Continuum Physics in d=1

We can understand a number of properties of one dimensional scattering by considering an off-diagonal current. We define

$$J_x = \frac{\hbar}{2mi}\left(\Psi_2^* \partial_x \Psi_1 - (\partial_x \Psi_2^*)\Psi_1\right)$$

and

$$\rho = \Psi_2^* \Psi_1.$$

Now if both Ψ_1 and Ψ_2 satisfy the time-dependent Schrödinger equation, we have.

$$\partial_x J_x + \partial_t \rho = 0$$

The current as defined with two different solutions is not necessarily a physical object. If we have the *same* two functions in the current, then it does have a physical meaning if we use properly normalized solutions of the Schrödinger equation. For now, we use continuum solutions which are not normalized in any particular way.

Now suppose both states are energy eigenstates with the same energy E.

$$\Psi_1 \sim \exp(-i\frac{Et}{\hbar})\ \Psi_2 \sim \exp(-i\frac{Et}{\hbar})$$

Then

$$\partial_t \rho = 0,$$

so we also have

$$\partial_x J_x = 0,$$

so the current must be independent of x.

To see what can happen, let us try some examples with free particle wave functions. First we try plane waves traveling in the same direction.

$$\Psi_1 = \exp(ikx)\ \Psi_2 = \exp(ikx)$$

This gives

$$J_x = \frac{\hbar k}{2m}$$

Next, try two plane waves traveling in opposite directions.

$$\Psi_1 = \exp(ikx)\ \Psi_2 = \exp(-ikx)$$

This gives

$$J_x = 0.$$

These two results will be useful in what follows. Now consider an eigenfunction when a potential is present. We take the potential to fall to zero as $|x| \to \infty$. The standard setup is to have a plane wave incident from $x = -\infty$, so the wave function takes the forms

$$\Psi_k(x) \to \exp(ikx) + R\exp(-ikx)\ \ x << 0,$$

and

$$\Psi_k(x) \to T\exp(ikx) \;\; x >> 0$$

In these notes R will be called the **reflection coefficient** and T will be called the **transmission coefficient**. The makes sense because they are *coefficients* of reflected and transmitted waves, respectively.

Let us see what we can learn by considering the current associated with Ψ_k.

$$J_x = \frac{\hbar}{2mi}\left(\Psi_k^*\partial_x\Psi_k - (\partial_x\Psi_k)^*\Psi_k\right)$$

Using our results from the two examples, we have

$$J_x = \frac{\hbar k}{m}(1-|R|^2) \quad x << 0,$$

and

$$J_x = \frac{\hbar k}{m}|T|^2 \quad x >> 0.$$

Since J_x must be independent of x, we have

$$1-|R|^2 = |T|^2$$

This simple result will contain extra factors of wave-vectors if the media at $x >> 0$ and $x << 0$ have different wave-vectors.

Wave Packets Although most of our attention will be on the solutions which have plane wave behavior at infinity, it is worthwhile to briefly consider the time dependence of a normalizable solution of the Schrödinger equation. We will concentrate on the region $x << 0$. The discussion for $x >> 0$ is completely analogous. Our scattering solutions with definite k or definite energy in this region have the behavior

$$\Psi_k(x) \to \exp(ikx) + R(k)\exp(-ikx)$$

In order to have a solution of the Schrödinger equation that would describe a real experimental situation, we need to form a wave packet by integrating over k. We write

$$\Psi(x,t) = \int dk\phi(k)\exp(-i\omega_k t)(\exp(ikx) + R(k)\exp(-ikx)),$$

where $\omega_k = (\hbar k^2)/2m$. We will assume that $\phi(k)$ is a smooth function, sharply peaked around $k = k_0$, such as

$$\phi(k) = N\exp(-\frac{\alpha(k-k_0)^2}{2}).$$

It is typically true in any scattering experiment that the functions that describe the scattering (in this case $R(k)$ and $T(k)$) are slowly varying in k compared to the variation

of $\phi(k)$. This makes it a good approximation to replace $R(k)$ by its value at $k = k_0$. Then we can get a good approximation to $\Psi(x,t)$ for $x << 0$ by computing the integral

$$\Psi(x,t) \sim \int dk\phi(k)\exp(-i\omega_k t)(\exp(ikx) + R(k_0)\exp(-ikx)).$$

Setting $k = k_0$ gives us standard Gaussian integrals to do. We have the formula

$$\Psi(x,t) \sim \left(\exp(-\frac{(x-v_0t)^2}{2(\alpha^2+\beta^2)}) + R(k_0)\exp(-\frac{(x+v_0t)^2}{2(\alpha^2+\beta^2)})\right), \tag{1}$$

where we have not written phase factors multiplying each term, and

$$\beta = \frac{\hbar t}{m}, \quad v_0 = \frac{\hbar k_0}{m}$$

The first term in Eq.(1) is negligible except in a narrow range around $x = v_0t$. The second term is negligible except in a narrow range around $x = -v_0t$. So for $x << 0$ and $t << 0$, only the first term is "on", while $x << 0$ and $t >> 0$ only the second term is "on." For the transmitted wave, the packet is negligible except near $x - v_0t$ and this term will be "on" for $x >> 0$ and $t >> 0$. This brief discussion shows that if packets are built up, the common sense behavior of scattering is obtained.

Parity Invariance We can obtain additional results when the potential is even under $x \to -x$,

$$V(x) - V(-x)$$

When this is true, the Hamiltonian is parity invariant, parity is a good quantum number, and solutions will be of definite parity, either even or odd. Let us consider the even parity case first. We define

$$\Psi_e(x) = \Psi_k(x) + \Psi_k(-x)$$

Using our previous large $|x|$ forms, we have

$$\Psi_e(x) \to (T+R)\exp(ikx) + \exp(-ikx) \quad x >> 0,$$

and

$$\Psi_e(x) \to (T+R)\exp(-ikx) + \exp(ikx) \quad x << 0.$$

Again, just as before, the current must be independent of x. Computing the current, we have

$$J_x = \frac{\hbar k}{2m}(|R+T|^2 - 1) \quad x >> 0,$$

and

$$J_x = \frac{\hbar k}{2m}(1 - |R+T|^2) \quad x << 0.$$

These two expressions must be equal. The only way this can happen is if both vanish, so we have

$$|R+T|^2 = 1.$$

This makes sense. An even parity solution sends in a particle from $x >> 0$ and one from $x << 0$ as well. What goes in must come out, so there can be no net current. The difference between this case and the standard one of a particle only incident from the left is *symmetry.*

Turning to odd or negative parity, we have

$$\Psi_o(x) \to (T-R)\exp(ikx) - \exp(-ikx) \;\; x >> 0,$$

and

$$\Psi_o(x) \to (R-T)\exp(-ikx) + \exp(ikx) \;\; x << 0.$$

Again computing the current, we get

$$J_x = \frac{\hbar k}{2m}(|R-T|^2 - 1) \quad x >> 0,$$

and

$$J_x = \frac{\hbar k}{2m}(1 - |R-T|^2) \quad x << 0.$$

Just as for even parity, the only way the current can be independent of x is for it to vanish, so we have

$$|T-R|^2 = 1$$

We have found that $T \pm R$ are both of unit modulus, so we can write them as follows:

$$T + R = z_e = \exp(2i\delta_e),$$

and

$$T - R = z_o = \exp(2i\delta_o).$$

The δ_e and δ_o are called *phase shifts.* The reason for the factor of 2 in the exponents will be explained later.

Even Parity Example To illustrate the discussion so far, we consider a square well potential and look at the even parity continuum solutions. The potential is initially taken to be repulsive, of strength V_0. We define

$$\kappa^2 = \frac{2mV_0}{\hbar^2}$$

The potential is zero for $|x| > a$, so we have the forms

$$\Psi_e = z_e \exp(ikx) + \exp(-ikx) \;\; x > a,$$

and

$$\Psi_e = A\cos(k'x) \;\; |x| < a.$$

The Schrödinger equation gives the relation

$$(k')^2 + \kappa^2 = k^2$$

It is useful in what follows to make the following definition.

$$\xi = \exp(ika) \;\; \bar{\xi} = \exp(-ika).$$

Now we must match the value and derivative of the wave function at $x = a$. This gives,

$$A\cos(k'a) = z_e\xi + \bar{\xi},$$

and

$$-k'A\sin(k'a) = ik(z_e\xi - \bar{\xi}).$$

Taking the ratio of these equations, we have

$$-k'\tan(k'a) = \frac{ik(z_e\xi - \bar{\xi})}{z_e\xi + \bar{\xi}}$$

Solving for z_e, we obtain

$$z_e = (\bar{\xi})^2\frac{ik - k'\tan(k'a)}{ik + k'\tan(k'a)}.$$

Note that $|z_e| = 1$ as it must.

So far we have studied the repulsive square well. However, our results can easily be adapted to the attractive case. We merely need to change the formula for k', so that it reads as follows:

$$(k')^2 - \kappa^2 = k^2$$

Our previous formula for z_e still applies. Now we know that the attractive square well always has a bound state. This can be seen in scattering quantities by taking

$$k \to i\alpha.$$

This takes $k^2 \to -\alpha^2$. i.e. we go from the scattering region to the bound state region. Doing this, we notice that

$$z_e(i\alpha) \to \infty$$

happens at

$$\alpha = k'\tan(k'a)$$

which is just the bound state condition for even parity in an attractive square well. To see what is going on in more detail, we multiply our even parity solution by $(ik + k'\tan(k'a))$, the factor that appears in the denominator of z_e. This gives

$$\Psi'_e = \exp(-ikx)(ik + k'\tan(k'a)) + \exp(ikx)(ik - k'\tan(k'a))(\bar{\xi})^2$$

Now let us let

$$k \to i\alpha.$$

We see that Ψ'_e becomes

$$\Psi'_e = \exp(\alpha x)(-\alpha + k' \tan(k'a)) + \exp(-\alpha x)(-\alpha - k' \tan(k'a))(\bar{\xi})^2$$

This is a solution of the Schrödinger equation, but is physically unacceptable unless the coefficient of the exploding exponential vanishes. When that does happen, we have a bound state. We see by looking at the equation for Ψ'_e, that the vanishing of this coefficient happens at

$$\alpha = k' \tan(k'a)$$

which we found previously as the condition for $z_e(i\alpha) = \infty$. **Summary:** By analytic continuation in k or the energy, scattering amplitudes reveal the presence of bound states of the system, if they exist.

Phase Shifts We will discuss the odd parity case, since it is of the same form as three dimensional scattering in the $l = 0$ state. Considering the large x behavior, we write

$$\Psi_o(x) \to \exp(2i\delta_o) \exp(ikx) - \exp(-ikx) = 2i \exp(i\delta_o) \sin(kx + \delta_o).$$

The reason for choosing $2\delta_o$ in the exponent of z_o is that the large x form then goes into a factor times $\sin(kx + \delta_o)$. The phase shift is a physically meaningful quantity, which is determined by the potential. If the phase shift is **positive**, the sin reaches each value at a *smaller* value of kx than it would for $\delta_o = 0$. It is as if the wave function is "pulled in" toward the origin. This case is characteristic of an *attractive* potential. Similarly, if the phase shift is negative, the sin reaches its argument later in kx than it would for $\delta_o = 0$, and we say the wave function is "pushed away" from the origin. This case is characteristic of a repulsive potential.

Integral Equation for Scattering The use of an integral equation for scattering is a way to automatically build in the required behavior at large x. The reflected and transmitted waves travel *away* from the region where the potential exists, and are therefore *outgoing* waves. The integral equation makes this behavior automatic.

Start with the Schrödinger equation,

$$(-\frac{\hbar^2}{2m}\partial_x^2 + V)\Psi = \frac{(\hbar k)^2}{2m}\Psi,$$

and re-arrange it to

$$(\partial_x^2 + k^2)\Psi = U(x)\Psi,$$

where

$$U(x) = \frac{2m}{\hbar^2}V(x).$$

The scattering situation can be represented as an input or zeroth order wave function, plus a scattered wave,

$$\Psi = \Psi^0 + \Psi_{sc}.$$

The zeroth order wave is a solution of the free Schrödinger equation,

$$(\partial_x^2 + k^2)\Psi^0 = 0,$$

while the scattered wave satisfies

$$(\partial_x^2 + k^2)\Psi_{sc} = U(x)\Psi.$$

These are both taken care of in the integral equation,

$$\Psi(x) = \Psi^0(x) + \int G_s(x - x')U(x')\Psi(x')dx'.$$

The free solution Ψ^0 can take various forms; $\exp(ikx)$ if the goal is to calculate R and T, or $\cos(kx)$ or $\sin(kx)$ if the goal is to work with definite parity solutions and obtain z_e or z_o. The function $G_s(x - x')$ is a scattering Green function, and must satisfy

$$(\partial_x^2 + k^2)G_s(x - x') = \delta(x - x') \tag{2}$$

From the integral equation, we see that the integration over x' is restricted to the region where the potential U is non-zero, essentially near the origin for a potential of restricted range. To obtain the correct large $|x|$ behavior for the wave function $\Psi_k(x)$, G_s must have the following behaviors;

$$G_s \sim \exp(ik(x - x')) \quad x >> x',$$

and

$$G_s \sim \exp(-ik(x - x')) \quad x << x'.$$

The final form of $G_s(x - x')$ which satisfies all requirements is

$$G_s = \frac{1}{2ik}\exp(ik|x - x'|). \tag{3}$$

The conditions on large $|x|$ behavior follow directly. The δ-function behavior is derived as follows. First compute a first derivative as $x \to x'$. We have

$$\partial_x G_s(x - x') = \frac{1}{2ik}\partial_x(1 + ik|x - x'| + \ldots) = \frac{1}{2ik}(ik(\theta(x) - \theta(-x)) + \ldots)$$

Computing a second derivative we obtain

$$\partial_x\partial_x G_s = \frac{1}{2ik}2ik\delta(x - x') = \delta(x - x'),$$

which shows that $G_s(x-x')$ contains the correct δ-function behavior. From Eq.(2) we have that $G_s(x-x')$ is the inverse of the operator $(\partial_x^2+k^2)$. Writing this as an equation, we have

$$G_s =< x|(\partial_x^2+k^2)^{-1}|x' > . \tag{4}$$

To spell this out in more detail, we first write the action of $(\partial_x^2+k^2)$, on a plane wave, which gives

$$(\partial_x^2+k^2) < x|k' >= (-(k')^2+k^2) < x|k' > .$$

It follows that $(\partial_x^2+k^2)^{-1}$ must produce

$$(\partial_x^2+k^2)^{-1} < x|k' >= (-(k')^2+k^2)^{-1} < x|k' > .$$

We may use this in Eq.(4) by sandwiching a complete set of wave-vector kets just after the $(\partial_x^2+k^2)^{-1}$ operation. The latter is ambiguous until we specify a prescription for handling the behavior when $k'=k$. This is done by an " $i\epsilon$" prescription, which gives the rule for detouring around the pole in the complex k' plane at $k'=\pm k$. The particular choice that is made is what guarantees that $G_s(x-x')$ will produce only outgoing waves. The final formula for $G_s(x-x')$ represented as an integral over k' is

$$G_s(x-x') = \int dk' < x|k' > \frac{1}{k^2+i\epsilon-(k')^2} < k'|x' >= \int \frac{dk'}{2\pi} \exp(ik'(x-x')) \frac{1}{k^2+i\epsilon-(k')^2}. \tag{5}$$

Verifying that this formula gives Eq.(3) when the k' integration is carried out is done by contour integration, a subject not required for Physics 580. However, let us extract the Fourier transform of G_s. We may write

$$G_s(x-x') = \int \frac{dk'}{2\pi} \exp(ik'(x-x'))\tilde{G}_s(k').$$

From Eq.(5) we find

$$\tilde{G}_s(k') = \frac{1}{k^2+i\epsilon-(k')^2}. \tag{6}$$

Propagator, Time Dependent and Scattering Green Functions In this section we relate three quantities which have been introduced thus far. For simplicity, we will take the case of a free particle with

$$H = -\frac{(\hbar\partial_x)^2}{2m}.$$

The quantity we have called the *propagator* is defined as

$$K(x,t;x',t') \equiv< x| \exp(-\frac{H(t-t')}{\hbar}|x' >,$$

and satisfies the equation,

$$(i\hbar\partial_t + \frac{(\hbar\partial_x)^2}{2m})K(x,t;x',t') = 0. \tag{7}$$

$K(x,t;x',t')$ is an object of interest in its own right, and of course is the basic quantity in Feynman's path integral formulation of quantum mechanics. Closely related to $K(x,t;x',t')$ is a quantity we can call the *time dependent Green function* defined as follows:

$$G_F(x,t;x',t') = -\frac{i}{\hbar}\theta(t-t')K(x,t;x',t'),$$

where the subscript F is for Feynman, and $\theta(t-t')$ is a step function, defined as follows:

$$\theta(t) = \begin{cases} 1 & t > 0 \\ 0 & t < 0 \end{cases}$$

The time dependent Green function satisfies a different equation than the propagator. We have

$$(i\hbar\partial_t + \frac{(\hbar\partial_x)^2}{2m})G_F(x,t;x',t') = \delta(t-t')K(x,t;x',t') + (i\hbar\partial_t + \frac{(\hbar\partial_x)^2}{2m})K(x,t;x',t')$$

$$= \delta(t-t')\delta(x-x')$$

To get the last equality, we used: (1) $\partial_t\theta(t-t') = \delta(t-t')$ (2)$K(x,t;x',) =< x|x' >= \delta(x-x')$ and (3) Eq.(7).

Let us Fourier analyze $G_F(x,t;x',t')$. We may write

$$G_F(x,t;x',t') = \int \frac{dk}{2\pi}\frac{d\omega}{2\pi}\exp(ik(x-x'))\exp(-i\omega(t-t'))\tilde{G}_F(k,\omega)$$

Applying the Schrödinger operator, we get

$$(i\hbar\partial_t + \frac{(\hbar\partial_x)^2}{2m})G_F(x,t;x',t') = \int \frac{dk}{2\pi}\frac{d\omega}{2\pi}\exp(ik(x-x'))\exp(-i\omega(t-t'))(\hbar\omega - \frac{(\hbar k)^2}{2m})\tilde{G}_F(k,\omega)$$

$$= \delta(t-t')\delta(x-x') = \int \frac{dk}{2\pi}\frac{d\omega}{2\pi}\exp(ik(x-x'))\exp(-i\omega(t-t'))$$

Comparing the last two equalities, we have

$$(\hbar\omega - \frac{(\hbar k)^2}{2m})\tilde{G}_F(k,\omega) = 1$$

Before dividing to get $\tilde{G}_F(k,\omega)$, it is necessary to give a prescription for what to do when $\hbar\omega = (\hbar k)^2/2m$. This is a so-called "i$\epsilon$" prescription. The correct formula for $\tilde{G}_F(k,\omega)$ is

$$\tilde{G}_F(k,\omega) = \frac{1}{(\hbar\omega + i\epsilon - \frac{(\hbar k)^2}{2m})}$$

The quantity $i\epsilon$ is an infinitesimal positive imaginary number, and says that the pole of $\tilde{G}_F(k,\omega)$ is located at

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

i.e. an infinitesimal amount in the lower half of the complex ω plane. This prescription will insure that in returning to real time by doing the integral over ω, the factor $\theta(t-t')$ will result. The relation between $\tilde{G}_F$ and $\tilde{G}_s$ will become clear if we use k' as the spacial Fourier variable in both cases. Doing this for $\tilde{G}_F$, we have

$$\frac{\hbar^2}{2m}\tilde{G}_F(\omega,k') = \frac{1}{\frac{2m\hbar\omega}{\hbar^2}+i\epsilon-k'^2}$$

Now if we set $\hbar\omega = (\hbar k)^2/2m$, we have from Eq.(6) that

$$\frac{\hbar^2}{2m}\tilde{G}_F(\frac{\hbar k^2}{2m},k') = \tilde{G}_s(k'),$$

or returning to configuration space, we have

$$G_s(x-x') = \frac{\hbar^2}{2m}\tilde{G}_F(\frac{\hbar k^2}{2m},x-x')$$

So G_s is related to G_F, or more accurately to the Fourier transform in time of G_F, with the frequency evaluated at the energy of the scattering process divided by $\hbar$. It should be noted that our notation for the scattering Green function always implies an energy for the scattering process. This is clear from the defining equation for G_s, Eq.(2).

The summary of this section is that G_F and G_s are closely related quantities. In practice, in discussing scattering from a static potential as covered in this section, G_s is the appropriate quantity to use. If the potential is time dependent, G_F is the appropriate quantity. In particle physics and condensed matter physics, the scattering is always time dependent. In that case the object which generalizes our G_F is the correct one to use.