## III. Exactly Solvable Problems

The systems for which exact QM solutions can be found are few in number and they are not particularly interesting in and of themselves; typical experimental systems are much more complicated than any exactly solvable Hamiltonian. However, we must understand these simple problems if we are to have any hope of attacking more complicated systems. For example, we will see later that one can develop very accurate approximate solutions by examining the difference between a given Hamiltonian and some exactly solvable Hamiltionian. The two problems we will deal with here are: the Harmonic Oscillator and Piecewise Constant Potentials.

## A. Operators and States in Real Space

To solve even simple one-dimensional problems, we need to be able to describe experiments in real space in terms of Hilbert space operators. The ansatz is fairly straightforward. A generic (classical) observable can be associated with some function of the position and momentum:

$$
A(p, q)
$$

Note that we assume (for now) that there is only one particle, so the observable only depends on one position and one momentum. The associated quantum operator is obtained by replacing the classical variables ( $p, q$ ) with the corresponding quantum operators $(\hat{p}, \hat{q})$ :

$$
\hat{A}=A(\hat{p}, \hat{q})
$$

The position and momentum operators satisfy the canonical commutation relation:

$$
[\hat{q}, \hat{p}]=i \hbar
$$

This association has a deep connection with the role of Poisson brackets in classical mechanics. Unfortunately, this connection is completely lost on the typical chemist, who is unfamiliar with Poisson brackets to begin with.

Now, the fact that $\hat{p}$ and $\hat{q}$ do not commute poses an immediate problem. What if we want to associate a quantum operator with a classical observable like $A(p, q)=p q$ ? We have more than one choice: we could choose $\hat{A}=\hat{p} \hat{q}$ or $\hat{A}=\hat{q} \hat{p}$. For this simple product
form, the dilemma is easily resolved by requiring $\hat{A}$ to be Hermitian, in which case the only possible choice is the symmetric form:

$$
\hat{A}=\frac{1}{2}(\hat{p} \hat{q}+\hat{q} \hat{p})
$$

You can verify for yourself that this operator is, indeed Hermitian. When $A(p, q)$ contains more complicated products of $\hat{p}$ and $\hat{q}$ (e.g. $\left.A(p, q)=p^{3} \cos (1-q)\right)$ the solution is, well, more complicated. In fact, there is no a general way to associate arbitrary (non-linear) products of $\hat{p}$ and $\hat{q}$ with a unique quantum operator. Fortunately, we will not be interested in classical observables that involve non-linear products of $\hat{p}$ and $\hat{q}$ in this course. Thus this is not a practical obstacle for us; however, there is an on-going debate within the physics community about how these products should be treated.

## B. The Harmonic Oscillator

Classically, a Harmonic oscillator is a system with a linear restoring force,

$$
-\nabla V(q)=-k q
$$

It is easily verified that the correct potential in this case is:

$$
V(q)=\frac{1}{2} k q^{2}=\frac{1}{2} m \omega^{2} q^{2} \quad \omega=\sqrt{\frac{k}{m}}
$$

where $k$ is the effective force constant and $\omega$ is the frequency of the oscillation. In QM, it is often more convenient to work in terms of this frequency, and this is what we will do. To begin with, we will be interested in the observable energies associated with this potential. In classical mechanics the total energy is generated by the Hamiltonian, which we can immediately associate with a quantum operator:

$$
H(p, q)=\frac{p^{2}}{2 m}+\frac{1}{2} m \omega^{2} q^{2} \Rightarrow \hat{H}=\frac{\hat{p}^{2}}{2 m}+\frac{1}{2} m \omega^{2} \hat{q}^{2}
$$

There are two main motivations for studying the harmonic oscillator. The first is that it has a deep relationship to many other exactly solvable problems in QM. You will sometimes even hear it said that all exactly solvable problems are the harmonic oscillator in disguise. This is because virtually every exactly solvable QM potential has some observable that evolves under a linear force; in the case of the harmonic oscillator, it is the position, but one can arrive at arbitrarily
complicated (but still exactly solvable) potentials by using different linear evolutions. Another justification for studying harmonic potentials is that even for a very anharmonic potential, the potential looks harmonic if one is near enough the minimum. Thus, if we expand around the minimum (and choose our zero of energy so that $V(0) \equiv 0)$ :

$$
V(\delta q)=\left.\frac{\partial V}{\partial q}\right|_{0} \delta q+\left.\frac{1}{2} \frac{\partial^{2} V}{\partial q^{2}}\right|_{0} \delta q^{2}+\left.\ldots \approx \frac{1}{2} \frac{\partial^{2} V}{\partial q^{2}}\right|_{0} \delta q^{2}
$$

And we see that the potential is approximately harmonic.
At this point, it is convenient to convert to reduced units by choosing our units of length, mass and energy so that $\hbar=m=\omega=1$. These units are merely out of convenience and in the end, once we have calculated an observable (such as the position) we will need to convert the result to a set of standard units (such as meters). We can do this by noting that, in reduced units:

$$
\text { Length: } 1=\sqrt{\frac{\hbar}{m \omega}} \quad \text { Energy: } 1=\hbar \omega
$$

The main benefit at the moment is that it removes the relatively unimportant factors of $\hbar, m$ and $\omega$ from our equations, so that in natural units:

$$
\hat{H}=\frac{\hat{p}^{2}}{2}+\frac{\hat{q}^{2}}{2}
$$

Notice that this is the most we can do; there are only three fundamental units, and so if there were a fourth constant (an anharmonicity, say) we would not be able to scale away this unit. Later, we will also very often be interested in only fixing some of our units (for example $\hbar=m=1$ ) and leaving others free. This will greatly simplify the algebra in many instances.

Now, define two operators:

$$
\hat{a}=\frac{1}{\sqrt{2}}(\hat{q}+i \hat{p}) \quad \text { and } \quad \hat{a}^{\dagger}=\frac{1}{\sqrt{2}}(\hat{q}-i \hat{p})
$$

As the notation suggests, these operators are Hermitian conjugates of one another. However, they do not commute

$$
\begin{align*}
\left\lfloor\hat{a}, \hat{a}^{\dagger}\right\rfloor= & \left.\frac{1}{2}[(\hat{q}+i \hat{p}),(\hat{q}-i \hat{p})]=\frac{1}{2}[\hat{q}, \hat{q}]+i[\hat{p}, \hat{q}]-i[\hat{q}, \hat{p}]+\left[\hat{p}, \hat{p_{4}}\right]\right) \\
& =i \frac{1}{2}[\hat{p}, \hat{q}]-i \frac{1}{2}[\hat{q}, \hat{p}]=1 \tag{0}
\end{align*}
$$

Now, we can re-write the Hamiltonian in terms of these operators if we notice that

$$
\hat{q}=\frac{1}{\sqrt{2}}\left(\hat{a}+\hat{a}^{\dagger}\right) \text { and } \hat{p}=\frac{-i}{\sqrt{2}}\left(\hat{a}-\hat{a}^{\dagger}\right)
$$

Then,

$$
\begin{aligned}
\hat{H}= & \frac{\hat{p}^{2}}{2}+\frac{\hat{q}^{2}}{2}=\frac{-\left(\hat{a}-\hat{a}^{\dagger}\right)^{2}}{4}+\frac{\left(\hat{a}+\hat{a}^{\dagger}\right)^{2}}{4} \\
& =-\left(\partial \hat{a}-\hat{a} \hat{a}^{\dagger}-\hat{a}^{\dagger} \hat{a}+\hat{d} \hat{a}^{\dagger}\right)+\left(\hat{d} \hat{a}+\hat{a} \hat{a}^{\dagger}+\hat{a} \hat{a}^{\dagger}+\hat{a} \hat{a}^{\dagger}\right) \\
& =\frac{1}{2}\left(\hat{a}^{\dagger} \hat{a}+\hat{a} \hat{a}^{\dagger}\right)
\end{aligned}
$$

We now make use of the commutation relations to write

$$
\hat{a} \hat{a}^{\dagger}-\hat{a}^{\dagger} \hat{a}=1 \Rightarrow \hat{a} \hat{a}^{\dagger}=1+\hat{a}^{\dagger} \hat{a}
$$

which leads to

$$
\hat{H}=\frac{1}{2}\left(\hat{a}^{\dagger} \hat{a}+\hat{a} \hat{a}^{\dagger}\right)=\frac{1}{2}\left(\hat{a}^{\dagger} \hat{a}+1+\hat{a}^{\dagger} \hat{a}\right)=\hat{a}^{\dagger} \hat{a}+\frac{1}{2}
$$

This leads us to our first key point: the eigenvalues of the harmonic oscillator Hamiltonian are all positive. To see this, note that for any state, $|\psi\rangle$, the average energy will be:

$$
\left.\langle\psi| \hat{H}|\psi\rangle=\langle\psi| \hat{a}^{\dagger} \hat{a}|\psi\rangle+\langle\psi| \frac{1}{2}|\psi\rangle=|\hat{a}| \psi\right\rangle\left.\right|^{2}+\frac{1}{2}
$$

Since the norm of a vector is always positive, we conclude the average energy is always positive. However, for an eigenstate the average energy is just the energy eigenvalue and the point is made. Next, define the number operator

$$
\hat{N}=\hat{a}^{\dagger} \hat{a}
$$

We will see later that this operator counts the number of quanta in our state, justifying the name. This operator commutes with the Hamiltonian, so it has the same eigenstates, and the eigenvalues of $\hat{H}$ will just be the eigenvalues $\hat{N}$ plus one half. Consider an eigenstate, $|n\rangle$, of the number operator such that

$$
\hat{N}|n\rangle=n|n\rangle
$$

Then, let us consider how $\hat{N}$ acts on the state $\hat{a}^{\dagger}|n\rangle$ :

$$
\begin{aligned}
\hat{N}\left(\hat{a}^{\dagger}|n\rangle\right) & \left.\left.=\left(\hat{a}^{\dagger} \hat{a}\right) \hat{a}^{\dagger}|n\rangle=\hat{a}^{\dagger}\left(\left[\hat{a}, \hat{a}^{\dagger}\right]+\hat{a}^{\dagger} \hat{a}\right) n\right\rangle=\hat{a}^{\dagger}\left(1+\hat{a}^{\dagger} \hat{a}\right) n\right\rangle \\
& \left.=\hat{a}^{\dagger}(1+\hat{N}) n\right\rangle=\hat{a}^{\dagger}(1+n)|n\rangle
\end{aligned}
$$

So, collapsing this result, we see that

$$
\hat{N}\left(\hat{a}^{\dagger}|n\rangle\right)=(n+1) \hat{a}^{\dagger}|n\rangle
$$

Thus, $\hat{a}^{\dagger}|n\rangle$ is also an eigenstate of the number operator with eigenvalue $(n+1)$, which we write concisely as:

$$
\hat{a}^{\dagger}|n\rangle=c|n+1\rangle
$$

For this reason $\hat{a}^{\dagger}$ is called the "raising" operator. The proportionality constant, $c$, just notes that by itself $\hat{a}^{\dagger}|n\rangle$ is not necessarily normalized. What does $\hat{a}$ do? Well

$$
\begin{gathered}
\hat{a}|n+1\rangle \propto \hat{a}\left(\hat{a}^{\dagger}|n\rangle\right)=\left(\left[\hat{a}, \hat{a}^{\dagger}\right]+\hat{a}^{\dagger} \hat{a}\right)|n\rangle=(n+1)|n\rangle \\
\Rightarrow \vec{a}|n+1\rangle=c|n\rangle
\end{gathered}
$$

Thus, $\hat{a}$ lowers the eigenvalue of $\hat{N}$ by 1 and we call it the "lowering" operator.

We can also easily determine the constants of proportionality in

$$
\hat{a}^{\dagger}|n\rangle \propto|n+1\rangle \quad \text { and } \quad \hat{a}|n+1\rangle \propto|n\rangle
$$

Taking the norm of the I.h.s. in each case

$$
\begin{gathered}
\left.\left|\hat{a}^{\dagger}\right| n\right\rangle\left.\right|^{2}=\langle n| \hat{a} \hat{a}^{\dagger}|n\rangle=\left\langlen \left(\left(\hat{a}^{\dagger} \hat{a}+1\right)|n\rangle=\langle n \mid(\hat{N}+1) n\rangle=n+1\right.\right. \\
|\hat{a}| n+1\rangle\left.\right|^{2}=\left\langle n+1 \hat{a}^{\dagger} \hat{a} \mid n+1\right\rangle=n+1
\end{gathered}
$$

Hence, we can define the normalized eigenstates in terms of the raising and lowering operators as:

$$
\hat{a}^{\dagger}|n\rangle=\sqrt{n+1}|n+1\rangle \quad \text { and } \quad \hat{a}|n+1\rangle=\sqrt{n+1}|n\rangle
$$

Now, notice that we can repeat this process. For example, starting from $|n\rangle$ we can apply the raising operator repeatedly to obtain

$$
\hat{a}^{\dagger}|n\rangle=\sqrt{n+1}|n+1\rangle, \hat{a}^{\dagger} \hat{a}^{\dagger}|n\rangle=\sqrt{n+1} \sqrt{n+2}|n+2\rangle \text {, etc. }
$$

Or, we can apply the lowering operator repeatedly to obtain

$$
\hat{a}|n\rangle=\sqrt{n}|n-1\rangle, \hat{a}|n\rangle=\sqrt{n} \sqrt{n-1}|n-2\rangle \text {, etc. }
$$

Thus, given an initial state $|n\rangle$, we can define an entire hierarchy of equally spaced states going upward and downward in $n$. Now, recall that the energy of the system is just $n+\frac{1}{2}$ and we concluded on physical grounds that the energy cannot be negative. This means that there must be a lowest state $\left|n_{0}\right\rangle$ within the given hierarchy. What happens if we apply the lowering operator to this lowest state? Well, as we have already showed $\hat{a}\left|n_{0}\right\rangle$ must be proportional to an eigenstate of $\hat{N}$ with eigenvalue $n_{0}-1$. Since such a state does not exist, the only possibility is that the constant of proportionality is 0 ; i.e. we must have the so-called "killer condition":

$$
\begin{gathered}
\hat{a}\left|n_{0}\right\rangle=0 \\
\Rightarrow \hat{a}\left|n_{0}\right\rangle=\sqrt{n_{0}}\left|n_{0}\right\rangle=0
\end{gathered}
$$

$$
\Rightarrow n_{0}=0
$$

Hence, the eigenvalues of $\hat{N}$ are just the non-negative integers $n=0,1,2,3 \ldots$ and the designation "number operator" is justified. As a consequence, we immediately deduce the eigenvalues of the Hamiltonian, which we will canonically represent with $E$ 's:

$$
E_{n}=\left(n+\frac{1}{2}\right) \hbar \omega \quad(n=0,1,2,3 \ldots)
$$

where we have multiplied by $\hbar \omega$ to convert back to conventional units. It can be shown that these states are non-degenerate (CTDL). In fact, one can show that the bound states of any one-dimensional potential are non-degenerate.

We now want to work out some important operator brackets between the harmonic oscillator eigenfunctions. First, we already have the brackets of the creation and destruction operators

$$
\begin{gathered}
\langle m| \hat{a}^{\dagger}|n\rangle=\sqrt{n+1}\langle m \mid n+1\rangle=\sqrt{n+1} \delta_{m, n+1} \\
\langle m| \hat{a}|n\rangle=\sqrt{n}\langle m \mid n-1\rangle=\sqrt{n} \delta_{m, n-1}
\end{gathered}
$$

Next, we wish to derive the representation of position and momentum. This can be done by expanding in terms of creation and destruction operators:

$$
\begin{aligned}
& \langle m| \hat{q}|n\rangle=\frac{1}{\sqrt{2}}\langle m|\left(\hat{a}^{\dagger}+\hat{a}\right)|n\rangle=\frac{1}{\sqrt{2}}\left(\sqrt{n+1} \delta_{m, n+1}+\sqrt{n} \delta_{m, n-1}\right) \\
& \langle m| \hat{p}|n\rangle=\frac{i}{\sqrt{2}}\langle m|\left(\hat{a}^{\dagger}-\hat{a}\right)|n\rangle=\frac{i}{\sqrt{2}}\left(\sqrt{n+1} \delta_{m, n+1}-\sqrt{n} \delta_{m, n-1}\right)
\end{aligned}
$$

Hence $\hat{q}$ and $\hat{p}$ connect states that differ by one quantum of excitation.

Now, if we take an arbitrary state and act on it with the destruction operator:

$$
|\varphi\rangle \equiv \hat{a}|\chi\rangle=\hat{a} \sum_{n} x_{n}|n\rangle=\sum_{n} x_{n} \hat{a}|n\rangle
$$

we can determine the coefficients of the resulting state:

$$
|\varphi\rangle \equiv \sum_{n} y_{n}|n\rangle
$$

by doing our standard trick of multiplying on the left by a bra state:

$$
\langle m \mid \varphi\rangle \equiv \sum_{n}\langle m| y_{n}|n\rangle=\sum_{n} y_{n} \delta_{m n}=y_{m}
$$

where, in the second equality we have used the orthogonality of the harmonic oscillator states and in the third equality, we have noted
that the delta function is zero except when $m=n$. On the other hand, we also have:

$$
\langle m \mid \varphi\rangle=\sum_{n} x_{n}\langle m| \hat{a}|n\rangle=\sum_{n} x_{n}\langle m| \hat{a}|n\rangle=\sum_{n} x_{n} \sqrt{n} \delta_{m, n-1}=x_{m+1} \sqrt{m+1}
$$

Comparing the two equations gives:

$$
y_{m}=x_{m+1} \sqrt{m+1} .
$$

As a more impressive example of the power of the creation and destruction operators, let us compute the representations of $\hat{q}^{2}$ and $\hat{p}^{2}$.

$$
\begin{aligned}
\langle m| \hat{q}^{2}|n\rangle & =\frac{1}{2}\langle m|\left(\hat{a}^{\dagger}+\hat{a}\right)^{2}|n\rangle=\frac{1}{2}\langle m|\left(\hat{a}^{\dagger} \hat{a}^{\dagger}+\hat{a} \hat{a}^{\dagger}+\hat{a}^{\dagger} \hat{a}+\hat{a} \hat{a}\right)|n\rangle \\
& =\frac{1}{2}\left(\sqrt{n+2} \sqrt{n+1} \delta_{m, n+2}+(2 n+1) \delta_{m, n}+\sqrt{n-1} \sqrt{n} \delta_{m, n-2}\right) \\
\langle m| \hat{p}^{2}|n\rangle & =-\frac{1}{2}\left\langle m\left(\hat{a}^{\dagger}-\hat{a}\right)^{2} \mid n\right\rangle=\frac{1}{2}\left\langle m\left(\hat{a}^{\dagger} \hat{a}^{\dagger}-\hat{a} \hat{a}^{\dagger}-\hat{a}^{\dagger} \hat{a}+\hat{a} \hat{a}\right) \mid n\right\rangle \\
& =-\frac{1}{2}\left(\sqrt{n+2} \sqrt{n+1} \delta_{m, n+2}-(2 n+1) \delta_{m, n}+\sqrt{n-1} \sqrt{n} \delta_{m, n-2}\right)
\end{aligned}
$$

Thus, $\hat{q}^{2}$ and $\hat{p}^{2}$ connect states that differ by zero or two quanta. We could continue this process to obtain higher and higher powers, but the pattern is clear: terms involving the $\mathrm{n}^{\text {th }}$ power will connect states that differ by $n, n-2, n-4, \ldots$ quanta of excitation.

We can apply these bracket formulae to study uncertainty in the harmonic oscillator. We define the Uncertainty (really the standard deviation) of an operator $\hat{O}$ by

$$
\Delta O \equiv \sqrt{\left\langle\hat{O}^{2}\right\rangle-\langle\hat{O}\rangle^{2}}
$$

where it is understood that the averages must be taken with some prescribed state $|\psi\rangle$. Note that if $|\psi\rangle$ is an eigenstate of $\hat{O}$ then the uncertainty is zero. For the Harmonic oscillator eigenstate $|n\rangle$, let us take a look at the uncertainties in position and momentum:

$$
\begin{aligned}
& \Delta q=\sqrt{\langle n| \hat{q}^{2}|n\rangle-\langle n| \hat{q}|n\rangle^{2}}=\sqrt{\left(n+\frac{1}{2}\right)-0}=\sqrt{\left(n+\frac{1}{2}\right)} \\
& \Delta p=\sqrt{\langle n| \hat{p}^{2}|n\rangle-\langle n| \hat{p}|n\rangle^{2}}=\sqrt{\left(n+\frac{1}{2}\right)-0}=\sqrt{\left(n+\frac{1}{2}\right)}
\end{aligned}
$$

So we see that (in natural units) the Harmonic oscillator eigenstates are an even tradeoff between uncertainty in $q$ and $p$. Further, we note that the uncertainty product (converted to normal units):

$$
\Delta q \Delta p=\left(n+\frac{1}{2}\right) \hbar
$$

increases as we go up the ladder of states. Finally, we note that for the ground state (converting back to normal units):

$$
\Delta q \Delta p=\frac{\hbar}{2} .
$$

Notice that these statements are true for any harmonic oscillator with any frequency and any particle mass. By working in natural units, the universality of these observations becomes more apparent.

Now, we could go on to discuss the position-space representation of the energy eigenfunctions, $\psi_{n}(q)$. However, these functions are of exceedingly little practical use. As we have (hopefully) seen, it is far easier to do the algebra using the raising and lowering operators than it would be using the real space wavefunctions. Further, the process of solving for these functions is quite tedious. Hence, we will not discuss the real space representation here. Suffice it to say that the eigenfunctions obey the qualitative rules we are familiar with; they are peaked near the classical turning points, each successive excited state has one additional node, the wavefunction decays rapidly in classically forbidden regions, etc.

## C. Position Representation and Wave Mechanics

For unbound problems, the abstract Dirac notation is not sufficient; one really wants to know where the particle is in real, physical, space. Two of the most commonly used bases in real space are the eigenstates of the position operator

$$
\hat{q}|q\rangle=q|q\rangle
$$

and the eigenstates of the momentum operator

$$
\hat{p}|p\rangle=p|p\rangle
$$

Since position and momentum are Hermitian operators, we immediately conclude that 1) their eigenvalues are real and 2) their eigenstates form an orthonormal basis. These are not the only bases we will work in, but they are two very important ones.

Unfortunately, these bases are not discrete. That is, we have no physical reason to expect that certain positions are "allowed" while others are forbidden. Instead, we expect a continuum of possible results. This requires two slight modifications of the Hilbert space rules we've used before, which implicitly assume a discrete basis.

The first is a change in how we define orthonormality. In the case of a discrete basis we had:

$$
\left\langle\phi_{i} \mid \phi_{j}\right\rangle=\delta_{i j}
$$

where $\delta_{i j}$ was the Kronecker delta. In the continuous case, we instead have:

$$
\left\langle q \mid q^{\prime}\right\rangle=\delta\left(q-q^{\prime}\right)
$$

Where $\delta(z)$ is the Dirac Delta Function. It is equal to 0 if $z \neq 0$ and it is equal to $\infty$ when $z=0$ in such a way that

$$
\int_{-\infty}^{\infty} f(z) \delta(z) d z=f(0)
$$

For any $f(z)$. This should be thought of as the extension of the Kronecker Delta to the case of a continuous argument.

We have already touched on the second step in converting to a continuous basis: we must replace every summation with an integration:

$$
\sum_{\alpha} \Rightarrow \int d \alpha
$$

This makes mathematical sense, since an integral is effectively the limit of a sum as one takes more and more small steps to cover the same interval. As an example, where before we represented an arbitrary function as a sum of the basis functions:

$$
|\psi\rangle=\sum_{i} c_{i}\left|\phi_{i}\right\rangle
$$

in real space we can write this as an integral over the $|q\rangle$ basis states:

$$
|\psi\rangle=\int_{-\infty}^{\infty} \psi\left(q^{\prime}\right)\left|q^{\prime}\right\rangle d q^{\prime}
$$

Now, we can do our favorite trick and take the inner product of both sides with $\langle q|$ :

$$
\langle q \mid \psi\rangle=\langle q| \int_{-\infty}^{\infty} \psi\left(q^{\prime}\right)\left|q^{\prime}\right\rangle d q^{\prime}=\int_{-\infty}^{\infty} \psi\left(q^{\prime}\right)\left\langle q \mid q^{\prime}\right\rangle d q^{\prime}=\int_{-\infty}^{\infty} \psi\left(q^{\prime}\right) \delta\left(q-q^{\prime}\right) d q^{\prime}=\psi(q)
$$

Thus, we see that knowing the state, $|\psi\rangle$, allows us to determine the coefficients, $\psi(q)$, using the second equation; meanwhile, knowledge of the coefficients suffices to re-construct the state using the first equation. Thus, we can switch between the two representations

$$
|\psi\rangle \leftrightarrow \psi(q) \quad\langle\psi| \leftrightarrow \psi^{*}(q)
$$

This representation is called wave mechanics and is probably familiar to many of you. In this formalism, operators in Hilbert space are replaced by differential operators on the function $\psi(q)$. For example, the position operator is easy to deal with; if we define $|\chi\rangle \equiv \hat{q}|\psi\rangle$ then we can obtain the coefficients associated with $|\chi\rangle$ by taking the inner product with $\langle q|$ :

$$
\langle q \mid \chi\rangle=\langle q| \hat{q}|\psi\rangle=q\langle q \mid \psi\rangle=q \psi(q)
$$

Hence, in wave mechanics, to determine the effect of $\hat{q}$ operating on a state $|\psi\rangle$, one need only multiply the coefficients by $q$ :

$$
\hat{q}|\psi\rangle \leftrightarrow q \psi(q)
$$

What about the momentum operator? What is the wave mechanics analog of $\hat{p}$ acting on $|\psi\rangle$ ? We would like to obtain the representation of $\hat{p}$ in, say, the position basis $\left(\left\langle q_{1}\right| \hat{p}\left|q_{2}\right\rangle\right)$. As shown in the following technical digression, it turns out that this can be done using just the commutation relations $[\hat{q}, \hat{p}]=i \hbar$ and the fact that we can give the system a boosted velocity without changing the results of our measurements. The result is that

$$
\left\langle q_{1}\right| \hat{p}\left|q_{2}\right\rangle=-i \hbar \frac{\partial}{\partial q_{1}} \delta\left(q_{1}-q_{2}\right) .
$$

In order to proceed rigorously, we need to make a formal definition of the derivative of the Dirac delta function. We use the definition

$$
\int_{-\infty}^{\infty} f(x) \delta^{\prime}(x) d x=-\int_{-\infty}^{\infty} f^{\prime}(x) \delta(x) d x+\left.f(x) \delta(x)\right|_{-\infty} ^{\infty}
$$

where we have used integration by parts to get from the left to the right. Clearly, the second term is zero, since $\delta(\infty)=\delta(-\infty)=0$ and we assume $f(x)$ is finite. Hence,

$$
\int_{-\infty}^{\infty} f(x) \delta^{\prime}(x) d x=-\int_{-\infty}^{\infty} f^{\prime}(x) \delta(x) d x=-f^{\prime}(0)
$$

where, in the second equality, we have used the definition of the delta function. If we make the definition $f(x)=x g(x)$, then we see that

$$
\int_{-\infty}^{\infty} g(x) x \delta^{\prime}(x) d x=-\left.\frac{\partial}{\partial x} x g(x)\right|_{x=0}=-g(0)+\left.x g^{\prime}(x)\right|_{x=0}=-g(0)
$$

$$
\Rightarrow \int_{-\infty}^{\infty} g(x) x \delta^{\prime}(x) d x=-g(0)
$$

If we compare this last equation with the definition of the delta function:

$$
\Rightarrow \int_{-\infty}^{\infty} g(x) \delta(x) d x=g(0)
$$

we immediately find that

$$
x \delta^{\prime}(x)=-\delta(x)
$$

This turns out to be the most useful definition of $\delta^{\prime}(x)$ for our purposes. It is not quite unique; note that another function that satisfies this equation is:

$$
x\left(\delta^{\prime}(x)+c \delta(x)\right)=-\delta(x)
$$

Thus, the above definition only fixes $\delta^{\prime}(x)$ up to an additional term proportional to $\delta(x)$. All the above relations (and many others) can be found in Appendix II of CTDL.

So, we now want to work out the bracket elements of $\hat{p}$. To do this, we use the canonical commutation relations, sandwiched between two position eigenstates:

$$
\begin{aligned}
& \left\langle q_{1}\right| \hat{q} \hat{p}-\hat{p} \hat{q}\left|q_{2}\right\rangle=i \hbar\left\langle q_{1} \mid q_{2}\right\rangle \\
\Rightarrow & \left\langle q_{1}\right| q_{1} \hat{p}-\hat{p} q_{2}\left|q_{2}\right\rangle=i \hbar \delta\left(q_{1}-q_{2}\right) \\
\Rightarrow & \left(q_{1}-q_{2}\right)\left\langle q_{1}\right| \hat{p}\left|q_{2}\right\rangle=i \hbar \delta\left(q_{1}-q_{2}\right)
\end{aligned}
$$

We see that this is very close to the definition of the derivative of the delta function. If we define $\left(q_{1}-q_{2}\right)=x$ then we have

$$
\Rightarrow x\left\langle q_{1}\right| \hat{p}\left|q_{2}\right\rangle=i \hbar \delta(x)
$$

Thus, if we can just show that $\left\langle q_{1}\right| \hat{p}\left|q_{2}\right\rangle$ is a function of $\left(q_{1}-q_{2}\right)$, then we are done. Note that this is not generally true; generally we must assume that $\left\langle q_{1}\right| \hat{O}\left|q_{2}\right\rangle$ is a function of $q_{1}$ and $q_{2}$ separately (i.e. $\left.f\left(q_{1}, q_{2}\right)\right)$ and not just on the difference between the two (i.e. $f\left(q_{1}-q_{2}\right)$ ). An operator whose bracket elements depend on $\left(q_{1}-q_{2}\right)$ alone is said to be translation-invariant. Hence, we need to prove that the momentum operator is translation-invariant, which is equivalent to proving that

$$
\left\langle q_{1}\right| \hat{p}\left|q_{2}\right\rangle=\left\langle q_{1}+c\right| \hat{p}\left|q_{2}+c\right\rangle
$$

where $c$ is an arbitrary constant.

To do this, we note that any property of the system must be the same if I give everything a boost in the $q$ direction. That is, if I start with a stationary system and move it rigidly at a constant velocity, $v$, and I shift my frame of reference to move at that velocity, as well, I must get the same answer for any experiment. This property is called Galillean Invariance. Pictorially,



The fact that the system is moving at a velocity $v$ means that the states transform as

$$
|q\rangle \rightarrow|q+v t\rangle .
$$

When I shift my frame of reference to one that is moving with velocity $v$, the apparent momentum of the particle decreases by $m v$ :

$$
\hat{p} \rightarrow \hat{p}-m v
$$

So, comparing the system at rest to the boosted system, we must have

$$
\begin{gathered}
\left\langle q_{1}\right| \hat{p}\left|q_{2}\right\rangle=\left\langle q_{1}+v t\right| \hat{p}-m v\left|q_{2}+v t\right\rangle \\
\Rightarrow\left\langle q_{1}\right| \hat{p}\left|q_{2}\right\rangle=\left\langle q_{1}+v t\right| \hat{p}\left|q_{2}+v t\right\rangle-m v\left\langle q_{1}+v t \mid q_{2}+v t\right\rangle \\
\Rightarrow\left\langle q_{1}\right| \hat{p}\left|q_{2}\right\rangle=\left\langle q_{1}+v t\right| \hat{p}\left|q_{2}+v t\right\rangle-m v \delta\left(q_{1}-q_{2}\right)
\end{gathered}
$$

Now, the right hand side must be the same for arbitrary $t$ :

$$
\begin{gathered}
\left\langle q_{1}+v t_{\alpha}\right| \hat{p}\left|q_{2}+v t_{\alpha}\right\rangle-m v \delta\left(q_{1}-q_{2}\right)=\left\langle q_{1}+v t_{\beta}\right| \hat{p}\left|q_{2}+v t_{\beta}\right\rangle-m v \delta\left(q_{1}-q_{2}\right) \\
\Rightarrow\left\langle q_{1}+v t_{\alpha}\right| \hat{p}\left|q_{2}+v t_{\alpha}\right\rangle=\left\langle q_{1}+v t_{\beta}\right| \hat{p}\left|q_{2}+v t_{\beta}\right\rangle
\end{gathered}
$$

If we choose $t_{\alpha}=0$ and $t_{\beta}=c / v$ :

$$
\Rightarrow\left\langle q_{1}\right| \hat{p}\left|q_{2}\right\rangle=\left\langle q_{1}+c\right| \hat{p}\left|q_{2}+c\right\rangle
$$

and the momentum operator is translation-invariant.
Returning to our original equation:

$$
x\left\langle q_{1}\right| \hat{p}\left|q_{2}\right\rangle=i \hbar \delta(x)
$$

we now conclude that we can write $\left\langle q_{1}\right| \hat{p}\left|q_{2}\right\rangle \equiv u\left(q_{1}-q_{2}\right)=u(x)$, in which case

$$
\Rightarrow x u(x)=i \hbar \delta(x)
$$

This leads us to the conclusion that $u(x)=-i \hbar\left(\delta^{\prime}(x)+c \delta(x)\right)$, or, switching back to Dirac notation,

$$
\left\langle q_{1}\right| \hat{p}\left|q_{2}\right\rangle=-i \hbar \frac{\partial}{\partial q_{1}} \delta\left(q_{1}-q_{2}\right)-i \hbar c \delta\left(q_{1}-q_{2}\right)
$$

It is easily verified that $\hat{p} \rightarrow \hat{p}-c$ (which corresponds to boosting the momentum to match the frame of reference of the system) gives the final result:

$$
\left\langle q_{1}\right| \hat{p}\left|q_{2}\right\rangle=-i \hbar \frac{\partial}{\partial q_{1}} \delta\left(q_{1}-q_{2}\right)
$$

We can use the bracket of $\hat{p}$ between position states to get more general operator brackets. For example,

$$
\langle q| \hat{p}|\psi\rangle=\int_{-\infty}^{\infty}\langle q| \hat{p}\left|q^{\prime}\right\rangle\left\langle q^{\prime} \mid \psi\right\rangle d q^{\prime}=-i \hbar \int_{-\infty}^{\infty} \frac{\partial}{\partial q} \delta\left(q-q^{\prime}\right) \psi\left(q^{\prime}\right) d q^{\prime}=-i \hbar \frac{\partial \psi(q)}{\partial q}
$$

where, in the first equality, we have inserted the identity in the form

$$
1=\int_{-\infty}^{\infty}|q\rangle\langle q| d q
$$

Collapsing the string of equalities, we find:

$$
\Rightarrow\langle q| \hat{p}|\psi\rangle=-i \hbar \frac{\partial \psi(q)}{\partial q} .
$$

Thus, in wave mechanics, we can compute the effect of $\hat{p}$ on a state as:

$$
\hat{p}|\psi\rangle \leftrightarrow-i \hbar \frac{\partial \psi(q)}{\partial q} \quad\langle\psi| \hat{p} \leftrightarrow i \hbar \frac{\partial \psi^{*}(q)}{\partial q}
$$

To put the final piece in the puzzle, we note that in wave mechanics, inner products should be replaced by integration over all space:

$$
\left\langle\psi \mid \psi^{\prime}\right\rangle=\int_{-\infty}^{\infty}\langle\psi \mid q\rangle\left\langle q \mid \psi^{\prime}\right\rangle d q=\int_{-\infty}^{\infty} \psi^{*}(q) \psi^{\prime}(q) d q
$$

where on the right we have just inserted the identity between the bra and ket states.

To summarize, in wave mechanics 1) states are $|\psi\rangle$ are replaced by functions $\psi(q) 2$ ) Operators are constructed by making the replacements $\hat{q} \rightarrow q$ and $\hat{p} \rightarrow-i \hbar \frac{\partial}{\partial q}$ (assuming the differentiation acts to the right) and 3) The brackets $\langle\psi| O(\hat{q}, \hat{p})\left|\psi^{\prime}\right\rangle$ are generated by $\int_{-\infty}^{\infty} \psi^{*}(q) O\left(q,-i \hbar \frac{\partial}{\partial q}\right) \psi^{\prime}(q) d q$. Wave mechanics is very useful in treating unbound problems, as we now show.

## D. Piecewise Constant Potentials

A particle subject to a harmonic potential has the key feature that the particle is bound; because the potential energy increases quadratically as the displacement increases, one can never achieve an infinite displacement without an infinite energy. In practice, one is often also interested in unbound motion; in this case, the particle can escape as long as its energy is larger than some characteristic value. This turns out to be the key feature of a scattering experiment. The simplest paradigm for unbound motion involves a particle that encounters a potential step. Pictorially, we can represent this situation as:


Mathematically, the potential is given by

$$
V(\hat{q})= \begin{cases}V_{L} & q<q_{0} \\ V_{R} & q>q_{0}\end{cases}
$$

and the Hamiltonian is of the standard form $\left(\frac{\hat{p}^{2}}{2 m}+V(\hat{q})\right)$. Once again, we are going to be interested in the energy eigenfunctions of this potential. Far to the left of the step, the energy eigenfunctions satisfy:

$$
\left(\frac{\hat{p}^{2}}{2 m}+V_{L}\right)\left|\phi_{\alpha}\right\rangle=E_{\alpha}\left|\phi_{\alpha}\right\rangle
$$

while to the right, we have:

$$
\left(\frac{\hat{p}^{2}}{2 m}+V_{R}\right)\left|\phi_{\alpha}\right\rangle=E_{\alpha}\left|\phi_{\alpha}\right\rangle .
$$

Since momentum is conserved everywhere except in the vanishingly small region near the step, it makes the most sense to express the energy eigenstates in terms of momentum eigenstates. It is clear that away from the step, each equation can be solved if $\left|\phi_{\alpha}\right\rangle$ is an eigenfunction of the momentum operator:

$$
\begin{aligned}
& \left(\frac{\hat{p}^{2}}{2 m}+V_{L}\right)\left|p_{L}\right\rangle=\left(\frac{p_{L}^{2}}{2 m}+V_{L}\right)\left|p_{L}\right\rangle \equiv E_{L}\left|p_{L}\right\rangle \\
& \left(\frac{\hat{p}^{2}}{2 m}+V_{R}\right)\left|p_{R}\right\rangle=\left(\frac{p_{R}^{2}}{2 m}+V_{R}\right)\left|p_{R}\right\rangle \equiv E_{R}\left|p_{R}\right\rangle
\end{aligned}
$$

In order to have an eigenfunction of the full Hamiltonian, we must have that the energies to the left and the right of the step are the same ( $E_{L}=E_{R} \equiv E$ ). This allows us to solve for the possible values of $p_{L}$ and $p_{R}$ :

$$
\left(\frac{p_{L}^{2}}{2 m}+V_{L}\right)=E \Rightarrow p_{L}= \pm \sqrt{E-V_{L}} \quad\left(\frac{p_{R}^{2}}{2 m}+V_{R}\right)=E \Rightarrow p_{R}= \pm \sqrt{E-V_{R}}
$$

Thus, for a given energy, there are two possible values of the momentum on either side of the step, as shown in the picture: one going toward the step and one going away from the step. According to the rules of QM , we can therefore write the eigenfunction of the Hamiltonian as a superposition of these two (degenerate) possibilities:

$$
\left|\psi_{L}\right\rangle=a_{L}\left|+p_{L}\right\rangle+b_{L}\left|-p_{L}\right\rangle \quad\left|\psi_{R}\right\rangle=a_{R}\left|+p_{R}\right\rangle+b_{R}\left|-p_{R}\right\rangle
$$

How do we choose the coefficients $a_{L}, b_{L}, a_{R}, b_{R}$ ? Well, it is clear that the coefficients to the right of the barrier need, in some sense, to "match" the coefficients on the left. We can choose the correct matching conditions by forcing the wavefunction to give sensible
answers when we make a measurement at the step. First, we require that the wavefunction be single-valued at the step; that is, we require that

$$
\begin{align*}
\left\langle q_{0} \mid \psi_{L}\right\rangle & =\left\langle q_{0} \mid \psi_{R}\right\rangle \\
\Rightarrow a_{L}\left\langle q_{0} \mid+p_{L}\right\rangle+b_{L}\left\langle q_{0} \mid-p_{L}\right\rangle & =a_{R}\left\langle q_{0} \mid+p_{R}\right\rangle+b_{R}\left\langle q_{0} \mid-p_{R}\right\rangle \tag{Eq. 1}
\end{align*}
$$

Second, we require that the momentum be well-defined at the step:

$$
\begin{gathered}
\left\langle q_{0}\right| \hat{p}\left|\psi_{L}\right\rangle=\left\langle q_{0}\right| \hat{p}\left|\psi_{R}\right\rangle \\
\Rightarrow a_{L}\left\langle q_{0}\right| \hat{p}\left|+p_{L}\right\rangle+b_{L}\left\langle q_{0}\right| \hat{p}\left|+p_{L}\right\rangle=a_{R}\left\langle q_{0}\right| \hat{p}\left|+p_{R}\right\rangle+b_{R}\left\langle q_{0}\right| \hat{p}\left|+p_{R}\right\rangle \\
\Rightarrow a_{L} p_{L}\left\langle q_{0} \mid+p_{L}\right\rangle-b_{L} p_{L}\left\langle q_{0} \mid-p_{L}\right\rangle=a_{R} p_{R}\left\langle q_{0} \mid+p_{R}\right\rangle-b_{R} p_{R}\left\langle q_{0} \mid-p_{R}\right\rangle \text { Eq. } 2
\end{gathered}
$$

It turns out that these two conditions suffice to define our eigenfunctions. In order to convince ourselves that this is true, we note that if there was no step ( $V_{L}=V_{R} \equiv V$ ), then we would just have a free particle Hamiltonian ( $\hat{H}=\frac{\hat{p}^{2}}{2 m}$ ). In this case, there are two degenerate states with energy $E$ : one that moves toward the right and one toward the left. Thus the most general eigenfunction without the step can be written as a linear combination of the degenerate states:

$$
|\psi\rangle=a|+p\rangle+b|-p\rangle
$$

Thus, there are two parameters ( $a$ and $b$ ) that determine the wavefunction. The key realization is that introducing the step should change the form of the eigenfunctions, but not the number of eigenfunctions. Thus, we should have exactly two free parameters in the step eigenfunction. Since we initially have four coefficients ( $a_{L}, b_{L}, a_{R}, b_{R}$ ) and there are two equations that constrain these coefficients (single valued wavefunction, well-defined momentum) the number of free parameters in the presence of the step is still $4-2=2$. Thus, these two conditions are exactly sufficient to specify the allowed coefficients.

In order to solve for the coefficients of the eigenfunctions, we need to know the form for the amplitude $\langle q \mid p\rangle$. That is, we need to know the inner produt between the momentum basis (which is natural away from the step) to the position basis (which is natural at the step).

Given the position space representation $\hat{p} \rightarrow-i \hbar \frac{\partial}{\partial q}$, it is fairly easy to derive the $\langle q \mid p\rangle \equiv \psi_{p}(q)$ overlaps:

$$
\begin{aligned}
& \hat{p}|p\rangle=p|p\rangle \\
& \Rightarrow\langle q| \hat{p}|p\rangle=\langle q| p|p\rangle=p\langle q \mid p\rangle \\
& \Rightarrow-i \hbar \frac{\partial}{\partial q} \psi_{p}(q)=p \psi_{p}(q)
\end{aligned}
$$

The solution to this differential equation is easily verified to be:

$$
\psi_{p}(q) \propto e^{i p q / \hbar}
$$

These states are commonly referred to as plane waves. Using these functions, we can succinctly re-write the matching conditions $\left(\Rightarrow a_{L}\left\langle q_{0} \mid+p_{L}\right\rangle+b_{L}\left\langle q_{0} \mid-p_{L}\right\rangle=a_{R}\left\langle q_{0} \mid+p_{R}\right\rangle+b_{R}\left\langle q_{0} \mid-p_{R}\right\rangle \quad\right.$ Eq. 1, $\Rightarrow a_{L} p_{L}\left\langle q_{0} \mid+p_{L}\right\rangle-b_{L} p_{L}\left\langle q_{0} \mid-p_{L}\right\rangle=a_{R} p_{R}\left\langle q_{0} \mid+p_{R}\right\rangle-b_{R} p_{R}\left\langle q_{0} \mid-p_{R}\right\rangle$ Eq. 2) (choosing units so that $\hbar=1$ from now on):

$$
\begin{aligned}
a_{L} e^{i p_{L} q_{0}}+b_{L} e^{-i i_{L} q_{0}} & =a_{R} e^{i p_{R} q_{0}}+b_{R} e^{-i p_{R} q_{0}} \\
a_{L} p_{L} e^{i_{L} q_{0}}-b_{L} p_{L} e^{-i p_{L} q_{0}} & =a_{R} p_{R} e^{i i_{R} q_{0}}-b_{R} p_{R} e^{-i p_{R} q_{0}}
\end{aligned}
$$

In order to solve these two equations, it is convenient to choose the origin so that $q_{0}=0$. This is equivalent to redefining the coefficients in the following way:

$$
a_{L} \rightarrow a_{L} e^{-i p_{L} q_{0}} \quad b_{L} \rightarrow b_{L} e^{i p_{L} q_{0}} \quad a_{R} \rightarrow a_{R} e^{-i p_{R} q_{0}} \quad b_{R} \rightarrow b_{R} e^{i p_{R} q_{0}}
$$

Clearly we can reverse this later, but for now it simplifies our equations to:

$$
\begin{aligned}
a_{L}+b_{L} & =a_{R}+b_{R} \\
a_{L} p_{L}-b_{L} p_{L} & =a_{R} p_{R}-b_{R} p_{R}
\end{aligned}
$$

defining $\alpha=\frac{p_{R}}{p_{L}}$ this can be simplified further:

$$
\begin{gathered}
a_{L}+b_{L}=a_{R}+b_{R} \\
a_{L}-b_{L}=\left(a_{R}-b_{R}\right) \alpha .
\end{gathered}
$$

Adding and subtracting the two equations gives expressions for $a_{L}$ and $b_{L}$ in terms of $a_{R}$ and $b_{R}$

$$
\begin{aligned}
& a_{L}=a_{R} \frac{1+\alpha}{2}+b_{R} \frac{1-\alpha}{2} \\
& b_{L}=a_{R} \frac{1-\alpha}{2}+b_{R} \frac{1+\alpha}{2}
\end{aligned}
$$

What does this mean? Given the wavefunction to the right of the barrier, we can now deduce the wavefunction to the left of the barrier. This is the fundamental point for unbound problems: rather than
defining the wavefunction by a quantization condition, one defines the wavefunction by a boundary condition. In this case the boundary condition is that we know $\left|\psi_{R}\right\rangle$ at the barrier and we need to solve for a $\left|\psi_{L}\right\rangle$ that is consistent with this boundary condition. This fundamentally arises because the energy eigenstates are degenerate, and we therefore must specify additional constraints to define the state we are interested in.

In order to illustrate how one applies the boundary conditions in practice, let us treat a particular case. It is useful to think about the particle hitting the step as a time dependent process (i.e. first this happens and then this happens) even though our equations are not time resolved. Thus, suppose our particle is hits the step from the left with initial momentum $+p_{L}$ and scatters off the potential. Physically, there is no way the particle can end up to the right of the barrier with a negative momentum; it would have to surmount the step and then decide to turn around, but momentum is conserved far from the barrier. Since $b_{R}$ tells us about the probability of finding the particle to the right of the barrier with momentum - $p_{R}$, we naturally choose the boundary condition $b_{R}=0$ for this situation. Then,

$$
\begin{aligned}
& a_{L}=a_{R} \frac{1+\alpha}{2}+0 \frac{1-\alpha}{2}=a_{R} \frac{1+\alpha}{2} \\
& b_{L}=a_{R} \frac{1-\alpha}{2}+0 \frac{1+\alpha}{2}=a_{R} \frac{1-\alpha}{2} .
\end{aligned}
$$

Note that these coefficients are not normalized; normalization turns out to be very tricky in this situation, and we will work to develop expressions where the norms cancel. What interesting measurements could we make on this system? One very basic quantity we might be interested in is the probability that the particle will end up to the left of the barrier traveling left:

$$
\begin{aligned}
\langle\psi| \hat{P}_{-p_{L}}|\psi\rangle & \propto\left\langle\psi \mid-p_{L}\right\rangle\left\langle-p_{L} \mid \psi\right\rangle \\
& =\left\langle\psi_{L} \mid-p_{L}\right\rangle\left\langle-p_{L} \mid \psi_{L}\right\rangle \\
& =\left|b_{L}\right|^{2}
\end{aligned}
$$

where, on the second line, we have noted that if the particle is to the left of the barrier (as we have assumed) $|\psi\rangle \equiv\left|\psi_{L}\right\rangle$. This equation illustrates the important point that the probability of finding the system in a given basis state is the square of the coefficient of that basis state. This holds as long as the basis is orthonormal. This allows us
to write the probabilities of finding the particle on either side of the barrier traveling right:

$$
\left\langle\psi_{L}\right| \hat{P}_{+p_{L}}\left|\psi_{L}\right\rangle \propto\left|a_{L}\right|^{2} \quad\left\langle\psi_{R}\right| \hat{P}_{+p_{R}}\left|\psi_{R}\right\rangle \propto\left|a_{R}\right|^{2}
$$

In the present case, these are all proportionalities, since we haven't normalized our state. However, if we take ratios of these, the constants cancel. For example, we might consider the following ratios that relate to the number of particles that are Reflected and Transmitted:


The question marks indicate that, as we shall see, these expressions are not quite correct. We now make use of our explicit solution for $a_{L}$ and $b_{L}$ in terms of $a_{R}$ :

$$
\begin{aligned}
& R^{?}=\frac{\left|b_{L}\right|^{2}}{\left|a_{L}\right|^{2}}=\frac{\left|\frac{1-\alpha}{2} a_{R}\right|^{2}}{\left|\frac{1+\alpha}{2} a_{R}\right|^{2}}=\left|\frac{1-\alpha}{1+\alpha}\right|^{2} \\
& T=\frac{2}{=} \frac{\left|a_{R}\right|^{2}}{\left|a_{L}\right|^{2}}=\frac{\left|a_{R}\right|^{2}}{\left|\frac{1+\alpha}{2} a_{R}\right|^{2}}=\left|\frac{2}{1+\alpha}\right|^{2}
\end{aligned}
$$

If these were really transmission and reflection probabilities, then they would sum to 1 , since the particle must either be transmitted or reflected. However:

$$
T+R \stackrel{2}{=}\left|\frac{2}{1+\alpha}\right|^{2}+\left|\frac{1-\alpha}{1+\alpha}\right|^{2}=\frac{3-2 \alpha+\alpha^{2}}{(1+\alpha)^{2}} \neq 1
$$

where we have used that $\alpha=\frac{p_{R}}{p_{L}}$ is real. What is wrong?


In order to obtain a reasonable answer, we must appeal to the timedependent picture once again. The measurements we made above simply counted the number of particles on one or the other side of the barrier in a given instant. A physical detector, on the other hand, must occupy a particular part of space and make a measurement for a given (typically long) period of time. Thus the experimental set up looks like the picture above and the relevant observable is not the total number of particles on one side of the barrier, but the number of particles per unit time that hit the detector. The first observable is density, the second is flux (or current). Simple arguments suffice to get from one observable to the other. For a given density, the flux of particles is proportional to their speed; the faster the particles move, the more particles will hit the detector per unit time. Thus, flux $=\mid$ velocity $\mid \times($ density $)$ and the reflected and transmitted fluxes are given by:

$$
\begin{gathered}
R=\frac{p_{L}\left|b_{L}\right|^{2}}{p_{L}\left|a_{L}\right|^{2}}=\frac{\left|b_{L}\right|^{2}}{\left|a_{L}\right|^{2}}=\left|\frac{1-\alpha}{1+\alpha}\right|^{2} \\
T=\frac{p_{R}\left|a_{R}\right|^{2}}{p_{L}\left|a_{L}\right|^{2}}=\frac{p_{R}}{p_{L}}\left|\frac{2}{1+\alpha}\right|^{2}=\alpha\left|\frac{2}{1+\alpha}\right|^{2}
\end{gathered}
$$

If we use these two expressions, we find that probability flux is conserved (assuming $\alpha$ is real):

$$
T+R=\alpha\left|\frac{2}{1+\alpha}\right|^{2}+\left|\frac{1-\alpha}{1+\alpha}\right|^{2}=\frac{4 \alpha}{(1+\alpha)^{2}}+\frac{1-2 \alpha+\alpha^{2}}{(1+\alpha)^{2}}=\frac{1+2 \alpha+\alpha^{2}}{(1+\alpha)^{2}}=1
$$

Now that we feel like we've got the right expressions for transmission and reflection, we make a few observations about our results. The first is that, even though the energy of the particle is above the barrier, there is still some probability that the particle will be reflected. Note that this would not be true for a classical particle; in that case, there would be $100 \%$ probability of transmission if the energy was above the barrier and $0 \%$ chance of reflection. The situation here is more reminiscent of classical waves, which typically split into two traveling waves whenever an obstacle is encountered. This "below barrier reflection" is another example of the particle-wave duality in QM .

Another good exercise is to examine the high- and low-energy limits of our expressions. When the energy is very high, the two momenta become almost equal, $p_{L} \approx p_{R}$, and $\alpha \approx 1$. As a result

$$
R=\left|\frac{1-\alpha}{1+\alpha}\right|^{2} \approx\left|\frac{1-1}{1+1}\right|^{2}=0
$$

Thus, at high energies, nothing gets reflected and the particle behaves like a classical particle. This is an example of quantumclassical correspondence: when the energy (or mass) is large enough, QM must recover the classical result, since we know that classical mechanics is correct for macroscopic objects. For energies just above the barrier, $p_{R} \approx 0$ and $\alpha \approx 0$ so that

$$
R=\left|\frac{1-\alpha}{1+\alpha}\right|^{2} \approx\left|\frac{1-0}{1+0}\right|^{2}=1
$$

and in this limit, the particle is always reflected.
Up until this point, we have made the tacit assumption that the energy is larger than $V_{R}$. For example, we have written down the momentum on the right as:

$$
p_{R}= \pm \sqrt{E-V_{R}} .
$$

However, if $E<V_{R}$ this is an imaginary number. Since it is not possible for a classical particle with energy $E<V_{R}$ to actually exist to the right of the barrier, this region is called the "classically forbidden" region. It turns out that all the equations we've written so far still hold (formally) in the classically forbidden region as long as we keep track
of complex conjugates. For example, we can still write out the momentum "eigenstate"

$$
\psi_{ \pm p}(q) \propto e^{ \pm i p q / \hbar}=e^{ \pm q q_{1} / h} \quad(\varphi=i p)
$$

where on the right we have taken care to write things in terms of the real variable $\varphi$. Note that, instead of oscillating forever, the momentum states with imaginary momentum grow or decay exponentially as a fuction of $q$, depending on the sign of $\varphi$. Now, we write the wavefunction to the right as

$$
\left|\psi_{R}\right\rangle=a_{R}\left|+\varphi_{R}\right\rangle+b_{R}\left|-\varphi_{R}\right\rangle
$$

and we see immediately that there will be a problem if $b_{R} \neq 0$, because then the wavefunction will grow beyond all bound in the classically forbidden region. Since we associate the square of the wavefunction with the probability of finding the particle at a particular point, this is clearly unphysical. Thus, we conclude that $b_{R}=0$ and the only solution to the right of the barrier is the one that decays. This is the source of the often-used blanket statement that "the wavefunction always decays exponentially in the classically forbidden region." This is not rigorously true, since the wavefunction can often decay either faster or slower than an exponential in a classically forbidden region. However, in general this idea is qualitatively correct. Note that, in the classically forbidden case there is no transmission. Because the wavefunction decays exponentially to the right of the barrier, the probability of finding the particle far to the right is vanishingly small. However, there is a small amount of barrier penetration; it is possible to find the particle just inside the barrier, before the decaying component has fallen to zero. This is called tunneling, and the characteristic distance that the particle can tunnel is given by $\hbar / \varphi$.

