in figure 2 we see immediately that two of them are zero (since they do not enclose any poles). If we choose to shift the contour down we get a result which is non-zero only for $t < 0$ (this is not what we want, it would mean propagation only backwards in time) but if we choose to shift the contour up we get a result which is non-zero only for $t > 0$ (which is exactly what we want since this is how we defined the Green function in the first place). The fact that physics tells us that we always have to shift the contour up can be nicely encoded in the way we write the momentum space propagator. Namely, write

$$
L(k, \omega) = \frac{i}{\omega - \frac{\hbar k^2}{2m} + i\epsilon},
\tag{53}
$$

where ϵ is an arbitrary small real number which we always let go to zero after the calculation. The fact that ϵ appears shifts the location of the pole from

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Figure 2: All possible contours

$\omega = \frac{\hbar k^2}{2m}$ to $\omega = \frac{\hbar k^2}{2m} - i\epsilon$ which means that the contour will not meet the pole and will naturally pass over it.

Finally, let us perform the integral in the case $t > 0$ which means that we have to choose to close the contour in the lower half plane so that there will be an extra minus from the clockwise orientation of the contour

$$-\int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{1}{\omega - \frac{\hbar k^2}{2m} + i\epsilon} e^{i\omega t} = -\oint \frac{d\omega}{2\pi i} \frac{1}{\omega - \frac{\hbar k^2}{2m} + i\epsilon} e^{i\omega t} =$$

$$\lim_{\epsilon \to 0} e^{-i\left(\frac{\hbar k^2}{2m} - i\epsilon\right)t} = e^{-\frac{i}{\hbar}\frac{\hbar^2 k^2}{2m} t}, \tag{54}$$

and inserting this in (50) we get

$$K(x,t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} e^{-\frac{i}{\hbar}\frac{\hbar^2 k^2}{2m} t} = \{p = \hbar k\} = \int_{-\infty}^{\infty} \frac{dp}{2\pi\hbar} e^{\frac{i}{\hbar} px} e^{-\frac{i}{\hbar}\frac{p^2}{2m} t}, \tag{55}$$

in which we recognize (36) which is indeed the expression for the one dimensional propagator that we derived independently in the previous section.

1.4 The spreading of a wave packet

Let us now try to calculate a more physical example using the one-dimensional free particle propagator. We saw previously that the sharply localized particle will spread out over all space infinitely fast. What about the perhaps more physical case where the initial particle (at time $t = 0$ say) is "smoothly" localized by a Gaussian "blob"

$$\psi_i(x, t = 0) = \left(\frac{2}{\pi}\right)^{\frac{1}{4}} e^{-x^2}. \tag{56}$$

The wave function at any later time is now given by

$$\psi(x, t) = \int dx' K(x, t; x', t' = 0)\psi_i(x'), \tag{57}$$

where $K(x, t; x', t')$ is the propagator for the physical situation we are interested in (in our case the free one-dimensional particle). Introducing the notation $\alpha = \frac{m}{2\hbar t}$ we write

$$\psi(x, t) = \left(\frac{2}{\pi}\right)^{\frac{1}{4}} \int dx' \sqrt{\frac{\alpha}{i\pi}} e^{i\alpha(x-x')^2} e^{-x'^2} =$$

$$\left(\frac{2}{\pi}\right)^{\frac{1}{4}} \sqrt{\frac{\alpha}{i\pi}} e^{i\alpha x^2} \int dx' e^{-(1-i\alpha)\left[x'^2 + \frac{2i\alpha}{1-i\alpha}xx'\right]}, \tag{58}$$

which, completing the squares in the exponential becomes

$$\psi(x, t) = \left(\frac{2}{\pi}\right)^{\frac{1}{4}} \sqrt{\frac{\alpha}{i\pi}} e^{i\alpha x^2} \int dx' e^{-(1-i\alpha)\left[(x' + \frac{i\alpha}{1-i\alpha}x)^2 + \frac{\alpha^2 x^2}{(1-i\alpha)^2}\right]}. \tag{59}$$

Shifting the integration variable $\tilde{x} = x' + \frac{i\alpha}{1-i\alpha}x$ we can perform the integration with the result

$$\psi(x, t) = \left(\frac{2}{\pi}\right)^{\frac{1}{4}} \sqrt{\frac{\alpha}{i\pi}} \sqrt{\frac{\pi}{1 - i\alpha}} e^{i\alpha x^2} e^{\frac{\alpha^2 x^2}{(1-i\alpha)^2}} =$$

$$\left(\frac{2}{\pi}\right)^{\frac{1}{4}} \sqrt{\frac{i\alpha}{i\alpha - 1}} e^{-\frac{i\alpha}{i\alpha - 1}x^2}, \tag{60}$$

which gives us the probability density

$$\rho = |\psi(x, t)|^2 = \sqrt{\frac{2\alpha^2}{\pi(1 + \alpha^2)}} e^{-\frac{2\alpha^2}{1+\alpha^2}x^2}. \tag{61}$$

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This is a normalized Gaussian of width $\sqrt{\frac{1+\alpha^2}{2\alpha^2}} = \sqrt{\frac{m^2+(2\hbar t)^2}{2m^2}}$. Taking the limit $t \to 0$ we get back the initial wave-function as we should but for large t we see that the width increases linearly with t so that the Gaussian wave-packet is smoothly spreading with time in correspondence with our intuition about this physical situation.

1.5 The path integral

The method we used to calculate the propagator in the free particle case was to insert a complete set of momentum eigenstates to turn the Hamiltonian operator into an ordinary function. However, this will work only for Hamiltonians depending on momenta *only*. For instance, if we try to use it in the case of a Hamiltonian of the form $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$ we have

$$\langle \mathrm{x}|e^{-\frac{i}{\hbar}t\hat{H}}|\mathrm{x}'\rangle = \int dp \langle \mathrm{x}|e^{-\frac{i}{\hbar}t\hat{H}}|\mathrm{p}\rangle\langle \mathrm{p}|\mathrm{x}'\rangle, \tag{62}$$

but now

$$\langle \mathrm{x}|e^{-\frac{i}{\hbar}t\hat{H}}|\mathrm{p}\rangle \neq e^{-\frac{i}{\hbar}t(\frac{p^2}{2m}+V(x))}\langle \mathrm{x}|\mathrm{p}\rangle. \tag{63}$$

I repeat: the left hand side and right hand side of the above equation *are not equal to each other*. To see this explicitly, try to evaluate the first few terms in a series expansion of the exponential on both sides (for the simple Hamiltonian $\hat{H} = \hat{p}^2 + \hat{x}^2$ for example). You will see that the problem is that the $\hat{p}^2$ part of the Hamiltonian does not commute with the $\hat{x}^2$ part. You will also see that the problem will appear at the quadratic (and higher) term in the expansion.

We therefore have to find some different way to calculate the propagator when the Hamiltonian is more complicated than the free particle. Instead, let us try to compute it for an infinitesimal time step. As before, the general case we can always get by putting together infinitely many infinitesimal steps. In the infinitesimal case we have

$$\langle \mathbf{x}|e^{-\frac{i}{\hbar}\hat{H}\Delta t}|\mathbf{x}'\rangle \approx \langle \mathbf{x}|\left(1 - \frac{i}{\hbar}\Delta t\hat{H}\right)|\mathbf{x}'\rangle. \tag{64}$$

Inserting a complete set of momentum eigenstates now is non problematic

$$K(\mathbf{x}, t+\Delta t; \mathbf{x}', t) = \tag{65}$$
$$\int d^3\mathbf{p} \left(\langle \mathbf{x}|\mathbf{p}\rangle\langle \mathbf{p}|\mathbf{x}'\rangle - \frac{i}{\hbar}\Delta t \langle \mathbf{x}|\frac{\hat{\mathbf{p}}^2}{2m}|\mathbf{p}\rangle\langle \mathbf{p}|\mathbf{x}'\rangle - \frac{i}{\hbar}\Delta t \langle \mathbf{x}|V(\hat{\mathbf{x}})|\mathbf{p}\rangle\langle \mathbf{p}|\mathbf{x}'\rangle \right),$$

giving us the result

$$K(\mathbf{x}, t + \Delta t; \mathbf{x}', t) = \tag{66}$$
$$\int d^3\mathbf{p} \left(1 - \frac{i}{\hbar}\Delta t \frac{\mathbf{p}^2}{2m} - \frac{i}{\hbar}\Delta t V(\mathbf{x})\right) \langle \mathbf{x}|\mathbf{p}\rangle\langle \mathbf{p}|\mathbf{x}'\rangle,$$

where now all the operators have been replaces by numbers. Notice that the last term can be rewritten

$$\int d^3\mathbf{p}\langle \mathbf{x}|V(\hat{\mathbf{x}})|\mathbf{p}\rangle\langle \mathbf{p}|\mathbf{x}'\rangle = \int d^3\mathbf{p}\langle \mathbf{x}|\mathbf{p}\rangle\langle \mathbf{p}|V(\hat{\mathbf{x}})|\mathbf{x}'\rangle, \tag{67}$$

giving us the possibility to write

$$K(\mathbf{x}, t + \Delta t; \mathbf{x}', t) = \tag{68}$$
$$\int d^3\mathbf{p} \left(1 - \frac{i}{\hbar}\Delta t \frac{\mathbf{p}^2}{2m} - \frac{i}{\hbar}\Delta t V(\mathbf{x})\right) \langle \mathbf{x}|\mathbf{p}\rangle\langle \mathbf{p}|\mathbf{x}'\rangle =$$
$$\int d^3\mathbf{p} \left(1 - \frac{i}{\hbar}\Delta t \frac{\mathbf{p}^2}{2m} - \frac{i}{\hbar}\Delta t V(\mathbf{x}')\right) \langle \mathbf{x}|\mathbf{p}\rangle\langle \mathbf{p}|\mathbf{x}'\rangle =$$
$$\int d^3\mathbf{p} \left(1 - \frac{i}{\hbar}\Delta t \frac{\mathbf{p}^2}{2m} - \frac{i}{\hbar}\Delta t V\left(\frac{\mathbf{x} + \mathbf{x}'}{2}\right)\right) \langle \mathbf{x}|\mathbf{p}\rangle\langle \mathbf{p}|\mathbf{x}'\rangle. \tag{69}$$

Again, to linear order in Δt we can write this as

$$K(\mathbf{x}, t + \Delta t; \mathbf{x}', t) = \int d^3\mathbf{p}\ e^{-\frac{i}{\hbar}\Delta t\left(\frac{\mathbf{p}^2}{2m} + V\left(\frac{\mathbf{x}+\mathbf{x}'}{2}\right)\right)} \langle \mathbf{x}|\mathbf{p}\rangle\langle \mathbf{p}|\mathbf{x}'\rangle = \tag{70}$$
$$\int d^3\mathbf{p}\ e^{-\frac{i}{\hbar}H\Delta t}\langle \mathbf{x}|\mathbf{p}\rangle\langle \mathbf{p}|\mathbf{x}'\rangle, \tag{71}$$

where now H is a number and not an operator. Inserting the expression for the wave functions we get

$$K(\mathbf{x}, t + \Delta t; \mathbf{x}', t) = \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3}\ e^{\frac{i}{\hbar}\Delta t\left(\frac{\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')}{\Delta t} - H\right)}. \tag{72}$$

Now remember that $\mathbf{x}$ is the position at time $t + \Delta t$ and that $\mathbf{x}'$ is the position at time t. This means that we can write

$$\frac{\mathbf{x} - \mathbf{x}'}{\Delta t} \approx \frac{d\mathbf{x}(t)}{dt}, \tag{73}$$

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giving us the expression for the infinitesimal propagator

$$K(\mathbf{x}, t + \Delta t; \mathbf{x}', t) = \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3} \, e^{\frac{i}{\hbar}\Delta t(\mathbf{p}\cdot\dot{\mathbf{x}} - H)}. \tag{74}$$

Here we recognize the combination $\mathbf{p} \cdot \dot{\mathbf{x}} - H$ as being the Lagrangian of classical mechanics (after performing a Legendre transform). In fact, we can transform this into the usual Lagrangian (which does not depend on $\mathbf{p}$ remember) by performing the $\mathbf{p}$ integration explicitly in the case where the Hamiltonian is of the form $H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x})$. Then we have

$$K(\mathbf{x}, t + \Delta t; \mathbf{x}', t) = e^{-\frac{i}{\hbar}\Delta t V} \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3} \, e^{\frac{i}{\hbar}\Delta t \left(\mathbf{p}\cdot\dot{\mathbf{x}} - \frac{\mathbf{p}^2}{2m}\right)} =$$

$$e^{-\frac{i}{\hbar}\Delta t V} \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3} \, e^{-\frac{i}{2\hbar m}\Delta t(\mathbf{p}^2 - 2m\mathbf{p}\cdot\dot{\mathbf{x}})}. \tag{75}$$

The integral is again Gaussian and can be performed with the tricks we have developed earlier. Namely, we write

$$\int \frac{d^3\mathbf{p}}{(2\pi\hbar)^2} \, e^{-\frac{i}{2\hbar m}\Delta t(\mathbf{p}^2 - 2m\mathbf{p}\cdot\dot{\mathbf{x}})} = \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^2} \, e^{-\frac{i}{2\hbar m}\Delta t[(\mathbf{p}-m\dot{\mathbf{x}})^2 - m^2\dot{\mathbf{x}}^2]}, \tag{76}$$

so that the integral (or integrals, there are three of them) can be performed by redefining the integration variable $\tilde{\mathbf{p}} = \mathbf{p} - m\dot{\mathbf{x}}$ and using the usual formula for the Gaussian integral (39). Doing this we finally get

$$K(\mathbf{x}, t + \Delta t; \mathbf{x}', t) = \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{3}{2}} e^{\frac{i}{\hbar}\Delta t\left(\frac{1}{2}m\dot{\mathbf{x}}^2 - V\right)}, \tag{77}$$

and we see that indeed it is the classical Lagrangian that appears in the exponential. Therefore we have the extremely nice result that the infinitesimal propagator can be written as

$$K(\mathbf{x}, t + \Delta t; \mathbf{x}', t) = \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{3}{2}} e^{\frac{i}{\hbar}\Delta t L} \tag{78}$$

where we have introduced the classical Lagrangian L. Observing that for an infinitesimal time interval $\Delta t L = S$, the classical *action* evaluated for the

straight line path between points $\mathbf{x}(t)$ and $\mathbf{x}(t + \Delta t)$[1].

Now let us try to evaluate the propagator for a finite time interval. In the same way as before we divide the interval (say from t_i to t_f) into infinitesimal pieces and in each piece we can use the infinitesimal expression. To this end define

$$
\begin{aligned}
\Delta t &= \frac{t_f - t_i}{N}, \\
t_k &= t_i + k\Delta t \ \ k \in [0 \dots N],
\end{aligned}
\tag{79}
$$

so that $t_N = t_f$ and $t_0 = t_i$. By taking N large we can make the time intervals as small as we like. Now let us compute the propagator by splitting it into these intervals

$$
K(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i) = \langle \mathbf{x}_f | \hat{U}(t_f, t_i) | \mathbf{x}_i \rangle =
\tag{80}
$$
$$
\lim_{N \to \infty} \langle \mathbf{x}_f | \hat{U}(t_N, t_{N-1}) \times \hat{U}(t_{N-1}, t_{N-2}) \times \dots \times \hat{U}(t_2, t_1) \times \hat{U}(t_1, t_0) | \mathbf{x}_i \rangle.
$$

Between each of the $\hat{U}$ operators we may insert $\hat{1}$ in the form of a complete set of position eigenstates giving us the expression

$$
K(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i) = \lim_{N \to \infty} \int d^3\mathbf{x}_{N-1} \int d^3\mathbf{x}_{N-2} \dots \int d^3\mathbf{x}_2 \int d^3\mathbf{x}_1
$$
$$
\langle \mathbf{x}_f | \hat{U}(t_N, t_{N-1}) | \mathbf{x}_{N-1} \rangle \langle \mathbf{x}_{N-1} | \hat{U}(t_{N-1}, t_{N-2}) | \mathbf{x}_{N-2} \rangle \times \dots
$$
$$
\dots \times \langle \mathbf{x}_2 | \hat{U}(t_2, t_1) | \mathbf{x}_1 \rangle \langle \mathbf{x}_1 | \hat{U}(t_1, t_i) | \mathbf{x}_i \rangle.
\tag{81}
$$

But now each of the $\langle \mathbf{x}_{k+1} | \hat{U}(t_{k+1}, t_k) | \mathbf{x}_k \rangle$ is an infinitesimal propagator which we just calculated. We know that it is simply given by the classical action calculated along the straight line constant velocity path going from point $\mathbf{x}_k$ at time t_k to the point $\mathbf{x}_{k+1}$ at time t_{k+1}. Or in formulas we have

$$
\langle \mathbf{x}_{k+1} | \hat{U}(t_{k+1}, t_k) | \mathbf{x}_k \rangle = \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{\frac{3}{2}} e^{\frac{i}{\hbar} \Delta t L(k+1, k)}.
\tag{82}
$$

---

[1]Remember that the action is a *functional* which means it is a function of a function. In other words, to compute $S[\mathbf{x}(t)]$, we need to specify the function $\mathbf{x}(t)$, that is we need to specify how the particle moves from the point $\mathbf{x}(t_1)$ to the point $\mathbf{x}(t_2)$. What we just showed is that we can write the *infinitesimal* propagator in terms of the path where the particle moves from the initial point to the final point in a straight line with constant speed.

Inserting this in the formula for the full propagator we have

$$K(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i) = \lim_{N \to \infty} \int d^3\mathbf{x}_{N-1} \int d^3\mathbf{x}_{N-2} \ldots \int d^3\mathbf{x}_2 \int d^3\mathbf{x}_1$$
$$\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{3N}{2}} e^{\frac{i}{\hbar}\Delta t L(N,N-1)} \times \ldots \times e^{\frac{i}{\hbar}\Delta t L(1,0)}. \tag{83}$$

Since the L functions are just numbers and not operators we may just as well write them all in the same exponential

$$K(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i) = \lim_{N \to \infty} \int d^3\mathbf{x}_{N-1} \int d^3\mathbf{x}_{N-2} \ldots \int d^3\mathbf{x}_2 \int d^3\mathbf{x}_1$$
$$\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{3N}{2}} e^{\frac{i}{\hbar}\Delta t(L(N,N-1)+L(N-1,N-2)+\ldots+L(2,1)+L(1,0))}. \tag{84}$$

The expression in the exponential is nothing but the integral $\frac{i}{\hbar}\int_{t_i}^{t_f} dt L(t)$ along the piecewise linear path given in figure 3 Notice that the fact that we

Figure 3: The piecewise path

integrate over all possible intermediate positions (i.e. over all intermediate $\mathbf{x}_k$) tells us that the propagator can essentially be calculated as the sum over all possible paths of the factor $e^{\frac{i}{\hbar}S[\text{path}]}$ where $S[\text{path}]$ is the classical action *functional* of the system. Sometimes this is written compactly as

$$K(\mathbf{x}_f, t_f; \mathbf{x}_i, t_i) = \int \mathcal{D}\mathbf{x} e^{\frac{i}{\hbar}S[\mathbf{x}]}, \tag{85}$$

where the funny symbol $\mathcal{D}\mathbf{x}$ stands for summing over all paths (including all the ugly factors which we have hidden).

The path-integral formulation of Quantum Mechanics gives a very nice interpretation of the theory and its classical limit. Namely, to calculate the probability amplitude that something will happen in Quantum Mechanics we have to include contribution from all possible ways it can happen, even over the ways which are forbidden classically. For most of these paths the action changes rapidly when we change the path a little bit. For instance, for a particular generic path leading to the action S_1 there is always a close lying path having the action $S_1 + \hbar\pi$. When we add the contribution $e^{\frac{i}{\hbar}S}$ of these two paths we will get zero. However, there also exist special paths for which the action does not change when we change the path a little bit. When we sum over such paths they will add up instead of canceling out. These paths are of course the paths which are solutions to the variational equation

$$\frac{\delta S}{\delta x} = 0, \tag{86}$$

i.e. the solutions to the classical equations of motion. So the classical limit of Quantum mechanics is essentially the limit where we sum over only the paths which are classically allowed.

1.6 The path integral evaluation of the harmonic oscillator

We will now illustrate the path integral method in an example. Namely, we want to calculate the probability amplitude (propagator) that we find the one dimensional harmonic oscillator at the point x_f at time t_f if we at time t_i have it localized at point x_i. We will use the definition in the form (83) so we first need to decompose the interval into N equal pieces. Thus we have $(x_i(t_i), t_i) = (x_0(t_0), t_0), \ldots, (x_N(t_N), t_N) = (x_f(t_f), t_f)$ and $\Delta t = \frac{t_N - t_0}{N} = t_{k+1} - t_k$. The definition now becomes

$$\langle f|i \rangle = \lim_{N \to \infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}} \int dx_{N-1} e^{\frac{im\Delta t}{2\hbar}\left(\frac{(x_N - x_{N-1})}{\Delta t^2} - \omega^2\left(\frac{x_N + x_{N-1}}{2}\right)^2\right)}$$

$$\times \ldots \times \int dx_1 e^{\frac{im\Delta t}{2\hbar}\left(\frac{(x_1 - x_0)}{\Delta t^2} - \omega^2\left(\frac{x_1 + x_0}{2}\right)^2\right)}. \tag{87}$$

Reshuffling the terms a bit and introducing the notation

$$A = \frac{m\Delta t}{2i\hbar}\left(\frac{1}{\Delta t^2} - \frac{\omega^2}{4}\right)$$

$$B = \frac{m\Delta t}{2i\hbar}\left(\frac{1}{\Delta t^2} + \frac{\omega^2}{4}\right), \tag{88}$$

we may write the path integral as

$$\langle f|i\rangle = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}}\int\prod_{k=1}^{N-1}dx_k e^{-Ax_N^2 - Ax_{N-1}^2 + 2Bx_N x_{N-1}}$$
$$\times \ldots \times e^{-Ax_1^2 - Ax_0^2 + 2Bx_1 x_0}. \tag{89}$$

This can be written even more compactly using matrix notation. We introduce the $N-1$ dimensional matrices

$$q = \begin{pmatrix} x_1 \\ \vdots \\ x_{N-1} \end{pmatrix}, \quad q_0 = \begin{pmatrix} Bx_0 \\ 0 \\ \vdots \\ 0 \\ Bx_N \end{pmatrix},$$

$$M = \begin{pmatrix} 2A & -B & 0 & 0 & \cdots \\ -B & 2A & -B & 0 & \cdots \\ 0 & -B & 2A & -B & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{90}$$

we may write the path integral very compactly as

$$\langle f|i\rangle = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}} e^{-A(x_0^2 + x_N^2)}\int\prod_{k=1}^{N-1}dx_k e^{-q^T M q + q^T q_0 + q_0^T q}. \tag{91}$$

The expression in the exponent can be rewritten as

$$-q^T M q + q^T q_0 + q_0^T q = -\left(q^T - q_0^T M^{-1}\right)M\left(q - M^{-1}q_0\right) + q_0^T M^{-1}q_0, \tag{92}$$

where we have used that M is nondegenerate and symmetric. We now use the fact that we may shift each of the integration variables x_k by an arbitrary constant without producing a (nontrivial) Jacobian. Thus we collectively define the new integration variables

$$y = \begin{pmatrix} y_1 \\ \vdots \\ y_{N-1} \end{pmatrix} = q - M^{-1}q_0, \tag{93}$$

which, when inserted in the path integral gives

$$\langle \mathrm{f}|\mathrm{i}\rangle = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}} e^{-A(x_0^2+x_N^2)} e^{+q_0^T M^{-1}q_0} \int \prod_{k=1}^{N-1} dy_k e^{-y^T My}. \qquad (94)$$

Since M is a symmetric ($N-1$ by $N-1$) matrix, we know that there exists an orthogonal matrix O with $\det O = 1$ such that $O^T MO$ is a diagonal matrix which we will call D. Thus, if we again change integration variables $Oz = y$ which produces a Jacobian $\det O = 1$ we may write the path integral as

$$\langle \mathrm{f}|\mathrm{i}\rangle = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}} e^{-A(x_0^2+x_N^2)} e^{+q_0^T M^{-1}q_0} \int \prod_{k=1}^{N-1} dz_k e^{-z^T O^T MOz}. \qquad (95)$$

Since $O^T MO = D$ we have decoupled the $N-1$ integrals into simple Gaussians which we are able to perform. Thus we have

$$\langle \mathrm{f}|\mathrm{i}\rangle = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}} e^{-A(x_0^2+x_N^2)} e^{+q_0^T M^{-1}q_0} \prod_{k=1}^{N-1} \int dz_k e^{-d_{kk}z_k^2} =$$

$$\lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}} e^{-A(x_0^2+x_N^2)} e^{+q_0^T M^{-1}q_0} \prod_{k=1}^{N-1} \sqrt{\frac{\pi}{d_{kk}}} =$$

$$\lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}} e^{-A(x_0^2+x_N^2)} e^{+q_0^T M^{-1}q_0} \sqrt{\frac{\pi^{N-1}}{\det D}} =$$

$$\lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}} e^{-A(x_0^2+x_N^2)} e^{+q_0^T M^{-1}q_0} \sqrt{\frac{\pi^{N-1}}{\det M}}, \qquad (96)$$

where we in the last line have used that $\det D = \det O^T MO = \det M$. This is quite a simple expression for the complicated path integral! It depends on the determinant and the inverse of the matrix M. Fortunately, because of the simple expression for q_0 (90) we only need to know the matrix elements $(M^{-1})_{11}$ and $(M^{-1})_{1\,N-1}$ of the inverse.

We will calculate the determinant recursively. Let us call the determinant of the $N-1$ times $N-1$ dimensional matrix M (90) I_{N-1}. Using the structure of M we may derive a recursion relation for I_N. Namely, we have that $I_{N+2} = 2AI_{N+1} - B^2 I_N$ with initial conditions $I_1 = 2A$ and $I_2 = 4A^2 - B^2$. Such a recursion relation can be conveniently solved by defining the generating function

$$f(\xi) = \sum_{n=0}^{\infty} I_n \frac{\xi^n}{n!}. \qquad (97)$$

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Multiplying the recursion relation by $\frac{\xi^n}{n!}$ and summing we get a differential equation for $f(\xi)$

$$f'' - 2Af' + f = 0, \tag{98}$$

with general solution

$$f(\xi) = c_1 e^{\omega_+ \xi} + c_2 e^{\omega_- \xi} \ , \quad \omega_\pm = A \pm \sqrt{A^2 - B^2} \tag{99}$$

Taylor expanding $f(\xi)$ we can read off the individual I_N. The initial conditions give equations for c_1 and c_2

$$c_1 \omega_+ + c_2 \omega_- = 2A$$
$$c_1 \omega_+^2 + c_2 \omega_-^2 = 4A^2 - B^2, \tag{100}$$

which can be solved to find $c_1 = \frac{\omega_+}{2\sqrt{A^2 - B^2}}$ and $c_2 = -\frac{\omega_-}{2\sqrt{A^2 - B^2}}$ which then gives us the general expression

$$I_N = \frac{1}{2\sqrt{A^2 - B^2}} \left(\omega_+^{N+1} - \omega_-^{N+1} \right). \tag{101}$$

To find the elements of M^{-1} we use Cramer's rule and the fact that we know the determinant of M of various dimensions. Straightforwardly we have

$$(M^{-1})_{11} = \frac{I_{N-2}}{I_{N-1}} \tag{102}$$

To calculate $(M^{-1})_{1\,N-1}$ is a bit more tricky. The minor one has to compute is an upper triangular matrix with $-B$ on the diagonal. Thus we have

$$(M^{-1})_{1\,N-1} = \frac{B^{N-2}}{I_{N-1}}. \tag{103}$$

Thus we have

$$\langle \mathrm{f}|\mathrm{i} \rangle = \lim_{N \to \infty} \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{\frac{N}{2}} e^{-A(x_0^2 + x_N^2)} e^{(x_0^2 + x_N^2) \frac{B^2 I_{N-2}}{I_{N-1}} + 2x_0 x_N \frac{B^{N-2}}{I_{N-1}}} \sqrt{\frac{\pi^{N-1}}{I_{N-1}}}. \tag{104}$$

Now we have to take the $N \to \infty$ limit in this expression. First let us have a look at the determinant. From the explicit expressions for $\omega_\pm$ (99) and the constants A and B (88) we have

$$\omega_\pm = \frac{m}{2i\hbar \Delta t} \left(1 \pm \frac{i\omega \Delta t}{2} \right)^2. \tag{105}$$

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Here the N dependence is hidden in $\Delta t = \frac{t_N - t_0}{N}$. Let us define $T = t_N - t_0$. Then we can write

$$\omega_\pm^N = \left(\frac{m}{2i\hbar\Delta t}\right)^N \left(1 \pm \frac{i\omega T}{2N}\right)^{2N} = \left(\frac{m}{2i\hbar\Delta t}\right)^N e^{2N\ln\left(1\pm\frac{i\omega T}{2N}\right)} \approx$$

$$\left(\frac{m}{2i\hbar\Delta t}\right)^N e^{2N\left(\pm\frac{i\omega T}{2N} - \frac{1}{2}\left(\frac{i\omega T}{2N}\right)^2\right)} \approx \left(\frac{m}{2i\hbar\Delta t}\right)^N e^{\pm i\omega T}\left(1 + \frac{\omega^2 T^2}{4N} + \mathcal{O}(\frac{1}{N^2})\right) \quad (106)$$

giving

$$I_{N-1} = \frac{2i\hbar}{m\omega}\left(\frac{m}{2i\hbar\Delta t}\right)^N \sin\omega T \left(1 + \frac{\omega^2 T^2}{4N} + \mathcal{O}(\frac{1}{N^2})\right) \quad (107)$$

A similar but slightly more involved calculation gives for

$$I_{N-2} = \frac{2i\hbar}{m\omega}\left(\frac{m}{2i\hbar\Delta t}\right)^{N-1}\left[\sin\omega T - \frac{\omega T}{N}\cos\omega T + \mathcal{O}(\frac{1}{N^2})\right] \times$$

$$\left(1 + \frac{\omega^2 T^2}{4N} + \mathcal{O}(\frac{1}{N^2})\right). \quad (108)$$

Similarly we have

$$B^N = \left(\frac{m}{2i\hbar\Delta t}\right)^N \left(1 + \mathcal{O}(\frac{1}{N^2})\right) \quad (109)$$

This is all we need to compute the relevant expressions in (104). They are

$$\frac{B^2 I_{N-2}}{I_{N-1}} - A = \left(\frac{m}{2i\hbar\Delta t}\right)\left(1 - \frac{\omega T}{N}\cot\omega T\right) - \left(1 - \frac{\omega^2 T^2}{4N^2}\right) =$$

$$-\left(\frac{\omega m}{2i\hbar}\right)\cot\omega T + \mathcal{O}(\frac{1}{N}), \quad (110)$$

and

$$\frac{B^N}{I_{N-1}} = \frac{m\omega}{2i\hbar}\frac{1}{\sin\omega T} + \mathcal{O}(\frac{1}{N}). \quad (111)$$

In these expressions we may now take the limit $N \to \infty$ since all potentially divergent terms have cancelled. Collecting all terms we have

$$\langle f|i\rangle = \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\Delta t}\right)^{\frac{N}{2}}\left(\frac{2\pi i\hbar\Delta t}{m}\right)^{\frac{N}{2}}\sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}}$$

$$e^{-\frac{m\omega}{2i\hbar}\left(\cot\omega T\left(x_0^2 + x_N^2\right) - \frac{2}{\sin\omega T}x_0 x_N + \mathcal{O}(\frac{1}{N^2})\right)}. \quad (112)$$

We see that indeed all the dangerous N dependence cancel and we can safely take the limit $N \to \infty$ which has the effect that we drop all terms $\mathcal{O}(\frac{1}{N})$. The final result is then

$$\langle x_f | x_i \rangle = \sqrt{\frac{m\omega}{2\pi i\hbar \sin \omega T}} e^{\frac{im\omega}{2\hbar}\left(\cot \omega T\left(x_i^2 + x_f^2\right) - \frac{2}{\sin \omega T}x_i x_f\right)} \tag{113}$$

2 Angular momentum

We know from experience that there is no preferred place or direction in the universe, that is, in more fancy language, that space is homogeneous and isotropic. (Homogeneous means that space is invariant under translations and isotropic means that it is invariant under rotations). This, in classical mechanics leads to the conservation of momentum and angular momentum respectively. This makes it important to study how physical objects transform under translations and rotations. This is also true in quantum mechanics. In this section we will study how physical systems behave under rotations in quantum mechanics.

The effect of a rotation of the physical system in quantum mechanics is of course represented by the action of an operator. Let us use the notation

$$\hat{R}_{\mathbf{n}}\left(\phi\right), \tag{114}$$

for the operator which performs a rotation by an angle ϕ around the unit vector $\mathbf{n}$.

One important property of the operator $\hat{R}$ we get from the fact that we cannot "lose" particles (or probability) when we do a rotation. This tells us that the state we get as a result of a rotation has to have the same norm as the initial state. In formulas we write

$$\langle \chi | \chi \rangle = \langle \chi' | \chi' \rangle = \langle \chi | \hat{R}^\dagger \hat{R} | \chi \rangle, \tag{115}$$

which implies that $\hat{R}^\dagger \hat{R} = \hat{1}$ or that the operator $\hat{R}$ is a *unitary* operator.

We can learn a lot from the fact that quantum mechanical rotations have to fulfill the properties of classical rotations. In particular, we know that any classical rotation can be built up from many infinitesimal rotations. That is, instead of rotating the system the angle ϕ around the axis $\mathbf{n}$ we can rotate it N times around the same axis, but each time only an angle $\frac{\phi}{N}$. Our experience

from classical physics tells us the the result of these two operations has to be the same. In quantum mechanics we write

$$\hat{R}_{\mathbf{n}}\left(\phi\right) = \left[\hat{R}_{\mathbf{n}}\left(\frac{\phi}{N}\right)\right]^{N}. \tag{116}$$

We also know that letting the angle with which we rotate become small, the "change" of the system becomes smaller and smaller. In quantum mechanics we could write this as

$$\lim_{\phi \to 0} \hat{R}\left(\phi\right) = \hat{1}, \tag{117}$$

or, introducing an operator $\hat{K}(\phi)$ with the property that $\lim_{\phi \to 0} \hat{K}\left(\phi\right) = 0$ we can for *infinitesimal* angles ϵ write

$$\hat{R}(\epsilon) = \hat{1} + \hat{K}\left(\epsilon\right) + \ldots. \tag{118}$$

Keeping the angle infinitesimal, and using (116) we can write

$$\hat{1} + \hat{K}(2\epsilon) = \hat{R}(2\epsilon) = \hat{R}(\epsilon)\hat{R}(\epsilon) = \left(\hat{1} + \hat{K}(\epsilon)\right)\left(\hat{1} + \hat{K}(\epsilon)\right) = \hat{1} + 2\hat{K}(\epsilon) + \ldots \tag{119}$$

That is, $\hat{K}(2\epsilon) = 2\hat{K}(\epsilon)$. This means that $\hat{K}$ depends on ϵ *linearly*. Let us therefore write

$$\hat{K}(\epsilon) = -\frac{i}{\hbar}\epsilon\hat{J}. \tag{120}$$

(The factor $-\frac{i}{\hbar}$ is introduced for convenience). Now we may also use that $\hat{R}$ is unitary to write

$$\hat{1} = \hat{R}^{\dagger}(\epsilon)\hat{R}(\epsilon) = \left(\hat{1} - \frac{i}{\hbar}\epsilon\hat{J}\right)^{\dagger}\left(\hat{1} - \frac{i}{\hbar}\epsilon\hat{J}\right) = \left(\hat{1} + \frac{i}{\hbar}\epsilon\hat{J}^{\dagger}\right)\left(\hat{1} - \frac{i}{\hbar}\epsilon\hat{J}\right)$$
$$\hat{1} + \frac{i}{\hbar}\epsilon(\hat{J}^{\dagger} - \hat{J}) + \mathcal{O}(\epsilon^2), \tag{121}$$

which leads us to deduce that $\hat{J} = \hat{J}^{\dagger}$ or, that $\hat{J}$ is a *hermitian* operator. $\hat{J}$ is called the *generator* of rotations[2].

---

[2]Here one can notice the reason for the extra factor of i in the definition of $\hat{J}$. Had it not been there the operator $\hat{J}$ would have been *anti*hermitian. Since we know that Hermitian operators are nice (they have real eigenvalues for instance) this is why we choose to define $\hat{J}$ as we did.

Since an arbitrary rotation can be thought of as being composed of an infinite number of infinitesimal rotations we can use the infinitesimal form found above to give the general form of the rotation operator. That is, we build up a rotation with angle ϕ as N rotations all with angle $\Delta\phi = \frac{\phi}{N}$. That is

$$\hat{R}(\phi) = \lim_{N\to\infty} \left[\hat{R}\left(\frac{\phi}{N}\right)\right]^N = \lim_{N\to\infty} \left[1 - \frac{i}{\hbar}\frac{\phi}{N}\hat{J}\right]^N. \tag{122}$$

Using a known formula for the exponential as $e^x = \lim_{N\to\infty}\left(1 + \frac{x}{N}\right)^N$ we find

$$\hat{R}(\phi) = e^{-\frac{i}{\hbar}\hat{J}\phi}, \tag{123}$$

in agreement with what we said about the operator $\hat{R}$ before.

It interesting to check that unitary operators can generally be written in terms of hermitian operators in this very convenient way. Namely, if we let $\hat{J}$ be an hermitian operator $\hat{J}^\dagger = \hat{J}$, the operator $\hat{R} = e^{-i\hat{J}}$ is always unitary since $\hat{R}^\dagger = \left(1 - i\hat{J} + \frac{(-i\hat{J})^2}{2!} + \dots\right)^\dagger = \left(1 + i\hat{J}^\dagger + \frac{(i\hat{J}^\dagger)^2}{2!} + \dots\right) = e^{i\hat{J}}$ and $e^{-i\hat{J}}e^{i\hat{J}} = 1$.

To summarize what we have found one can say that the operator of rotations with angle ϕ around an axis $\mathbf{n}$ can be written as

$$\hat{R}_{\mathbf{n}}(\phi) = e^{-\frac{i}{\hbar}\phi\hat{J}_{\mathbf{n}}}, \tag{124}$$

where $\hat{J}_{\mathbf{n}}$ is a hermitian operator called the generator of rotations around axis $\mathbf{n}$. If physics is invariant under rotations around $\mathbf{n}$ it is represented by a state $|\psi\rangle$ which has to be an eigenstate of the generator of rotations.

Another classical property of rotations is that they do not commute. That is a rotation around the x-axis followed by a rotation around the y-axis is not the same as a rotation around the y-axis followed by a rotation around the x-axis. This is however true only in the non infinitesimal case. One can for instance check that two (classical) rotations with angle ϵ around the x and y axises commute when taking into account terms linear in epsilon only. To see the non-commutativity one has to also keep terms quadratic in ϵ. Mathematically we may write

$$R_x(\epsilon)R_y(\epsilon) - R_y(\epsilon)R_x(\epsilon) = R_z(\epsilon^2) - 1 + \mathcal{O}(\epsilon^3). \tag{125}$$

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Let us check how this goes in the quantum mechanical case. Writing the rotation operators in terms of generators we have on the left hand side

$$\hat{R}_x \hat{R}_y - \hat{R}_y \hat{R}_x = \left(1 - \frac{i}{\hbar} \hat{J}_x \epsilon - \frac{1}{2\hbar^2} \hat{J}_x^2 \epsilon^2\right) \left(1 - \frac{i}{\hbar} \hat{J}_y \epsilon - \frac{1}{2\hbar^2} \hat{J}_y^2 \epsilon^2\right) -$$
$$\left(1 - \frac{i}{\hbar} \hat{J}_y \epsilon - \frac{1}{2\hbar^2} \hat{J}_y^2 \epsilon^2\right) \left(1 - \frac{i}{\hbar} \hat{J}_x \epsilon - \frac{1}{2\hbar^2} \hat{J}_x^2 \epsilon^2\right) + \mathcal{O}(\epsilon^3) =$$
$$-\frac{\epsilon^2}{\hbar^2} \left[\hat{J}_x, \hat{J}_y\right] + \mathcal{O}(\epsilon^3). \quad (126)$$

This should be compared to the right hand side which becomes

$$\hat{R}_z\left(\epsilon^2\right) - 1 = -\frac{i}{\hbar} \hat{J}_z \epsilon^2. \quad (127)$$

Thus we see that for rotations in quantum mechanics to have the properties of classical rotations, we need to require

$$\left[\hat{J}_x, \hat{J}_y\right] = \frac{\hbar^2}{\epsilon^2} \left(\frac{i}{\hbar} \hat{J}_z \epsilon^2\right) = i\hbar \hat{J}_z. \quad (128)$$

Since the axis around which we performed the rotation is really arbitrary in this example, we can immediately generalize this to the commutation relations

$$\left[\hat{J}_i, \hat{J}_k\right] = i\hbar \epsilon_{ikl} \hat{J}_l, \quad (129)$$

where we have introduced the notation $\hat{J}_1 = \hat{J}_x$, $\hat{J}_2 = \hat{J}_y$, $\hat{J}_3 = \hat{J}_z$ and the totally antisymmetric tensor ϵ_{ikl}.

2.1 An example

As an illustration of the use of rotations in quantum mechanics consider the following situation. The "elementary" particle Λ_0 (with spin $\frac{1}{2}$) decays into a π^- meson (with spin 0) and a proton p^+ (with spin $\frac{1}{2}$). Assume that the initial Λ_0 particle is in a state where the spin is pointing upwards along the z-axis and let us call this state $|+\rangle$ (as opposed to the state with spin projection down which we will call $|-\rangle$). Our task is to calculate the angular distribution of the final p^+ (because of momentum conservation the p^+ and the π^- always go out back to back so we do not need to worry about the

π^- in what follows). What "angular distribution" means is that we want to calculate the probability that the proton p^+ comes out at an angle θ with the z-axis. This seems almost impossible since it seems that we do not have enough information to calculate this but the answer is essentially given by rotation invariance. Calculate as follows: assume that we know the probability for the proton to go out along the z-axis. To be concrete, let us say that the probability amplitude is a if the initial Λ_0 has spin up $|+\rangle$ and b if the initial Λ_0 has spin down $|-\rangle$. Because of angular momentum conservation the proton comes out with spin up in the first case and with spin down in the second case. To calculate the probability amplitude for the proton to go out at an angle θ we take the original Λ_0 and rotate it. In the rotated system we want to calculate the probability for the proton to go straight up (since this is at an angle θ with the original Λ_0). To find out the effect of a rotation on Λ_0 we need to know how the rotation operator acts on spin $\frac{1}{2}$ states. This will be shown later in great detail so let me just quote the result for a rotation around the y-axis

$$\hat{R}_y(\theta)|+\rangle = \cos\left(\frac{\theta}{2}\right)|+\rangle + \sin\left(\frac{\theta}{2}\right)|-\rangle, \qquad (130)$$

so in the rotated system the probability amplitude that the proton goes straight up with spin up is

$$a\cos\left(\frac{\theta}{2}\right), \qquad (131)$$

and the probability amplitude that the proton goes straight up with spin down is

$$b\sin\left(\frac{\theta}{2}\right). \qquad (132)$$

The probability that the proton comes out with spin up is

$$|a|^2\cos^2\left(\frac{\theta}{2}\right), \qquad (133)$$

and with spin down it is given by

$$|b|^2\sin^2\left(\frac{\theta}{2}\right). \qquad (134)$$

The total probability that the proton comes out at an angle θ (if we do not observe the spin) is given by the sum of these two probabilities

$$\frac{|a|^2 + |b|^2}{2} \left(1 + \frac{|a|^2 - |b|^2}{|a|^2 + |b|^2} \cos(\theta)\right). \tag{135}$$

So we see that from just rotation invariance we have been able to say that the probability that the proton goes out at an angle θ is given by a formula of the type

$$\alpha \left(1 + \beta \cos(\theta)\right), \tag{136}$$

for some constants α and β.

2.2 The angular momentum algebra

The angular momentum algebra can abstractly be written as

$$\left[\hat{J}_i, \hat{J}_k\right] = i\hbar\epsilon_{ikl} \, \hat{J}_l, \tag{137}$$

where ϵ_{ijk} is the completely antisymmetric symbol and repeated indices are summed over. This is a compact form of writing the following three commutation relations

$$\begin{aligned}
\left[\hat{J}_1, \hat{J}_2\right] &= i\hbar\hat{J}_3, \\
\left[\hat{J}_2, \hat{J}_3\right] &= i\hbar\hat{J}_1, \\
\left[\hat{J}_3, \hat{J}_1\right] &= i\hbar\hat{J}_2,
\end{aligned} \tag{138}$$

$$\tag{139}$$

where we can interpret $\hat{J}_1 = \hat{J}_x$, $\hat{J}_2 = \hat{J}_y$ and $\hat{J}_3 = \hat{J}_z$. It is possible to form an operator which commutes with all $\hat{J}_i$. Namely, define $\hat{\mathbf{J}}^2 = \hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2$. Then it is easy to check that $\left[\hat{J}_i, \hat{\mathbf{J}}^2\right] = 0$ for all i. This means that we can always choose states to be simultaneous eigenstates of $\hat{\mathbf{J}}^2$ and $\hat{J}_i$ for one fixed i. Let us choose $\hat{J}_3 = \hat{J}_z$ to be concrete. Then we can choose states $|a, b\rangle$ such that

$$\begin{aligned}
\hat{J}_3|a, b\rangle &= a|a, b\rangle, \\
\hat{\mathbf{J}}^2|a, b\rangle &= b|a, b\rangle.
\end{aligned} \tag{140}$$

To find out what $\hat{J}_1$ and $\hat{J}_2$ do with this state we define the operators $\hat{J}_\pm = \hat{J}_1 \pm i\hat{J}_2$. Since the operators $\hat{J}_\pm$ are just linear combinations of $\hat{J}_{1,2}$ we may equivalently work with them or, in other words, the algebra in terms of $\hat{J}_+, \hat{J}_-, J_3$ contains the same information (is equivalent to) the algebra in terms of $\hat{J}_1, \hat{J}_2, \hat{J}_3$. In terms of these new operators the algebra looks like

$$
\begin{aligned}
\left[\hat{J}_3, \hat{J}_\pm\right] &= \pm\hbar\hat{J}_\pm, \\
\left[\hat{J}_+, \hat{J}_-\right] &= 2\hbar\hat{J}_3.
\end{aligned}
\tag{141}
$$

We may also rewrite $\hat{\mathbf{J}}^2$ in terms of the new operators. By inserting their definitions it is straightforward to confirm that $\hat{\mathbf{J}}^2 = \frac{1}{2}\left\{\hat{J}_+, \hat{J}_-\right\} + \hat{J}_3^2$ where we have introduced the *anti*-commutator $\left\{\hat{A}, \hat{B}\right\} = \hat{A}\hat{B} + \hat{B}\hat{A}$.

We will now try to find out what the operators $\hat{J}_\pm$ does to the states $|a, b\rangle$. In fact, running ahead a bit, we will see that they map these states into each other, that is acting with $\hat{J}_\pm$ on an eigenstate of $\hat{J}_3, \hat{\mathbf{J}}^2$ gives us back a (generally different) eigenstate of $\hat{J}_3, \hat{\mathbf{J}}^2$. In formulas we have

$$
\begin{aligned}
\hat{J}_3\hat{J}_\pm|a, b\rangle &= \left(\left[\hat{J}_3, \hat{J}_\pm\right] + \hat{J}_\pm\hat{J}_3\right)|a, b\rangle \\
&= \left(\pm\hbar\hat{J}_\pm + \hat{J}_\pm a\right)|a, b\rangle \\
&= (a \pm \hbar)\,\hat{J}_\pm|a, b\rangle,
\end{aligned}
\tag{142}
$$

which tells us that $\hat{J}_\pm|a, b\rangle$ is an eigenstate of $\hat{J}_3$ with eigenvalue $(a \pm \hbar)$. Let us check that $\hat{J}_\pm|a, b\rangle$ is an eigenstate of also $\hat{\mathbf{J}}^2$. This is even easier; since $\hat{\mathbf{J}}^2$ commutes with *all* $\hat{J}_i$ it also commutes with $\hat{J}_\pm$ which are just linear combinations of the $\hat{J}_i$ operators. Thus we have that $\hat{\mathbf{J}}^2\hat{J}_\pm|a, b\rangle = \hat{J}_\pm\hat{\mathbf{J}}^2|a, b\rangle = b\hat{J}_\pm|a, b\rangle$ showing that $\hat{J}_\pm|a, b\rangle$ is an eigenstate of *both* $\hat{J}_3$ and $\hat{\mathbf{J}}^2$ with eigenvalues $a \pm \hbar$ and b. That is, that $\hat{J}_\pm|a, b\rangle \propto |a \pm \hbar, b\rangle$. Notice that the action of $\hat{J}_1$ or $\hat{J}_2$ does not give back states of the type $|a, b\rangle$. This is the explanation why we choose to work with $\hat{J}_\pm$.

Acting more times with $\hat{J}_\pm$ and using the argument repeatedly we have that $\left(\hat{J}_\pm\right)^n|a, b\rangle \propto |a \pm n\hbar, b\rangle$ and it looks like we can go on forever like this. However, this cannot be true which we can see by studying the operator $\hat{\mathbf{J}}^2 - \hat{J}_3^2$. According to a previous formula, this can be written as

$$
\hat{\mathbf{J}}^2 - \hat{J}_3^2 = \frac{1}{2}\left\{\hat{J}_+, \hat{J}_-\right\} = \frac{1}{2}\left(\hat{J}_-\hat{J}_+ + \hat{J}_+\hat{J}_-\right),
\tag{143}
$$

and using that $\hat{J}_{\pm} = \left(\hat{J}_{\mp}\right)^{\dagger}$ we can write this as

$$\mathbf{\hat{J}}^2 - \hat{J}_3^2 = \frac{1}{2}\left(\hat{J}_+^{\dagger}\hat{J}_+ + \hat{J}_-^{\dagger}\hat{J}_-\right). \tag{144}$$

Taking the expectation value of this relation in a $|\mathrm{a,b}\rangle$ state we have on the left hand side

$$\langle \mathrm{a,b}| \left(\mathbf{\hat{J}}^2 - \hat{J}_3^2\right)|\mathrm{a,b}\rangle = b - a^2, \tag{145}$$

and on the right hand side we get

$$\frac{1}{2}\langle \mathrm{a,b}|\left(\hat{J}_+^{\dagger}\hat{J}_+ + \hat{J}_-^{\dagger}\hat{J}_-\right)|\mathrm{a,b}\rangle = \frac{1}{2}\left(\left|\hat{J}_+|\mathrm{a,b}\rangle\right|^2 + \left|\hat{J}_-|\mathrm{a,b}\rangle\right|^2\right) \geq 0, \tag{146}$$

which leads to the inequality

$$b - a^2 \geq 0. \tag{147}$$

Here is a lot of information hidden. First of all, b has to be positive. Second of all, a cannot be arbitrary large but there exists a maximal $a = a_{\max}$ such that

$$\begin{aligned} b &\geq& a_{\max}^2, \\ b &<& (a_{\max} + \hbar)^2, \end{aligned} \tag{148}$$

and equivalently a minimal $a = a_{\min}$ such that

$$\begin{aligned} -b &\leq& a_{\min}^2, \\ -b &>& (a_{\min} - \hbar)^2. \end{aligned} \tag{149}$$

In order for the $\left(\hat{J}_{\pm}\right)^n |\mathrm{a,b}\rangle \propto |\mathrm{a} \pm \mathrm{m}\hbar, \mathrm{b}\rangle$ iteration to stop at $a_{\max}$ (resp. $a_{\min}$), we need

$$\begin{aligned} \hat{J}_+|\mathrm{a_{\max},b}\rangle &=& 0, \\ \hat{J}_-|\mathrm{a_{\min},b}\rangle &=& 0. \end{aligned} \tag{150}$$

This we may now use in the following way

$$0 = \hat{J}_-\hat{J}_+|\mathrm{a_{\max},b}\rangle = \left(\hat{J}_1 - i\hat{J}_2\right)\left(\hat{J}_1 + i\hat{J}_2\right)|\mathrm{a_{\max},b}\rangle =$$
$$\left(\hat{J}_1^2 + \hat{J}_2^2 + i\left[\hat{J}_1,\hat{J}_2\right]\right)|\mathrm{a_{\max},b}\rangle = \left(\hat{J}_1^2 + \hat{J}_2^2 - \hbar\hat{J}_3\right)|\mathrm{a_{\max},b}\rangle = \tag{151}$$
$$\left(\mathbf{\hat{J}}^2 - \hat{J}_3^2 - \hbar\hat{J}_3\right)|\mathrm{a_{\max},b}\rangle = \left(b - a_{\max}^2 - \hbar a_{\max}\right)|\mathrm{a_{\max},b}\rangle,$$

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which tells us that $b = a_{\max} (a_{\max} + \hbar)$. The same calculation starting with $0 = \hat{J}_+ \hat{J}_- |a_{\min}, b\rangle$ gives $b = a_{\min} (a_{\min} - \hbar)$ which tells us that $a_{\min} = -a_{\max}$.

Starting from $|a_{\min}, b\rangle = |-a_{\max}, b\rangle$ and acting with $\hat{J}_+$ we should reach $|a_{\max}, b\rangle$ after a finite number of steps, let us say n (where n of course is an integer). Thus we have $-a_{\max} + n\hbar = a_{\max}$, or $a_{\max} = \frac{n}{2}\hbar$. Thus, the representation is characterized by the half-integer $\frac{n}{2}$. Let us call it j for simplicity (and we have to remember that j can be both integer and half-integer). Then we have

$$
\begin{aligned}
b &= \hbar^2 j (j + 1), \\
a &\in \hbar [-j, -j + 1, \ldots, j - 1, j].
\end{aligned}
\tag{152}
$$

In the following we will forget about the $\hbar$ factors in the way we denote the states $|a, b\rangle$ and denote them just by the half-integer j and by $m = \frac{a}{\hbar}$ so that an arbitrary state will look like $|j, m\rangle$ where $m \in [-j, \ldots, j]$. The action by the operators on these states are

$$
\begin{aligned}
\hat{\mathbf{J}}^2 |j, m\rangle &= \hbar^2 j (j + 1) |j, m\rangle, \\
\hat{J}_3 |j, m\rangle &= \hbar m |j, m\rangle, \\
\hat{J}_\pm |j, m\rangle &\propto |j, m \pm 1\rangle.
\end{aligned}
\tag{153}
$$

In the last relation, we can even compute the coefficient of proportionality. Namely, if we have $\hat{J}_+ |j, m\rangle = C_{j,m} |j, m + 1\rangle$ we can compute the absolute value of $C_{j,m}$ since we know that the $|j, m\rangle$ states are normalized. Thus

$$
\begin{aligned}
|C_{j,m}| = \left| \hat{J}_+ |j, m\rangle \right|^2 &= \langle j, m | \hat{J}_+^\dagger \hat{J}_+ |j, m\rangle = \langle j, m | \hat{J}_- \hat{J}_+ |j, m\rangle = \\
&\langle j, m | \left(\hat{J}_1^2 + \hat{J}_2^2 + i \left[\hat{J}_1, \hat{J}_2 \right] \right) |j, m\rangle = \\
&\langle j, m | \left(\hat{\mathbf{J}}^2 - \hat{J}_3^2 - \hbar \hat{J}_3 \right) |j, m\rangle = \\
&\hbar^2 (j (j + 1) - m (m + 1)),
\end{aligned}
\tag{154}
$$

so if we choose $C_{j,m}$ to be real and positive by convention we have

$$
\hat{J}_+ |j, m\rangle = \hbar \sqrt{j (j + 1) - m (m + 1)} |j, m + 1\rangle.
\tag{155}
$$

A similar calculation for $\hat{J}_-$ gives

$$
\hat{J}_- |j, m\rangle = \hbar \sqrt{j (j + 1) - m (m - 1)} |j, m - 1\rangle.
\tag{156}
$$

Notice that the proportionality factor indeed vanishes for the case $\hat{J}_+ |j, j\rangle$ or $\hat{J}_- |j, -j\rangle$ so that the iteration indeed stops as we claimed before.

2.3 The rotation operator in general

We are now equipped to study the rotation operator in general. From the previous section we know that any action of the $\hat{J}$ operators on a state with fixed quantum number j gives back states with the same quantum number j (but in general with different values of the quantum number m). In more physical language this corresponds to the fact that if we take a spin j particle and rotates it, it stays a spin j particle. In mathematical language we say that the states with spin j constitutes a *irreducible representation* of the rotation group[3]. In other words, the rotation operator acts in a block diagonal way on the different irreducible representations. This means that we can study how the rotation operator looks like for the different representations (or spins if you like) separately. For instance, for the spin 0 representation the rotation operator acts trivially (since there is only one state there is not much that *can* happen) so the first non-trivial example is for the spin half ($j = \frac{1}{2}$) representation. From the previous section we know that there are two states in this representation

$$|\frac{1}{2}, \frac{1}{2}\rangle \equiv |+\rangle,$$
$$|\frac{1}{2}, -\frac{1}{2}\rangle \equiv |-\rangle. \tag{157}$$

The action of the generators on these states is given by

$$
\begin{aligned}
\hat{J}_z|\pm\rangle &= \pm\frac{\hbar}{2}|\pm\rangle, \\
\hat{J}_+|+\rangle &= 0, \\
\hat{J}_-|+\rangle &= \hbar\sqrt{\frac{3}{4} + \frac{1}{4}}|-\rangle = \hbar|-\rangle, \\
\hat{J}_+|-\rangle &= \hbar\sqrt{\frac{3}{4} + \frac{1}{4}}|+\rangle = \hbar|+\rangle, \\
\hat{J}_-|-\rangle &= 0.
\end{aligned}
\tag{158}
$$

From the action of the $\hat{J}_\pm$ operators we find the action of the $\hat{J}_x$ and $\hat{J}_y$ operators as

$$\hat{J}_x|+\rangle = \frac{\hbar}{2}|-\rangle,$$

---

[3]An irreducible representation is the minimal set of states that transform into each other under an arbitrary operation of the group

$$\hat{J}_x|-\rangle = \frac{\hbar}{2}|+\rangle, \tag{159}$$

$$\hat{J}_y|+\rangle = -\frac{\hbar}{2i}|-\rangle,$$

$$\hat{J}_y|-\rangle = \frac{\hbar}{2i}|+\rangle.$$

Equivalently, we can give the matrix elements of the operators as

$$\begin{pmatrix} \langle+|\hat{J}|+\rangle & \langle+|\hat{J}|-\rangle \\ \langle-|\hat{J}|+\rangle & \langle-|\hat{J}|-\rangle \end{pmatrix}. \tag{160}$$

Doing this we have

$$J_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$J_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{161}$$

$$J_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

(Here you might recognize the Pauli matrices!) This matrix notation is very efficient if we want to find matrix elements of powers of operators. For instance, finding the matrix elements of the operator $\hat{O}\hat{K}$ one proceeds as follows. An arbitrary matrix element is

$$\langle i|\hat{O}\hat{K}|k\rangle = \sum_n \langle i|\hat{O}|n\rangle\langle n|\hat{K}|k\rangle, \tag{162}$$

where we have inserted $\hat{1}$ in terms of a complete set of states between the operators. We see that the matrix elements of the product operator is given by the product of the *matrices* $\langle i|\hat{O}|n\rangle$ and $\langle n|\hat{K}|k\rangle$. Thus we can evaluate any power of the operators $\hat{J}_i$ by taking the power of their matrix representatives. To be concrete, let us take $\hat{J}_y$ as an example. We now compute

$$J_y^2 = \left(\frac{\hbar}{2}\right)^2\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \left(\frac{\hbar}{2}\right)^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{163}$$

Now it is easy to generalize to arbitrary power, we get

$$J_y^{2n} = \left(\frac{\hbar}{2}\right)^{2n}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$J_y^{2n+1} = \left(\frac{\hbar}{2}\right)^{2n+1}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{164}$$

This we can use to compute the matrix representative of the rotation operator $\hat{R}_y$ since

$$R_y(\theta) = e^{-\frac{i}{\hbar} J_y \theta} = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar} J_y \theta \right)^n =$$

$$1 - \frac{i\theta}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \frac{1}{2!} \left(-\frac{i\theta}{2} \right)^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \dots . \tag{165}$$

We see that the odd and even dimensional powers decouple when we add up the matrices. The sum is

$$R_y(\theta) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \sum_{n=0}^{\infty} \frac{1}{(2n)!} \left(-\frac{i\theta}{2} \right)^{2n} + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \sum_{n=0}^{\infty} \frac{1}{(2n+1)!} \left(-\frac{i\theta}{2} \right)^{2n+1} \tag{166}$$

and using that

$$\sum_{n=0}^{\infty} \frac{1}{(2n)!} \left(-\frac{i\theta}{2} \right)^{2n} = \cos \frac{\theta}{2},$$

$$\sum_{n=0}^{\infty} \frac{1}{(2n+1)!} \left(-\frac{i\theta}{2} \right)^{2n+1} = -i \sin \frac{\theta}{2}, \tag{167}$$

we get

$$R_y(\theta) = \begin{pmatrix} \cos \frac{\theta}{2} & -\sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{pmatrix}, \tag{168}$$

which we interpret to mean in the operator language that

$$\hat{R}_y(\theta) \left| + \right\rangle = \cos \frac{\theta}{2} \left| + \right\rangle + \sin \frac{\theta}{2} \left| - \right\rangle,$$

$$\hat{R}_y(\theta) \left| - \right\rangle = -\sin \frac{\theta}{2} \left| + \right\rangle + \cos \frac{\theta}{2} \left| - \right\rangle \tag{169}$$

Needless to say, this method to compute the action of an arbitrary rotation becomes very cumbersome when the representations (or the spins if you prefer) become large since the matrices then become very big. There is another nice way to compute the action of a rotation for arbitrary spin. We start by observing that any state state with fixed spin j and *maximal* spin projection $m = j$ can be constructed by putting $2j$ spin $\frac{1}{2}$ states, all with

spin up, next to each other. Another way of saying it is that if we have $2j$ spin $\frac{1}{2}$ particles, all with spin up, the system as a whole is in the state $|j,j\rangle$[4]. Mathematically we would write

$$|+\rangle \otimes |+\rangle \otimes \ldots \otimes |+\rangle = |j,j\rangle. \tag{170}$$

The action of the rotation operator on $|j,j\rangle$ is now given by the fact that we know how a rotation acts on each of the $|+\rangle$ states. (We just computed the $\hat{R}_y$ action, remember). Since we know that the rotation operator does not give us states with different spin, we can classify what we get by computing m. This method can be used to compute the rotation operator for arbitrary spin but let us illustrate the method by using it to compute $\hat{R}_y$ in the spin 1 representation. In that case we have

$$|1,1\rangle = |+\rangle \otimes |+\rangle, \tag{171}$$

which, when we act on it with the rotation operator becomes

$$\hat{R}_y(\theta)|1,1\rangle = \left(\cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}|-\rangle\right) \otimes \left(\cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}|-\rangle\right). \tag{172}$$

We know that the result of a rotation has to be a linear combination of states with the same j but different m so we can write for some constants a, b and c

$$\hat{R}_y(\theta)|1,1\rangle = a|1,1\rangle + b|1,0\rangle + c|1,-1\rangle. \tag{173}$$

Comparing both equations we see that

$$
\begin{aligned}
|1,1\rangle &= |+\rangle \otimes |+\rangle, \\
|1,0\rangle &= \frac{1}{\sqrt{2}}\left(|+\rangle \otimes |-\rangle + |-\rangle \otimes |+\rangle\right), \\
|1,-1\rangle &= |-\rangle \otimes |-\rangle,
\end{aligned}
\tag{174} \tag{175}
$$

and, consequently that

$$
\begin{aligned}
a &= \cos^2\frac{\theta}{2}, \\
b &= \sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}, \\
c &= \sin^2\frac{\theta}{2}.
\end{aligned}
\tag{176} \tag{177}
$$

---

[4]This will be discussed in great detail in the subsection about addition of angular momenta

Since we now know how the $|1,0\rangle$ state looks like, we can find out how a rotation acts on that state

$$\hat{R}_y|1,0\rangle = \frac{1}{\sqrt{2}}\left(\left(\cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}|-\rangle\right)\otimes\left(-\sin\frac{\theta}{2}|+\rangle + \cos\frac{\theta}{2}|-\rangle\right)+\right.$$
$$\left.\left(-\sin\frac{\theta}{2}|+\rangle + \cos\frac{\theta}{2}|-\rangle\right)\otimes\left(\cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}|-\rangle\right)\right),(178)$$

leading to

$$\hat{R}_y|1,0\rangle = -\sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}|1,1\rangle + \left(\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}\right)|1,0\rangle +$$
$$\sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}|1,-1\rangle, \qquad (179)$$

and on the $|1,-1\rangle$ we similarly find

$$\hat{R}_y|1,-1\rangle = \sin^2\frac{\theta}{2}|1,1\rangle - \sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2}|1,0\rangle + \cos^2\frac{\theta}{2}|1,-1\rangle, \qquad (180)$$

leading to the matrix representation of the spin 1 rotation operator

$$\langle 1,m'|\hat{R}_y|1,m\rangle = \begin{pmatrix} \cos^2\frac{\theta}{2} & -\sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2} & \sin^2\frac{\theta}{2} \\ \sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2} & \cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2} & -\sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2} \\ \sin^2\frac{\theta}{2} & \sqrt{2}\sin\frac{\theta}{2}\cos\frac{\theta}{2} & \cos^2\frac{\theta}{2} \end{pmatrix} (181)$$

One can check that this matrix is unitary as it should be.

2.4 The rotation operator in coordinate representation and spherical harmonics

We can now ask what is the coordinate representation of the generators of the rotation operator. We do this in the same way as one can do to find the coordinate representation of the momentum operator. Namely, let us consider the (infinitesimal) action of (say) $\hat{R}_z$ on an arbitrary state

$$\hat{R}_z(\Delta\phi)|\psi\rangle. \qquad (182)$$

The coordinate representation of this is of course

$$\langle\mathbf{x}|\hat{R}_z(\Delta\phi)|\psi\rangle = \left(\langle\psi|\hat{R}_z^\dagger(\Delta\phi)|\mathbf{x}\rangle\right)^* = \left(\langle\psi||\mathrm{x}+\Delta\phi\mathrm{y}, \mathrm{y}-\Delta\phi\mathrm{x}, \mathrm{z}\rangle\right)^* =$$
$$\langle\mathrm{x}+\Delta\phi\mathrm{y}, \mathrm{y}-\Delta\phi\mathrm{x}, \mathrm{z}||\psi\rangle = \langle\mathbf{x}|\psi\rangle + \Delta\phi\left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right)\langle\mathbf{x}|\psi\rangle, (183)$$

where we have used that $\hat{R}$ is unitary so that $\hat{R}^\dagger(\theta) = \hat{R}(-\theta)$. Since $\Delta\phi$ is infinitesimal we can expand $\hat{R}_z(\Delta\phi) = 1 - \frac{i\Delta\phi}{\hbar}\hat{J}_z + \ldots$. Reading off terms up to first order we get that

$$\hat{J}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right). \tag{184}$$

This is the coordinate representation of the generator $\hat{J}_z$. In an exactly analogous fashion we can compute the general formula

$$\hat{J}_i = -i\hbar\epsilon_{ijk}x_j\frac{\partial}{\partial x_k}. \tag{185}$$

In spherical coordinates we can write the action of the (infinitesimal) rotation operator as

$$\begin{aligned}
\hat{R}_x(\epsilon)|\theta,\phi\rangle &= |\theta - \epsilon\sin\phi, \phi - \epsilon\cot\theta\cos\phi\rangle, \\
\hat{R}_y(\epsilon)|\theta,\phi\rangle &= |\theta + \epsilon\cos\phi, \phi - \epsilon\cot\theta\sin\phi\rangle, \\
\hat{R}_z(\epsilon)|\theta,\phi\rangle &= |\theta, \phi + \epsilon\rangle.
\end{aligned} \tag{186}$$

So in that case the coordinate representation becomes

$$\begin{aligned}
\langle\mathbf{x}|\hat{R}_x(\epsilon)|\psi\rangle &= \langle\theta + \epsilon\sin\phi, \phi + \epsilon\cot\theta\cos\phi|\psi\rangle, \\
\langle\mathbf{x}|\hat{R}_y(\epsilon)|\psi\rangle &= \langle\theta - \epsilon\cos\phi, \phi + \epsilon\cot\theta\sin\phi|\psi\rangle, \\
\langle\mathbf{x}|\hat{R}_z(\epsilon)|\psi\rangle &= \langle\theta, \phi - \epsilon|\psi\rangle,
\end{aligned} \tag{187}$$

and Taylor expanding in ϵ we get the coordinate representation of the generators

$$\begin{aligned}
-\frac{i}{\hbar}\langle\mathbf{x}|\hat{J}_x|\psi\rangle &= \left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)\langle\mathbf{x}|\psi\rangle, \\
-\frac{i}{\hbar}\langle\mathbf{x}|\hat{J}_y|\psi\rangle &= \left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)\langle\mathbf{x}|\psi\rangle, \\
-\frac{i}{\hbar}\langle\mathbf{x}|\hat{J}_z|\psi\rangle &= -\frac{\partial}{\partial\phi}\langle\mathbf{x}|\psi\rangle,
\end{aligned} \tag{188}$$

or, in other words

$$J_x = -i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right),$$

$$J_y = -i\hbar \left(\cos\phi \frac{\partial}{\partial\theta} - \cot\theta \sin\phi \frac{\partial}{\partial\phi} \right), \tag{189}$$

$$J_z = -i\hbar \frac{\partial}{\partial\phi}.$$

From these expressions we may also find the coordinate representations of the ladder operators

$$J_\pm = -i\hbar e^{\pm i\phi} \left(\pm i \frac{\partial}{\partial\theta} - \cot\theta \frac{\partial}{\partial\phi} \right). \tag{190}$$

Having the coordinate representation of the operators we may now proceed to find the coordinate representation of the states. In other words, we want to find the wave functions $\langle\theta, \phi| l, m\rangle$. Let us first assume that l is an integer (the half integer case we will be commented on in the end). First we notice that the equation

$$m\hbar\langle\theta, \phi| l, m\rangle = \langle\theta, \phi| \hat{J}_z| l, m\rangle = -i\hbar \frac{\partial}{\partial\phi} \langle\theta, \phi| l.m\rangle, \tag{191}$$

can be immediately solved to tell us that the wave function can be written as

$$\langle\theta, \phi| l, m\rangle = e^{im\phi} f_l(\theta), \tag{192}$$

for some function $f_l(\theta)$. Now we know that for $m = l$ we have

$$0 = \langle\theta, \phi| \hat{J}_+| l, l\rangle = -i\hbar e^{i(l+1)\phi} \left(i \frac{\partial f_l}{\partial\theta} - il \cot\theta f_l \right), \tag{193}$$

or, that

$$\frac{\partial f_l}{\partial\theta} = l \cot\theta f_l. \tag{194}$$

This is a first order differential equation which is easy to solve. The result is

$$f_l = c_l \sin^l \theta, \tag{195}$$

for some normalization constant c_l. To determine it we have to do the integral

$$1 = |c_l|^2 \int \sin\theta d\theta d\phi \, |f_l|^2 = 2\pi |c_l|^2 \int_{-1}^{1} d(\cos\theta) \left(1 - \cos^2\theta \right)^l =$$

$$2\pi |c_l|^2 \frac{\Gamma(l+1)\Gamma(\frac{1}{2})}{\Gamma(l+\frac{3}{2})} = |c_l|^2 \, 4\pi \frac{2^{2l} l!^2}{(2l+1)!}, \tag{196}$$

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leading to

$$c_l = \frac{(-1)^l}{2^l l!} \sqrt{\frac{(2l+1)!}{4\pi}}. \tag{197}$$

Here the choice of the phase factor $(-1)^l$ is purely conventional.

Having the coordinate representation of the highest weight states it is an easy task to find all states. We just proceed as we did before by acting with $\hat{J}_-$ to take us from one state to the other. To be explicit we have

$$\hbar\sqrt{l(l+1) - m(m-1)}\langle\theta,\phi|l,m-1\rangle = \langle\theta,\phi|\hat{J}_-|l,m\rangle =$$
$$-i\hbar e^{-i\phi}\left(-i\frac{\partial}{\partial\theta} - im\cot\theta\right)\langle\theta,\phi|l,m\rangle. \tag{198}$$

The states come out automatically normalized and orthogonal to each other. These wave functions are conventionally denoted $Y_l^m(\theta,\phi) = \langle\theta,\phi|l,m\rangle$ and are called *Spherical harmonics*. They form a complete basis of functions in the angular variables θ and ϕ so that in problems with spherical symmetry they are often used to Fourier expand the functions.

Let us try the method out for $l=1$. In this case we know that

$$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi}. \tag{199}$$

To find Y_1^0 we act with $\hat{J}_-$ to get

$$\hbar\sqrt{2}Y_1^0 = -i\hbar e^{-i\phi}\left(-i\frac{\partial}{\partial\theta} - i\cot\theta\right)(-1)\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi}, \tag{200}$$

giving us

$$Y_1^0 = \sqrt{\frac{3}{16\pi}}\left(\cos\theta + \cos\theta\right) = \sqrt{\frac{3}{4\pi}}\cos\theta. \tag{201}$$

Acting once more we have

$$\hbar\sqrt{2}Y_1^{-1} = -i\hbar e^{-i\phi}\left(-i\frac{\partial}{\partial\theta}\right)\sqrt{\frac{3}{4\pi}}\cos\theta, \tag{202}$$

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which gives us

$$Y_1^{-1} = \sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\phi}. \tag{203}$$

One can try what happens if one assumes that l is half integer. For simplicity let us assume $l = \frac{1}{2}$. Then the above program leads us to the wave function

$$Y_{1/2}^{1/2} = c_{\frac{1}{2}} \sqrt{\sin\theta} e^{\frac{i}{2}\phi}. \tag{204}$$

Acting on this with the $\hat{J}_-$ operator we get

$$Y_{1/2}^{-1/2} = -c_{\frac{1}{2}} \cot\theta \sqrt{\sin\theta} e^{-\frac{i}{2}\phi}. \tag{205}$$

There are (at least) two problems with this (tentative) expression for the half integer wave functions. Firstly it is singular at $\theta = 0, \pi$. Secondly, if we act with $\hat{J}_-$ again *we do not get zero* as we should!! This leads us to the conclusion that only the integer value angular momentum wave functions have a coordinate representation. The half integer wave functions should be understood as an internal property of the system and can not be understood as "something rotating around something else" in normal space.

Finally, let us return to the rotation matrix now that we have found the coordinate representation of the generators. Let us consider a rotation matrix that takes a vector pointing in the z direction and rotates it to a vector that point in the θ, ϕ direction. This can be done by first making a rotation around y with angle θ and then a rotation around z with angle ϕ. In other words, let us look at the operator

$$\hat{R}(\theta, \phi) = \hat{R}_z(\phi)\hat{R}_y(\theta). \tag{206}$$

This operator takes a state $|\hat{z}\rangle \equiv |\theta = 0, \phi\rangle$ and rotates it to the state $|\hat{n}\rangle \equiv |\theta, \phi\rangle$. (Here $\hat{n}$ is a unit vector in the ϕ, θ direction). In formulas we have

$$\hat{R}|\hat{z}\rangle = |\hat{n}\rangle. \tag{207}$$

In this relation we insert a $\hat{1}$ as follows

$$|\hat{n}\rangle = \sum_{l', m'} \hat{R}|l', m'\rangle\langle l', m'|\hat{z}\rangle. \tag{208}$$

Hitting everything from the left with a $\langle l, m|$ gives

$$\langle l, m|\hat{n}\rangle = \sum_{l', m'} \langle l, m|\hat{R}|l', m'\rangle \langle l', m'|\hat{z}\rangle. \tag{209}$$

Since we know that a rotation just mixes the m quantum numbers but not the l quantum numbers, the sum over l' is trivial, and we get

$$\langle l, m|\hat{n}\rangle = \sum_{m'} \langle l, m|\hat{R}|l, m'\rangle \langle l, m'|\hat{z}\rangle. \tag{210}$$

Now we can use that we know the coordinate representation of the $|l, m\rangle$ states. Namely, we know that

$$\langle \hat{n}|l, m\rangle = Y_l^m(\theta, \phi), \tag{211}$$

which in particular means that

$$\langle \hat{z}|l, m\rangle = Y_l^m(\theta = 0, \phi) = \sqrt{\frac{2l + 1}{4\pi}} \delta_{m,0}. \tag{212}$$

Here we have used that we know that $Y_l^m(\theta = 0, \phi)$ vanishes for $m \neq 0$[5] and the explicit form of Y_l^0. This implies that

$$(Y_l^m(\theta, \phi))^* = \sum_{m'} \langle l, m|\hat{R}|l, m'\rangle \left(\sqrt{\frac{2l + 1}{4\pi}} \delta_{m',0} \right)^* = \langle l, m|\hat{R}|l, 0\rangle \sqrt{\frac{2l + 1}{4\pi}} \tag{213}$$

or

$$\langle l, m|\hat{R}|l, 0\rangle = \sqrt{\frac{4\pi}{2l + 1}} (Y_l^m(\theta, \phi))^*, \tag{214}$$

so the matrix elements in the coordinate representation of the rotation matrix are essentially given by the spherical harmonics!

2.5 Addition of angular momentum

We now turn to the problem of how systems of many spins (or angular momenta) behave under rotations. Technically what happens is that a system of many spins does *not* transform irreducibly under rotations and one has to

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[5]This can be seen from the fact that $\hat{J}_z|\hat{z}\rangle = 0$ since then $0 = \langle \hat{z}|\hat{J}_z|l, m\rangle = \hbar m \langle \hat{z}|l, m\rangle$

decompose it into pieces that do transform irreducibly. In more physical words, under a rotation the states of the system get mixed up. However, since the representation is reducible all states do not transform into all other states. It is possible to find subsets of states which transform into each other and only into each other. One reason why this is important is that these subgroups of states have similar physical properties. For instance, if our physics is rotationally invariant we must have that

$$\hat{R}\hat{U}|\psi\rangle = \hat{U}\hat{R}|\psi\rangle, \tag{215}$$

or, in words that we get the same thing if we first rotate the system and then wait a little time or if we first wait and then rotate. this means that $\hat{R}^\dagger \hat{U}\hat{R} = \hat{U}$ or, infinitesimally, that $\left[\hat{\mathbf{J}}, H\right] = 0$. This means that we can find a set of mutually commuting operators $\hat{J}_z, \hat{\mathbf{J}}^2, H$ whose eigenvalues we can use to label the states $|\mathrm{n,j,m}\rangle$. Also, since any rotation on the states $|\mathrm{n,j,m}\rangle$ just mixes the m quantum numbers (this is of course because any $\hat{J}_i$ commutes with both $\hat{\mathbf{J}}^2$ and $\hat{H}$), the j and the n quantum number stay the same, that is *all* states in a given angular momentum representation must have the same energy! This is in general true for the spectrum of any operator that commutes with rotations and since rotations and rotational symmetry is such a common phenomenon in physics, it is very important to investigate how these composite states decompose into states that transform irreducibly.

For instance, let us say that we have a system of two independent spin $\frac{1}{2}$ spins. The Hilbert space of states are given by tensor products of states of the single spins

$$|+\rangle \otimes |+\rangle, \ |+\rangle \otimes |-\rangle, \ |-\rangle \otimes |+\rangle, \ |-\rangle \otimes |-\rangle. \tag{216}$$

We may define operators that act on the whole space as follows

$$\hat{\mathbf{S}} = \hat{\mathbf{S}}_{\mathbf{1}} \otimes \hat{1} + \hat{1} \otimes \hat{\mathbf{S}}_{\mathbf{2}}. \tag{217}$$

Here $\hat{O}\otimes\hat{P}$ means an operator which acts on the state $|\mathrm{a}\rangle\otimes|\mathrm{b}\rangle$ as $\hat{O}|\mathrm{a}\rangle\otimes\hat{P}|\mathrm{b}\rangle$. With some abuse of notation, we often write $\hat{\mathbf{S}}_{\mathbf{1}} \equiv \hat{\mathbf{S}}_{\mathbf{1}} \otimes \hat{1}$ and $\hat{\mathbf{S}}_{\mathbf{2}} \equiv \hat{1} \otimes \hat{\mathbf{S}}_{\mathbf{2}}$. Let us assume that the (rotationally invariant) Hamiltonian of the system is given by

$$\hat{H} = \alpha\hat{\mathbf{S}}_{\mathbf{1}} \cdot \hat{\mathbf{S}}_{\mathbf{2}} = \alpha\left(\hat{S}_{1x} \otimes \hat{S}_{2x} + \hat{S}_{1y} \otimes \hat{S}_{2y} + \hat{S}_{1z} \otimes \hat{S}_{2z}\right). \tag{218}$$

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We can straightforwardly compute the matrix elements of the Hamiltonian as

$$\langle \pm, \pm | \hat{H} | \pm, \pm \rangle = \frac{\alpha \hbar^2}{4} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{219}$$

We see that the Hamilton is not diagonal and hence the $|\pm, \pm \rangle$ states are not the "correct" states to use. We can diagonalize the Hamiltonian with the result that it has one eigenstate $\frac{1}{\sqrt{2}} \left(|+\rangle \otimes |-\rangle - |-\rangle \otimes |+\rangle \right)$ with eigenvalue $-\frac{3\alpha\hbar^2}{4}$ and three eigenstates $|+\rangle \otimes |+\rangle$, $\frac{1}{\sqrt{2}} \left(|+\rangle \otimes |-\rangle + |-\rangle \otimes |+\rangle \right)$ and $|-\rangle \otimes |-\rangle$ which each have eigenvalue $\frac{\alpha\hbar^2}{4}$. The single eigenstate corresponds to a one-dimensional representation of the rotation group (a spin 0 representation) and the group of three eigenstates correspond to a three dimensional representation (a spin 1 rep.). The states in each representations transform into each other under rotations but they do not mix.

Let us now investigate how this work in general. Assume that we have two independent arbitrary spins j_1 and j_2. Again we define the states of the system with the help of the tensor product as $|j_1, m_1 \rangle \otimes |j_2, m_2 \rangle$. We also define the operators

$$\hat{\mathbf{J}} = \hat{\mathbf{J}}_1 \otimes \hat{1} + \hat{1} \otimes \hat{\mathbf{J}}_2 \equiv \hat{\mathbf{J}}_1 + \hat{\mathbf{J}}_2. \tag{220}$$

One can check that the operator thus defined also satisfies the angular momentum algebra

$$\left[\hat{J}_i, \hat{J}_k \right] = i\hbar \epsilon_{ikl} \hat{J}_l. \tag{221}$$

Since we have two spins, the states of the system are completely given by four quantum number. For instance the eigenvalues of $J_{1z}, \hat{\mathbf{J}}_1^2, J_{2z}, \hat{\mathbf{J}}_2^2$ (which leads to the tensor product states $|j_1, m_1 \rangle \otimes |j_2, m_2 \rangle$). However, if one instead takes the four operators $\hat{\mathbf{J}}_1^2, \hat{\mathbf{J}}_2^2, \hat{\mathbf{J}}^2, \hat{J}_z$ one can show that they also mutually commute. For instance, that $\hat{\mathbf{J}}^2$ and $\hat{J}_z$ commutes follows from the fact that they satisfy the usual angular momentum commutation relations. That $\hat{\mathbf{J}}_1^2$ and $\hat{\mathbf{J}}_2^2$ commutes follows from the fact that they act on independent spaces. In formulas we would write

$$\hat{\mathbf{J}}_1^2 \hat{\mathbf{J}}_2^2 \equiv \left(\hat{\mathbf{J}}_1^2 \otimes \hat{1} \right) \left(\hat{1} \otimes \hat{\mathbf{J}}_2^2 \right) = \hat{\mathbf{J}}_1^2 \otimes \hat{\mathbf{J}}_2^2 = \hat{\mathbf{J}}_2^2 \hat{\mathbf{J}}_1^2, \tag{222}$$

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so the commutator is indeed zero. Lastly we see that $\hat{\mathbf{J}}_1^2$ (and similarly also $\hat{\mathbf{J}}_2^2$) commutes with all other operators since $\hat{\mathbf{J}}_1^2$ commutes with any $\hat{J}_{1i}$ (this is the usual relation $\left[\hat{J}_i, \hat{\mathbf{J}}^2\right] = 0$ which holds for any spin) and also with any $\hat{J}_{2i}$ (since they act on different spins).

Thus we can instead choose $\hat{\mathbf{J}}_1^2, \hat{\mathbf{J}}_2^2, \hat{\mathbf{J}}^2, \hat{J}_z$ as the operators which will classify our states. These are states $|j, m, j_1, j_2\rangle$ given by the *total* angular momentum j and its projection m plus the individual spins j_1 and j_2. Notice that the individual spin projections m_1 and m_2 in this basis are not certain. This is because $\left[\hat{\mathbf{J}}^2, \hat{J}_{1z}\right] \neq 0$ (and similarly for $\hat{J}_{2z}$ so that one cannot at the same time give total spin and individual spin projections. To be completely clear, let us give the action of the operators on their eigenstates. First the states which are eigenstates of the individual spins

$$
\begin{aligned}
\hat{\mathbf{J}}_1^2|j_1, m_1; j_2, m_2\rangle &= \hbar^2 j_1(j_1+1)|j_1, m_1; j_2, m_2\rangle, \\
\hat{\mathbf{J}}_2^2|j_1, m_1; j_2, m_2\rangle &= \hbar^2 j_2(j_2+1)|j_1, m_1; j_2, m_2\rangle, \\
\hat{J}_{1z}|j_1, m_1; j_2, m_2\rangle &= \hbar m_1|j_1, m_1; j_2, m_2\rangle, \\
\hat{J}_{2z}|j_1, m_1; j_2, m_2\rangle &= \hbar m_2|j_1, m_1; j_2, m_2\rangle.
\end{aligned}
\tag{223}
$$

$$
\begin{aligned}
\hat{\mathbf{J}}_1^2|j_1, j_2; j, m\rangle &= \hbar^2 j_1(j_1+1)|j_1, j_2; j, m\rangle, \\
\hat{\mathbf{J}}_2^2|j_1, j_2; j, m\rangle &= \hbar^2 j_2(j_2+1)|j_1, j_2; j, m\rangle, \\
\hat{\mathbf{J}}^2|j_1, j_2; j, m\rangle &= \hbar^2 j(j+1)|j_1, j_2; j, m\rangle, \\
\hat{J}_z|j_1, j_2; j, m\rangle &= \hbar m|j_1, j_2; j, m\rangle
\end{aligned}
\tag{224}
$$

To find how a state transforms in the general case what we need to do is to write any state where the individual particles have fixed angular momenta $|j_1, m_1; j_2, m_2\rangle$ in terms of states $|j_1, j_2; j, m\rangle$ which have well defined properties under rotation. Actually we will do the opposite (write $|j_1, j_2; j, m\rangle$ as a linear combination of $|j_1, m_1; j_2, m_2\rangle$) but that does not matter since the transformation is invertible. Also, to avoid cluttering the formulas we will not write j_1 and j_2 everywhere since they are the same for all states and to keep track of which states are of which type we introduce the notation

$$
\begin{aligned}
|j, m\rangle &\equiv |j_1, j_2; j, m\rangle, \\
|m_1, m_2\rangle\rangle &\equiv |j_1, m_1; j_2, m_2\rangle.
\end{aligned}
\tag{225}
$$

Our goal is now to find the relation between these states

$$
|j, m\rangle = \sum_{m_1, m_2} c_{m_1, m_2}|m_1, m_2\rangle\rangle.
\tag{226}
$$

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This we will do in several steps. First let us see that the space of all $|m_1, m_2\rangle$ is finite dimensional with a total number of $(2j_1 + 1)(2j_2 + 1)$ states. This is because each spin (j_1 and j_2) can separately have $2j_1 + 1$ and $2j_2 + 1$ different values of the m quantum number respectively. However, we do not need to sum over all these states in the sum (226) since for fixed m we can use that $\hat{J}_z = \hat{J}_{1z} + \hat{J}_{2z}$ and since we know that

$$
\begin{aligned}
\hat{J}_z |j, m\rangle &= m |j, m\rangle, \\
\left(\hat{J}_{1z} + \hat{J}_{2z} \right) |m_1, m_2\rangle\rangle &= (m_1 + m_2) |m_1, m_2\rangle\rangle,
\end{aligned}
\tag{227}
$$

we immediately see that $\langle\langle m_1, m_2 | j, m\rangle = 0$ if $m \neq m_1 + m_2$. This follows from the fact that

$$
0 = \langle\langle m_1, m_2| \left(\hat{J}_z - \hat{J}_{1z} - \hat{J}_{2z} \right) |j, m\rangle = (m - m_1 - m_2) \langle\langle m_1, m_2 | j, m\rangle. \tag{228}
$$

So for each fixed m on the left hand side of the equation (226) we need only states with $m_1 + m_2 = m$ on the right hand side. It is useful to know exactly how many states with $m_1 + m_2 = m$ there are for each fixed m. To find this we draw the allowed states as points in the (m_1, m_2) plane. Here each diagonal

Figure 4: The allowed states for $j_1 = 7/2$ and $j_2 = 2$

line going from upper left to lower right goes through points with the same value of $m_1 + m_2$. From the picture it is immediately obvious that there is always only one state with maximal value of $m_{\max} = m_1 + m_2 = j_1 + j_2$. When we go down one level to states with $m = j_1 + j_2 - 1$ there are two states, $|j_1 - 1, j_2\rangle\rangle$ and $|j_1, j_2 - 1\rangle\rangle$. Going down in m once more gives us one more state and so on. However, from the picture we see that something happens when we get to the diagonal which hits the lower right corner (that is, assuming that $j_1 \geq j_2$ as is true in the picture, for $m = (j_1 + j_2) - 2j_2 = j_1 - j_2 \geq 0$). After that, going down in m does not give new states but the number of states is constant for each new m. When we get to the diagonal which hits the upper left corner (this is for $m = j_2 - j_1 \leq 0$) something again happens, after that the number of states starts to decrease with one each time until we reach the single state in the lower left corner which has $m = -j_1 - j_2$. Thus we can write for the number of $|m_1, m_2\rangle\rangle$ states (in the $j_1 \geq j_2$ case)

$$
0 \quad \text{if} \quad |m| > j_1 + j_2,
$$

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$$j_1 + j_2 + 1 - |m| \quad \text{if} \quad j_1 + j_2 \geq |m| \geq j_1 - j_2, \qquad (229)$$
$$2j_2 + 1 \quad \text{if} \quad j_1 - j_2 \geq |m| \geq 0.$$

Let us now look at the $|j, m\rangle$ states. From the above discussion we found that the maximal m that we can have is $m_{\text{max}} = j_1 + j_2$. Therefore we see that there can be no $|j, m\rangle$ states with $j > j_1 + j_2$ (if there were, there would be states states with $m = j > j_1 + j_2$ which we just showed that there are not). The question is how many of each states with $j \leq j_1 + j_2$ we can have. Let us start with the *unique* state with maximal $m = j_1 + j_2$. From our discussion we know that it has to be the state $|j_1 + j_2, j_1 + j_2\rangle$ or, in other words, that it is the highest weight state in the $j = j_1 + j_2$ representation. We can get all the states in the representation by acting repeatedly with $\hat{J}_-$ on this state. At the next level with $m = m_{\text{max}} - 1$ we already have one state, namely the state we got by acting with $\hat{J}_-$ on $|j_1 + j_2, j_1 + j_2\rangle$ (that is $|j_1 + j_2, j_1 + j_2 - 1\rangle$). However, we know from our counting of $|m_1, m_2\rangle\rangle$ states that at this level there should be two states. The other state thus have to be the highest weight state in a representation with $j = j_1 + j_2 - 1$, that is a state which we can write as $|j_1 + j_2 - 1, j_1 + j_2 - 1\rangle$. We can continue in this fashion going down in m and filling out the states we find in the figure When we get to the point where $m = j_1 - j_2$ we know that there are no new states at the next m level. This we have to interpret that we do not get any new representations going lower in m. In fact, we can check that what we have is everything by *counting* the states. Since we know that we have $(2j_1 + 1)(2j_2 + 1)$ states of $|m_1, m_2\rangle\rangle$ type, we should have the same number of states of $|j, m\rangle$ type. In fact we have (again we assume $j_1 \geq j_2$)

$$\sum_{j=j_1-j_2}^{j_1+j_2} (2j + 1) = \sum_{j'=1}^{2j_2+1} \left(2\left(j' + j_1 - j_2 - 1\right) + 1\right) = (2j_1 + 1)(2j_2 + 1), \quad (230)$$

so everything seems to work out.

We have thus learned that in a system with two independent angular momenta j_1 and j_2 the total angular momenta j of the system has to satisfy $|j_1 - j_2| \leq j \leq j_1 + j_2$ and that there is one and only one state with a particular value of j and m.

2.6 Clebsh-Gordan coefficients

Let us continue what we did in the last section and try to find explicitly the expansion coefficients c_{m_1, m_2} in the expansion (226). Actually, the notation we will use is $\langle\langle m_1, m_2 | j, m \rangle$. These numbers are called *Clebsh-Gordan* coefficients. Sometimes one also sees in the literature the so called 3j-symbols. They are related to the Clebsh-Gordan coefficients by

$$\langle\langle m_1, m_2 | j, m \rangle = (-1)^{j_1 - j_2 + m} \sqrt{2j+1} \left(\begin{array}{ccc} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{array} \right), \qquad (231)$$

but we will not use them here. The Clebsh-Gordan coefficients are conventionally chosen to be real so that

$$\langle\langle m_1, m_2 | j, m \rangle = \langle j, m | m_1, m_2 \rangle\rangle. \qquad (232)$$

Also, since the states $|m_1, m_2 \rangle\rangle$ or the states $|j, m\rangle$ form a complete basis in the subspace of states of two angular momenta j_1 and j_2 we have the following relations (in this subspace)

$$\hat{1} = \sum_{m_1, m_2} |m_1, m_2 \rangle\rangle\langle\langle m_1, m_2 | = \sum_{j,m} |j, m\rangle\langle j, m|, \qquad (233)$$

where the sums are over the "allowed" values of the eigenvalues only. This leads to the following relations between the Clebsh-Gordan coefficients

$$\delta_{j,j'} \delta_{m,m'} = \langle j, m | j', m' \rangle = \sum_{m_1, m_2} \langle j, m | m_1, m_2 \rangle\rangle\langle\langle m_1, m_2 | j', m' \rangle =$$

$$\sum_{m_1, m_2} \langle\langle m_1, m_2 | j, m \rangle\langle\langle m_1, m_2 | j', m' \rangle, \qquad (234)$$

and similarly

$$\delta_{m_1, m_1'} \delta_{m_2, m_2'} = \langle\langle m_1, m_2 | m_1', m_2' \rangle\rangle = \sum_{j,m} \langle\langle m_1, m_2 | j, m \rangle\langle j, m | m_1', m_2' \rangle\rangle =$$

$$\sum_{j,m} \langle\langle m_1, m_2 | j, m \rangle\langle\langle m_1', m_2' | j, m \rangle. (235)$$

It is certainly possible to calculate arbitrary formulas for the Clebsh-Gordan coefficients. For instance, the 3j-symbols are often listed in tables. However, I will not present such a formula which is often hard to read and does not say very much. Instead I will give you a prescription how to calculate

them yourselves in any given case. The method is built on the way we calculated the allowed states in the previous section. To be concrete, let us use our example of the previous section of adding a spin $\frac{7}{2}$ and a spin 2. The state with the highest value of $m = j_1 + j_2$ ($\frac{11}{2}$ in our case) is given to us for free. Since there is only one $|j, m\rangle$ state as well as $|m_1, m_2\rangle\rangle$ state they must be equal. That is

$$|\frac{11}{2}, \frac{11}{2}\rangle = |\frac{7}{2}, 2\rangle\rangle, \tag{236}$$

and the Clebsh-Gordan coefficient is of course

$$\langle\langle \frac{7}{2}, 2|\frac{11}{2}, \frac{11}{2}\rangle = 1. \tag{237}$$

Notice that the arbitrary phase factor that could have appeared in (236) was eliminated by requiring that the Clebsh-Gordan coefficients are real (and in this case positive). To find the other states in the $\frac{11}{2}$ representation we can act on (236) with the lowering operator $\hat{J}_- = \hat{J}_x - i\hat{J}_y$. The action on the left hand side is easy to find. Using the regular formulas we get

$$\hat{J}_-|\frac{11}{2}, \frac{11}{2}\rangle = \hbar\sqrt{11}|\frac{11}{2}, \frac{9}{2}\rangle. \tag{238}$$

To find the action of $\hat{J}_-$ on the right hand side of (236) we have to use that

$$\hat{J}_- = \hat{J}_x - i\hat{J}_y = \left(\hat{J}_{1x} + \hat{J}_{2x}\right) - i\left(\hat{J}_{1y} + \hat{J}_{2y}\right) = \hat{J}_{1-} + \hat{J}_{2-}, \tag{239}$$

which tells us that

$$\hat{J}_-|\frac{7}{2}, 2\rangle\rangle = \left(\hat{J}_{1-}|\frac{7}{2}, \frac{7}{2}\rangle\right) \otimes |2, 2\rangle + |\frac{7}{2}, \frac{7}{2}\rangle \otimes \left(\hat{J}_{2-}|2, 2\rangle\right) =$$
$$\left(\hbar\sqrt{7}|\frac{7}{2}, \frac{5}{2}\rangle\right) \otimes |2, 2\rangle + |\frac{7}{2}, \frac{7}{2}\rangle \otimes \left(\hbar 2|2, 1\rangle\right) = \hbar\left(\sqrt{7}|\frac{5}{2}, 2\rangle\rangle + 2|\frac{7}{2}, 1\rangle\rangle\right). \tag{240}$$

Equating the left and right hand sides we find

$$|\frac{11}{2}, \frac{9}{2}\rangle = \sqrt{\frac{7}{11}}|\frac{5}{2}, 2\rangle\rangle + \sqrt{\frac{4}{11}}|\frac{7}{2}, 1\rangle\rangle, \tag{241}$$

which gives us the non-zero Clebsh-Gordan coefficients

$$\langle\langle \frac{5}{2}, 2|\frac{11}{2}, \frac{9}{2}\rangle = \sqrt{\frac{7}{11}},$$
$$\langle\langle \frac{7}{2}, 1|\frac{11}{2}, \frac{9}{2}\rangle = \sqrt{\frac{4}{11}}. \tag{242}$$

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It is gratifying to see that the state (241) comes out automatically normalized as it should. Using $\hat{J}_-$ we could now continue to find all 12 states in the spin $\frac{11}{2}$ representation but we will not do so here. Instead let us look at the next to highest $m = j_1 + j_2 - 1$ ($\frac{9}{2}$ in our case). We know that there are two states with this value of m but we have only found one so far (241). We also know that the second state is the highest weight state in a new (in this case spin $\frac{9}{2}$ representation. We should therefore be able to write

$$|\frac{9}{2}, \frac{9}{2}\rangle = a|\frac{5}{2}, 2\rangle\rangle + b|\frac{7}{2}, 1\rangle\rangle, \tag{243}$$

for some unknown constants a and b. The constants we can determine by acting with $\hat{J}_+$ on both sides of the equation. Exactly similar to how we found the $\hat{J}_-$ action we now find

$$0 = \hat{J}_+|\frac{9}{2}, \frac{9}{2}\rangle = \hbar\left(a\sqrt{7}|\frac{7}{2}, 2\rangle\rangle + b2|\frac{7}{2}, 2\rangle\rangle\right). \tag{244}$$

In order for this to be true we have to have

$$\sqrt{7}a + 2b = 0 \tag{245}$$

Together with the requirement that the state should be normalized we get

$$|\frac{9}{2}, \frac{9}{2}\rangle = \sqrt{\frac{7}{11}}|\frac{7}{2}, 1\rangle\rangle - \sqrt{\frac{4}{11}}|\frac{5}{2}, 2\rangle\rangle, \tag{246}$$

where we again have fixed an arbitrary phase by the requirement that the Clebsh-Gordan coefficients should all be real and by the convention that the state with the maximum m_1 value should also be positive. Notice that this state comes out automatically orthogonal to (241) as it should. This result gives rise to the non-zero Clebsh-Gordan coefficients

$$\langle\langle\frac{7}{2}, 1|\frac{9}{2}, \frac{9}{2}\rangle = \sqrt{\frac{7}{11}},$$
$$\langle\langle\frac{5}{2}, 2|\frac{9}{2}, \frac{9}{2}\rangle = -\sqrt{\frac{4}{11}}. \tag{247}$$

By using the ladder operators $\hat{J}_\pm$ in this way we can go on and find all the non-zero Clebsh-Gordan coefficients. You can as an exercise try to find the expression for the $|\frac{3}{2}, \frac{1}{2}\rangle$ state in terms of the $|m_1, m_2\rangle\rangle$ states. The calculation is not too difficult. You need to act once with $\hat{J}_+$ once with $\hat{J}_-$ and use the normalization condition. The answer I believe should be
$|\frac{3}{2}, \frac{1}{2}\rangle = \sqrt{\frac{3}{14}}|\frac{5}{2}, -2\rangle\rangle - \sqrt{\frac{2}{7}}|\frac{3}{2}, -1\rangle\rangle + \sqrt{\frac{9}{35}}|\frac{1}{2}, 0\rangle\rangle - \sqrt{\frac{6}{35}}|-\frac{1}{2}, 1\rangle\rangle + \sqrt{\frac{1}{14}}|-\frac{3}{2}, 2\rangle\rangle.$

2.6.1 An application

As an application of the above formalism, let us consider a system of two nucleons (a nucleon is particle that you find in the nucleus of the atom, that is a neutron or a proton). The system is described by the relative coordinate of the two nucleons $\mathbf{r}$ and furthermore each of the two nucleons carry spin $\frac{1}{2}$ (let us call the spin operators acting on each spin $\hat{\mathbf{S}}_1$ and $\hat{\mathbf{S}}_2$ respectively). The nucleons interact in several ways. First of all there is a regular (strong) force between them, second of all their spins interact with the orbital angular momenta $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ and finally there is an interaction between the spins themselves. The system should be rotationally invariant so that the Hamiltonian should be rotationally invariant. If the mass of a nucleon is M and with the definition $\hat{\mathbf{S}} = \hat{\mathbf{S}}_1 + \hat{\mathbf{S}}_2$ then we can write the Hamiltonian as

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{M} + V_1(r) + V_2(r)\hat{\mathbf{L}} \cdot \hat{\mathbf{S}} + V_3(r)\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2, \qquad (248)$$

for some functions $V_i(r)$. $V_1(r)$ describe the force interaction, $V_2(r)$ describes the spin-orbit interaction and $V_3(r)$ describes the spin-spin interaction. There are other possible interaction terms but we will not consider them here. This is a pretty complicated system so it is important to find the "correct" variables in which the description is as simple as possible. To do this we will try to find as many (hermitian) operators as possible which commute with the Hamiltonian. Then these can be used to classify the eigenstates, or in other words, using eigenstates of these operators, the Hamiltonian will take the simplest possible form. We see that the Hamiltonian commutes with the operators $\hat{\mathbf{L}}^2, \hat{\mathbf{S}}_1^2, \hat{\mathbf{S}}_2^2, \hat{\mathbf{S}}^2$ and defining the operator $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$ we see that the Hamiltonian also commutes with $\hat{\mathbf{J}}^2$ and $\hat{J}_z$. Notice however that it does *not* commute with the operators $\hat{S}_{1z}, \hat{S}_{2z}$ or $\hat{L}_z$ since the $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}$ term contains for instance $\hat{L}_x(\hat{S}_{1x} + \hat{S}_{2x})$. We can therefore use the states

$$|\mathrm{l}, \mathrm{s}; \mathrm{j}, \mathrm{m}\rangle, \qquad (249)$$

which are eigenstates of $\hat{\mathbf{L}}^2, \hat{\mathbf{S}}^2, \hat{\mathbf{J}}^2, \hat{J}_z$ (and also of $\hat{\mathbf{S}}_1^2, \hat{\mathbf{S}}_2^2$) as our basis. Now we use that we can write

$$\begin{aligned} 2\hat{\mathbf{S}}_1 \cdot \hat{\mathbf{S}}_2 &= \hat{\mathbf{S}}^2 - \hat{\mathbf{S}}_1^2 - \hat{\mathbf{S}}_2^2 \\ 2\hat{\mathbf{L}} \cdot \hat{\mathbf{S}} &= \hat{\mathbf{J}}^2 - \hat{\mathbf{L}}^2 - \hat{\mathbf{S}}^2. \end{aligned} \qquad (250)$$

That means that when we act with the Hamiltonian on one of the basis states we get

$$\hat{H}|\text{l},\text{s};\text{j},\text{m}\rangle =$$

$$\left(\frac{\hat{\mathbf{p}}^2}{M} + V_1(r) + \frac{\hbar^2}{2}V_2(r)\left(j(j+1) - l(l+1) - s(s+1)\right) + \right. \tag{251}$$

$$\left. \frac{\hbar^2}{2}V_3(r)\left(s(s+1) - s_1(s_1+1) - s_2(s_2+1)\right)\right)|\text{l},\text{s};\text{j},\text{m}\rangle. \tag{252}$$

From our discussion about addition of angular momenta we know that since $s_1 = s_2 = \frac{1}{2}$, s can be only 0 or 1. Thus when the Hamiltonian acts on $s = 0$ states we have

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{M} + V_1(r) + \frac{\hbar^2}{2}V_2(r)\left(j(j+1) - l(l+1)\right) - \frac{3\hbar^2}{4}V_3(r), \tag{253}$$

and when it acts on $s = 1$ states we have

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{M} + V_1(r) + \frac{\hbar^2}{2}V_2(r)\left(j(j+1) - l(l+1) - 2\right) + \frac{\hbar^2}{4}V_3(r), \tag{254}$$

which is a considerable simplification. Thus we will try to find eigenfunctions of the Hamiltonian which are also eigenstates of $\hat{\mathbf{L}}^2, \hat{\mathbf{S}}^2, \hat{\mathbf{J}}^2$ and $\hat{J}_z$ An ansatz would be

$$|\psi\rangle = |\text{E}_{\text{l},\text{s},\text{j},\text{m}}\rangle \otimes |\text{l},\text{s};\text{j},\text{m}\rangle. \tag{255}$$

The state $|\text{E}_{\text{l},\text{s},\text{j},\text{m}}\rangle$ contains all the radial dependence of the wave function while the $|\text{l},\text{s};\text{j},\text{m}\rangle$, since it contains all the information about rotations, contain all the angular dependence. We can now take the coordinate representation of the eigenvalue equation

$$\langle\mathbf{x}|\hat{H}|\psi\rangle = \hbar^2 \sum_{m_l, m_s} \left\{-\frac{1}{M}\left(\frac{1}{r}\frac{d^2}{dr^2}r - \frac{l(l+1)}{r^2}\right) + V_{\text{l},\text{s},\text{j}}\right\} \times$$

$$\text{f}_{\text{l},\text{s},\text{j},\text{m}}(r)\langle\theta, \phi|\text{l},\text{s},\text{j},\text{m}\rangle, \tag{256}$$

where $f_{l,s,j,m}(r) = \langle\text{r}|\text{E}_{\text{l},\text{s},\text{j},\text{m}}\rangle$ is the coordinate representation of radial part of the wave function and where $V_{l,s,j}(r)$ is an effective potential of the form

$$V_{l,s,j} = \frac{1}{\hbar^2}V_1(r) + \frac{V_2(r)}{2}\left(j(j+1) - l(l+1) - s(s+1)\right)$$

$$+ \frac{V_3(r)}{2}\left(s(s+1) - \frac{3}{2}\right). \tag{257}$$

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To derive this result we also used that the coordinate representation of the operator $\hat{\mathbf{p}}^2$ can be written

$$\langle \mathbf{x}|\hat{\mathbf{p}}^2|\psi\rangle = -\frac{\hbar^2}{r}\frac{d^2}{dr^2}\left(r\langle \mathbf{x}|\psi\rangle\right) + \frac{1}{r^2}\langle \mathbf{x}|\hat{\mathbf{L}}^2|\psi\rangle, \tag{258}$$

and that the action of $\hat{\mathbf{L}}^2$ on the state is known. When we want to find the eigenfunctions of the Hamiltonian what is left for us to do is therefore solve the one dimensional differential equation

$$\left(-\frac{1}{M}\frac{1}{r}\frac{d^2}{dr^2}r + V_{l,s,j}(r)\right)f_{l,s,j,m}(r) = \frac{E}{\hbar^2}f_{l,s,j,m}(r). \tag{259}$$

where the potential depends on the quantum number j, s and l

$$\begin{aligned}
V(r) &= \left(\frac{V_1}{\hbar^2} - \frac{3V_3}{4}\right) + l(l+1)\left(\frac{1}{Mr^2} - \frac{V_2}{2}\right)\\
&\quad + s(s+1)\left(\frac{V_3}{2} - \frac{V_2}{2}\right) + j(j+1)\frac{V_2}{2}.
\end{aligned} \tag{260}$$

Since the effective potential do not depend on the quantum number m the wave functions $f_{l,s,j,m}$ will also not depend on m and the spectrum will be degenerate in m, that is, each energy eigenvalue will be $(2j+1)$ times degenerate.

To find the explicit angular dependence of the states $\langle \theta,\phi|l,s;j,m\rangle$ one has to use the Clebsh-Gordan composition of the state $|l,s;j,m\rangle = |j,m\rangle$ into the $|l,s;m_l,m_s\rangle = |m_l,m_s\rangle\rangle$ basis. Namely, since we know $\langle \theta,\phi|l,m_l\rangle = Y_l^{m_l}(\theta,\phi)$ we have

$$\langle \theta,\phi|l,s;j,m\rangle = \sum_{m_l,m_s} Y_l^{m_l}(\theta,\phi)|s,m_s\rangle\langle\langle m_l,m_s|j,m\rangle, \tag{261}$$

where the last factor are the Clebsh-Gordan coefficients for the decomposition of the $|j.m\rangle$ states into $|m_l,m_s\rangle\rangle$ states.

2.7 Tensor operators

Until now we have been interested in how states transform under rotations. Now we will take a look at how *operators* transform under rotations. A tensor operator is really a set of operators whose expectation values transform into each other in exactly the same way as classical tensors when one performs

a rotation of the system. The simplest case is a *scalar* operator. In this case the set contains only one operator which consequently transforms into itself under rotation (i.e. it does not transform at all). The simplest non-trivial example is given by a *vector* operator. It is given by a set of three operators, let us call them $\hat{V}_x, \hat{V}_y$ and $\hat{V}_z$, or, collectively as $\hat{V}_i$. To find out how it transforms under rotations we first notice that under a rotation any state $|\alpha\rangle$ transforms into $\hat{R}|\alpha\rangle$ and thus we find the quantum mechanical transformation of an arbitrary expectation value as

$$\langle\alpha|\hat{V}_i|\alpha\rangle \rightarrow \langle\alpha|\hat{R}^\dagger\hat{V}_i\hat{R}|\alpha\rangle. \tag{262}$$

The requirement that this should transform as a classical vector for the expectation value of *any* state $|\alpha\rangle$ now gives us

$$\hat{R}^\dagger\hat{V}_i\hat{R} = \sum_k R_i{}^k\hat{V}_k, \tag{263}$$

where $R_i{}^k$ is the *classical* rotation matrix. To be concrete, let us do this explicitly for an infinitesimal rotation around the z-axis. We have

$$\begin{aligned}
\left(1 + \frac{i}{\hbar}\epsilon\hat{J}_z\right)\hat{V}_x\left(1 - \frac{i}{\hbar}\epsilon\hat{J}_z\right) &= \hat{V}_x - \epsilon\hat{V}_y, \\
\left(1 + \frac{i}{\hbar}\epsilon\hat{J}_z\right)\hat{V}_y\left(1 - \frac{i}{\hbar}\epsilon\hat{J}_z\right) &= \hat{V}_y + \epsilon\hat{V}_x, \\
\left(1 + \frac{i}{\hbar}\epsilon\hat{J}_z\right)\hat{V}_z\left(1 - \frac{i}{\hbar}\epsilon\hat{J}_z\right) &= \hat{V}_z.
\end{aligned} \tag{264}$$

Expanding and equating terms of order ϵ on both sides gives us the commutation relations

$$\begin{aligned}
\left[\hat{J}_z, \hat{V}_x\right] &= i\hbar\hat{V}_y, \\
\left[\hat{J}_z, \hat{V}_y\right] &= -i\hbar\hat{V}_x, \\
\left[\hat{J}_z, \hat{V}_z\right] &= 0.
\end{aligned} \tag{265}$$

The same calculation for infinitesimal rotations around the x and the y axis gives the complete commutation relations

$$\left[\hat{J}_i, \hat{V}_j\right] = i\hbar\epsilon_{ijk}\hat{V}_k. \tag{266}$$

In fact, we can now turn things around and take this as the definition of a vector operator. Here it is interesting to observe that the *classical* rotation

matrix is the same as the spin 1 representation of the *quantum* operator $\hat{R}^\dagger$ (notice the hermitian conjugation) although written in complex notation. Namely, if we reshuffle the components of $\hat{V}_i$ a bit and define

$$
\begin{aligned}
\hat{V}_{+1} &= -\frac{1}{\sqrt{2}}\left(V_x + iV_y\right), \\
\hat{V}_0 &= V_z, \\
\hat{V}_{-1} &= \frac{1}{\sqrt{2}}\left(V_x - iV_y\right),
\end{aligned}
\tag{267}
$$

we can write the classical rotation as

$$
\hat{R}^\dagger \hat{V}_q \hat{R} = \sum_{q'=-1}^{1} \hat{V}_{q'} \, \langle 1, q'|\hat{R}^\dagger|1, q\rangle.
\tag{268}
$$

Let us try it explicitly in the rotation around the z-axis that we computed in (264). Classically we can compute that the rotation should give

$$
\begin{aligned}
\hat{V}_{+1} &\rightarrow \hat{V}_{+1} + i\epsilon\hat{V}_{+1}, \\
\hat{V}_0 &\rightarrow \hat{V}_0, \\
\hat{V}_{-1} &\rightarrow \hat{V}_{-1} - i\epsilon\hat{V}_{-1},
\end{aligned}
\tag{269}
$$

which we can write in matrix form

$$
\begin{pmatrix} \hat{V}_{+1} & \hat{V}_0 & \hat{V}_{-1} \end{pmatrix} \rightarrow \begin{pmatrix} \hat{V}_{+1} & \hat{V}_0 & \hat{V}_{-1} \end{pmatrix} \begin{pmatrix} 1+i\epsilon & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1-i\epsilon \end{pmatrix},
\tag{270}
$$

in which we indeed recognize the infinitesimal form of the spin 1 representation of the rotation matrix $\hat{R}_z^\dagger = e^{\frac{i}{\hbar}\hat{J}_z\epsilon} \approx 1 + \frac{i}{\hbar}\hat{J}_z\epsilon$. This property can similarly be checked for the other rotations around the x or the y axis. (Do it as an exercise!)

We may now similarly define other types of tensor operators. For instance, a classical tensor $T_{ijk...}$ transform under classical rotations as

$$
T_{ijk...} \rightarrow \sum_{i'j'k'} R_i^{\;i'} R_j^{\;j'} R_k^{\;k'} \cdots T_{i'j'k'...},
\tag{271}
$$

so the definition of a tensor operator would be that

$$
\hat{R}^\dagger \hat{T}_{ijk...} \hat{R} = \sum_{i'j'k'} R_i^{\;i'} R_j^{\;j'} R_k^{\;k'} \cdots \hat{T}_{i'j'k'...},
\tag{272}
$$

or, infinitesimally

$$\left[\hat{J}_a, \hat{T}_{ijk\ldots}\right] = i\hbar \left(\epsilon_{ai}{}^{i'}\hat{T}_{i'jk\ldots} + \epsilon_{aj}{}^{j'}\hat{T}_{ij'k\ldots} + \epsilon_{ak}{}^{k'}\hat{T}_{ijk'\ldots} + \ldots\right). \qquad (273)$$

This is all fine except for one thing. It turns out that the components of an arbitrary tensor operator $\hat{T}_{ijk\ldots}$ do not transform into each other *irreducibly*. That is, there are subgroups of components which transform into each other and do not mix with the other components. This indicates that the tensor operators defined in this way are not the tensors we should use if we want to consider operators that transform as simple as possible under rotations. In other words, we need to decompose the tensor operators as defined above into their irreducible subsets just as we needed to decompose the angular momentum states into irreducible subsets. However, the example above with the vector operator teaches us how to find the irreducible subsets. Namely, we need tensors such that the classical rotation can be written using an *irreducible* representation of the rotation operator. That is that we can write

$$\hat{T}_q^{(k)} \rightarrow \sum_{q'} \hat{T}_{q'}^{(k)} \langle k, q' | \hat{R}^\dagger | k, q \rangle, \qquad (274)$$

for some fixed k so that the rotation operator is in the k (that is the $2k+1$ dimensional) representation. A tensor $\hat{T}_q^{(k)}$ that transforms in this irreducible way is called an *irreducible* tensor or a *spherical* tensor. Thus, the defining equation for spherical tensors of rank k is

$$\hat{R}^\dagger \hat{T}_q^{(k)} \hat{R} = \sum_{q'} \hat{T}_{q'}^{(k)} \langle k, q' | \hat{R}^\dagger | k, q \rangle, \qquad (275)$$

or infinitesimally

$$\left[\hat{J}_i, \hat{T}_q^{(k)}\right] = \sum_{q'} \hat{T}_{q'}^{(k)} \langle k, q' | \hat{J}_i | k, q \rangle. \qquad (276)$$

Since the matrix elements of $\hat{J}_\pm$ are nicer, let us write the commutation relations in terms of them as

$$\left[\hat{J}_\pm, \hat{T}_q^{(k)}\right] = \sum_{q'} \hat{T}_{q'}^{(k)} \langle k, q' | \hat{J}_\pm | k, q \rangle =$$
$$\sum_{q'} \hbar\sqrt{k(k+1) - q(q \pm 1)} \hat{T}_{q'}^{(k)} \langle k, q' | k, q \pm 1 \rangle, \qquad (277)$$

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and using the orthogonality of the angular momentum eigenstates we have

$$\left[\hat{J}_\pm, \hat{T}_q^{(k)}\right] = \hbar\sqrt{k(k+1) - q(q\pm 1)}\hat{T}_{q\pm 1}^{(k)}. \tag{278}$$

For $\hat{J}_z$ we similarly have

$$\left[\hat{J}_z, \hat{T}_q^{(k)}\right] = \sum_{q'} \hat{T}_{q'}^{(k)}\langle k, q'|\hat{J}_z|k, q\rangle = \sum_{q'}\hat{T}_{q'}^{(k)}\hbar q\langle k, q'|k, q\rangle = \hbar q\hat{T}_q^{(k)}. \tag{279}$$

Thus we see that the commutation relations are very similar to the way the angular momentum operators act on the angular momentum eigenstates.

One may ask if it is always possible to decompose an ordinary tensor operator transforming according to (271) into "sub tensors" transforming according to (274). That this is true one may argue as follows. We know that each $R_i{}^{i'}$ is a spin 1 representation of the rotation operator. Thus $T_{ijk\ldots}$ actually transform like a collection of independent spin 1 spins so that the problem of decomposing the tensor is the same as finding the total angular momenta when one adds a number of independent spin 1 spins. This we have shown how to do in the previous section, it is essentially done by finding the Clebsh-Gordan coefficients. Let us illustrate this with a simple example. We can make a two index tensor by multiplying two vectors. That is define

$$T_{ij} = U_i V_j. \tag{280}$$

This is usually decomposed in the following suggestive way

$$T_{ij} = \frac{\mathbf{U}\cdot\mathbf{V}}{3}\delta_{ij} + \frac{(U_iV_j - V_iU_j)}{2} + \left(\frac{(U_iV_j + V_iU_j)}{2} - \frac{\mathbf{U}\cdot\mathbf{V}}{3}\delta_{ij}\right). \tag{281}$$

The first term in this "expansion" is just the scalar product of the two vectors $\mathbf{U}$ and $\mathbf{V}$. It is clear that it is *invariant* under rotations. Thus, it forms an invariant subgroup of tensor components. The second term is nothing but the cross product $\mathbf{U} \times \mathbf{V}$ which transforms like a vector so it also forms an irreducible subcomponent. The third term is a symmetric and traceless tensor. It can be shown to form a spin 2 representation. Now let us try to see the same thing by using the "sum of spins" idea. The spin 0 wave function that we get when we add two spin 1 spins we find using the methods introduced earlier to be

$$|0, 0\rangle = \frac{1}{\sqrt{3}}\left(|1, -1\rangle\rangle - |0, 0\rangle\rangle + |-1, 1\rangle\rangle\right). \tag{282}$$

Thus we expect that the combination

$$T_{+1,-1} - T_{0,0} + T_{-1,+1}, \tag{283}$$

should transform like a scalar (that is, not transform at all). Using (267) we can see that this combination is indeed equal to (minus) the scalar product of **U** and **V** so that this is indeed true. The other components can be verified similarly (exercise!).

2.8 The Wigner-Eckart theorem

So far we have been looking at how the spherical tensor operators transform under rotations. Now let us take a look at how they act on states. This information is contained in (infinitesimal version of) their definition as derived in the previous section

$$
\begin{aligned}
\left[\hat{J}_{\pm}, \hat{T}_q^{(k)}\right] &= \hbar\sqrt{k(k+1) - q(q\pm 1)}\hat{T}_{q\pm 1}^{(k)}, \\
\left[\hat{J}_z, \hat{T}_q^{(k)}\right] &= \hbar q \hat{T}_q^{(k)}.
\end{aligned}
\tag{284}
$$

Using these relations we may first of all, find the rotational properties of states created by $\hat{T}_q^{(k)}$ acting on states that do not transform under rotations (that is on the state $|0,0\rangle$). Namely, using the commutation relations above and that $\hat{J}$ acts trivially on $|0,0\rangle$, we have

$$
\begin{aligned}
\hat{J}_{\pm}\hat{T}_q^{(k)}|0,0\rangle &= \left[\hat{J}_{\pm}, \hat{T}_q^{(k)}\right]|0,0\rangle = \hbar\sqrt{k(k+1) - q(q\pm 1)}\hat{T}_{q\pm 1}^{(k)}|0,0\rangle, \\
\hat{J}_z\hat{T}_q^{(k)}|0,0\rangle &= \left[\hat{J}_z, \hat{T}_q^{(k)}\right]|0,0\rangle = \hbar q \hat{T}_q^{(k)}|0,0\rangle.
\end{aligned}
\tag{285}
$$

Thus we see that the angular momentum operators act on $\hat{T}_q^{(k)}|0,0\rangle$ in exactly the same way as on a state $|j, m\rangle$ with $j = k$ and $m = q$. That also tells us something about the matrix elements of the operator $\hat{T}_q^{(k)}$. Namely, since $\langle j, m|k, q\rangle \neq 0$ only if $j = k$ and $q = m$ we have

$$\langle j, m|\hat{T}_q^{(k)}|0,0\rangle \neq 0 \ \text{ iff } \ j = k, \ m = q. \tag{286}$$

This (including the generalization to other states than $|0,0\rangle$) is essentially the Wigner-Eckart theorem. To be able to state it in all generality, we need

now study what $\hat{T}_q^{(k)}$ does to an arbitrary state $|j,m\rangle$. In the same way as above we find

$$\hat{J}_z\hat{T}_q^{(k)}|j,m\rangle = \hat{T}_q^{(k)}\hat{J}_z|j,m\rangle + \left[\hat{J}_z,\hat{T}_q^{(k)}\right]|j,m\rangle =$$
$$\hbar m\hat{T}_q^{(k)}|j,m\rangle + \hbar q\hat{T}_q^{(k)}|j,m\rangle \qquad (287)$$
$$\hat{J}_\pm\hat{T}_q^{(k)}|j,m\rangle = \hat{T}_q^{(k)}\hat{J}_\pm|j,m\rangle + \left[\hat{J}_\pm,\hat{T}_q^{(k)}\right]|j,m\rangle =$$
$$\hbar\sqrt{j(j+1)-m(m\pm1)}\hat{T}_q^{(k)}|j,m\pm1\rangle +$$
$$\hbar\sqrt{k(k+1)-q(q\pm1)}\hat{T}_{q\pm1}^{(k)}|j,m\rangle.$$

Compare this to how the angular momentum operators act on a product state $|j,m\rangle \otimes |k,q\rangle$ (that is, on a state describing two independent spins, one with spin j and one with spin k). Then we have

$$\hat{J}_z\left(|j,m\rangle \otimes |k,q\rangle\right) = \left(\hat{J}_z|j,m\rangle\right) \otimes |k,q\rangle + |j,m\rangle \otimes \left(\hat{J}_z|k,q\rangle\right) =$$
$$(\hbar m + \hbar q)\,|j,m\rangle \otimes |k,q\rangle, \qquad (288)$$
$$\hat{J}_\pm\left(|j,m\rangle \otimes |k,q\rangle\right) = \left(\hat{J}_\pm|j,m\rangle\right) \otimes |k,q\rangle + |j,m\rangle \otimes \left(\hat{J}_\pm|k,q\rangle\right) =$$
$$\hbar\sqrt{j(j+1)-m(m\pm1)}|j,m\pm1\rangle \otimes |k,q\rangle +$$
$$\hbar\sqrt{k(k+1)-q(q\pm1)}|j,m\rangle \otimes |k,q\pm1\rangle. \qquad (289)$$

Comparing these two results we see that they are exactly analogous!! This means that we can expect that the state $\hat{T}_q^{(k)}|j,m\rangle$ behaves (from the point of view of rotations) like the product state $|m,q\rangle\rangle = |j,m\rangle \otimes |k,q\rangle$. From our previous discussion we know that we can decompose this into irreducible components

$$|J,M\rangle = \sum_{m,q} c_{m,q}|m,q\rangle\rangle, \qquad (290)$$

where the constants $c_{m,q}$ are the Clebsh-Gordan coefficients. Thus we may for instance expect that $\langle J,M|\hat{T}_q^{(k)}|j,m\rangle \neq 0$ iff the Clebsh-Gordan coefficient $\langle\langle m,q|J,M\rangle$ is non-zero. As we know, this requires that $|j-k| \leq J \leq j+k$ and $M = m+q$.

Let us now try to prove this a little bit more carefully. To this end define

$$|A(J,M)\rangle = \sum_{q',m'} \hat{T}_{q'}^{(k)}|j,m'\rangle\langle\langle m',q'|J,M\rangle. \qquad (291)$$

Then we have

$$\sum_{J,M} |A(J, M)\rangle\langle J, M|m, q\rangle\rangle = \tag{292}$$

$$\sum_{m',q'} \hat{T}_{q'}^{(k)}|j, m'\rangle\langle\langle m', q'| \left(\sum_{J,M} |J, M\rangle\langle J, M|\right)|m, q\rangle\rangle.$$

and since $\sum_{J,M} |J, M\rangle\langle J, M| = \hat{1}$ in each subspace of fixed J, we have

$$\hat{T}_q^{(k)}|j, m\rangle = \sum_{J,M} |A(J, M)\rangle\langle J, M|m, q\rangle\rangle, \tag{293}$$

or, that

$$\langle J, M|\hat{T}_q^{(k)}|j, m\rangle = \sum_{J',M'} \langle J, M|A(J', M')\rangle\langle J', M'|m, q\rangle\rangle. \tag{294}$$

We need to find what kind of state $|A(J, M)\rangle$ is. This we do by acting with the angular momentum operators on it. Using the commutation relations of $\hat{J}$ with $\hat{T}$ we get

$$\hat{J}_z|A(J, M)\rangle = \sum_{q,m} \hbar (q + m) \hat{T}_q^{(k)}|j, m\rangle\langle\langle m, q|J, M\rangle. \tag{295}$$

Since we know that the Clebsh-Gordan coefficient is non-zero if and only if $q + m = M$ we may write this as

$$\hat{J}_z|A(J, M)\rangle = \hbar M|A(J, M)\rangle. \tag{296}$$

Similarly we have

$$\hat{J}_\pm|A(J, M)\rangle = \sum_{q,m} \left(\hbar\sqrt{j(j+1) - m(m \pm 1)}\hat{T}_q^{(k)}|j, m \pm 1\rangle\langle\langle m, q|J, M\rangle + \right.$$

$$\left.\hbar\sqrt{k(k+1) - q(q \pm 1)}\hat{T}_{q\pm 1}^{(k)}|j, m\rangle\langle\langle m, q|J, M\rangle\right) \tag{297}$$

By shifting the sums we may write this as

$$\sum_{q,m} \hat{T}_q^{(k)}|j, m\rangle \left(\hbar\sqrt{(j(j+1) - m(m \mp 1)}\langle\langle m \mp 1, q|J, M\rangle\right.$$

$$\left.+\hbar\sqrt{k(k+1) - q(q \mp 1)}\langle\langle m, q \mp 1|J, M\rangle\right). \tag{298}$$

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Now we can use a property of the Clebsh-Gordan coefficients which can be easily proved using the angular momentum commutation relations

$$
\sqrt{j(j+1)-m(m \mp 1)}\langle\!\langle \mathrm{m} \mp 1, \mathrm{q}|\mathrm{J}, \mathrm{M}\rangle +
$$
$$
\sqrt{k(k+1)-q(q \mp 1)}\langle\!\langle \mathrm{m}, \mathrm{q} \mp 1|\mathrm{J}, \mathrm{M}\rangle =
$$
$$
\sqrt{J(J+1)-M(M \pm 1)}\langle\!\langle \mathrm{m}, \mathrm{q}|\mathrm{J}, \mathrm{M} \pm 1\rangle. \tag{299}
$$

This gives us

$$
\hat{J}_{\pm}|\mathrm{A}(\mathrm{J}, \mathrm{M})\rangle = \hbar\sqrt{J(J+1)-M(M \pm 1)}|\mathrm{A}(\mathrm{J}, \mathrm{M} \pm 1)\rangle. \tag{300}
$$

Thus we see that $|\mathrm{A}(\mathrm{J}, \mathrm{M})\rangle$ fulfills exactly the same relations as the state $|\mathrm{J}, \mathrm{M}\rangle$. Thus $|\mathrm{A}(\mathrm{J}, \mathrm{M})\rangle$ must be proportional to $|\mathrm{J}, \mathrm{M}\rangle$ with a constant of proportionality that does not depend on M but only on J! That is, the constant of proportionality can be different for different J but for each fixed J it is the same for all M. We thus have

$$
\langle \mathrm{J}, \mathrm{M}|\mathrm{A}(\mathrm{J}', \mathrm{M}')\rangle = \delta_{J,J'}\delta_{M,M'}\frac{\langle J||\hat{T}^{(k)}||j\rangle}{\sqrt{2j+1}}, \tag{301}
$$

where we (conventionally) have introduced the so called *reduced* matrix element $\langle J||\hat{T}^{(k)}||j\rangle$ to write the constant of proportionality. As indicated it depends on the j, J quantum number and of course on the tensor $\hat{T}^{(k)}$, but it does not depend on the particular M, m and q quantum numbers. The factor $\frac{1}{2j+1}$ is purely conventional. This enables us to state the Wigner-Eckart theorem

$$
\langle \mathrm{J}, \mathrm{M}|\hat{T}_q^{(k)}|\mathrm{j}, \mathrm{m}\rangle = \frac{\langle J||\hat{T}^{(k)}||j\rangle}{\sqrt{2j+1}}\langle\!\langle \mathrm{m}, \mathrm{q}|\mathrm{J}, \mathrm{M}\rangle. \tag{302}
$$

This tells us many important things about the matrix elements of spherical tensors. First of all, the matrix element is zero unless $|j-k| \leq J \leq j+k$ and $M = m+q$ and secondly, for fixed J and j, the rotational properties of the spherical tensor $\hat{T}^{(k)}$ are completely contained in the Clebsch-Gordan coefficients $\langle\!\langle \mathrm{m}, \mathrm{q}|\mathrm{J}, \mathrm{M}\rangle$. In particular, we need only to calculate one matrix element for some given (preferably particularly simple) values of M, m and q and the other matrix elements follow automatically.

3 Scattering theory

Let us now turn our attention to scattering theory. In scattering theory we study quantum mechanical problems where we have some incoming free particles (state) which scatter on something located at some particular point in space. This means that the Hamiltonian in these problems is always of the type

$$\hat{H} = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}), \tag{303}$$

where the potential $V(\mathbf{x})$ is non-zero only in the small region of space where the interaction (scattering) takes place. Thus the Schrödinger equation can almost everywhere be written

$$\frac{\mathbf{p}^2}{2m}|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle, \tag{304}$$

which is just the Schrödinger equation for a free particle with the usual plane wave solutions. We thus expect that the full solution should look very much like a plane wave. We will study only elastic scattering which means that the energy (and probability) will be conserved in the process and we will study the static problem by throwing a continuous stream of particles at the target rather than particles one by one. The question will thus be: if I have a certain incident stream of particles, what out-coming stream of particles will I have. This makes it possible to study the time independent Schrödinger equation which simplifies things considerably.

3.1 The Lippman-Schwinger equation

Let us thus study the (time independent) Schrödinger equation

$$\left(\hat{H}_0 + \hat{V}\right)|\psi\rangle = E|\psi\rangle, \tag{305}$$

where $\hat{V}$ is non-zero only in a small region of space. Formally, if we knew how to "divide" by an operator, we could write the (implicit) solution to this equation as

$$|\psi\rangle = \frac{1}{E - \hat{H}_0}\hat{V}|\psi\rangle + |\phi\rangle. \tag{306}$$

Here $|\phi\rangle$ is an arbitrary state which satisfies $\hat{H}_0|\phi\rangle = E|\phi\rangle$. This ensures that when we hit both sides of the equation with the operator $E - \hat{H}_0$ we get back the original equation. In the limit where the potential vanishes we get that $|\psi\rangle = |\phi\rangle$. This way of writing the Schrödinger equation is known as the Lippman-Schwinger equation. In the form it has now it is purely formal since the operator $\frac{1}{E-\hat{H}_0}$ is singular when acting on for instance $|\phi\rangle$. To make sense of it, we need to give a prescription how make the inverse operator always well defined. This we do in a fashion inspired by the propagator in the first section. Namely, we let

$$\frac{1}{E - \hat{H}_0} \to \lim_{\epsilon \to 0} \frac{1}{E - \hat{H}_0 \pm i\epsilon}, \tag{307}$$

which means that we do all calculations with $\epsilon \neq 0$, giving us a well defined inverse operator, and only in the end do we let $\epsilon \to 0$. The sign of ϵ we will have to determine from the physical situation, just as in the propagator case in the first section. In the coordinate basis we can therefore write this equation as

$$\langle \mathbf{x}|\psi\rangle = \langle \mathbf{x}|\phi\rangle + \langle \mathbf{x}|\frac{1}{E - \hat{H}_0 \pm i\epsilon}\hat{V}|\psi\rangle, \tag{308}$$

and, inserting the unit operator in the form $\hat{1} = \int d^3\mathbf{x}|\mathbf{x}\rangle\langle\mathbf{x}|$ we get

$$\langle \mathbf{x}|\psi\rangle = \langle \mathbf{x}|\phi\rangle + \int d^3\mathbf{x}'\langle \mathbf{x}|\frac{1}{E - \hat{H}_0 \pm i\epsilon}|\mathbf{x}'\rangle\langle \mathbf{x}'|\hat{V}|\psi\rangle. \tag{309}$$

To be able to use this expression we need to know the form of the inverse operator in the coordinate basis

$$\langle \mathbf{x}|\frac{1}{E - \hat{H}_0 \pm i\epsilon}|\mathbf{x}'\rangle = \int d^3\mathbf{p}d^3\mathbf{p}'\langle \mathbf{x}|\mathbf{p}\rangle\langle \mathbf{p}|\frac{1}{E - \hat{H}_0 \pm i\epsilon}|\mathbf{p}'\rangle\langle \mathbf{p}'|\mathbf{x}'\rangle. \tag{310}$$

Using the explicit form of the wave function $\langle \mathbf{x}|\mathbf{p}\rangle = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}}e^{\frac{i}{\hbar}\mathbf{x}\cdot\mathbf{p}}$ and that the states $|\mathbf{p}\rangle$ are eigenstates of the Hamiltonian $\hat{H}_0 = \frac{\mathbf{p}^2}{2m}$ we get

$$\langle \mathbf{x}|\frac{1}{E - \hat{H}_0 \pm i\epsilon}|\mathbf{x}'\rangle = \int d^3\mathbf{p}d^3\mathbf{p}' \frac{e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{x}}}{(2\pi\hbar)^{\frac{3}{2}}} \frac{\delta^{(3)}(\mathbf{p} - \mathbf{p}')}{\left(E - \frac{\mathbf{p}'^2}{2m} \pm i\epsilon\right)} \frac{e^{\frac{i}{\hbar}\mathbf{p}'\cdot\mathbf{x}'}}{(2\pi\hbar)^{\frac{3}{2}}} =$$

$$\frac{1}{(2\pi\hbar)^3} \int d^3\mathbf{p} \frac{e^{\frac{i}{\hbar}\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')}}{\left(E - \frac{\mathbf{p}^2}{2m} \pm i\epsilon\right)}. \tag{311}$$

It is easy to see that this is in fact the Fourier transform of the free space propagator of the first section. Namely, in the first section we computed

$$
\begin{aligned}
K(\mathbf{x}, t) &= K(\mathbf{x}, t; \mathbf{x}', 0) = \int \frac{d^3\mathbf{p}}{(2\pi\hbar)^3} e^{-\frac{i}{\hbar}t\frac{\mathbf{p}^2}{2m} + \frac{i}{\hbar}\mathbf{p}\cdot(\mathbf{x}-\mathbf{x}')} \quad t > 0, \\
K(\mathbf{x}, t) &= 0 \quad t < 0.
\end{aligned} \tag{312}
$$

The Fourier transform (in the time coordinate) of this is

$$
L(x, E) = \int_0^\infty dt K(x, t) e^{\frac{i}{\hbar}Et}, \tag{313}
$$

and performing the integral gives exactly the inverse operator (311). The expression we have found is thus the propagator, but not from one particular time to another but rather for particles with a fixed energy. This is appropriate for our problem where we study the static situation with a steady flow of particles, all with the same energy E.

The integral in (311) can be performed using exactly the same methods as when we found the original propagator. The result is

$$
\langle\mathbf{x}|\frac{1}{E - \hat{H}_0 \pm i\epsilon}|\mathbf{x}'\rangle = -\frac{2m}{4\pi\hbar^2}\frac{e^{\pm i|\mathbf{x}-\mathbf{x}'|k}}{|\mathbf{x} - \mathbf{x}'|}. \tag{314}
$$

Here the $\pm$ signs refer to the $\pm i\epsilon$ signs and k is related to the energy by $E = \frac{\hbar^2 k^2}{2m}$. Using this we may now write the Lippman-Schwinger equation as

$$
\langle\mathbf{x}|\psi\rangle = \langle\mathbf{x}|\phi\rangle - \frac{2m}{\hbar^2}\int d^3\mathbf{x}'\frac{e^{\pm i|\mathbf{x}-\mathbf{x}'|k}}{4\pi|\mathbf{x} - \mathbf{x}'|}\langle\mathbf{x}'|\hat{V}|\psi\rangle. \tag{315}
$$

Written in this form, the equation has a very nice interpretation but to emphasize it more clearly, let us make the assumption that the potential is local. This means that $\langle\mathbf{x}|\hat{V}|\mathbf{x}'\rangle = V(\mathbf{x})\delta^{(3)}(\mathbf{x} - \mathbf{x}')$. This is not a very severe restriction, for instance, all potentials which depend only on coordinates are in this class. For local potentials, we may write

$$
\langle\mathbf{x}|\hat{V}|\psi\rangle = \int d^3\mathbf{x}'\langle\mathbf{x}|\hat{V}|\mathbf{x}'\rangle\langle\mathbf{x}'|\psi\rangle =
$$
$$
V(\mathbf{x})\int d^3\mathbf{x}'\delta^{(3)}(\mathbf{x} - \mathbf{x}')\langle\mathbf{x}'|\psi\rangle = V(\mathbf{x})\langle\mathbf{x}|\psi\rangle, \tag{316}
$$

which, inserted in the Lippman-Schwinger equation, leads to

$$
\langle\mathbf{x}|\psi\rangle = \langle\mathbf{x}|\phi\rangle - \frac{2m}{\hbar^2}\int d^3\mathbf{x}'\frac{e^{\pm i|\mathbf{x}-\mathbf{x}'|k}}{4\pi|\mathbf{x} - \mathbf{x}'|}V(\mathbf{x}')\langle\mathbf{x}'|\psi\rangle. \tag{317}
$$

The interpretation is as follows, on the left hand side we have the full wave function observed at the point $\mathbf{x}$. It is given, on the right hand side as the sum of $\langle \mathbf{x}|\phi\rangle$ which is the coordinate representation of a free wave, representing the incoming particles[6], and the second term which represent the interaction with the potential. The integral is over points where $V(\mathbf{x}') \neq 0$ since if $V = 0$ there are no interactions. The interaction also depends on the magnitude of the wave function at the point $\mathbf{x}'$. If the wave function is zero at $\mathbf{x}'$, there is no particle there which can interact with the potential. After the wave function has interacted with the potential at $\mathbf{x}'$ it is propagated out to $\mathbf{x}$ using the *free* propagator. The integral sums over all possible points of interaction.

With this interpretation in the back of our minds, we can go on and simplify the Lippman-Schwinger equation even further. That is, let us assume that the point $\mathbf{x}$ where we observe the wave function is far away from the region where the potential is non-zero. We can choose the origin of our coordinates precisely in this region which, since $\mathbf{x}'$ is also in this region, leads to the assumption $|\mathbf{x}| \gg |\mathbf{x}|'$. In this limit we have

$$|\mathbf{x} - \mathbf{x}'| = \sqrt{r^2 + r'^2 - 2rr'\cos\alpha} = r\sqrt{1 - 2\frac{r'}{r}\cos\alpha + \frac{r'^2}{r^2}} \approx$$
$$r - r'\cos\alpha = r - \frac{\mathbf{x}\cdot\mathbf{x}'}{r}. \qquad (318)$$

Using this approximation, the expression for the propagator simplifies to

$$\frac{e^{\pm i|\mathbf{x}-\mathbf{x}'|k}}{4\pi|\mathbf{x}-\mathbf{x}'|} \approx \frac{e^{\pm ikr}e^{\mp ik\frac{\mathbf{x}\cdot\mathbf{x}'}{r}}}{4\pi r}. \qquad (319)$$

Since we know that the energy is not changed in the scattering process (elastic scattering, remember) we know that the momentum of the outgoing wave is the same as the momentum of the incoming wave. The only thing that changes is the direction of the momenta. Thus we know that the outgoing wave-number $\mathbf{k}' = k\frac{\mathbf{x}}{r}$. Using this and that $|\phi\rangle = |\mathbf{k}\rangle$ we can write

$$\langle \mathbf{x}|\psi\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{\frac{3}{2}}} - \frac{2m}{\hbar^2}\frac{e^{\pm ikr}}{4\pi r}\int d^3\mathbf{x}'e^{\mp i\mathbf{k}'\cdot\mathbf{x}'}V(\mathbf{x}')\langle \mathbf{x}'|\psi\rangle. \qquad (320)$$

---

[6]Remember that $|\phi\rangle$ is a solution to the free Schrödinger equation $\hat{H}_0|\phi\rangle = E|\phi\rangle$. We will choose it to be $|\phi\rangle = |\mathbf{k}\rangle$, that is, an incoming plane wave with wavenumber $\mathbf{k}$ related to the momentum $\mathbf{k} = \frac{\mathbf{p}}{\hbar}$

The first term on the right hand side is again the incoming plane wave with momentum $\mathbf{p} = \hbar\mathbf{k}$. The second term is a spherical wave (times the integral which does not depend on $\mathbf{x}$ anymore). The sign in the exponential of the spherical wave tells us if it is moving outwards ($+$ sign) or inwards ($-$ sign) and since the physical situation that we want to describe is that the second term represents the wave coming *out* after scattering on the potential we have to choose the $+$ sign (which also tells us to choose the $+$ sign in the original expression for the inverse operator). Thus we see that Lippman-Schwinger tells us that in *any* scattering problem the wave-function (at large distance from where the scattering takes place) *must* take the following form

$$\langle \mathbf{x}|\psi\rangle = \frac{1}{(2\pi)^{\frac{3}{2}}}\left[e^{i\mathbf{k}\cdot\mathbf{x}} + \frac{e^{ikr}}{r}f(\mathbf{k}, \mathbf{k}')\right], \qquad (321)$$

where the first term on the right hand side is the incoming wave and the second term represents the scattered, outgoing wave. The function $f(\mathbf{k}, \mathbf{k}')$ is a function of the incoming ($\mathbf{k}$) and outgoing ($\mathbf{k}'$) wave numbers. In fact, since $|\mathbf{k}| = |\mathbf{k}'| = k$ it is just a function of k and the angle between the vectors $\mathbf{k}$ and $\mathbf{k}'$. The explicit expression for it is given by

$$f(\mathbf{k}, \mathbf{k}') = -\frac{(2\pi)^{\frac{3}{2}}}{4\pi}\frac{2m}{\hbar^2}\int d^3\mathbf{x}' e^{-i\mathbf{k}'\cdot\mathbf{x}'}\langle \mathbf{x}'|\hat{V}|\psi\rangle =$$

$$-\frac{(2\pi)^3}{4\pi}\frac{2m}{\hbar^2}\int d^3\mathbf{x}'\langle \mathbf{k}'|\mathbf{x}\rangle\langle \mathbf{x}'|\hat{V}|\psi\rangle = -\frac{(2\pi)^3}{4\pi}\frac{2m}{\hbar^2}\langle \mathbf{k}'|\hat{V}|\psi\rangle \qquad (322)$$

3.2 The cross section

In the experimental situation one is usually interested in shooting a continuous stream of particles at a target and then measuring how much of the stream of particles is deflected. However, the outgoing flow of particles is of course dependent on the incoming flow. The more particles we throw in, the more we get out. To get a number which is independent of the particular flow we chose to use in the experiment, people have invented the concept of *cross-section*. Simply said it is just the outgoing flow divided by the incoming flow. That is, we define the differential cross section as

$$\frac{d\sigma}{d\Omega}d\Omega = \frac{\#\text{ outgoing particles going through d}\Omega\text{ per unit time}}{\#\text{ incoming particles per unit time and unit area}} \qquad (323)$$

To be able to calculate the cross section for any process that we are interested in, we need to figure out what the incoming and outgoing flows are in our case.

To be able to do this we remember that the density of probability (which can be interpreted as the density of particles) is given by $\rho(\mathbf{x}) = |\psi(\mathbf{x})|^2$. The time derivative of the probability density is

$$\frac{\partial \rho}{\partial t} = \frac{\partial \psi^\dagger}{\partial t} \psi + \psi^\dagger \frac{\partial \psi}{\partial t}, \tag{324}$$

and using the Schrödinger equation (for the free particle) and its complex conjugate

$$\begin{aligned} i\hbar \frac{\partial \psi}{\partial t} &= -\frac{\hbar^2 \nabla^2}{2m} \psi, \\ -i\hbar \frac{\partial \psi^\dagger}{\partial t} &= -\frac{\hbar^2 \nabla^2}{2m} \psi^\dagger, \end{aligned} \tag{325}$$

we can write this as

$$\frac{\partial \rho}{\partial t} = \frac{i\hbar}{2m} \left(-\left(\nabla^2 \psi^\dagger\right) \psi + \psi^\dagger \left(\nabla^2 \psi\right) \right) = \frac{i\hbar}{2m} \nabla \left(\psi^\dagger \nabla \psi - \nabla \psi^\dagger \psi \right). \tag{326}$$

We see that if we define the current $\mathbf{j} = \frac{i\hbar}{2m} \left(\nabla \psi^\dagger \psi - \psi^\dagger \nabla \psi \right)$, the above equation takes the suggestive form

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0. \tag{327}$$

This is nothing but the equation of continuity for the probability density so we must interpret $\mathbf{j}$ as the probability current which is what measures the flow of particles. To see this even more explicitly, let us write the integral form of the continuity equation. If we call the number of particles in a volume N it takes the form

$$\frac{dN}{dt} + \oint_A \mathbf{n} \cdot \mathbf{j} = 0. \tag{328}$$

This we interpret to mean that the change of the number of particles per unit term (the first term) equals the flow of particles per unit time through the surface (the second term). We read off from the second term that the flow per unit time and unit area must be $\mathbf{n} \cdot \mathbf{j}$. This is therefore the flux! This we can use to compute the incoming flux for a wave function $\frac{e^{ikz}}{(2\pi)^{\frac{3}{2}}}$ representing free particle moving in the z direction

$$\begin{aligned} j_z &= \frac{i\hbar}{2m(2\pi)^3} \left(\left(-ike^{-ikz} \right) e^{ikz} - e^{-ikz} \left(ike^{ikz} \right) \right) = \frac{\hbar k}{m(2\pi)^3}, \\ j_x &= j_y = 0. \end{aligned} \tag{329}$$

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On the other hand, if we have a wave function

$$\frac{e^{ikr}}{(2\pi)^{\frac{3}{2}}r}f(\mathbf{k},\mathbf{k}'),\tag{330}$$

which represents a spherical wave propagating outwards, we can compute the flux through the area element $r^2 d\Omega$ by computing $\hat{\mathbf{r}}\cdot\mathbf{j}$ at some large value of r. Using

$$\nabla\psi=\hat{\mathbf{r}}\frac{\partial\psi}{\partial r}+\hat{\theta}\frac{1}{r}\frac{\partial\psi}{\partial\theta}+\hat{\phi}\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\phi},\tag{331}$$

we find

$$\hat{\mathbf{n}}\cdot\mathbf{j}=\frac{\hbar k}{(2\pi)^3 m}\frac{|f|^2}{r^2}.\tag{332}$$

This is the flux through the area element $r^2 d\Omega$ which means that through the space angle $d\Omega$ we have $\frac{\hbar k}{(2\pi)^3 m}|f|^2$ particles per unit time giving us the expression for the differential cross section

$$\frac{d\sigma}{d\Omega}=|f|^2.\tag{333}$$

Thus we see what we have to do to calculate the cross section. We just find the full static wave function of the problem with the correct boundary conditions (the incoming wave is a plane wave) and write it in such a way that we can identify $f(\mathbf{k},\mathbf{k}')$. This we now proceed to do in various ways.

3.3   The Born approximation

The simplest and most intuitive way to find the wave function is when the potential $\hat{V}$ is in some sense "small" and can be thought of as a perturbation. Then we make the ansatz

$$|\psi\rangle=|\psi^{(0)}\rangle+|\psi^{(1)}\rangle+|\psi^{(2)}\rangle+\ldots,\tag{334}$$

where $|\psi^{(\mathrm{n})}\rangle$ should be thought of as being of order $\hat{V}^n$. Inserting this into the Lippman-Schwinger equation we get

$$|\psi^{(0)}\rangle+|\psi^{(1)}\rangle+|\psi^{(2)}\rangle+\ldots=|\phi\rangle+$$
$$\frac{1}{E-\hat{H}_0+i\epsilon}\hat{V}\left(|\psi^{(0)}\rangle+|\psi^{(1)}\rangle+|\psi^{(2)}\rangle+\ldots\right).\tag{335}$$

Equating terms of the same order on each side of the equations gives us a set of recursion relations

$$
\begin{aligned}
|\psi^{(0)}\rangle &= |\phi\rangle, \\
|\psi^{(1)}\rangle &= \frac{1}{E - \hat{H}_0 + i\epsilon} \hat{V} |\psi^{(0)}\rangle, \\
|\psi^{(2)}\rangle &= \frac{1}{E - \hat{H}_0 + i\epsilon} \hat{V} |\psi^{(1)}\rangle, \\
&\vdots \qquad\qquad \vdots \\
|\psi^{(\mathrm{n})}\rangle &= \frac{1}{E - \hat{H}_0 + i\epsilon} \hat{V} |\psi^{(\mathrm{n}-1)}\rangle, \\
&\vdots \qquad\qquad \vdots
\end{aligned}
\tag{336}
$$

which can be easily solved to any given order since we know that $|\phi\rangle$ is a plane wave. Then we have

$$
\begin{aligned}
|\psi^{(0)}\rangle &= |\phi\rangle, \\
|\psi^{(1)}\rangle &= \frac{1}{E - \hat{H}_0 + i\epsilon} \hat{V} |\phi\rangle, \\
|\psi^{(1)}\rangle &= \frac{1}{E - \hat{H}_0 + i\epsilon} \hat{V} \frac{1}{E - \hat{H}_0 + i\epsilon} \hat{V} |\phi\rangle, \\
&\vdots \qquad\qquad \vdots
\end{aligned}
\tag{337}
$$

Written in this way the expansion have a very nice interpretation. Namely, since we know that $\frac{1}{E-\hat{H}_0+i\epsilon}$ is the free particle propagator we get the interpretation that $|\psi^{(0)}\rangle$ is just the non-interacting incoming wave, $|\psi^{(1)}\rangle$ is the incoming wave interacting once with the potential and then propagating to the position where we observe the wave function. In general $|\psi^{(\mathrm{n})}\rangle$ is interpreted as the incoming wave interacting for the first time with the potential, propagating like a free particle, interacting for the second time with the potential, propagating like a free particle, interacting again and so on n times.

Let us compute the explicit form of the cross section (or rather of $f(\mathbf{k}, \mathbf{k}')$) to lowest non-trivial order. This result is known as the first Born approximation. In the coordinate basis we have

$$
\langle \mathbf{x} | \psi^{(1)} \rangle = \langle \mathbf{x} | \frac{1}{E - \hat{H}_0 + i\epsilon} \hat{V} |\mathbf{k}\rangle = \int d^3\mathbf{x}' \langle \mathbf{x} | \frac{1}{E - \hat{H}_0 + i\epsilon} |\mathbf{x}'\rangle \langle \mathbf{x}' | \hat{V} |\mathbf{k}\rangle, \tag{338}
$$

where we have inserted a unit operator. This is easy to evaluate since we have already calculated the coordinate space representation of the propagator (314). Furthermore using that the potential is local we write

$$\langle \mathbf{x} | \psi^{(1)} \rangle = -\frac{2m}{4\pi\hbar^2} \int d^3\mathbf{x}' \frac{e^{ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} V(\mathbf{x}') \frac{e^{i\mathbf{k}\cdot\mathbf{x}'}}{(2\pi)^{\frac{3}{2}}}, \tag{339}$$

which, in the $|\mathbf{x}| \gg |\mathbf{x}'|$ can be further simplified to

$$\langle \mathbf{x} | \psi^{(1)} \rangle \approx -\frac{2m}{4\pi\hbar^2} \frac{e^{ikr}}{(2\pi)^{\frac{3}{2}} r} \int d^3\mathbf{x}' e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}'} V(\mathbf{x}'). \tag{340}$$

Thus, to this order of approximation, the full wave function in the coordinate representation and far away from the center of scattering is

$$\langle \mathbf{x} | \psi^{(0)} \rangle + \langle \mathbf{x} | \psi^{(1)} \rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} \left(e^{i\mathbf{k}\cdot\mathbf{x}} - \frac{2m}{4\pi\hbar^2} \frac{e^{ikr}}{r} \int d^3\mathbf{x}' e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}'} V(\mathbf{x}') \right), \tag{341}$$

which, when we compare it to the general form of the wave function (321) we can read off what f is

$$f(\mathbf{k}, \mathbf{k}') = -\frac{2m}{4\pi\hbar^2} \int d^3\mathbf{x}' e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}'} V(\mathbf{x}'). \tag{342}$$

We see that f to lowest non-trivial order is essentially the Fourier transform of the potential.

This procedure can of course be continued. At the next order we get

$$\langle \mathbf{x} | \psi^{(2)} \rangle = \int d^3\mathbf{x}' \int d^3\mathbf{x}'' \langle \mathbf{x} | \frac{1}{E - \hat{H}_0 + i\epsilon} | \mathbf{x}' \rangle V(\mathbf{x}') \times$$
$$\langle \mathbf{x}' | \frac{1}{E - \hat{H}_0 + i\epsilon} | \mathbf{x}'' \rangle V(\mathbf{x}'') \langle \mathbf{x}'' | \mathbf{k} \rangle. \tag{343}$$

Notice that here we can only simplify the propagator between $\mathbf{x}'$ and $\mathbf{x}$ since both $\mathbf{x}'$ and $\mathbf{x}''$ is in the region where $V \neq 0$ and thus are of the same order of magnitude.

Let us evaluate the cross section at lowest order for a concrete potential. We take the potential to be

$$V(r) = V_0 \frac{e^{-\mu r}}{\mu r}. \tag{344}$$

This potential is local and for small r ($r \ll \frac{1}{\mu}$) it looks just like the Coulomb potential $\frac{1}{r}$. For large r ($r \gg \frac{1}{\mu}$) however, the exponential suppression makes it effectively zero. Thus the range where the potential is non-zero is for $r < \frac{1}{\mu}$. Now let us calculate the cross-section. We have

$$f(\mathbf{k}, \mathbf{k}') = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int d^3\mathbf{x}\, e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}}V(\mathbf{x}), \qquad (345)$$

which, since V is a function only of r, we can write as

$$f(\mathbf{k}, \mathbf{k}') = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int_0^{2\pi} d\phi \int_0^{\pi} d\theta\sin\theta \int_0^{\infty} dr\, r^2 e^{iqr\cos\theta}V(r) =$$
$$-\frac{2mV_0}{\mu\hbar^2 q}\int_0^{\infty} dr\, e^{-\mu r}\sin qr, \qquad (346)$$

where we have introduced the vector $\mathbf{q} = \mathbf{k} - \mathbf{k}'$. The final integral over r can be performed by using that we know that $e^{iqr} = \cos qr + i\sin qr$ and thus rewriting the integral as

$$f(\mathbf{k}, \mathbf{k}') = -\frac{2mV_0}{\mu\hbar^2 q}\Im\left[\int_0^{\infty} dr\, e^{-\mu r}e^{iqr}\right] = -\frac{2mV_0}{\mu\hbar^2 q}\Im\left[\frac{1}{\mu - iq}\right] =$$
$$-\frac{2mV_0}{\mu\hbar^2\left(\mu^2 + q^2\right)}. \qquad (347)$$

To calculate q^2 we use that we know that $|\mathbf{k}| = |\mathbf{k}'| = k$ and assume that the scattered angle is θ, that is that the angle between $\mathbf{k}$ and $\mathbf{k}'$ is θ. This gives us

$$q^2 = |\mathbf{k} - \mathbf{k}'|^2 = k^2 + k'^2 - 2kk'\cos\theta = 2k^2 - 2k^2\cos\theta = 4k^2\sin^2\frac{\theta}{2}. \quad (348)$$

Everything together now gives us the differential cross section

$$\frac{d\sigma}{d\Omega} = |f|^2 = \left(\frac{2mV_0}{\mu\hbar^2}\frac{1}{\mu^2 + 4k^2\sin^2\frac{\theta}{2}}\right)^2 \qquad (349)$$

We can compare this with something we know (scattering on the Coulomb potential or Rutherford scattering) by taking the limit $\mu \to 0$ keeping $\frac{V_0}{\mu}$ fixed. Then our potential reduces to the Coulomb potential and the cross section goes to

$$\left(\frac{2mV_0}{\mu\hbar^2}\right)^2\frac{1}{16k^4\sin^4\frac{\theta}{2}}, \qquad (350)$$

which indeed is the Rutherford cross section.

Since this way of solving the scattering problem is an approximation, it is important to ask ourselves how far we can trust it. Our basic assumption was all the time that the successive wave functions $|\psi^{(n)}\rangle$ become smaller and smaller for each successive n. In particular this has to hold in the region where the potential is non zero since what we do in the first Born approximation is really to replace $|\psi\rangle$ in (315) with $|\phi\rangle$. Therefore, to check this we should evaluate the wave functions at $\mathbf{x} = 0$ for a "typical" potential and see for which data (range of the potential, energy of the incoming particles etc) the approximation breaks down (i.e. where the perturbation to the wave function $|\psi^{(1)}\rangle$ becomes of the same order as the whole wave function. To this end let us assume that we have a potential which is non-zero for $r < a$ for some number a and in the non-zero region it has average value V_0. We have

$$
\begin{aligned}
\left| \langle \mathbf{x} | \psi^{(0)} \rangle \right| &= \left| \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{\frac{3}{2}}} \right| = \frac{1}{(2\pi)^{\frac{3}{2}}} \\
\left| \langle \mathbf{x} = 0 | \psi^{(1)} \rangle \right| &= \left| \frac{2mV_0}{(2\pi)^{\frac{3}{2}} 4\pi\hbar^2} \int_0^a d^3\mathbf{x}' \frac{e^{ik|\mathbf{x}|'}}{|\mathbf{x}|'} e^{i\mathbf{k}\cdot\mathbf{x}'} \right|.
\end{aligned}
\tag{351}
$$

We see that for the approximation to be good, we need that $\left| \langle \mathbf{x} = 0 | \psi^{(0)} \rangle \right| \gg \left| \langle \mathbf{x} = 0 | \psi^{(1)} \rangle \right|$ or, in other words, that

$$
\left| \frac{2mV_0}{4\pi\hbar^2} \int_0^a d^3\mathbf{x}' \frac{e^{ik|\mathbf{x}|'}}{|\mathbf{x}|'} e^{i\mathbf{k}\cdot\mathbf{x}'} \right| \ll 1
\tag{352}
$$

First let us assume that the energy of the incoming particles (given by k) is small compared to the range of the potential (given by a). That is, assume that $ka \ll 1$. Since $|\mathbf{x}'|$ in the integral is always less than a we can put $e^{ik|\mathbf{x}|'} \approx e^{i\mathbf{k}\cdot\mathbf{x}'} \approx 1$. Then the integral is easily done

$$
\left| \frac{2mV_0}{4\pi\hbar^2} \int_0^a d^3\mathbf{x}' \frac{e^{ik|\mathbf{x}|'}}{|\mathbf{x}|'} e^{i\mathbf{k}\cdot\mathbf{x}'} \right| \approx \left| \frac{2mV_0}{4\pi\hbar^2} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \int_0^a dr' r'^2 \frac{1}{r'} \right| =
$$
$$
\left| \frac{mV_0 a^2}{\hbar^2} \right|. \tag{353}
$$

The requirement is therefore $|V_0| \ll \frac{\hbar^2}{ma^2}$ which means that the potential cannot be too strong (i.e. V_0 big) or of too long range (i.e. a big) if the Born

approximation should be good at *low* energy. At high energy ($ka \gg 1$) on the other hand, we have the requirement

$$1 \gg \left| \frac{2mV_0}{4\pi\hbar} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \int_0^a dr' r'^2 \frac{e^{ikr'\cos\theta} e^{ikr'}}{r'} \right|. \qquad (354)$$

Doing the integral over the angles, we get

$$\left| \frac{mV_0}{ik\hbar^2} \int_0^a dr' \left(e^{2ikr'} - 1 \right) \right|, \qquad (355)$$

and then the integral over r' gives us

$$\left| \frac{mV_0}{2k^2\hbar^2} \left(2ika - e^{2ika} + 1 \right) \right| \approx \left| \frac{V_0 ma}{k\hbar^2} \right|, \qquad (356)$$

where we have used that $ka \gg 1$. This leads to the requirement

$$|V_0| \ll \frac{\hbar^2}{ma^2} ka. \qquad (357)$$

Notice that this is the same requirement as in the low energy case, but multiplied with the (large) factor ka. Thus we see that the Born approximation becomes better and better when we increase the energy. This can be intuitively understood since for high energy (which is equivalent to high velocity) the particles go through the potential region very fast and there is no time to interact many times with the potential. Thus the first order Born approximation (which is, as you remember, given by restricting the number of interactions to one) should be good.

3.4   Partial waves

In view of the above restrictions of the Born approximation, it is important to find other, non equivalent, approximations in which the scattering problem can be solved. One such methods starts by the assumption that the potential is spherically symmetric (but there is no assumption that the potential is "small" or of finite range as in the Born approximation). That the potential is spherically symmetric means that it is invariant under rotations, which, as we know from our discussions on angular momenta means that $\hat{V}$ commutes with $\hat{\mathbf{L}}$ and in particular with $\hat{\mathbf{L}}^2$ and $\hat{L}_z$. Since $\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + \hat{V}$ and $\hat{\mathbf{p}}^2$ also commutes with the angular momentum operator we can choose energy eigenstates that

are simultaneously eigenstates of $\hat{\mathbf{L}}^2$ and $\hat{L}_z$. Therefore, let us use these eigenstates to expand an arbitrary wave function with energy $E = \frac{\hbar^2 k^2}{2m}$ in the coordinate basis as

$$\psi_k(x) = \sum_{l,m} R_{k,l}(r) Y_l^m(\theta, \phi). \tag{358}$$

In fact, in our problems, since we can always choose the incoming wave to be a plane wave moving in the z direction, the fact that the potential is spherically symmetric tells us that no wave function can depend on ϕ. The only Y_l^m independent of ϕ is $Y_l^0 = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta)$ so the wave function can actually be written even simpler as

$$\psi_k(x) = \sum_l f_{k,l}(r) Y_l^0(\theta, \phi) = \sum_l R_{k,l}(r) \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta). \tag{359}$$

In fact, any function of only θ can be decomposed in such a way, in particular $f(\mathbf{k}, \mathbf{k}')$ which depends only on θ in the case where the potential is spherically symmetric is usually expanded in the following way

$$f(\mathbf{k}, \mathbf{k}') = f(\theta) = \sum_l^\infty (2l+1) f_l(k) P_l(\cos\theta). \tag{360}$$

The factor $(2l+1)$ is purely conventional and could be included in f_l for instance.

3.4.1 The resolution of a plane wave

Also the incoming wave function $\propto e^{ikz} = e^{ikr\cos\theta}$ is a function of only θ and can be expanded in this way. There are quick and dirty ways to find this expansion, but let us do it more carefully. Let us first find the basis functions we want to use. That is, let us solve the *free* Schrödinger equation in spherical coordinates

$$-\frac{\hbar^2}{2m} \nabla^2 \psi_k(x) = \frac{\hbar^2 k^2}{2m} \psi_k(x). \tag{361}$$

Making the ansatz $\psi_k(x) = R_{kl}(r) Y_l^m(\theta, \phi)$ and using that the Laplacian in spherical coordinates can be written

$$\nabla^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \left(\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial}{\partial r} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2} \right)$$

$$= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{\hat{\mathbf{L}}^2}{\hbar^2 r^2}, \tag{362}$$

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we see that the Schrödinger equation reduces to the radial equation

$$\left(-\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{d}{dr} R_{kl} \right) + \frac{l(l+1)}{r^2} R_{kl} \right) = k^2 R_{kl}, \tag{363}$$

or

$$\frac{d^2 R_{kl}}{dr^2} + \frac{2}{r} \frac{dR_{kl}}{dr} + \left(k^2 - \frac{l(l+1)}{r^2} \right) R_{kl} = 0. \tag{364}$$

This equation has the solution

$$R_{kl}^{(1)} = (-1)^l (kr)^l \left(\frac{1}{kr} \frac{d}{d(kr)} \right)^l \frac{\sin kr}{kr} \equiv j_l(kr), \tag{365}$$

and the linearly independent solution

$$R_{kl}^{(2)} = (-1)^{(l+1)} (kr)^l \left(\frac{1}{kr} \frac{d}{d(kr)} \right)^l \frac{\cos kr}{kr} \equiv n_l(kr), \tag{366}$$

which is however singular for $r = 0$. These functions are known as *spherical Bessel functions*. They are related to the ordinary Bessel functions by

$$
\begin{aligned}
j_l(x) &= \left(\frac{\pi}{2x} \right)^{\frac{1}{2}} J_{l+\frac{1}{2}}(x), \\
n_l(x) &= (-1)^{(l+1)} \left(\frac{\pi}{2x} \right)^{\frac{1}{2}} J_{-l-\frac{1}{2}}(x).
\end{aligned}
\tag{367}
$$

Their asymptotic properties are given by

$$
\begin{aligned}
\lim_{x \to 0} j_l(x) &= \frac{x^l}{(2l+1)!!}, \\
\lim_{x \to 0} n_l(x) &= -\frac{(2l-1)!!}{x^{l+1}},
\end{aligned}
\tag{368}
$$

and

$$
\begin{aligned}
\lim_{x \to \infty} j_l(x) &= \frac{1}{x} \cos \left[x - \frac{\pi(l+1)}{2} \right], \\
\lim_{x \to \infty} n_l(x) &= \frac{1}{x} \sin \left[x - \frac{\pi(l+1)}{2} \right].
\end{aligned}
\tag{369}
$$

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Thus we have found that any solution with energy $E = \frac{\hbar^2 k^2}{2m}$ of the free Schrödinger equation can be written as

$$\psi_k(x) = \sum_{lm} \left(c_{lm}^{(1)} j_l(kr) + c_{lm}^{(2)} n_l(kr) \right) Y_l^m(\theta, \phi). \tag{370}$$

In the cases we are interested in there is no dependence on ϕ so $m = 0$ and since n_l is singular at the origin we can set $c^{(2)} = 0$ for solutions which are non singular at the origin. In particular, turning back to our plane wave, we can write

$$e^{ikz} = e^{ikr\cos\theta} = \sum_l c_l j_l(kr) P_l(\cos\theta), \tag{371}$$

for some constants c_l. The coefficients can be determined by comparing terms on both sides of the equation. To make it simpler, let us compare for $r \to 0$. On the left hand side we have a power series in $(kr\cos\theta)$ which the coefficient of the l-th term being $\frac{i^l}{l!}$. On the right hand side j_l goes like $\frac{(kr)^l}{(2l+1)!!}$ and from P_l we need the $\cos^l\theta$ term which can be found from the formula

$$P_l(\cos\theta) = \frac{1}{2^l l!} \frac{d^l}{d(\cos\theta)^l} (\cos^2\theta - 1)^l, \tag{372}$$

to have coefficient $\frac{(2l)!}{2^l l! l!}$ which tells us that on the right hand side the coefficient multiplying the $(kr\cos\theta)^l$ term is $c_l \frac{(2l)!}{(2l+1)!! 2^l l! l!} = c_l \frac{(2l)!}{(2l+1)!! l!}$. Equating this we get

$$c_l = i^l (2l + 1), \tag{373}$$

which gives us the final expression

$$e^{ikz} = \sum_l (2l + 1) i^l j_l(kr) P_l(\cos\theta). \tag{374}$$

It is interesting to see how this expression looks like for large r. Using the asymptotic expressions for the spherical Bessel functions we can write

$$e^{ikz} \approx \sum_l \frac{(2l+1)i^l}{kr} \cos\left[kr - \frac{\pi(l+1)}{2} \right] P_l(\cos\theta) =$$

$$\sum_l \frac{(2l+1)i^l}{2kr} \left(e^{ikr - i\frac{\pi(l+1)}{2}} + e^{-ikr + i\frac{\pi(l+1)}{2}} \right) P_l(\cos\theta) = \tag{375}$$

$$\sum_l \frac{(2l+1)i^l}{2kr} \left((-i)^{l+1} e^{ikr} + i^{l+1} e^{-ikr} \right) P_l(\cos\theta) =$$

$$\sum_l \frac{(2l+1)}{2ikr} \left(e^{ikr} - e^{-i(kr-\pi l)} \right) P_l(\cos\theta).$$

We thus see the interesting fact that a *plane* wave can be written as a linear combination of one incoming and one outgoing *spherical* wave.

3.4.2 General formalism

Having everything written in spherical coordinates we can now proceed and solve the scattering problem. The general solution of the wave function (321) can now be written, using (374) to write the incoming part and (360) to write the outgoing part, as

$$\langle \mathbf{x}|\psi\rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_l (2l+1) P_l(\cos\theta) \left(i^l j_l(kr) + \frac{e^{ikr}}{r} f_l(k) \right). \qquad (376)$$

At large values of r (we observe the wave function far away from the scatterer remember), using (375) this simplifies to

$$\langle \mathbf{x}|\psi\rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_l \frac{(2l+1)}{2ik} P_l(\cos\theta) \left(-\frac{e^{-i(kr-l\pi)}}{r} + \frac{e^{ikr}}{r} (1 + 2ik f_l(k)) \right) (377)$$

We see that the full wave function is, in the same way as the plane wave in the previous section, just a linear combination of an incoming and an outgoing spherical wave. The only thing which changed as compared to the plan wave (375) is that the coefficient of the outgoing wave changed from 1 to $S_l = 1 + 2ik f_l(k)$.

One way to get some hold on what $f_l(k)$ can be without doing any calculation is to observe the simple principle that "what goes in must come out" (in the case of elastic scattering of course). This means that the flow of probability into the region must be the same as the flow out. Now we can use that in (332) we found an expression for the radial probability current for an arbitrary wave function. That is, for a general spherical wave $g \frac{e^{\pm ikr}}{r}$ (g cannot depend on r) the probability current is

$$j_r = \frac{\hbar k}{mr^2} |g|^2, \qquad (378)$$

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or, the flow through the area element $r^2 d\Omega$ is $\frac{\hbar k}{m} |g|^2 d\Omega$. From this we find that the requirement that the probability is conserved leads in our case to the requirement that the coefficient in front of the outgoing wave has the same absolute value as the coefficient in front of the incoming wave. Because of angular momentum conservation, this has to be true for each l separately. This means that for each l we have

$$1 = |1 + 2ikf_l(k)|. \tag{379}$$

This condition is easily solved by saying that S_l is a pure phase, i.e. that

$$S_l = 1 + 2ikf_l(k) = e^{2i\delta_l}. \tag{380}$$

Inserting this back in the wave function we have

$$\langle \mathbf{x}|\psi\rangle = \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_l \frac{(2l+1)}{2ik} P_l(\cos\theta) \left(-\frac{e^{-i(kr-l\pi)}}{r} + \frac{e^{ikr+2i\delta_l}}{r} \right). \tag{381}$$

We see that the only thing that the potential does is to change the phase of the outgoing wave with δ_l being the phase shift. To be complete we also express f_l in terms of the phase shift. We have

$$f_l = \frac{S_l - 1}{2ik} = \frac{e^{2i\delta_l} - 1}{2ik} = \frac{e^{i\delta_l}\sin\delta_l}{k} = \frac{1}{k\cot\delta_l - ik}. \tag{382}$$

As a consequence of this we can relate the imaginary part of $f(\theta = 0)$ to the total cross section. It is known as the *optical theorem* and it follows from just the conservation of probability (which is the only thing we have used) so it holds quite generally. Namely, since the differential cross section is $\frac{d\sigma}{d\Omega} = |f|^2$ we may calculate the total cross section as

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega} = \int d\Omega \sum_{ll'} (2l+1)(2l'+1) f_{l'}^\star f_l P_{l'}(\cos\theta) P_l(\cos\theta). \tag{383}$$

Then we may use the orthogonality properties of the Legendre polynomials

$$\int d\Omega P_{l'}(\cos\theta) P_l(\cos\theta) = \delta_{l,l'} \frac{4\pi}{2l+1}, \tag{384}$$

to find

$$\sigma = 4\pi \sum_l (2l+1) |f_l|^2. \tag{385}$$

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On the other hand we can calculate the imaginary part of f evaluated at $\theta = 0$ (forward scattering). This we calculate to be

$$\Im f(\theta = 0) = \sum_l (2l+1) P_l(1) \Im f_l(k) = \sum_l (2l+1) \Im f_l(k). \qquad (386)$$

But now comes the trick. We have used the conservation of probability to show that we may write f_l as

$$f_l = \frac{e^{i\delta_l} \sin \delta_l}{k}, \qquad (387)$$

and from this we derive

$$
\begin{aligned}
|f_l|^2 &= \frac{\sin^2 \delta_l}{k^2}, \\
\Im f_l &= \frac{\sin^2 \delta_l}{k} = k\,|f_l|^2 .
\end{aligned}
\qquad (388)
$$

Thus we find that

$$\Im f(\theta = 0) = \frac{k\sigma}{4\pi}, \qquad (389)$$

which is known as the optical theorem.

It is now clear how to find the cross section using the method of partial waves. We need to find the wave function far away from the scattering area. We have shown that it always looks like in (381) so writing it in this form we can just read off the phase shift δ_l and then we have

$$f(\theta) = \sum_l (2l+1) \frac{e^{i\delta_l} \sin \delta_l}{k} P_l(\cos \theta), \qquad (390)$$

which gives us the cross section through $\frac{d\sigma}{d\Omega} = |f|^2$. To find the wave function we have to solve the (radial) Schrödinger equation which can be done in many ways. If the potential is simple enough it might be possible to do it exactly. If the potential has finite range so that for large r it is equal to zero, we can solve the radial Schrödinger equation (even numerically, if necessary) in the region where the potential is non-zero and in the region where it is zero separately. In the region where it is zero we have in fact already solved it since in that region the Schrödinger equation is the equation for a free particle which has as its most general solution (370). To get the full solution we need the inner

solution with the outer solution (wave functions and their derivatives should
be equal) at some point $r = R$ and we are done. In formulas we have the
outer wave function (we conventionally redefine the constants as compared
to (370))

$$\psi_k(x) = \sum_l (2l+1)i^l \left(c_l^{(1)}j_l(kr) + c_l^{(2)}n_l(kr)\right) P_l(\cos\theta), \qquad (391)$$

where we find $c_l^{(1)}$ and $c_l^{(2)}$ by matching to the inner solution. The asymptotic
expressions for the spherical Bessel functions give us an expression for the
asymptotic form of the wave function

$$\psi_k(x) = \frac{1}{(2\pi)^{\frac{3}{2}}} \sum_l \frac{(2l+1)(c_l^{(1)} + ic_l^{(2)})}{2ikr} P_l(\cos\theta)$$
$$\left(-\frac{e^{-i(kr-l\pi)}}{r} + \frac{c_l^{(1)} - ic_l^{(2)}}{c_l^{(1)} + ic_l^{(2)}} \frac{e^{ikr}}{r}\right). \qquad (392)$$

Comparing this to (377) we find that

$$\begin{aligned}
c_l^{(1)} + ic_l^{(2)} &= 1, \\
\frac{c_l^{(1)} - ic_l^{(2)}}{c_l^{(1)} + ic_l^{(2)}} &= e^{2i\delta_l},
\end{aligned} \qquad (393)$$

or

$$\begin{aligned}
c_l^{(1)} &= \frac{e^{i\delta_l}\cos\delta_l}{2}, \\
c_l^{(2)} &= -\frac{e^{i\delta_l}\sin\delta_l}{2}
\end{aligned} \qquad (394)$$

so finding the coefficients $c_l^{(1)}$ and $c_l^{(2)}$ immediately gives us the cross section.

3.4.3 Applications

As an illustration of this let us find the scattering on a "hard sphere" potential

$$V(r) = \begin{cases} \infty & \text{for} \quad r < R, \\ 0 & \text{for} \quad r > R. \end{cases} \qquad (395)$$

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Solving for the wave function in the inner region $r < R$ is easy. Because the potential is infinite there the wave function has to be zero. Matching the outer wave function to the inner one tells us that we have to find $c_l^{(1)}$ and $c_l^{(2)}$ such that

$$c_l^{(1)} j_l(kR) + c_l^{(2)} n_l(kR) = 0, \qquad (396)$$

and using (394) we find

$$\tan \delta_l = -\frac{c_l^{(2)}}{c_l^{(1)}} = \frac{j_l(kR)}{n_l(kR)}. \qquad (397)$$

We can now find the phase shift (and thus the cross section) for each l separately but to keep it simple, let us do so in the low energy $(kR \ll 1)$ limit only. Then we have

$$\tan \delta_l = \lim_{kR \to 0} \frac{j_l(kR)}{n_l(kR)} = \frac{\frac{(kR)^l}{(2l+1)!!}}{-\frac{(2l-1)!!}{(kR)^{l+1}}} = -\frac{(kR)^{2l+1}}{(2l+1)!!(2l-1)!!}. \qquad (398)$$

Since kR is small we see that $\delta_0 \approx -kR$ and all higher δ_l rapidly become smaller for larger l. Therefore to a good approximation $f(\theta)$ is given by the $l = 0$ term as

$$f(\theta) \approx f_0 P_0(\theta) = \frac{e^{i\delta_0} \sin \delta_0}{k} \approx -R, \qquad (399)$$

giving us the differential cross section

$$\frac{d\sigma}{d\Omega} = |f|^2 = R^2. \qquad (400)$$

Notice that this gives a total cross section (by integrating over $d\Omega$) of $4\pi R^2$ which is *four* times as large as the geometrical cross section that one would expect classically. Notice also that the differential cross section is independent of any angles. This is the case for all scattering where only $l = 0$ contributes since $P_0(\cos \theta) = 1$.

Another interesting potential that we may consider is the square well potential

$$V(r) = \begin{cases} V_0 & \text{for} \quad r < R, \\ 0 & \text{for} \quad r > R. \end{cases}, \qquad (401)$$

where V_0 is some positive *or* negative constant. If V_0 is positive, the potential is repulsive and if V_0 is negative the potential is attractive. For attractive enough potential (V_0 negative enough) the potential develops bound states. Let us study only the $l = 0$ case which should be the relevant case at low energy. The outer wave function (valid in the $r > R$ region) may in this case be written

$$\psi_k(x) = \left(c_0^{(1)} j_0(kr) + c_0^{(2)} n_0(kr) \right). \tag{402}$$

Inserting the expressions for the Bessel functions and using (394) we can rewrite this as

$$\psi_k(x) = \frac{e^{i\delta_0} \sin\left(kr + \delta_0\right)}{kr}. \tag{403}$$

Remember that this is the solution of the radial Schrödinger equation for the free particle (364) in the $l = 0$ case. In the presence of a potential, the radial Schrödinger equation becomes

$$\frac{d^2 R_{kl}}{dr^2} + \frac{2}{r}\frac{dR_{kl}}{dr} + \left(\frac{2mE}{\hbar^2} - \frac{2mV(r)}{\hbar^2} - \frac{l(l+1)}{r^2} \right) R_{kl} = 0, \tag{404}$$

which for our potential and in the $l = 0$ case leads to the equation that needs to be solved in the inner region

$$\frac{d^2 R_{k0}}{dr^2} + \frac{2}{r}\frac{dR_{k0}}{dr} + \frac{2m(E - V_0)}{\hbar^2} R_{k0} = 0. \tag{405}$$

which can be rewritten even more nicely as

$$\frac{d^2}{dr^2}(rR_{k0}) + \frac{2m(E - V_0)}{\hbar^2}(rR_{k0}) = 0. \tag{406}$$

We see immediately that the solution which is regular at $r = 0$ can in the $V_0 > E$ case (which implies $V_0 > 0$ since $E > 0$) be written as

$$rR_{k0} \;\; = \;\; a \sinh \kappa r \quad \kappa^2 = \frac{2m(V_0 - E)}{\hbar^2}, \tag{407}$$

and in the $E > V_0$ case we have

$$rR_{k0} \;\; = \;\; b \sin k' r \quad k'^2 = \frac{2m(E - V_0)}{\hbar^2}, \tag{408}$$

for some constants a and b. Let us concentrate on the attractive case $E > V_0 = -|V_0|$ in the following. Then as we saw we have the inner wave function $\frac{b \sin k'r}{r}$ and the outer wave function $\frac{e^{i\delta_0} \sin(kr+\delta_0)}{kr}$ and they need to be matched at $r = R$. That is, their values need to be equal there

$$\frac{b \sin k'R}{R} = \frac{e^{i\delta_0} \sin(kR + \delta_0)}{kR}, \tag{409}$$

and their first derivatives also need to be equal there

$$b \left(\frac{k' \cos k'R}{R} - \frac{\sin k'R}{R^2} \right) = e^{i\delta_0} \left(\frac{\cos(kR + \delta_0)}{R} - \frac{\sin(kR + \delta_0)}{kR^2} \right). \tag{410}$$

Dividing these two equation with each other b and $e^{i\delta_0}$ drop out and we get

$$k'R \cot k'R - 1 = kR \cot(kR + \delta_0) - 1, \tag{411}$$

or

$$\frac{\tan(kR + \delta_0)}{kR} = \frac{\tan k'R}{k'R}. \tag{412}$$

This is a rather complicated equation which we need to solve for δ_0. We can simplify it a bit by using the addition formula for the tangent

$$\tan(A + B) = \frac{\tan A + \tan B}{1 - \tan A \tan B}, \tag{413}$$

to write

$$\tan \delta_0 = \frac{kR \tan k'R - k'R \tan kR}{k'R + kR \tan kR \tan k'R}. \tag{414}$$

This allows us to analyze the scattering behavior qualitatively as a function of V_0. Starting at $V_0 = 0$ which means no potential at all we have $k = k'$ and thus $\tan \delta_0 = 0$ which means that $\delta_0 = 0$ and there is no scattering as should be expected. Increasing $|V_0|$ (that is decreasing V_0 or making the potential more attractive) one will get $k' > k$ and $\tan \delta_0 \neq 0$ which gives a non-zero value for δ_0 and thus for the cross section. The cross section

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \approx f_0(k) P_0(\cos \theta) = \frac{\sin^2 \delta_0}{k^2}, \tag{415}$$

will increase and reach its maximum at $\delta_0 = \frac{\pi}{2}$. This happens when $\tan\delta_0 = \infty$, which means that $k'R + kR\tan kR\tan k'R = 0$. Increasing $|V_0|$ even more we again will come to a point where $kR\tan k'R - k'R\tan kR = 0$ (this means that $\delta_0 = \pi$ and $k'R \approx \frac{3\pi}{2}$ which paradoxically leads to the fact that cross section is *zero* even thought the potential is far from being zero! This is known as the Ramsauer-Townsend effect and can be experimentally observed in scattering of electrons on rare gas atoms.