A. PROPAGATORS IN QUANTUM THEORY

In elementary Q.M., we are typically presented with the wave-function or state vector $|\psi_\alpha(t)\rangle$ as the fundamental quantity of interest. But often we are more interested in the transitions between states, and the time evolution of such transitions. Thus we may wish to know what is the TRANSITION AMPLITUDE for a system to go from state $|\psi_\alpha(t_1)\rangle$ at time t_1 to another state $|\psi_\beta(t_2)\rangle$ at time t_2.

Let us assume a CLOSED system, which can therefore be described by a time-independent Hamiltonian $\mathcal{H}$, satisfying the Schrodinger differential eqtn

$$(\hat{\mathcal{H}} - i\hbar \hat{I} \partial_t)\,\psi(t) = 0 \qquad (1)$$

where we make explicit the fact that $i\hbar\partial_t$ is multiplied by the unit operator $\hat{I}$.

We can then invert (1) to write, for the time evolution of $\psi(t)$, that

$$|\psi(t_2)\rangle = e^{-i/\hbar\,\hat{H}(t_2 - t_1)}\,|\psi(t_1)\rangle \qquad (2)$$

Moreover we can always decompose $\psi(t)$ into a sum over the eigenstates $|n(t)\rangle$ of $\hat{\mathcal{H}}$, ie., we write

$$|\psi(t)\rangle = \sum_n c_n(t)|\phi_n(t)\rangle \equiv \sum_n c_n|n\rangle \qquad (3)$$

such that $\hat{\mathcal{H}}|n\rangle = \epsilon_n|n\rangle \qquad (4)$

from which it follows that $|\phi_n(t_2)\rangle = e^{-i/\hbar\,\epsilon_n(t_2 - t_1)}|\phi_n(t_1)\rangle \qquad (5)$

The key operator that emerges from this is the TIME EVOLUTION OPERATOR $\hat{G}(t)$, which we define here as*

$$\boxed{\hat{G}(t) = e^{-i/\hbar\,\hat{H}t}} \qquad (6)$$

and which generates the time evolution of the state vector $|\psi(t)\rangle$ in the Schrodinger representation.

A.1: PROPERTIES of $\hat{G}(t)$:

We can always sandwich the operator $\hat{G}(t)$ between any set of complete states $|\alpha\rangle = |\phi_\alpha\rangle$, to define the Green function or propagator

$$\boxed{\begin{aligned} G_{\alpha\beta}(t) &= \langle\alpha|\hat{G}(t)|\beta\rangle \\ &\equiv \langle\alpha|e^{-i/\hbar\,\hat{H}t}|\beta\rangle \end{aligned}} \qquad (7)$$

One can always define a Green function of this kind, for any linear differential

* Note that in the literature $\hat{G}(t)$ is often called $\hat{U}(t)$; but we will reserve this symbol for denote time-dependent external field operators.

operator, and it is important to be aware of, and have a general understanding of, the theory of Green functions for differential equations.

Typically the operator $\hat{\mathcal{H}}$ will be composed of separate parts that do not commute with each other, and so we have to treat the exponential in (6) with care. But lets first establish some general properties of $\hat{G}(t)$ and of its matrix elements $G_{\alpha\beta}(t)$.

It is common to split $\hat{G}(t)$ into its retarded and advanced parts, viz.,

$$\hat{G}(t) = \hat{G}^{+}(t) + \hat{G}^{-}(t) \tag{8}$$

where

$$\left.\begin{aligned} \hat{G}^{+}(t) &= \hat{G}(t)\,\Theta(t) \qquad &&(\text{Retarded}) \\ G^{-}(t) &= \hat{G}(t)\,\Theta(-t) \qquad &&(\text{Advanced}) \end{aligned}\right\} \tag{9}$$

We will typically deal with the retarded form, and it is easy to see from combining (1) and (9) that the retarded Green operator satisfies the differential equation

$$\boxed{(\hat{\mathcal{H}} - i\hbar\partial_t)\,\hat{G}^{+}(t-t') = -i\hbar\,\delta(t-t')} \tag{10}$$

where the "δ-function kick" at $t=t'$ comes from integrating over the $\Theta(t-t')$ function in (9). This equation has a simple interpretation - one sees that $G^{+}(t)$ satisfies the Schrodinger differential eqtn in (1), everywhere in time except at $t=t'$; at $t=t'$, the system receives an instantaneous impulse or kick. Thus the object $\hat{G}^{+}(t)$ can be looked at in 2 ways, viz.

(a) As an operator defined by: $\qquad \int dt''\,\hat{L}(t,t'')\,\hat{G}(t'',t') = -i\hbar\,\hat{I}(t,t') \qquad (11)$

where $\hat{L}(t,t'') = (\hat{\mathcal{H}} - i\hbar\partial_t)\,\hat{I}(t,t'') \qquad (12)$

and $\hat{I}(t,t') = \delta(t-t') \qquad (13)$

is a "unit operator", diagonal in the time coordinates - from this we see that $\hat{G}(t)$ is the INVERSE OPERATOR to $\hat{L}(t)$; and

(b) We can think of $G^{+}(t)$ as a simple function, satisfying the eqtn.

$$\hat{L}(t)\,G^{+}_{t_0}(t) = -i\hbar\,\delta(t-t_0) \tag{14}$$

where $\hat{L}(t)$ is again given by (12), and is diagonal in t-space.

The reason that both of these pictures work is that $L(t,t'')$ is diagonal in time space, and so we can then think of the time t_0 in (14) as a parameter rather than a variable - with $\hat{L}(t)$ now operating on the function $G_{t_0}(t)$, a function of the time variable t only. On the other hand the operator eqtn. (11) treats time t as a kind of ket $|t\rangle$, with the operator L sandwiched between time states, according to

$$\hat{L}(t,t') = \langle t|\hat{L}|t'\rangle = (\hat{\mathcal{H}} - i\hbar\partial_t)\,\delta(t-t') \tag{15}$$

The reason for the rather peculiar status afforded to time here is that we are dealing with non-relativistic QM, where time t is a parameter, but position $\hat{r}$ is associated with a state vector $|\underline{r}\rangle$. Below I will briefly discuss what happens in a relativistic theory, where this distinction between time and space is no longer made.

A.1 (a) MATRIX ELEMENTS $G_{\beta\alpha}(t)$:

We consider now a single non-relativistic system which is again isolated, so that again, $H(t)$ is independent of t.

Then the simplest set of transition matrix elements is that between eigenstates. We again assume eigenstates $|\phi_n(t)\rangle = |n(t)\rangle$, and using (8) we have

$$G_{nn}(t) = \langle n| e^{-\frac{i}{\hbar}\hat{H}t} |n\rangle = e^{-\frac{i}{\hbar}\epsilon_n t} \qquad (16)$$

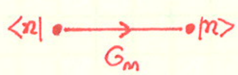
and moreover we can expand the operator $\hat{G}(t)$ in terms of the $|n(t)\rangle$, writing

$$\boxed{\begin{aligned} \hat{G}(t) &= e^{-\frac{i}{\hbar}\hat{H}t} \\ &= \sum_n |n\rangle e^{-\frac{i}{\hbar}\epsilon_n t} \langle n| \end{aligned}} \qquad (17)$$

and we also notice that $G_{nn'}(t) = 0$ if $n \neq n'$, so we can write in compact form that

$$G_{nn'}(t) = \delta_{nn'} e^{-\frac{i}{\hbar}\epsilon_n t} \qquad (18)$$

These results are often expressed in diagrammatic form - we will look at this in much more detail later, but simply show how the diagram for $G_{nn'}(t)$ is represented in this notation. We see that the rule for this diagram is that we associate the factor $\delta_{nn'} e^{-\frac{i}{\hbar}\epsilon_n t}$ with the line.



Eqtn. (17) is extremely useful as a representation of $G(t)$ just because it is diagonal - it can be sandwiched between other operators, as we will see.

Now consider the situation where we are dealing with a single particle and a time-independent Hamiltonian. We must sandwich the operator between 2 position eigenstates - we therefore define

$$G(\underline{r},\underline{r}'; t,t') = \langle \underline{r}| \hat{G}(t-t') |\underline{r}'\rangle \qquad (19)$$

If we now use the representation (17) for $\hat{G}(t)$, we immediately get

$$\boxed{\begin{aligned} G(\underline{r}\underline{r}'; tt') &= \langle r|n\rangle \langle n| \hat{G}(t-t') |n\rangle \langle n|\underline{r}'\rangle \\ &\equiv \sum_n \phi_n(r)\, \phi_n^*(r')\, e^{-\frac{i}{\hbar}\epsilon_n (t-t')} \end{aligned}} \qquad (20)$$

where we use the summation convention (over the $|n\rangle$) in the 1st line. Thus we have projected the eigenfunction expansion (17) of $\hat{G}(t)$ onto position states, and thereby represented the amplitude $G(r,r' tt')$ as a sum over a set of eigenstates written in real-space representation, along with the time evolution factor $e^{-i/\hbar\, \epsilon_n (t-t')}$.

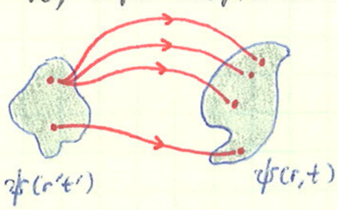
Now suppose we do the same thing with the time evolution eqtn. (2) for the state vector $\psi(t)$. From (2) we have

$$\left.\begin{aligned} \psi(r,t) &= \langle \underline{r}|\psi(t)\rangle = \langle \underline{r}| e^{-i/\hbar \hat{H}(t-t')}|\psi(t')\rangle = \langle r|\hat{G}(t-t')|\psi(t')\rangle \\ \text{which from the def}^{\underline{n}} \text{ of } G(rr'tt') \text{ is just } &\quad \langle r|\psi(t)\rangle = \langle \underline{r}|\hat{G}(t-t')|r'\rangle\langle r'|\psi(t')\rangle \end{aligned}\right\} (21)$$

(now using summation convention over $|r'\rangle$); this is written more explicitly as

$$\boxed{\psi(\underline{r},t) = \int d^3r'\, G(r,r';tt')\,\psi(r't')} \qquad (22)$$

which is not only a form of central importance in the theory, but which also has a very simple interpretation, as follows: suppose at time t' the wave-function $\psi(r't')$ is spread over some region, as shown at left. Then if we pick a particular point $\underline{r}'$, at time t', the amplitude for it to go to another point $\underline{r}$ at time t is just $G(r,r';tt')$. But it does not have to go to the point $\underline{r}$ at time t; it can go to some other point, and indeed there will be some amplitude, which we can call $G(R,r';t,t')$, for it go to some other point $\underline{R}$ at time t. In this way one builds up the wave function at a later time.



If the particle definitely starts at position $\underline{r}_0$ at time t', its later wave-fn. will be

$$\psi(\underline{r}_0 t') \rightarrow G(r,r_0;t,t') = \psi(\underline{r},t) \qquad (23)$$

which we can see by writing the initial wave-fn as $\psi(\underline{r}'t') = \delta(\underline{r}'-r_0)$. Thus we arrive at the picture shown above, where the wave-function evolves by summing over all initial bits of the wave-fn. $\psi(\underline{r}',t')$, and adding the contributions of the propagator from each bit - this gives the integral in (22).

$$\langle r'| \bullet \xrightarrow[G(rr')]{} \bullet |r\rangle = \sum_n \langle r'|n\rangle G_{nn} \langle n|r\rangle$$
$$= \langle r'|n\rangle \bullet \xrightarrow[n]{} \bullet \langle n|\underline{r}\rangle$$

We can also represent $G(\underline{r}\underline{r}';tt')$ as a diagram, shown at left. The amplitude to go from r' to r is given by the sum over amplitudes to go in any state $|n\rangle$, multiplied by the overlaps between $|n\rangle$ and $|r'\rangle$ (at time t') and between $|n\rangle$ and $|r\rangle$ (at time t). This diagram, in this form, is then just representing eqtn. (20).

A.1.(b): THE S-MATRIX:

The use of the S-matrix is typically associated with scattering theory, but it is actually more general. Consider again the transition amplitude $G^+_{\beta\alpha}(t,t')$ between an initial state at time t' and a final state at time t; we now assume explicitly that we have $t > t'$, so we employ $\hat{G}^+(t,t')$.

Suppose now that we extend t' back to the distant past, and t to the distant future. Formally we will imagine that $t' < T'$, and that $t > T$, where

T' is a large negative time, and T a large positive time. Then the S-matrix $S_{\beta\alpha}$ is defined as

$$S_{\beta\alpha} = \lim_{\substack{t'<T' \\ t>T}} \langle\beta|G^{+}(t-t')|\alpha\rangle \tag{24}$$

with the assumption that this limit exists. This sort of function is useful in several contexts, notably the following

(a) When the initial and final states are simple "asymptotic" states. This happens in particular when we deal with a Hamiltonian having some potential confined to a spatial region, and $|\alpha\rangle$ and $|\beta\rangle$ are far from this region, so they don't feel the potential (ie., they are free particle states). Then $S_{\beta\alpha}$ tells us about the scattering between these states, by the potential, during the time period $T'<t<T$.

(b) In the case where some time-dependent term $\hat{U}(t)$ is added to the time-independent H, during the period $T'<t<T$, but is zero outside this time window. Then $S_{\beta\alpha}$ tells us the total transition amplitude between $|\alpha\rangle$ and $|\beta\rangle$, caused by the application of $U(t)$ (in this case, one would typically assume that $|\alpha\rangle$ and $|\beta\rangle$ were eigenstates of $\mathcal{H}$).

The principal application of the S-matrix is in scattering theory. We can think of $S_{\beta\alpha}$ as the matrix element of the operator

$$\hat{S} = \lim_{\substack{t'<T' \\ t>T}} \hat{G}^{+}(t-t') \tag{25}$$

and write it in a position expansion as

$$\hat{S} = \lim_{\substack{t'<T' \\ t>T}} \int d^D\underline{r} \int d^D\underline{r}' \, |\underline{r}\rangle G(\underline{r}\underline{r}';tt') \langle\underline{r}'| \tag{26}$$

Since the Green operator $\hat{G}(t)$ is clearly a unitary operator (it causes the time evolution of $|\psi\rangle$), then so is $\hat{S}$, ie., we have

$$\hat{S}\hat{S}^{+} = 1. \tag{27}$$

which is a special case of the relation $\quad \hat{G}(t)\hat{G}^{+}(t) = 1 \qquad (28)$

which follows from the definition (6) of $\hat{G}(t)$; here $\hat{G}^{+}$ is the Hermitian conjugate of $\hat{G}(t)$

A.2 : PROPERTIES of $\hat{G}(\omega)$ & $\hat{G}(z)$:

It is, when the system is closed, so that $\mathcal{H}$ is independent of time and energy is conserved, much more useful to Fourier transform $\hat{G}(t)$ to frequency space. This can be done in completely straightforward way, by just taking the Fourier transform; or in a more general & satisfactory way by looking at the operator as defined throughout the complex frequency plane. The results obtained are very general, and only acquire definite physical meaning when applied to specific systems – one simple example, for single particles, being that provided by scattering theory.

A.2 (a) THE RESOLVENT OPERATOR $\hat{G}(z)$

: Suppose we just naively take the Fourier transform of $\hat{G}^+(t)$, defined by (9). Then we would have

$$\left.\begin{aligned} \hat{G}^+(\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t}\, \hat{G}^+(t) \\ &\rightarrow \int_0^{\infty} dt\, e^{i(\omega - \hat{H}/\hbar)t} \end{aligned}\right\} \tag{29}$$

which would give the simple result
$$\hat{G}^+(\omega) = \frac{i}{\omega - \hat{H}/\hbar} \tag{30}$$

If interpreted in the right way, this expression can be used to get sensible results – but we can see immediately that this requires care, because as defined, $\hat{G}^+(\omega)$ is singular – the denominator vanishes when $\omega\hbar = \hat{H}$. To see this more clearly, we take matrix elements of $G^+(\omega)$, to find that

$$\left.\begin{aligned} G_{\beta\alpha}(\omega) &= \langle\beta|G^+(\omega)|\alpha\rangle \\ &= \sum_n \langle\beta|n\rangle\, G^+_{nn}(\omega)\, \langle n|\alpha\rangle \end{aligned}\right\} \tag{31}$$

where we have
$$G^+_{nn}(\omega) = \frac{i\hbar}{\hbar\omega - \epsilon_n} \tag{32}$$

and the expansion
$$G^+(\omega) = |n\rangle \frac{i\hbar}{\hbar\omega - \epsilon_n} \langle n| \tag{33}$$

The expression is clearly undefined when $\hbar\omega = \epsilon_n$; but this is obviously because we are dealing with simple poles of an expression defined throughout the complex frequency plane.

Accordingly we consider a COMPLEX FREQUENCY z, and define the "resolvent operator"

$$\boxed{\hat{G}(z) = \frac{1}{z - \hat{H}}} \tag{34}$$

where it is assumed that this inverse operator exists, so that we also write

$$(z - \hat{H})\,\hat{G}(z) = 1 \tag{35}$$

and we can resolve $\hat{G}(z)$ as

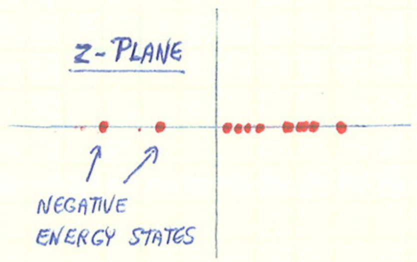
$$\boxed{\hat{G}(z) = |n\rangle \frac{1}{z - \epsilon_n} \langle n|} \tag{36}$$

where the usual summation convention applies. We see that $G(z)$ is a complex meromorphic variable, characterized entirely by the set of simple poles at $z = \epsilon_n$. For a finite quantum system this is all that needs to be said

A.2(b) Analytic Properties of $G(z)$

: Now let's look at the resolvent operator in a diagonal basis, ie, consider the function

$$\left.\begin{aligned} G(z) \equiv G_{nn}(z) &= \langle n|\hat{G}(z)|n\rangle \\ &\equiv \sum_n \frac{1}{z-\epsilon_n} \end{aligned}\right\} \quad (37)$$

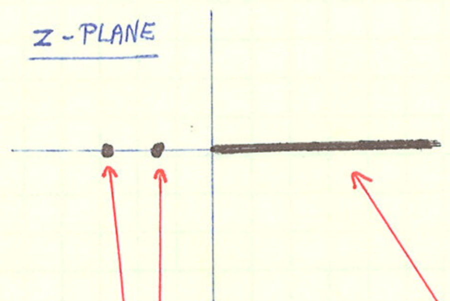


in more detail.

We see a plot in the z-plane of the positions of the poles of $G(z)$ along the real energy axis at positions $z = \epsilon_n$. Notice that for z very close to some pole at ϵ_j, we will have $G(z) \sim A_j/(z-\epsilon_j)$, where A_j is some constant. Thus the behaviour near ϵ_j, in the case where all the poles are separated by finite energy gaps. However all of this is just for a finite system with discrete energies.

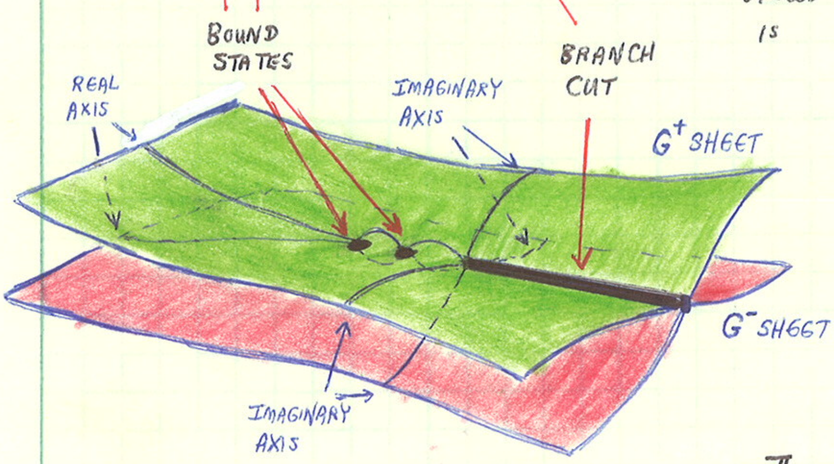
Now consider what happens for an infinite system. We are dealing here just with a single particle, not an N-body system. Nevertheless we encounter a new situation, because if we put our particle in a box of size L, and then let $L \to \infty$, the character of the poles in $G(z)$ changes - the gaps between them tend to 0, and we need to do things a little differently.

In what follows we shall establish the following picture for $G(z)$.



(i) In the continuum limit $L \to \infty$, the spectrum of the system splits into sets of discrete states and sets of continuum states. The continuum states are extended in space and their poles merge into a BRANCH CUT in $G(z)$. If the magnitude of the branch cut at energy $z \to E$ is $A(E)$, then the density of states (the level density) per unit volume is

$$N(E) = \frac{-1}{\pi} A(E) \qquad (38)$$



where $A(E)$ defines the jump in $G(z)$ as we cross the branch cut, such that

$$\left.\begin{aligned} \Delta G(E) &= G(E+i\delta) - G(E-i\delta) \\ &= 2iA(E) \\ &= -2\pi i N(E) \end{aligned}\right\} \quad (39)$$

The discrete states are as described above.

(ii) The complex variable $G(z)$ is defined on a pair of Rieman sheets, which are connected to each other at the branch cuts and poles. To be more precise it is useful to subtract off the contribution of $G(z)$ as $z \to \infty$, defining

$$\tilde{G}(z) = G(z) - G(\infty) \qquad (40)$$

which works provided $G(z)$ falls off fast enough as $z \to \infty$ (if it doesn't, we employ "subtraction" techniques). Let us write now two functions $\tilde{G}^{\pm}(z)$, according to

$$\tilde{G}^{\pm}(E) = \tilde{G}(z \to E \pm i\delta) = \sum_{n \in n_B} \frac{1}{E - \epsilon_n \pm i\delta} + \frac{\mathbb{P}}{\pi} \int_{-\infty}^{\infty} dx \, \frac{A(x)}{x - E} \qquad (41)$$

these functions existing close to the real axis on the 2 Rieman sheets shown on the last page. These results can be written in terms of the real & imaginary parts of (41) as

$$\boxed{\begin{aligned} Re\, \tilde{G}^{+}(E) &= \sum_{n \in n_B} \frac{1}{E - \epsilon_n} + \frac{\mathbb{P}}{\pi} \int_{-\infty}^{\infty} dx \, \frac{Im\, \tilde{G}^{+}(x + i\delta)}{x - E} \\ Im\, \tilde{G}^{+}(E) &= \sum_{n \in n_B} \frac{1}{E - \epsilon_n} - \frac{\mathbb{P}}{\pi} \int_{-\infty}^{\infty} dx \, \frac{Re\, \tilde{G}^{+}(x + i\delta)}{x - E} \end{aligned}} \qquad (42)$$

and these relations are usually known as the Kramers - Kronig relations. They are in fact a consequence of causality - we will not pause to show this here. They are used throughout physics — any correlation function or response function $X(\omega)$ will satisfy similar relations in the complex plane.

To see how one establishes the above results, consider first the situation where the continuum states can be written as

$$|n\rangle = |E, m\rangle \, \delta(\epsilon_n - E) \qquad \text{(continuum)} \qquad (43)$$

ie, we have a set of states $|m\rangle$ at energy E that are all degenerate, & which make up a sub-manifold of states $|Em\rangle$. Assume that the total # of states is $N(E)$, at this energy. This is a very naive way of treating the continuum limit. Then we have

$$\hat{G}(z) = \sum_n |n\rangle \frac{1}{z - \epsilon_n} \langle n| \implies \int_{-\infty}^{\infty} dE \sum_m |Em\rangle \frac{1}{z - \epsilon} \langle Em| \qquad (44)$$

and for any pair of states $|\alpha\rangle, |\beta\rangle$, the matrix element

$$\langle \beta | \hat{G}(z) | \alpha \rangle = G_{\beta\alpha}(z) = \int_{-\infty}^{\infty} d\epsilon \sum_m \langle \beta | \epsilon m \rangle \frac{1}{z - \epsilon} \langle \epsilon m | \alpha \rangle \qquad (45)$$

In particular, we have

$$\Delta \hat{G}(E) = \hat{G}(E + i\delta) - \hat{G}(E - i\delta) = \int dx \sum_m |xm\rangle \langle xm| \left[\frac{1}{E - x + i\delta} - \frac{1}{E - x - i\delta} \right] \qquad (46)$$

ie., we have

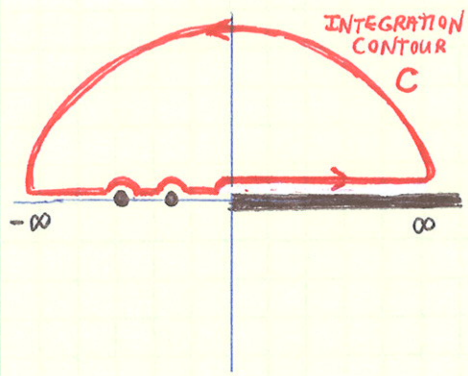
$$\Delta\hat{G}(E) = -2\pi i \sum_m |E m\rangle\langle m E| \tag{47}$$

which is an operator acting at the energy E. We can write a function $\Delta G(E)$ by sandwiching this between all states, to get

$$\Delta G(E) = \sum_n \langle n|\Delta\hat{G}(E)|n\rangle = -2\pi i N(E) \tag{48}$$

which is just the result (39) given previously.

To understand the analytic properties, let's go to the function $\tilde{G}(E)$ defined in (40). Now, by Cauchy's theorem, we can write the function in the form



$$\tilde{G}(E) = \frac{1}{2\pi i}\oint_C dz\, \frac{\tilde{G}(z)}{E-z} \tag{49}$$

which, for the contour shown at left, is

$$\left.\begin{aligned}\tilde{G}(E) &= \sum_{n\in n_B} \frac{1}{E-\epsilon_n} + \frac{1}{\pi}\int dx\, \frac{\operatorname{Im}\tilde{G}(x+i\delta)}{x-E} \\ &= \sum_{n\in n_B} \frac{1}{E-\epsilon_n} + \frac{1}{\pi}\int dx\, \frac{A(x)}{x-E}\end{aligned}\right\} \tag{50}$$

by our previous def^{n} of $A(x)$. Now, to get the result (41) above, we let $E \to E \pm i\delta$, and note that for any function $f(z)$, vanishing sufficiently quickly as $z\to\infty$, we have

$$2\pi i\, f(E\pm i\delta) = \int_{-\infty}^{\infty} dx\, \frac{f(x)}{x-E\mp i\delta} = \mathbb{P}\int dx\, \frac{f(x)}{x-E} \pm i\pi f(E) \tag{51}$$

a result well known from complex variable theory.

The multi-sheeted structure allows us to pass smoothly from one function $G^+(z)$ to another $G^-(z)$. Let's consider the relationship to the functions $G^\pm(t)$ defined in (9). It will be obvious that we extend the Fourier transform in (29) to the complex plane of frequency, ie., write

$$\hat{G}^+(z) = \int_{-\infty}^{\infty} dt\, e^{izt}\, \hat{G}^+(t) = \int_0^{\infty} dt\, e^{izt}\, \hat{G}(t) \tag{52}$$

then this function can have no poles in the upper half-plane (the integral in (52) converges when $\operatorname{Im} z > 0$). Thus the function $G^+(E)$ given in (41) and (42) is just the Fourier transform of $G^+(t)$ in (9). To get $G^-(E)$ we just close the contour in the lower half-plane.

Finally, let us note that in scattering theory - not covered here, but see notes on scattering theory - the functions $T(z)$ and $S(z)$ are used. Since these are linearly related to $G(z)$, they have the same analytic structure.

A.3: DYSON EQUATION

: This famous eqtn. is nothing but a natural consequence of a perturbative expansion of the propagator in powers of a potential perturbation. We write the 1-particle Hamiltonian as

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \hat{V} \tag{53}$$

and expand the 1-particle propagator $G_{\beta\alpha} = G(\beta, \alpha ; t_\beta, t_\alpha)$ in powers of the interaction V. Thus we have

$$\left.\begin{aligned} G_{\beta\alpha}[V] &= \int_\alpha^\beta \mathcal{D}x(\tau)\, e^{\frac{i}{\hbar}\int_{t_\alpha}^{t_\beta} d\tau\, (L_0(x\dot{x}) - V(x\tau))} \\ &= G_0(\beta,\alpha) \sum_{k=0}^{\infty} \left(\frac{-i}{\hbar}\right)^k \frac{1}{k!} \left(\int_{t_\alpha}^{t_\beta} d\tau\, V(x(\tau)) \right)^k \end{aligned}\right\} \tag{54}$$

where the non-interacting propagator is $$G_0(\beta,\alpha) = \int_\alpha^\beta \mathcal{D}x(\tau)\, e^{\frac{i}{\hbar}\int_{t_\alpha}^{t_\beta} d\tau\, L_0(x\dot{x})} \tag{55}$$

and where we use the shorthand

$$\int_\alpha^\beta \mathcal{D}x(\tau) = \int dx_1 \int dx_2 \langle \beta | x_1 \rangle \langle x_2 | \alpha \rangle \int_{x_1}^{x_2} \mathcal{D}x(\tau) \tag{56}$$

Let's write (54) as

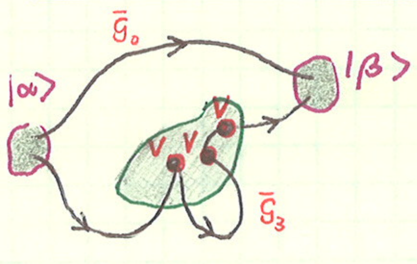
$$G_{\beta\alpha}[V] = \sum_{k=0}^{\infty} \bar{\mathcal{G}}_k(\beta, \alpha | V) \tag{57}$$

and we immediately see that the $\bar{\mathcal{G}}_k$ satisfy the recursion relation

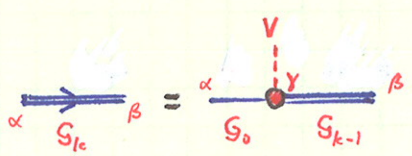
$$\bar{\mathcal{G}}_k(\beta\alpha) = -\frac{i}{\hbar}\int_{t_\alpha}^{t_\beta} d\tau \int dy(\tau)\; G_0(\beta, y ; t_\beta, \tau)\, V(y(\tau))\, \bar{\mathcal{G}}_{k-1}(y, \alpha ; \tau, t_\alpha) \tag{58}$$

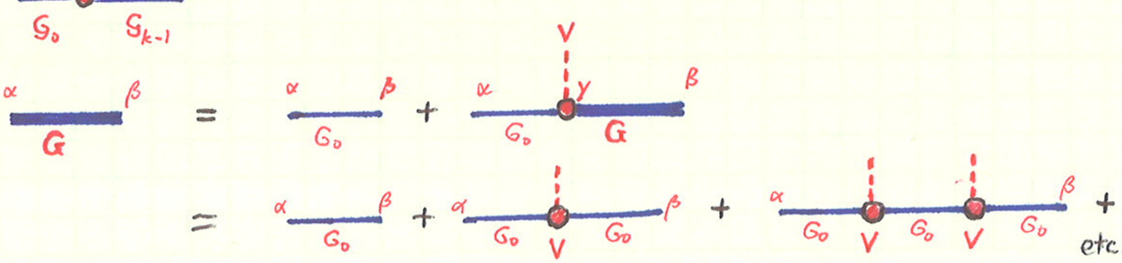
which is just another way of saying that $G_{\beta\alpha}$ satisfies the integral eqtn:

$$\boxed{G_{\beta\alpha} = G^0_{\beta\alpha} - \frac{i}{\hbar}\int_{t_\alpha}^{t_\beta} d\tau \int dy(\tau)\, G^0(\beta, y ; t_\beta, \tau)\, V(y(\tau))\, G(y, \alpha ; \tau, t_\alpha)} \tag{59}$$



There are a number of ways to think about this eqtn. Let's first look at the paths in real space. Two paths are shown at left - one is for the non-interacting contribution $\mathcal{G}_0(\beta,\alpha)$, the other is for the 3rd-order term $\mathcal{G}_3(\beta\alpha)$. The sum in (57) is over all paths, in which we have divided these paths into classes depending on how often the interaction $V(q(\tau))$ appears in them. At left we show the recursion relation (55), and below we see (59).





The way we have written the Dyson eqtn (59) is quite general, but is messy because of our choice of real-space representation for the propagators. Suppose instead we choose to represent these functions in terms of the eigenfunctions $|m\rangle$ of $\mathcal{H}_0$ and G_0, so that both of them are then diagonal. We then have

$$G_{mm'}(tt') = G^0_m(tt') - \tfrac{i}{\hbar}\int d\tau\, G^0_m(t,\tau)\, V_{mm''}\, G_{m''m'}(\tau,t') \tag{60}$$

and if we now Fourier transform this in time (a good move since energy conservation means that G_0 and G will be diagonal in frequency space) we get

$$G_{mm'}(\epsilon) = G^0_m(\epsilon)\,\delta_{mm'} + G^0_m(\epsilon)\, V_{mm''}\, G_{m''m'}(\epsilon) \tag{61}$$

However this is nothing but the representation in the $|m\rangle, |m'\rangle$ basis of the operator eqtn:

$$\boxed{\hat{G}(\epsilon) = \hat{G}_0(\epsilon) + \hat{G}_0(\epsilon)\,\hat{V}\,\hat{G}(\epsilon) = \frac{\hat{G}_0(\epsilon)}{\hat{1} - \hat{V}\hat{G}_0(\epsilon)}} \tag{62}$$

which is a more typical form for the Dyson eqtn. The "bare" Green function $\hat{G}_0(\epsilon)$ is given by

$$G_0(\epsilon) = \frac{i}{\omega - \mathcal{H}_0/\hbar} \tag{63}$$

(cf (30)).

We can also rewrite this Dyson eqtn in the form of a "scattering eqtn". Suppose we write the solutions to the full Hamiltonian as

$$\hat{\mathcal{H}}|\psi\rangle = (\hat{\mathcal{H}}_0 + \hat{V})|\psi\rangle = E|\psi\rangle. \tag{64}$$

Now rewrite (62) as

$$(\hat{1} - \hat{V}\hat{G}_0(\epsilon))\,\hat{G}(\epsilon) = G_0(\epsilon) \tag{65}$$

and operate on $|m\rangle$, to get

$$\left[1 - \frac{\hat{V}}{\epsilon - \mathcal{H}_0/\hbar}\right]|\psi\rangle = |m\rangle \tag{66}$$

where we use the fact that

$$\hat{G}|m\rangle = |\psi\rangle \tag{67}$$

(which can be seen as a defining property of $\hat{G}(\epsilon)$). Thus we get the integral eqtn:

$$|\psi\rangle = |m\rangle + \frac{\hat{V}}{\omega - \hat{\mathcal{H}}_0/\hbar}|\psi\rangle \tag{68}$$

which in scattering theory is known as the Lippmann-Schwinger eqtn, although we see that it is just another form of the Dyson eqtn. The Lippmann-Schwinger eqtn.

is more usually written not as an operator eqtn, but in the real space reprentation, as

$$\psi^{\pm}(\underline{r}) = \phi_k^{\pm}(\underline{r}) + \int d^3r' \, G_0^{\pm}(r-r') \langle r' | V | \psi^{\pm} \rangle \tag{69}$$

or in momentum space as

$$\psi_k^{\pm} = \phi_k + G_0^{\pm}(k) \sum_{k'} V_{kk'} \psi_{k'}^{\pm} \tag{70}$$

where we assume that $|m\rangle \to |\underline{k}\rangle$, ie., a momentum eigenstate, and we define incoming and outgoing states $|\phi_k^{\pm}\rangle$ and $|\psi^{\pm}\rangle$ (also called "retarded" and "advanced" states); these correspond to the states $G^{\pm}$ defined earlier, so that in energy representation we have

$$G_0^{\pm}(\epsilon) = \frac{1}{\epsilon - \hat{H}_0/\hbar \pm i\delta} \tag{71}$$

These eqtns form the basis for standard 1-particle scattering theory.