38 Green's Function: Diffusion Equation

The Green's function method to solve the general initial-boundary value problem for diffusion equations is given. The Markovian property of the free-space Green's function (= heat kernel) is the key to construct Feynman-Kac path integral representation of Green's functions.

Key words: reciprocity, general solution formula, eigenfunction expansion, Markovian property, Feynman-Kac formula, path integral.

Summary:
(1) The reader should roughly remember the strategy for constructing Green's function, and its use (→**38.9**, **38.7**).
(2) The relation between the heat kernel and random walk is extremely important.[445] Many important properties of the heat kernel can be derived and/or understood with the aid of this interpretation.
(3) The Markovian property (→**38.10**) of the heat kernel is crucial in developing path integrals (→**38.11**).
(4) Functional integrals are staple for theoreticians. Cf. Glimm and Jaffe.[446]

38.1 Summary up to this point. We have constructed the free-space Green's function, and used it to solve the initial value-problem in **16B.1**, **16B.10**. The image source method is explained in **16B.9** to construct Green's functions for various simple regions.

38.2 The most general diffusion problem. The general form of the problem on the region Ω is

$$(\partial_t - D\Delta)u(x,t) = \varphi(x,t) \quad \text{on} \quad \Omega \tag{38.1}$$

with the boundary condition, a Dirichlet or a Neumann condition on $\partial\Omega$ for $t > 0$, and the initial condition $u(0,x) = f(x)$. It is a standard trick

[445] See **16B.8**. An elementary (and classic) introduction is: S. Chandrasekhar. Rev. Mod. Phys. **15**, 1 (1943). This does not use δ-function at all. If you use it, you can rewrite the review in a more concise way. To make a modern version is a good exercise (was good to the lecturer as an undergrad).

[446] J. Glimm and A. Jaffe, *Quantum Physics, a functional integral point of view*, (Springer, 1987). However, the book is not recommended to a casual reader.

that the initial condition can be written as a source term as (→**16B.5**)

$$(\partial_t - D\Delta)u(x,t) = \varphi(x,t) + f(x)\delta(t) \quad \text{on } \Omega. \tag{38.2}$$

Hence, we have only to solve the homogeneous initial value problem.

38.3 Green's function. The solution to

$$(\partial_t - D\Delta)G(x,t|y,s) = \delta(t-s)\delta(x-y) \tag{38.3}$$

with the homogeneous boundary condition is called the *Green's function.*

38.4 Existence of Dirichlet Green's function. We have constructed the Green's function G_0 for the free space in **16B.1**. Now we wish to determine the Green's function for the homogeneous Dirichlet problem. Note that $u \equiv G(x,t|x',t') - G_0(x,t|x',t')$ obeys the diffusion equation with the boundary condition

$$u(t,x|t',x') = -w(x,t|x',t') \quad \text{on } \partial\Omega, t > t' \tag{38.4}$$

and the initial condition $u = 0$ for $t = t'$ (or $t \le t'$). The unique existence of the solution has been discussed (heuristically **1.18**; **28.3**). Hence, the existence of Green's functions is guaranteed at least for a compact domain.

The Neumann condition can also be treated analogously.

38.5 Counterpart of Green's formula. Let $\mathcal{L} \equiv \partial_t - D\Delta$ and $\mathcal{L}^+ \equiv -\partial_t - D\Delta$. Then for u which is zero for $t \le 0$[447] and also $u \to 0$ in the $t \to \infty$ limit we have

$$\int_0^\infty dt \int_\Omega dx[(\mathcal{L}u)v - u\mathcal{L}^+v] = -D\int_0^\infty dt \int_{\partial\Omega} d\sigma \cdot (v\nabla u - u\nabla v). \tag{38.5}$$

This is essentially Green's theorem and can be proved quite analogously (→**16A.19**).

Exercise. Prove this.

38.6 Reciprocity relations. Notice that the Green's function is a function of $t-s$ (time translational symmetry), so that $G(x,t-\tau|y,s-\tau) = G(x,t|y,s)$. If we choose $\tau = t+s$, we get

$$G(x,t|y,s) = G(x,-s|y,-t). \tag{38.6}$$

[447]Since the solution to the diffusion equation is very smooth, we may put the initial condition at $t = 0+$ instead of $t = 0$.

We have

$$\left(-\frac{\partial}{\partial t} - D\Delta_x\right) G(x,-t|y,-s) = \delta(x-y)\delta(t-s) \tag{38.7}$$

as can easily be seen from the change of variables $t \to -t$ and $s \to -s$. Hence, (38.6) implies

$$\mathcal{L}^+ G = \left(-\frac{\partial}{\partial t} - D\Delta_x\right) G(x,s|y,t) = \delta(x-y)\delta(t-s). \tag{38.8}$$

If we set $u = G(z,\tau|y,s)$ and $v = G(z,t|x,\tau)$ in (38.5), we obtain, regarding u and v as functions of z and τ

$$\int_0^\infty d\tau \int_\Omega dz[(\mathcal{L}G(z,\tau|y,s))G(z,t|x,\tau) - G(z,\tau|y,s)\mathcal{L}^+ G(z,t|x,\tau)] = 0. \tag{38.9}$$

(Here the operators act on the functions of z and τ.) That is, with the aid of (38.8)

$$G(y,t|x,s) = G(x,t|y,s). \tag{38.10}$$

38.7 Solution to general boundary value problem. In terms of the Green's function the solution to

$$(\partial_t - D\Delta)u(x,t) = \varphi(x,t) \tag{38.11}$$

under the initial condition $u(x,0) = f(x)$ and an appropriate boundary condition (inhomogeneous Dirichlet or Neumann that may depend on time) reads

$$\begin{aligned} u(t,x) &= \int_0^t ds \int_\Omega dy\, G(x,t|y,s)\varphi(y,s) + \int_\Omega dy G(x,t|y,0)f(y) \\ &+ D\int_0^t ds \int_{\partial\Omega} d\sigma(y)\left[G(x,t|y,s)\frac{\partial u(y,s)}{\partial n(y)} - u(y,s)\frac{\partial}{\partial n(y)}G(x,t|y,s)\right]. \end{aligned} \tag{38.12}$$

Here the surface term simplifies if we specialize the formula to Dirichlet or Neumann cases.

[Demo] In the analogue of Green's theorem **38.5** we set u to be the solution to the problem, and G to be the Green's function for the corresponding homogeneous boundary condition. We know $\mathcal{L}^+G(x,s|y,t) = \mathcal{L}^+G(y,s|x,t) = \mathcal{L}^+G(x,t|y,s) = \delta(x-y)(t-s)$ (→**38.6**).

38.8 Steady source problem, recurrence of random walk. Let us assume that the source term $\varphi(x,t)$ is time-independent point source $\delta(x)$, and the problem is in the free space with 0 initial condition. Then, (38.12) gives

$$u(x,t) = \int_0^t G(x,t|0,s)ds, \tag{38.13}$$

which is increasing without limit for $d \leq 2$ and finite for $d > 2$. This distinct behaviors for $d > 2$ or not can be understood as the recurrence property of the random walks.

38.9 Eigenfunction expansion of Green's function. (cf. **35.22**) Let λ_n be the n-th eigenvalue of $-\Delta$ on Ω with a homogeneous boundary condition (Dirichlet or Neumann), and u_n be the corresponding normalized eigenfunction. Then the Green's function for the diffusion equation with the same boundary condition $G(x,t|x',t')$ reads

$$G(x,t|x',t') = \sum_n u_n(x)\overline{u_n(x')}e^{-\lambda_n(t-t')}\Theta(t-t'). \tag{38.14}$$

Notice that in this case the zero eigenvalue existing for the Neumann condition is not excluded (this is required by the conservation of the total mass).

Exercise.
Find the Green's function for the following equation on the unit 3-cube $[0,1] \times [0,1] \times [0,1]$

$$\frac{\partial u}{\partial t} = \frac{1}{2}\Delta u - cu, \tag{38.15}$$

where c is a positive constant, with a homogeneous Dirichlet boundary condition.

38.10 Markov property revisited. (→**16B.7**) For the heat kernel G_0 (→**16B.1**),

$$G_0(x,t|x_0,t_0) = \int_{\boldsymbol{R}^d} dx_1 G_0(x,t|x_1,t_1)G_0(x_1,t_1|x_0,t_0), \tag{38.16}$$

[Demo] Note the 'translation symmetry' (38.6) allows (38.16) to be rewritten with the introduction of $g(x,t) = G_0(x,t|0,0)$ as

$$g(x,t) = \int_{\boldsymbol{R}^d} dy\, g(x-y,t-s)g(y,s). \tag{38.17}$$

(There is NO integral with respect to time.) Introducing the Fourier transform $\hat{g}$ of g with respect to x, this reads $\hat{g}(k,t) = \hat{g}(k,t-s)\hat{g}(k,s)$ (→**33.8**). This is obvious from

$$\hat{g}(k,t) = e^{-Dk^2t}. \tag{38.18}$$

which is directly obtainable from $(\partial_t - D\Delta)g(x,t) = \delta(t)\delta(x)$.[448]

38.11 Feynman-Kac formula for the heat kernel. Using (38.16) repeatedly to divide the time axis into pieces, we get

$$g(x,t) = \prod_{i=1}^{N-1} \int_{\mathbf{R}^d} dx_i \prod_{i=1}^{N} g(x_i - x_{i-1}, t_i - t_{i-1}), \tag{38.19}$$

where $t_N \equiv t$, $t_0 \equiv 0$, $x_N \equiv x$ and $x_0 \equiv 0$. Let us choose the equal spacing of the time axis $\Delta t = t_i - t_{i-1}$ for all i, and let $\Delta x_i \equiv x_i - x_{i-1}$. Then (38.19) and (448) imply

$$g(x,t) = \prod_{i=1}^{N-1} \int dx_i (4\pi D\Delta t)^{-3/2} \exp[-\sum_{i=1}^{N} (\Delta x_i)^2/4D\Delta t]. \tag{38.20}$$

If Δt is sufficiently small, then, formally,

$$\sum_{i=1}^{N} \frac{(\Delta x_i)^2}{\Delta t} \to \int_0^t dt \left(\frac{dx}{dt}\right)^2. \tag{38.21}$$

Therefore, formally, (38.20) converges to

$$g(x,t) = \int_{x(0)=0}^{x(t)=x} \mathcal{D}[x(\cdot)] \exp\left[-\frac{1}{4D}\int_0^t dt \left(\frac{dx}{dt}\right)^2\right], \tag{38.22}$$

where $\mathcal{D}$ is the 'uniform measure'[449] on the set of continuous functions $[0,t] \to \boldsymbol{R}^3$. This is the *Feynman-Kac formula* for the heat kernel.

38.12 Feynman-Kac path integral. The Green's function for

$$(\partial_t - D\Delta + V)u = 0 \tag{38.23}$$

with $u \to 0$ in the $|x| \to \infty$ limit can be written as

$$g(x,t) = \int_{x(0)=0}^{x(t)=x} \mathcal{D}[x(\cdot)] \exp\left[-\int_0^t dt \left(\frac{1}{4D}\left(\frac{dx}{dt}\right)^2 + V(x(t))\right)\right], \tag{38.24}$$

[448] We can invert this to get

$$g(x,t) = (4\pi Dt)^{-3/2} e^{-x^2/4Dt}.$$

[449] This is a very delicate object, but is definable in a certain sense. However, in these days. mathematicians seem to avoid this altogether. Cf. **20.2** Discussion (1).

where V is a function bounded from below.[450]

[450] A good introductory book on this subject may be R. P. Feynman, *Statistical Mechanics*, Chapter 3 (Benjamin, 1972). This path integral is well defined as a Lebesgue integral on the set of continuous functions. For Schrödinger equation, we must replace t with it. This replacement completely destroys the currently available justification of the formula as a Lebesgue integral.