

Quantum Many Body Theory

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Week 1

1 Green's functions of the Schrödinger equation

1.1 Retarded Green's function

The retarded Green's function of the Schrödinger equation $G^R(x_f, x_i; t_f, t_i)$ is defined (up to a factor of $-i$) as a probability amplitude of a particle to hop from the point x_i at a time t_i to the point x_f at a time t_f , where $t_f > t_i$. In other words, the Green's function coincides with a wave function $\psi(x, t)$ of a particle evaluated at a point $x = x_f$ and time $t = t_f$ whose wave function at time t_i was $\psi(x, t_i) = -i\delta(x - x_i)$ (The coefficient $-i$ is introduced because of a standard convention). At the same time, if $t_f < t_i$, the retarded Green's function is identically zero. The regarded Green's function, by construction, must satisfy the Schrödinger equation

$$i \frac{\partial G^R(x, x_i; t, t_i)}{\partial t} = \hat{H}(x, t) G(x, x_i; t, t_i), \quad t > t_i. \quad (1.1)$$

It must also satisfy the boundary condition

$$\lim_{t_f \rightarrow t_i + 0} G(x_f, x_i; t_f, t_i) = -i\delta(x_f - x_i). \quad (1.2)$$

It is easy to check that the retarded Green's function has the following expression in terms of the eigenfunctions ψ_n and the eigenvalues E_n of the Hamiltonian, as long as $t_f \geq t_i$ (the assumption here is that the Hamiltonian does not change in time):

$$G^R(x_f, x_i; t_f, t_i) = -i \sum_n \exp(-iE_n(t_f - t_i)) \psi_n(x_f) \psi_n^*(x_i). \quad (1.3)$$

Indeed, if $t_f > t_i$, this expression explicitly satisfies the Schrodinger equation. At the same time, if $t_f \rightarrow t_i$, then using a well known relation

$$\sum_n \psi_n(x_f) \psi_n^*(x_i) = \delta(x_f - x_i) \quad (1.4)$$

gives us (1.2).

It follows from this definition that, if a particle's wave function is $\psi_i(x)$ at time $t = t_i$, its wave function at $t = t_f > t_i$ is

$$\psi_f(x) = i \int dy G^R(x, y; t_f, t_i) \psi_i(y). \quad (1.5)$$

The Green's function of a time independent Hamiltonian depends only on the time difference $t = t_f - t_i$. Often it is emphasized by writing it as a function of that difference only, $G^R(x_f, x_i, t)$. Notice that $G^R = 0$ if $t < 0$.

The Fourier transform of the Green's function is very useful. In case of the retarded Green's function, this is defined by

$$G^R(x_f, x_i, E) = \int_0^\infty dt e^{iEt} G^R(x_f, x_i, t). \quad (1.6)$$

Substituting (1.3) we observe that we need to compute integrals of the form $\int_0^\infty dt e^{iEt}$, and these are not well defined if E is real. However, if E is complex, and if its imaginary part is positive, then this integral is well defined. It is customary to denote the real part of E simply by E , and the imaginary part by ϵ . This gives

$$G^R(x_f, x_i, E) = \sum_n \frac{\psi_n(x_f) \psi_n^*(x_i)}{E + i\epsilon - E_n}. \quad (1.7)$$

It is easy to see that

$$(E + i\epsilon - \hat{H}(x)) G^R(x, x_i, \omega) = \delta(x - x_i). \quad (1.8)$$

Formally this means that the Green's function can be understood as an operator

$$\hat{G}^R = \frac{1}{E + i\epsilon - \hat{H}}. \quad (1.9)$$

It is often interesting to know the limit of the Green's function in the limit when ϵ vanishes. This is denoted by

$$\hat{G}^R(E) = \lim_{\epsilon \rightarrow +0} \frac{1}{E + i\epsilon - \hat{H}} \equiv \frac{1}{E + i0 - \hat{H}}. \quad (1.10)$$

1.2 Advanced Green's function

Advanced Green's function is the wave function of a particle at a time $t_f < t_i$, such that at the time t_i the particle's wave function is $i\delta(x_f - x_i)$. If $t_f > t_i$, it is equal to zero. Thus it is given by

$$G^A(x_f, x_i; t_f, t_i) = i \sum_n \exp(-iE_n(t_f - t_i)) \psi_n(x_f) \psi_n^*(x_i), \quad t_f < t_i. \quad (1.11)$$

Introducing $t_f - t_i = t$, as before, we find the Fourier transform of the retarded Green's function

$$G^A(x_f, x_i, E) = \int_{-\infty}^0 dt e^{itE} G^A(x_f, x_i, t). \quad (1.12)$$

This time E must have a negative imaginary part in order for this integral to exist. Denoting it by $-\epsilon$, we find

$$G^A = \sum_n \frac{\psi_n(x_f) \psi_n^*(x_i)}{E - i\epsilon - E_n}. \quad (1.13)$$

Often one is interested in the limit when ϵ approaches zero. Then we find

$$\hat{G}^A(E) = \frac{1}{E - i0 - \hat{H}}. \quad (1.14)$$

Notice that this is essentially the same expression as (1.10). The difference is just in how the limit is approached.

1.3 Simplest Applications of Green's functions

Green's functions have poles at values of E which approach the values of discrete energy spectrum E_n . They have cuts at values of E where the spectrum is continuous. Knowing Green's functions allows to determine where the discrete states are. If the spectrum is continuous, it allows to determine the density of states. This is defined as

$$\rho(E) = \frac{1}{L} \sum_n \delta(E - E_n), \quad (1.15)$$

where L is the length of the system (or volume, if it is multidimensional). With the help of a well known expression

$$\frac{1}{x + i\epsilon} = -i\pi\delta(x) + \text{something real} \quad (1.16)$$

one finds

$$\rho(E) = -\frac{1}{L} \int dx \frac{1}{\pi} \text{Im} G^R(x, x, E) = \frac{1}{L} \int dx \frac{i}{2\pi} (G^R(x, x, E) - G^A(x, x, E)). \quad (1.17)$$

The quantity

$$\rho(x, E) = \frac{i}{2\pi} (G^R(x, x, E) - G^A(x, x, E)) \quad (1.18)$$

is called the local density of states.

Second well known application concerns the probability of finding a particle at a position x_f at time t_f which was at a point x_i at a time t_i . This is given by, if $t = t_f - t_i$

$$P(x_f, t_f; x_i, t_i) = |G^R(x_f, t_f; x_i, t_i)|^2 = G^R(x_f, t_f; x_i, t_i) G^A(x_i, t_i; x_f, t_f). \quad (1.19)$$

Writing it in this form

$$|G^R(x_f, x_i, t)|^2 = G^R(x_f, x_i, t) G^A(x_i, x_f, -t) \quad (1.20)$$

allows us to deduce that

$$P(x_f, x_i, E) = \int_{-\infty}^{\infty} d\omega G^R\left(x_f, x_i, \omega + \frac{E}{2}\right) G^A\left(x_i, x_f, \omega - \frac{E}{2}\right) \quad (1.21)$$

1.4 Examples

1.4.1 Green's functions of a free particle in 1D

Consider a 1D free particle living on a line of length L with the spectrum and normalized wavefunctions

$$E_k = \frac{k^2}{2m}, \quad \psi_k(x) = \frac{1}{L} e^{ikx}. \quad (1.22)$$

The Green's function is given by

$$G^R(x_f, x_i, E) = \frac{1}{L} \sum_k \frac{e^{ik(x_f - x_i)}}{E + i0 - \frac{k^2}{2m}}. \quad (1.23)$$

The summation over k can be replaced by an integral if the system size is large, by recalling that the summation really goes over integer n such that $k_n = 2\pi n/L$. That gives

$$G^R(x_f, x_i, E) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{e^{ik(x_f - x_i)}}{E + i0 - \frac{k^2}{2m}}. \quad (1.24)$$

It is customary to omit the steps leading to (1.24), yet often useful to remember what stood behind it.

Correspondingly, the advanced Green's function is given by

$$G^A(x_f, x_i, E) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{e^{ik(x_f - x_i)}}{E - i0 - \frac{k^2}{2m}}. \quad (1.25)$$

If $E < 0$, there is no difference between advanced and retarded Green's functions because the integral is not sensitive to whether $+i0$ or $-i0$ sits in the denominator.

To calculate the integral over k , suppose $E < 0$. Then the denominator vanishes if $k = \pm i\sqrt{2m|E|}$.

If $x_f > x_i$, the integral must be closed in the upper half plane. We find

$$G(x_f, x_i, E) = -\sqrt{\frac{m}{2}} \frac{e^{-\sqrt{-2mE}|x_f - x_i|}}{\sqrt{-E}}, \quad E < 0. \quad (1.26)$$

This expression is analytic if $E < 0$. However, if $E > 0$, it is not well defined (can take one of two possible values). Thus to find its value, one needs to analytically continue the Green's function to positive E over upper half plane for retarded function, or over lower half plane for advanced function.

For retarded function, we find

$$G^R(x_f, x_i, E) = \sqrt{\frac{m}{2}} \frac{e^{i\sqrt{2mE}|x_f - x_i|}}{i\sqrt{E}}. \quad (1.27)$$

We can use this to find the density of states via (1.17). It is

$$\rho(E) = \frac{i}{2\pi L} \int dx G^R(x, x, E) = \frac{\sqrt{m}}{2\pi\sqrt{2E}}. \quad (1.28)$$

Let us check this expression via the direct definition of the density of states.

$$\rho(E) = \int \frac{dk}{2\pi} \delta(E - k^2/(2m)) = \frac{\sqrt{m}}{2\pi\sqrt{2E}}. \quad (1.29)$$

Since the Green's function depends only on the difference $x = x_f - x_i$, it is possible to Fourier transform it into four different forms, $G^R(x, E)$, $G^R(k, E)$, $G^R(x, t)$, $G^R(k, t)$. The expression for $G^R(k, E)$ is especially simple

$$G^R(k, E) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} \frac{dk'}{2\pi} \frac{e^{i(k'-k)x}}{E + i0 - \frac{k'^2}{2m}} = \frac{1}{E + i0 - \frac{k^2}{2m}}. \quad (1.30)$$

This expression can also be thought of as the matrix elements of the operator $\hat{G}(E)$ with respect to the definite momentum wave functions, with one subtlety: the absence of the delta-function present in the matrix elements.

$$\langle k | \frac{1}{E + i0 - \hat{H}} | k' \rangle = \frac{2\pi\delta(k - k')}{E + i0 - \frac{k^2}{2m}} \quad (1.31)$$

1.4.2 A particle in 1D in a delta-function potential: bound states

Consider

$$\hat{H} = -\frac{1}{2m} \frac{\partial^2}{\partial x^2} + \lambda\delta(x). \quad (1.32)$$

It is possible to find its Green's functions by calculating its eigenfunctions and eigenvalues. But there is a direct way which is actually faster. Denote $\hat{H}_0 = 1/(2m)\partial^2/\partial x^2$. Introduce

$$\hat{G}_0^R = \frac{1}{E + i0 - \hat{H}_0}, \quad (1.33)$$

which was calculated in the previous section. Now we can write

$$\hat{G}^R = \frac{1}{E + i0 - \hat{H}_0 - \hat{V}} = \hat{G}_0^R + \hat{G}_0^R \hat{V} \hat{G}_0^R + \hat{G}_0^R \hat{V} \hat{G}_0^R \hat{V} \hat{G}_0^R + \dots \quad (1.34)$$

It is common to introduce the following “ T -matrix”. It is defined in the following way:

$$\hat{T} = \hat{V} + \hat{V} \hat{G}_0^R \hat{V} + \hat{V} \hat{G}_0^R \hat{V} \hat{G}_0^R \hat{V} + \dots \quad (1.35)$$

Knowing T -matrix gives the Green's function as in

$$\hat{G}^R = \hat{G}_0^R + \hat{G}_0^R \hat{T} \hat{G}_0^R. \quad (1.36)$$

Its meaning is the following: it looks like interactions which, when taken into account in the first Born approximation, produce the exact answer.

Let us calculate $\langle k | \hat{T} | k' \rangle$. We observe that

$$\langle k | \hat{V} | k' \rangle = \lambda. \quad (1.37)$$

We calculate the sum by inserting the complete set of states, for example, by writing

$$\langle k | \hat{V} \hat{G}_0^R \hat{V} | k' \rangle = \int \frac{dk''}{2\pi} \frac{dk'''}{2\pi} \langle k | \hat{V} | k'' \rangle \langle k'' | \hat{G}_0^R | k''' \rangle \langle k''' | \hat{V} | k' \rangle. \quad (1.38)$$

An important expression which appears within the expression above is

$$\int \frac{dk}{2\pi} \frac{dk'}{2\pi} \langle k | \hat{G}_0^R | k' \rangle = \int \frac{dk}{2\pi} \frac{1}{E + i0 - \frac{k^2}{2m}} = -\frac{\sqrt{m}}{\sqrt{-2E}} \equiv \Pi \quad (1.39)$$

This integral has been calculated earlier (1.26) and has to be understood as an analytic continuation from $E < 0$.

Thus we find

$$\langle k | \hat{T} | k' \rangle = \lambda + \lambda^2 \Pi + \dots = \frac{\lambda}{1 - \lambda \Pi} = \frac{1}{\frac{1}{\lambda} - \Pi} = \frac{1}{\frac{1}{\lambda} + \sqrt{\frac{m}{-2E}}}. \quad (1.40)$$

The poles of T coincide with the poles of G^R . Thus its poles signify the presence of bound states. If $\lambda > 0$, there are no poles in T . If $\lambda < 0$, then there is a pole at

$$E = -\frac{\lambda^2 m}{2}. \quad (1.41)$$

This is the famous bound state in a 1D delta-function potential.