# Causality of the diffusion propagator

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## 1 Diffusion equation

We first establish the diffusion equation. By Fick's first law, we have

$$\mathbf{J}(t, \mathbf{r}) = -D(\mathbf{r})\partial_{\mathbf{r}}\rho(t, \mathbf{r}). \tag{1}$$

Given an arbitrary source $f(t, \mathbf{r})$, by the continuity equation, we have

$$\partial_t \rho(t, \mathbf{r}) + \partial_{\mathbf{r}}\mathbf{J}(t, \mathbf{r}) = f(t, \mathbf{r}). \tag{2}$$

Combining (1) and (2), we have

$$[\partial_t - \partial_{\mathbf{r}} D(\mathbf{r})\partial_{\mathbf{r}}]\rho(t, \mathbf{r}) = f(t, \mathbf{r}). \tag{3}$$

Now, to solve the partial differential equation in (3), we notice that it is translation-invariant in time, in which case, the fundamental solution $\mathcal{G}(t; \mathbf{r}, \mathbf{r}_0)$ satisfies

$$[\partial_t - \partial_{\mathbf{r}} D(\mathbf{r})\partial_{\mathbf{r}}]\mathcal{G}(t; \mathbf{r}, \mathbf{r}_0) = \delta(t)\delta(\mathbf{r} - \mathbf{r}_0). \tag{4}$$

Hence, we get the solution to (3) by convolution, i.e.,

$$\rho(t, \mathbf{r}) = \int dt_0 d^d\mathbf{r}_0 \; \mathcal{G}(t - t_0; \mathbf{r}, \mathbf{r}_0) f(t_0, \mathbf{r}_0). \tag{5}$$

## 2 Causality

For the rest of the note, we focus on the case of uniform diffusion, i.e., consider $D(\mathbf{r}) = D_0 \; \forall \mathbf{r}$. Now, the fundamental solution $G(t, \mathbf{r})$ satisfies

$$[\partial_t - D_0\partial_{\mathbf{r}}^2]G(t, \mathbf{r}) = \delta(t)\delta(\mathbf{r}). \tag{6}$$

Notice that no particle is introduced to the system until $t = 0$. Hence, $G(t, \mathbf{r}) = 0 \ \forall t < 0$, which demonstrates causality. However, the notion of causality can also be illustrated in the Fourier domain.

Indeed, we apply Fourier transform to both sides of (6). It is clear that the right hand side is 1. To simplify the left hand side, we use integration by parts. Notice that

$$(\mathcal{F}\partial_t G)(\omega, \mathbf{q}) = \int dt \int d^d\mathbf{r} \ \partial_t G(t, r) e^{i\omega t - i\mathbf{q}\mathbf{r}} \tag{7}$$

$$= -\int dt \int d^d\mathbf{r} \ G(t, r)(i\omega) e^{i\omega t - i\mathbf{q}\mathbf{r}}, \tag{8}$$

where we drop the boundary term, assuming $G(t, \mathbf{r}) \to 0$ as $t \to \pm\infty$. Hence, we have

$$(\mathcal{F}\partial_t G)(\omega, \mathbf{q}) = -i\omega(\mathcal{F}G)(\omega, \mathbf{q}). \tag{9}$$

Similarly, applying integration by parts twice, we have

$$(\mathcal{F}\partial_{\mathbf{r}}^2 G)(\omega, \mathbf{q}) = \int dt \int d^d\mathbf{r} \ \partial_{\mathbf{r}}^2 G(t, r) e^{i\omega t - i\mathbf{q}\mathbf{r}} \tag{10}$$

$$= \int dt \int d^d\mathbf{r} \ \partial_{\mathbf{r}} G(t, r)(i\mathbf{q}) e^{i\omega t - i\mathbf{q}\mathbf{r}} \tag{11}$$

$$= \int dt \int d^d\mathbf{r} \ G(t, r)(i\mathbf{q})^2 e^{i\omega t - i\mathbf{q}\mathbf{r}}, \tag{12}$$

where we drop the boundary term, assuming additionally that $\partial_{\mathbf{r}} G(t, \mathbf{r}) \to 0$ as $t \to \pm\infty$. Hence, we have

$$(\mathcal{F}\partial_{\mathbf{r}}^2 G)(\omega, \mathbf{q}) = -\mathbf{q}^2(\mathcal{F}G)(\omega, \mathbf{q}). \tag{13}$$

Therefore, equation (6) in the Fourier domain is given by

$$[-i\omega + D_0\mathbf{q}^2]G(\omega, \mathbf{q}) = 1, \tag{14}$$

whose solution is given by

$$G(\omega, \mathbf{q}) = \frac{1}{-i\omega + D_0\mathbf{q}^2}. \tag{15}$$

Notice that the only singularity of $G(\omega, \mathbf{q})$ is given by $\omega = -iD_0 q^2$. Applying the inverse Fourier transform back to the time ($t$) domain, we have

$$G(t, \mathbf{q}) = \int \frac{d\omega}{2\pi} \ \frac{e^{-i\omega t}}{-i\omega + D_0\mathbf{q}^2} = \frac{1}{2\pi i} \int d\omega \ \frac{-e^{-i\omega t}}{\omega + iD_0\mathbf{q}^2}. \tag{16}$$

At this point, we wish to apply Cauchy's integral theorem or Cauchy's integral formula to compute $G(t, \mathbf{q})$. In particular, we can view the inverse Fourier transform above as an integration along the equator of the Riemann sphere. Then, for each $t$, we can shrink the contour either toward the upper or the lower half of the complex plane depending on whether $e^{-\omega t} \to 0$ in the upper or the lower half by Jordan's lemma.

1. For $t < 0$, we see that $e^{-i\omega t} \to 0$ when $\Im\omega > 0$. So, we shink the contour toward the upper half of the complex plane. By Cauchy's integral theorem, we see that

$$G(t, \mathbf{q}) = \frac{1}{2\pi i} \int d\omega \; \frac{-e^{-i\omega t}}{\omega + iD_0\mathbf{q}^2} = 0. \tag{17}$$

2. For $t > 0$, we we see that $e^{-i\omega t} \to 0$ when $\Im\omega < 0$. So, we shrink the contour toward the lower half of the complex plane. By Cauchy's integral formula, we see that

$$G(t, \mathbf{q}) = \frac{1}{2\pi i} \int d\omega \; \frac{-e^{-i\omega t}}{\omega + iD_0\mathbf{q}^2} = -e^{-D_0\mathbf{q}^2 t}. \tag{18}$$

This agrees with our previous observation that the uniform diffusion propagator preserves causality since $G(t, \mathbf{q}) = 0 \; \forall t < 0$.