Chapter 8

Green's functions

8.1 "Classical" Green's functions

The Green's function method is a very useful method in the theory of ordinary and partial differential equations. It has a long history with numerous applications.

To illustrate the idea of the method let us consider the familiar problem of finding the electrical potential ϕ given a fixed charge distribution, ρ_e, i.e. we want to solve Poisson's equation

$$\nabla^2\phi(\mathbf{r}) = -\frac{1}{\varepsilon_0}\rho_e(\mathbf{r}). \tag{8.1}$$

It turns out to be a good idea instead to look for the solution G of a related but simpler differential equation

$$\nabla^2_{\mathbf{r}} G(\mathbf{r}) = \delta(\mathbf{r}), \tag{8.2}$$

where $\delta(\mathbf{r})$ is the Dirac delta function. $G(\mathbf{r})$ is called the Green's function for the Laplace operator, $\nabla^2_{\mathbf{r}}$. This is a good idea because once we have found $G(\mathbf{r})$, the electrical potential follows as

$$\phi(\mathbf{r}) = -\frac{1}{\varepsilon_0}\int d\mathbf{r}'\, G(\mathbf{r}-\mathbf{r}')\rho_e(\mathbf{r}'). \tag{8.3}$$

That this is a solution to Eq. (8.1) is easily verified by letting $\nabla^2_{\mathbf{r}}$ act directly on the integrand and then use Eq. (8.2).

The easiest way to find $G(\mathbf{r})$ is by Fourier transformation, which immediately gives

$$-k^2 G(\mathbf{k}) = 1 \qquad \Rightarrow \qquad G(\mathbf{k}) = -\frac{1}{k^2}, \tag{8.4}$$

and hence

$$G(\mathbf{r}) = \int \frac{d\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} G(\mathbf{k}) = -\int \frac{d\mathbf{k}}{(2\pi)^3}\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{k^2} = -\frac{1}{4\pi r}. \tag{8.5}$$

When inserting this into (8.3) we obtain the well-known potential created by a charge distribution

$$\phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0}\int d\mathbf{r}'\frac{\rho_e(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}. \tag{8.6}$$

8.2 Green's function for the one-particle Schrödinger equation

Green's functions are particular useful for problems where one looks for perturbation theory solutions. Consider for example the Schrödinger equation

$$[H_0(\mathbf{r}) + V(\mathbf{r})]\,\Psi_E = E\Psi_E, \tag{8.7}$$

where we know the eigenstates of H_0, and where we want to treat V as a perturbation. Here we consider the case of an open system, i.e. there is a continuum of states and hence we are free to choose any E. This situation is relevant for scattering problems where a flux of incoming particles (described by H_0) interacts with a system (described by V). The interaction induces transitions from the incoming state to different outgoing states. The procedure outlined below is then a systematic way of calculating the effect of the interaction between the "beam" and the "target" on the outgoing states.

In order to solve the Schrödinger equation, we define the corresponding Green's function by the differential equation

$$[E - H_0(\mathbf{r})]\,G_0(\mathbf{r},\mathbf{r}',E) = \delta(\mathbf{r}-\mathbf{r}'), \tag{8.8}$$

with the boundary condition, $G_0(\mathbf{r},\mathbf{r}') = G_0(\mathbf{r}',\mathbf{r})$. It is natural to identify the operator $[E - H_0(\mathbf{r})]$ as the inverse of $G_0(\mathbf{r},\mathbf{r}')$ and therefore we write[1]

$$G_0^{-1}(\mathbf{r},E) = E - H_0(\mathbf{r}) \quad \text{or} \quad G_0^{-1}(\mathbf{r},E)\,G_0(\mathbf{r},\mathbf{r}',E) = \delta(\mathbf{r}-\mathbf{r}'). \tag{8.9}$$

Now the Schrödinger equation can be rewritten as

$$\left[G_0^{-1}(\mathbf{r},E) - V(\mathbf{r})\right]\Psi_E = 0, \tag{8.10}$$

and by inspection we see that the solution may be written as an integral equation

$$\Psi_E(\mathbf{r}) = \Psi_E^0(\mathbf{r}) + \int d\mathbf{r}'\,G_0(\mathbf{r},\mathbf{r}',E)V(\mathbf{r}')\Psi_E(\mathbf{r}'), \tag{8.11}$$

where Ψ_E^0 is the eigenstate to H_0. This is verified by inserting ψ_E from Eq. (8.11) into the $G_0^{-1}\psi_E$ term of Eq. (8.10) and then using Eq. (8.9). One can now solve the integral equation Eq. (8.11) by iteration, and up to first order in V the solution is

$$\Psi_E(\mathbf{r}) = \Psi_E^0(\mathbf{r}) + \int d\mathbf{r}'\,G_0(\mathbf{r},\mathbf{r}',E)V(\mathbf{r}')\Psi_E^0(\mathbf{r}') + \mathcal{O}\left(V^2\right), \tag{8.12}$$

where Ψ_E^0 is an eigenstate to H_0 with eigenenergy E. What we have generated by the iteration procedure is nothing but the ordinary (non-degenerate) perturbation theory. The next leading terms are also easily found by continuing the iteration procedure. The Green's

[1] In order to emphasize the matrix structure we could have written this as $\int d\mathbf{r}''G_0^{-1}(\mathbf{r},\mathbf{r}'')\,G_0(\mathbf{r}'',\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')$, where the inverse Green's function is a function of two arguments. But in the $\mathbf{r}$-representation it is in fact diagonal $G_0^{-1}(\mathbf{r},\mathbf{r}') = (E - H_0(\mathbf{r}))\delta(\mathbf{r}-\mathbf{r}')$.

function method is thus useful for this kind of iterative calculations and one can regard the Green's function of the unperturbed system, G_0, as simple building blocks from which the solutions of more complicated problems can be build.

Before we introduce the many-body Green's function in the next section, we continue to study the case of non-interacting particles some more and include time dependence. Again we consider the case where the Hamiltonian has a free particle part H_0 of some perturbation V, $H = H_0 + V$. The time dependent Schrödinger equation is

$$[i\partial_t - H_0(\mathbf{r}) - V(\mathbf{r})]\,\Psi(\mathbf{r},t) = 0. \tag{8.13}$$

Similar to Eq. (8.8) we define the Green's functions by

$$[i\partial_t - H_0(\mathbf{r})]\,G_0(\mathbf{r}t,\mathbf{r}'t') = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t'). \tag{8.14a}$$
$$[i\partial_t - H_0(\mathbf{r}) - V(\mathbf{r})]\,G(\mathbf{r}t,\mathbf{r}'t') = \delta(\mathbf{r}-\mathbf{r}')\delta(t-t'). \tag{8.14b}$$

The inverse of the Green's functions are thus

$$G_0^{-1}(\mathbf{r},t) = i\partial_t - H_0(\mathbf{r}) \tag{8.15a}$$
$$G^{-1}(\mathbf{r},t) = i\partial_t - H_0(\mathbf{r}) - V(\mathbf{r}). \tag{8.15b}$$

From these building blocks we easily build the solution of the time dependent Schrödinger equation. First we observe that the following expression is a solution to Eq. (8.13)

$$\Psi(\mathbf{r},t) = \Psi^0(\mathbf{r},t) + \int d\mathbf{r}' \int dt'\; G_0(\mathbf{r}t,\mathbf{r}'t')V(\mathbf{r}')\Psi(\mathbf{r}',t'), \tag{8.16}$$

or in terms of the full Green's function

$$\Psi(\mathbf{r},t) = \Psi^0(\mathbf{r},t) + \int d\mathbf{r}' \int dt'\; G(\mathbf{r},\mathbf{r}';t,t')V(\mathbf{r}')\Psi^0(\mathbf{r}',t'), \tag{8.17}$$

which both can be shown by inspection, see Exercise 8.1. As for the static case in Eq. (8.11) we can iterate the solution and get

$$\begin{aligned}\Psi &= \Psi^0 + G_0V\Psi^0 + G_0VG_0V\Psi^0 + G_0VG_0VG_0V\Psi^0 + \cdots \\ &= \Psi^0 + \big(G_0 + G_0VG_0 + G_0VG_0VG_0 + \cdots\big)V\Psi^0,\end{aligned} \tag{8.18}$$

where the integration variables have been suppressed. By comparison with Eq. (8.17), we see that the full Green's function G is given by

$$\begin{aligned}G &= G_0 + G_0VG_0 + G_0VG_0VG_0 + \cdots \\ &= G_0 + G_0V\big(G_0 + G_0VG_0 + \cdots\big).\end{aligned} \tag{8.19}$$

Noting that the last parenthesis is nothing but G itself we have derived the so-called Dyson equation

$$G = G_0 + G_0VG. \tag{8.20}$$

This equation will play and important role when we introduce the Feynman diagrams later in the course. The Dyson equation can also be derived directly from Eqs. (8.14) by multiplying Eq. (8.14b) with G_0 from the left.

The Green's function $G(\mathbf{r}t, \mathbf{r}'t')$ we have defined here is the non-interacting version of the retarded single particle Green's function that will be introduced in the following section. It is also often called a propagator because it propagates the wavefunction, i.e. if the wavefunction is know at some time, t' then the wavefunction at a later time, t is given by

$$\Psi(\mathbf{r}, t) = \int d\mathbf{r}' \, G(\mathbf{r}t, \mathbf{r}'t')\Psi(\mathbf{r}', t'), \tag{8.21}$$

which can be checked by inserting Eq. (8.21) into the Schrödinger equation and using the definition Eq. (8.14b).[2]

That the Green's function is nothing but a propagator is immediately clear when we write is it as

$$G(\mathbf{r}t, \mathbf{r}'t') = -i\theta(t - t')\langle \mathbf{r}|e^{-iH(t-t')}|\mathbf{r}'\rangle, \tag{8.22}$$

which indeed is a solution of the partial differential equation defining the Green's function, Eq. (8.14b), the proof being left as an exercise; see Exercise 8.2. Looking at Eq. (8.22) the Green's function expresses the amplitude for the particle to be in state $|\mathbf{r}\rangle$ at time t, given that it was in the state $|\mathbf{r}'\rangle$ at time t'. We could of course calculate the propagator in a different basis, e.g. suppose it was in a state $|\phi_{n'}\rangle$ and time t' then the propagator for ending in state $|\phi_n\rangle$ is

$$G(nt, n't') = -i\theta(t - t')\langle \phi_n|e^{-iH(t-t')}|\phi_{n'}\rangle. \tag{8.23}$$

The Green's function are related by a simple change of basis

$$G(\mathbf{r}t, \mathbf{r}'t') = \sum_{nn'} \langle \mathbf{r}|\phi_n\rangle G(nt, n't')\langle \phi_{n'}|\mathbf{r}'\rangle. \tag{8.24}$$

If we choose the basis state $|\phi_n\rangle$ as the eigenstates of the Hamiltonian, then the Green's function becomes

$$G(\mathbf{r}t, \mathbf{r}'t') = -i\theta(t - t') \sum_{n} \langle \mathbf{r}|\phi_n\rangle\langle \phi_n|\mathbf{r}'\rangle e^{-iE_n(t-t')}. \tag{8.25}$$

Propagation from one point to another in quantum mechanics is generally expressed in terms of transmission amplitudes. As a simple example we end this section by a typical scattering problem in one dimension. Consider an electron incident on a barrier, located between $x > 0$ and $x < L$, the incoming wave is for $x < 0$ given by $\exp(ikx)$ while the outgoing wave on the other side $x > L$ is given $t \exp(ikx)$. Here t is the transmission amplitude. The eigenstates are for this example thus given by

$$\psi(\mathbf{k}) = \begin{cases} \exp(ikx), & \text{for} \quad x < 0, \\ t \exp(ikx), & \text{for} \quad x > L. \end{cases} \tag{8.26}$$

[2] Another way to write Eq. (8.21)) is: $\int d\mathbf{r}' \langle \mathbf{r}|e^{-iH(t-t')}|\mathbf{r}'\rangle\langle \mathbf{r}'|\Psi(t')\rangle = \langle \mathbf{r}|\Psi(t)\rangle$.

When this is inserted into Eq. (8.25) we see that the Green's function for the $x > L$ and $x' < 0$ precisely describes propagator across the scattering region becomes

$$G(xt, x't') = t\, G_0(x, x'; t, t'), \quad x > L \quad \text{and} \quad x' < 0. \tag{8.27}$$

where G_0 is the Green's function in the absence of the scattering potential. From this example it is evident that the Green's function contains information about the transmission amplitudes for the particle. See also Exercise 12.2.

8.3 Single-particle Green's functions of many-body systems

In many-particle physics we adopt the Green's function philosophy and define some simple building blocks, also called Green's functions, from which we obtain solutions to our problems. The Green's functions contain only part of the full information carried by the wave functions of the systems but they include the relevant information for the given problem. When we define the many-body Green's functions it is not immediately clear that they are solutions to differential equations as for the Schrödinger equation Green's functions defined above. But as you will see later they are in fact solutions of equations of motions with similar structure justifying calling them Green's functions. Let us simply carry on and define the different types of Green's functions that we will be working with.

There are various types of single-particle Green's functions. The retarded Green's function is defined as[3]

$$G^R(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = -i\theta(t-t')\langle[\Psi_\sigma(\mathbf{r}t), \Psi^\dagger_{\sigma'}(\mathbf{r}'t')]_{B,F}\rangle, \quad \left\{ \begin{array}{ll} B: & \text{bosons} \\ F: & \text{fermions} \end{array} \right\} \tag{8.28}$$

where the (anti-) commutator $[\cdots, \cdots]_{B,F}$ is defined as

$$\begin{array}{ll} [A,B]_B = & [A,B] = AB - BA, \\ [A,B]_F = & \{A,B\} = AB + BA. \end{array} \tag{8.29}$$

Similarly, we define a advanced Green's function as

$$G^A(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = i\theta(t'-t)\langle[\Psi_\sigma(\mathbf{r}t), \Psi^\dagger_{\sigma'}(\mathbf{r}'t')]_{B,F}\rangle, \tag{8.30}$$

Notice the similarity between the many-body Green's function Eq. (8.28) and the one for the propagator for the one particle wavefunction, in Eq. (8.22). For non-interacting particles they are indeed identical.

The second type of single-particle Green's functions is the so-called greater and lesser Green's functions

$$G^>(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = -i\langle\Psi_\sigma(\mathbf{r}t)\Psi^\dagger_{\sigma'}(\mathbf{r}'t')\rangle, \tag{8.31a}$$

$$G^<(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = -i\,(\pm 1)\,\langle\Psi^\dagger_{\sigma'}(\mathbf{r}'t')\Psi_\sigma(\mathbf{r}t)\rangle. \tag{8.31b}$$

[3] remember the definition of the thermal average defined in Eq. (1.119).

We see that the retarded and advanced Green's function can be written in terms of these two functions as

$$G^R(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = \theta(t-t')\left[G^>(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') - G^<(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t')\right], \tag{8.32a}$$

$$G^A(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') = \theta(t'-t)\left[G^<(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t') - G^>(\mathbf{r}\sigma t, \mathbf{r}'\sigma' t')\right]. \tag{8.32b}$$

Even though we call these Green's functions for "single-particle Green's functions", they are truly many-body objects because they describe the propagation of single particles governed by the full many-body Hamiltonian. Therefore the single-particle functions can include all sorts of correlation effects.

The Green's functions in Eqs. (8.28), (8.31a), and (8.31b) are often referred to as propagators. The reason is that they give the amplitude of a particle inserted in point $\mathbf{r}'$ at time t' to propagate to position $\mathbf{r}$ at time t. In this sense G^R has its name "retarded" because it is required that $t > t'$.

The relation between the real space retarded Green's function and the corresponding one in a general $|\nu\rangle$-basis as defined in Eq. (1.71) is

$$G^R(\sigma\mathbf{r}t, \sigma\mathbf{r}'t') = \sum_{\nu\nu'} \psi_\nu(\sigma\mathbf{r}) G^R(\nu\sigma t, \nu'\sigma' t') \psi^*_{\nu'}(\sigma'\mathbf{r}'), \tag{8.33}$$

where

$$G^R(\nu\sigma t, \nu'\sigma' t') = -i\theta\left(t-t'\right)\langle[a_{\nu\sigma}(t), a^\dagger_{\nu'\sigma'}(t')]_{B,F}\rangle, \tag{8.34}$$

and similarly for $G^>$ and $G^<$.

8.3.1 Green's function of translation-invariant systems

For a system with translation-invariance the usual $\mathbf{k}$-representation is a natural basis set. Since the system is translation-invariant $G(\mathbf{r}, \mathbf{r}')$ can only depend on the difference $\mathbf{r} - \mathbf{r}'$ and in this case

$$\begin{aligned} G^R(\mathbf{r}-\mathbf{r}', \sigma t, \sigma' t') &= \frac{1}{\mathcal{V}} \sum_{\mathbf{k}\mathbf{k}'} e^{i\mathbf{k}\cdot\mathbf{r}} G^R(\mathbf{k}\sigma t, \mathbf{k}'\sigma' t') e^{-i\mathbf{k}'\cdot\mathbf{r}'}, \\ &= \frac{1}{\mathcal{V}} \sum_{\mathbf{k}\mathbf{k}'} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} G^R(\mathbf{k}\sigma t, \mathbf{k}'\sigma' t') e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}'}. \end{aligned} \tag{8.35}$$

However, because the right hand side cannot explicitly dependent on the origin and on $\mathbf{r}'$, it follows that $G(\mathbf{k},\mathbf{k}') = \delta_{\mathbf{k},\mathbf{k}'} G(\mathbf{k})$, allowing us to write

$$G^R(\mathbf{r}-\mathbf{r}', \sigma t, \sigma' t') = \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} G^R(\mathbf{k}, \sigma t, \sigma' t'), \tag{8.36a}$$

$$G^R(\mathbf{k}, \sigma t, \sigma' t') = -i\theta\left(t-t'\right)\langle[a_{\mathbf{k}\sigma}(t), a^\dagger_{\mathbf{k}\sigma'}(t')]_{B,F}\rangle. \tag{8.36b}$$

The other types of Green's functions have similar forms.