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 Ω.

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

$$\int_\Omega \mathrm{dr}\,\phi_n{}^*(r)\,\phi_m(r) = \delta_{n\,m}$$

$$\sum_n\ \phi_n(r)\ \phi_n{}^*(r\,') = \delta(\,r - r\,'\,)$$

where the sum $\sum_n$ is to be replaced by integration $\int \mathrm{d}\lambda$ 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 ϕ_n.

Dirac Notations

$\phi_n(r) \equiv\ <r\,|\,\phi_n>\ =\ <r\,|\,n>$
$\phi_n(r)^* \equiv\ <\phi_n\,|\,r>\ =\ <n\,|\,r>$
$\delta(r - r\,'\,)\,L(r) \equiv\ <r\,|\,L\,|\,r\,'>$
$G(r - r\,'\,)\ \equiv\ <r\,|\,G\,|\,r\,'>$

The basis vectors $|\,r>$ are othogonal, δ normalized & complete:

$<r\,|\,r\,'>= \delta(r - r\,'\,)$
$\int \mathrm{dr}\ \left|\,r>\ <r\,\right| =\ 1$

The eqs involved in the definition of G becomes:

$L\,|\,\phi_n>= \lambda_n\,|\,\phi_n>$ or $L\,|\,n>= \lambda_n\,|\,n>$
$(\,z - L\,)\,G(z) = 1$
$<\phi_n\,|\,\phi_m>= \delta_{n\,m}$ or $<n\,|\,m>= \delta_{n\,m}$
$\sum_n \left|\,\phi_n>\ <\phi_n\,\right| =\ 1$ or $\sum_n \left|\,n>\ <n\,\right| =\ 1$

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:

$$(\,z - L\,)\,G(z) = 1$$

$$\longrightarrow\quad <r\,|\,(\,z - L\,)\,G(z)\,|\,r\,'>=\ <r\,|\,r\,'>$$

$$\int \mathrm{dr}\,''<r\,\left|\,(\,z - L\,)\,\right|r\,''>\ <r\,''\left|\,G(z)\,\right|r\,'>= \delta(r - r\,')$$

$$=\ \int \mathrm{dr}\,''\ \ \delta(r - r\,'')\,[\,z\ - L(r)\,]\,G(r\,'',\ r\,';\,z)$$

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

- **Properties**

$$(z - L)\, G(z) = 1$$

$$\longrightarrow \quad G(z) = \frac{1}{z - L} \qquad \text{if } z \neq \lambda_n$$

$$= \sum_n \left| n > \frac{1}{z - L} < n \right|$$

$$= \sum_n \frac{|n><n|}{z - \lambda_n}$$

$$= \int d\lambda \, \frac{|\lambda><\lambda|}{z - \lambda} \qquad \text{for continuous spectrum}$$

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

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

Since L is hermitian, λ_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 λ_n.

For continuous eigenvalues λ, 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

$$G^{\pm}(\lambda) \equiv \lim_{s \to 0_+} G(\lambda \pm i\, s) \qquad \lambda,\ s = \text{real}$$

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

$$\tilde{G}(\lambda) \equiv G^{+}(\lambda) - G^{-}(\lambda)$$

- **Discrete spectrum**

Define

$$G^{\pm}(\lambda) \equiv \lim_{s \to 0_+} G(\lambda \pm i\, s) \qquad \lambda,\ s = \text{real}$$

Using the identity

$$\lim_{y\to 0_+} \frac{1}{x \pm i\, y} = \text{PV}\, \frac{1}{x} \mp i\, \pi\, \delta(x)$$

we have:

$$G^{\pm}(\lambda) = \sum_n \frac{|n><n|}{\lambda - \lambda_n \pm i\, s}$$

$$= \text{PV} \sum_n \frac{|n><n|}{\lambda - \lambda_n} \mp i\, \pi \sum_n \delta(\lambda - \lambda_n) \left| n > < n \right|$$