Connections between diffusion and electrostatics

Consider
\[ \begin{align*}
C_t &= D \nabla^2 C \\
C(\vec{r}, t=0) &= \delta(\vec{r} - \vec{r}_0) \\
C(\vec{r} \in B) &= 0 \quad \text{absorbing boundary}
\end{align*} \]

Then
\[ \vec{j}(\vec{r}_B, t) = -D \nabla C \quad \text{is the flux into the boundary at } \vec{r}_B, \]

and
\[ \int_0^\infty \int_{\vec{r}_B \in B} \frac{\partial}{\partial t} \phi(\vec{r}_B, t) = 1 \]

To simplify the problem, consider
\[ \phi(\vec{r}) = \int_0^\infty \int_{\vec{r}_B \in B} \frac{\partial}{\partial t} C(\vec{r}, t). \]

Then
\[ \int_0^\infty \int_{\vec{r}_B \in B} \frac{\partial}{\partial t} C_t = C(\vec{r}, \infty) - C(\vec{r}, 0) = \delta(\vec{r} - \vec{r}_0), \]

and we have
\[ -\delta(\vec{r} - \vec{r}_0) = D \nabla^2 \phi. \]

So \( \phi \) is like the electrostatic potential, and
\( E(\vec{r}_b) \) is like electric field for a point charge of magnitude \( q_0 = \frac{1}{D \omega_d} \)

surface area of a unit sphere in \( d \) dim's, e.g. \( 4\pi \) in 3D

Indeed, \( E(\vec{r}_b) = \int_0^\infty dt \overset{\infty}{\int} j(\vec{r}_b, t) = \)

\(-D \int_0^\infty dt \partial_t \overset{\infty}{\int} C = -D \partial_n \overset{\infty}{\int} C \).

The boundary is grounded (\( \overset{\infty}{\int} C = 0 \)) due to absorbing BCs.

**Semi-infinite 1D Line**

**QA:**

1. What is the prob. of hitting \( x = 0 \) at \( t \) for the 1st time?
2. What is the average hitting time?

Here, \( \begin{cases} C_t = DC_{xx}, \\ C(x, t=0) = \delta(x-x_0), \\ C(x=0, t) = 0 \end{cases} \)
Let's use the image method.

\[ \frac{x_0}{\text{antiparticle}} \rightarrow \frac{x}{\text{particle}} \rightarrow x \]

Then \( C(x, t) = \frac{1}{\sqrt{4\pi D t}} \left[ e^{-(x-x_0)^2/4Dt} - e^{-(x+x_0)^2/4Dt} \right] \)

satisfies the eq'n & the BCS.

Note that
\[
\frac{\partial C}{\partial x} \bigg|_{x=0} = \frac{1}{\pi^{1/2} (4Dt)^{3/2}} x
\]

\[
x \left[ -2(x-x_0) e^{-(x-x_0)^2/4Dt} + 2(x+x_0) e^{-(x+x_0)^2/4Dt} \right] \bigg|_{x=0} = \frac{x_0}{(4\pi)^{1/2} (Dt)^{3/2}} e^{-x_0^2/4Dt}
\]

Then \( j(x=0, t) = -D \frac{\partial C}{\partial x} \bigg|_{x=0} = -\frac{x_0}{\sqrt{4\pi D t^{3/2}}} e^{-x_0^2/4Dt} \)

Eventual exit prob. is given by

\[ L(x=0) = \int_0^\infty dt \left| j(x=0, t) \right| = \]

\[ = + \frac{x_0}{\sqrt{4\pi D}} \int_0^\infty \frac{dt}{t^{3/2}} e^{-x_0^2/4Dt} \]

\[ = 2 \int_0^\infty du e^{-u^2/4D} \]

\( \left\{ \begin{array}{l}
    u^2 = \frac{1}{t}, \\
    dt = -2 \frac{du}{u^2}
\end{array} \right. \)

\[ = \frac{x_0}{\sqrt{4\pi D}} \int_0^\infty du e^{-u^2/4D} = 1, \text{ as expected} \]

\[ = \int_0^\infty du \ldots = \frac{\sqrt{4\pi D}}{x_0} \]

-3-
Moreover,
\[
\langle t \rangle = \frac{\int_0^\infty dt \, t \, j(x=0,t)}{\int_0^\infty dt \, j(x=0,t)} = \infty
\]
on average, takes infinite time to get absorbed.

Indeed, \( \int_0^\infty dt \, t \, j(x=0,t) \sim \int_0^\infty dt \, \frac{x^2}{4D} \, t \) diverges.

Higher moments diverge as well.

**Finite 1D interval**

\[x=0 \quad x_0 \quad L\]

**QQ:**

1. What is the survival prob. \( S(t) \)?
2. What is the 1st passage prob. (FPP) to \( 0 \) or \( L \), at time \( t \)?
3. What are the eventual exit probs. to \( 0 \) or \( L \)?
4. What is the average time \( t(x_0) \) to reach \( 0 \) or \( L \)?
5. What are the conditional average times to reach \( L \) (\( t+(x_0) \)) or \( 0 \) (\( t-(x_0) \))?
We have
\[
\begin{cases}
C_t = DC_{xx}, \\
C(x, t=0) = \delta(x-x_0), \\
C(0, t) = C(L, t) = 0
\end{cases}
\]

The diff'\n eq\n' n is like a time-dep.
SE in a square-well potential:
\[
\begin{cases}
V(x) = 0, & 0 < x < L \\
V(x) = \infty & \text{otherwise}
\end{cases}
\]

with \( D \leftrightarrow -\frac{h^2}{2m} \)

So we can use SE technique to solve this eq'n.

1. Survival prob. \( S(t) \).

Try variable separation on \( \phi(x, t) \):
\[
\phi(x, t) = f(t) g(x)
\]

Then \( f'g = Dg'' \), or
\[
\frac{f'}{f} = D \frac{g''}{g} \Rightarrow D^{-1} \frac{f'}{f} = \frac{g''}{g} \equiv -\frac{k}{\text{const}}
\]

This gives \( g'' = -kg \), or
\[
g \sim \sin \left( \frac{n\pi}{L} x \right), \ n \in \mathbb{Z}
\]

to satisfy the BCS
Furthermore,
\[ \dot{f} = -D_k f \] gives
\[ f \sim e^{-D \left( \frac{\pi n}{L} \right)^2 t} \]

So,
\[ C(x, t) = \frac{2}{L} \sum_{n=1}^{\infty} \sin \left( \frac{n \pi x}{L} \right) \sin \left( \frac{n \pi x_0}{L} \right) e^{-D \left( \frac{\pi n}{L} \right)^2 t} \]
\[ \times \quad \ast \]

Note that \( C(0, t) = C(L, t) = 0 \) by construction.
Also, the \( n=0 \) term is \( \theta \) everywhere
and the expression is symm. wrt \( n \).

Indeed, consider
\[ C(x, 0) = \delta(x-x_0) = \sum_{n=1}^{\infty} \sin \left( \frac{n \pi x}{L} \right) \]
dact with
\[ \int_0^L dx \sin \left( \frac{n' \pi x}{L} \right) \ast \quad \text{on both sides:} \]
\[ h' = 1, 2, 3, \ldots \]

\[ \sin \left( \frac{n' \pi x_0}{L} \right) = \sum_{n=1}^{\infty} A_n \int_0^L dx \sin \left( \frac{n' \pi x}{L} \right) \sin \left( \frac{n \pi x}{L} \right) = \]
\[ = \sum_{n=1}^{\infty} A_n \frac{1}{2} \int_0^L dx \left[ \cos \left( \frac{n \pi x}{L} (n-n') \right) - \cos \left( \frac{n \pi x}{L} (n+n') \right) \right] \]
\[ \text{will always give } \theta \] since \( n, n' > 0 \)
\[ \int_0^L \cos \left( \frac{\pi x}{L} (n-n') \right) \frac{L}{\pi(n-n')} \sin(\pi(n-n')) = \begin{cases} 0 & n \neq n' \\ L & n = n' \end{cases} \]

But then \( \sin \frac{n\pi x_0}{L} = A_n \frac{L}{2} \), or

\[ A_n = \frac{2}{L} \sin \frac{n\pi x_0}{L} \text{, which gives } (*) \]

Finally, \( S(t) = \int_0^L dx \ C(x,t) \sim e^{-\frac{D \pi^2 t}{L^2}} \sim e^{-\frac{t}{\tau}} \),

where \( \tau \sim \frac{L^2}{D} \) is the slowest decaying mode \( n=1 \) the diffusion time-scale.

(2) FPP \Rightarrow use Laplace domain

\[ C(x,s) = \int_0^\infty dt \ e^{-st} C(x,t) \]

\[ \int_0^\infty dt \ e^{-st} \frac{\partial C(x,t)}{\partial t} = e^{-st} C(x,t) \bigg|_0^\infty + \]

\[ + \int_0^\infty dt \ e^{-st} C(x,t) = -C(x,0) + SC(x,s). \]

With \( C \equiv C(x,s) \), we have:

\[ \int \left[ SC - \delta(x-x_0) \right] = DC, \]

\[ C(0,s) = C(L,s) = 0 \]
This is solved by

\[ C(x, s) = \frac{1}{\gamma DS} \frac{\sinh \left( \sqrt{\frac{S}{D}} x_2 \right) \sinh \left( \sqrt{\frac{S}{D}} (L - x_0) \right)}{\sinh \left( \sqrt{\frac{S}{D}} L \right)} \]

\[
\begin{cases}
  x_2 = \min(x, x_0) \\
  x_0 = \max(x, x_0)
\end{cases}
\]

Indeed, \( C(0, S) = C(L, S) = 0 \).

\[ [C(x, s)] = \frac{T}{L} \text{ in } 1D \]

\[ [s] = \frac{1}{T} \Rightarrow \left[ \frac{1}{\gamma DS} \right] = \frac{1}{\sqrt{L^2/T^2}} = \frac{T}{L}, \]

as expected.

Finally,

\[ \lim_{\varepsilon \to 0} D \frac{DC'}{x_0^\pm \varepsilon} = D \frac{1}{\gamma DS} \left[ \frac{\sinh \left( \sqrt{\frac{S}{D}} x_0 \right)}{\sinh \left( \sqrt{\frac{S}{D}} L \right)} \left( -\sqrt{\frac{S}{D}} \cosh \left( \sqrt{\frac{S}{D}} (L - x_0) \right) \right) \\
- \sqrt{\frac{S}{D}} \cosh \left( \sqrt{\frac{S}{D}} x_0 \right) \frac{\sinh \left( \sqrt{\frac{S}{D}} (L - x_0) \right)}{\sinh \left( \sqrt{\frac{S}{D}} L \right)} \right] = \]

\[ = -\frac{1}{\sinh \left( \sqrt{\frac{S}{D}} L \right)} \sinh \left( \sqrt{\frac{S}{D}} (x_0 + L - x_0) \right) = -1, \]

as expected.

\[ \int_{x_0 - \varepsilon}^{x_0 + \varepsilon} \delta(x - x_0) = -1. \]
But then

\[ \tilde{j}_+(s) = - D \left. \frac{\partial c(x,s)}{\partial x} \right|_{x=L} = \]

\[ = \frac{1}{T D s} \frac{\sinh \left( \sqrt{\frac{s}{D}} x_0 \right)}{\sinh \left( \sqrt{\frac{s}{D}} L \right)} \sqrt{\frac{s}{D}} (-1) = \]

\[ = \frac{\sinh \left( \sqrt{\frac{s}{D}} x_0 \right)}{\sinh \left( \sqrt{\frac{s}{D}} L \right)}. \]

\[ \tilde{j}_-(s) = - D \left. \frac{\partial c(x,s)}{\partial x} \right|_{x=0} = - \frac{\sinh \left( \sqrt{\frac{s}{D}} (L-x_0) \right)}{\sinh \left( \sqrt{\frac{s}{D}} L \right)}. \]

Eventual exit prob.:

\[ \xi_-(x_0) = \left| \int_0^\infty dt j_-(0,t) e^{-st} \right|_{s=0} = \]

\[ = \left| \tilde{j}_-(S=0) \right| = 1 - \frac{x_0}{L}. \]

Likewise,

\[ \xi_+(x_0) = \left| \tilde{j}_+(S=0) \right| = \frac{x_0}{L}. \]

Note that \( \xi_+(x_0) + \xi_-(x_0) = 1 \), as expected.
Finally, consider

$$t(x) = \frac{\int_0^\infty dt \left[ j_-(t) + j_+(t) \right]}{\int_0^\infty dt \left[ j_-(t) + j_+(t) \right]}$$

average time to reach \(0\) or \(L\) starting from \(x\)

since you leave the system eventually

\[ \Rightarrow \quad \int_0^\infty dt t j(t) e^{-st} \bigg|_{s=0} = \left( -\frac{\partial}{\partial s} \int_0^\infty dt j(t) e^{-st} \right) \bigg|_{s=0} = -\frac{\partial \tilde{j}(s)}{\partial s} \bigg|_{s=0} \]

In this way, one can obtain

$$t(x) = \frac{x(L-x)}{2D}, \quad \text{as well as} \quad t_+(x) \quad \& \quad t_-(x).$$

However, there is a more straightforward approach, as discussed next.