Green Function

E.N. Economou, "Green's Functions in Quantum Physics", 2nd ed. (83)

Definition

Consider a time-independent, linear, Hermitian differential operator \( L(r) \) where \( r \) is the spatial vector. The complete set of eigenfunctions of \( L \) satisfies the differential eq.

\[
L(r) \phi_n(r) = \lambda_n \phi_n(r)
\]

and some boundary conditions on the surface \( S \) of some domain \( \Omega \).

The set \( \{ \phi_n(r) \} \) is assumed to be orthonormal & complete, i.e.

\[
\int_{\Omega} \text{d}\lambda \phi_m^*(r) \phi_n(r) = \delta_{nm}
\]

\[
\sum_n \phi_n(r) \phi_n(r') = \delta( r - r' )
\]

where the sum \( \sum_n \) is to be replaced by integration \( \int d\lambda \) for continuous eigen spectrum.

The corresponding green function \( G \) is defined by

\[
[ z - L(r) ] G(r, r'; z) = \delta( r - r' )
\]

subjected to the same boundary conditions as \( \phi_n \).

Dirac Notations

\[
\phi_n(r) \equiv < r | \phi_n > = < r | n >
\]

\[
\phi_n(r') = < \phi_n | r > = < n | r >
\]

\[
\delta(r-r') L(r) \equiv < r | L | r' >
\]

\[
G(r-r') \equiv < r | G | r' >
\]

The basis vectors \( | r > \) are orthogonal, \( \delta \) normalized & complete:

\[
< r | r' > = \delta( r - r' )
\]

\[
\int \text{d}r \ | r > < r | = 1
\]

The eqs involved in the definition of \( G \) becomes:

\[
L | \phi_n > = \lambda_n | \phi_n > \quad \text{or} \quad L | n > = \lambda_n | n >
\]

\[
( z - L ) G(z) = 1
\]

\[
< \phi_n | \phi_m >= \delta_{nm} \quad \text{or} \quad < n | m >= \delta_{nm}
\]

\[
\sum_n < \phi_n > < \phi_n > = 1 \quad \text{or} \quad \sum_n | n > < n | = 1
\]

In these forms, these eqs are called operator eqs.

The original defining eqs are said to be written in the \( r \)-representation. They are simply the matrix elements of the operator eqs. For example:

\[
( z - L ) G(z) = 1
\]

\[
\rightarrow \quad < r | ( z - L ) G(z) | r' > = < r | r' >
\]

\[
\int \text{d}r'' < r | ( z - L ) | r'' > < r'' | G(z) | r' > = \delta( r - r' )
\]

\[
= \int \text{d}r'' \delta( r - r' ) [ z - L(r) ] G(r'', r'; z)
\]

\[
= [ z - L(r) ] G(r, r'; z)
\]
Properties

\[(z - L) G(z) = 1\]

\[
\rightarrow \quad G(z) = \frac{1}{z - L} \quad \text{if} \quad z \neq \lambda_n
\]

\[
= \sum_n \left[ n > \frac{1}{z - L} < n \right]
\]

\[
= \sum_n \left[ n > \frac{1}{z - \lambda_n} \right]
\]

\[
= \int d\lambda \ \frac{|\lambda| \left< \lambda \right|}{z - \lambda_n} \quad \text{for continuous spectrum}
\]

\[
G(r, r'; z) = \sum_n \frac{\phi_n(r) \phi_n^*(r')}{z - \lambda_n}
\]

\[
G(r, r'; z)^* = \sum_n \frac{\Delta_n(r') \Delta_n(r)}{z^* - \lambda_n} = G(r', r; z^*)
\]

Since \(L\) is hermitian, \(\lambda_n\) are real.

\(*\) \(G(z)\) is analytic off the real axis.

Poles of \(G(z)\) are at discrete eigenvalues of \(L\).

Order of these poles equals the degeneracy of \(\lambda_n\).

For continuous eigenvalues \(\lambda\), we have 2 situations:

1. extended states: \(\phi(r) \neq 0\) as \(|r| \to \infty\)
   \(G(\lambda \pm i s)\) exists as \(s \to 0\).
   The real axis is a branch cut.

2. localized states: \(\phi(r) \to 0\) as \(|r| \to \infty\)
   \(G(\lambda \pm i s)\) does not exist as \(s \to 0\).
   The real axis is a natural boundary.

Our discussion will be restricted to extended states only.

Extended states

Define

\[
G^\pm(\lambda) = \lim_{s \to 0} G(\lambda \pm i s) \quad \lambda, \ s = \text{real}
\]

From \(G(r, r'; z)^* = G(r', r; z^*)\)

we have

\[
G^+(r, r'; \lambda)^* = G(r, r'; \lambda + i s)^*
= G(r', r; \lambda - i s) = G^-(r', r; \lambda)
\]

Hence

\[
\text{Re} \ G^+(r, r ; \lambda) = \text{Re} \ G^-(r, r ; \lambda)
\]

\[
\text{Im} \ G^+(r, r ; \lambda) = -\text{Im} \ G^-(r, r ; \lambda)
\]

Define

\[
\tilde{G}(\lambda) = G^+(\lambda) - G^-(\lambda)
\]

Discrete spectrum

Define

\[
G^\pm(\lambda) = \lim_{s \to 0} G(\lambda \pm i s) \quad \lambda, \ s = \text{real}
\]
Using the identity
\[ \lim_{y \to 0} \frac{1}{x \mp iy} = \text{PV} \frac{1}{x} \mp i \pi \delta(x) \]
we have:
\[
G(\lambda) = \sum_n \frac{|n > n|}{\lambda - \lambda_n \pm i\varepsilon} = \text{PV} \sum_n \frac{|n > n|}{\lambda - \lambda_n} \mp i \pi \sum_n \delta(\lambda - \lambda_n) \quad \text{where} \quad n > n
\]