Applications of Quantum Mechanics: RMT, Brownian Motion and All That

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Outline

▶ First Lecture (Basic): Brownian Motion in Quantum Mechanics formalism

▶ Second Lecture (Basic): Basic RMT ensembles

▶ Third Lecture (Basic): Vicious Brownian paths in Quantum Mechanics formalism and connections to RMT (Part I)

▶ Fourth Lecture (Advanced): Vicious Brownian paths in Quantum Mechanics formalism and connections to RMT (Part II)

▶ Fifth Lecture (Advanced): the one-dimensional Lieb-Liniger gas and Brownian paths with mixed boundary conditions
First Lecture (Basic): Brownian Motion in Quantum Mechanics formalism
Outline

- Diffusion equation. Einstein’s derivation (two ways).
- Wiener Process (Langevin approach).
- Examples:
  - Diffusive particle on the real line.
  - Diffusive particle on the semi-infinite line with absorbing/reflecting boundary conditions at \( x = 0 \) (method of images).
  - Diffusive particle in a box (method of images).
- Path integral approach (Derivation from discrete Wiener Process).
- Operator formalism.
- Propagator in terms of eigenfunctions and eigenvalues.
- Diffusive particle in a box revisited and connection to the method of images.
- Take Home Message
- Recommended Reading
Diffusion equation. Einstein’s derivation (two ways)

In 1905, Einstein’s *On the movement of small particles suspended in stationary liquids required by the molecular-kinetic theory of heat*

▶ Quantitative description of Brownian motion.

▶ Two parts:

I A fluctuation-dissipation relation: it relates the fluctuations of microscopic movements with macroscopic observables/parameters (viscosity, temperature)

II A beautiful derivation of the diffusion equation

\[
\frac{\partial \rho(x, t)}{\partial t} = D \frac{\partial^2 \rho(x, t)}{\partial x^2}
\]

Foundation of the field of stochastic processes.
Diffusion equation. Einstein’s derivation (two ways)

First part:

- Particles are in a gravitational field
- Diluted gas of non-interacting Brownian particles in a solvent under a constant external volume force \( F_0 \) (gravity).
- \( x \)-axis to be the vertical axis
- Recall: an ideal gas we have that \( pV = Nk_B T \). We assume

\[
\rho(x) = k_B T \rho(x)
\]

- Force is due to pressure

\[
F = -\frac{\partial p(x)}{\partial x} = -k_B T \frac{\partial \rho(x)}{\partial x}
\]

- System at equilibrium \( \Rightarrow \) force must be equal to \( \rho(x)F_0 \)

\[
\rho(x)F_0 = -k_B T \frac{\partial \rho(x)}{\partial x} \Rightarrow \rho_{eq}(x) = \rho(0)e^{-\left(F/k_B T\right)x}
\]
Diffusion equation. Einstein’s derivation (two ways)

Also, we must have two currents:

- **Diffusion**
  \[ J_{\text{diff}} = -D \frac{\partial \rho}{\partial x} \]

- **Drift**
  \[ J_{\text{drift}} = \rho(x)v \]

where \( v \) is the velocity.

- But \( F_0 = -\Gamma v \), where \( \Gamma \) is a friction coefficient.

- **Equilibrium** \( \Rightarrow \) zero total current
  \[ 0 = J_{\text{total}} = -D \frac{\partial \rho}{\partial x} - \rho(x) \frac{F_0}{\Gamma} \Rightarrow \rho(x) = \rho(0)e^{\frac{-F_0}{\Gamma D}x} \]

- Comparing both expressions:
  \[ D = \frac{k_B T}{\Gamma}, \quad \text{Sutherland-Einstein relation} \]
Diffusion equation. Einstein’s derivation (two ways)

- Use Stoke’s relation $\Gamma = 6\pi \eta a$ for a particle of radius $a$ to obtain
  $$D = \frac{k_B T}{6\pi \eta a}$$

- If the viscosity $\eta$ increases, the diffusion decreases

- If the radius of the particles decreases, the diffusion coefficient $D$ increases
Diffusion equation. Einstein’s derivation (two ways)

Second part (about diffusion process)
- We treat the one-dimensional case
- Analysis easily extendable to higher dimensions.
- Consider \( \rho(x, t) \) the density of particles at \( x \) at time \( t \).
- The particles are non-interacting.
- We can think of \( \rho(x, t) \) as the Prob that the particle is at \( x \) at time \( t \).
- We start from:

\[
P(x, t + \Delta t) = \int_{-\infty}^{\infty} P(x - \Delta x, t) \phi_{\Delta t}(\Delta x) d(\Delta x)
\]

where \( \phi_{\Delta t}(\Delta x) \) is a normalised pdf of jumps \( \Delta x \).
Diffusion equation. Einstein’s derivation (two ways)

Second part (about diffusion process)

- Graphically

\[ P(x, t + \Delta t) = \int_{-\infty}^{\infty} P(x - \Delta x, t) \phi_{\Delta t}(\Delta x)d(\Delta x) \]
Diffusion equation. Einstein’s derivation (two ways)

By expanding in Taylor series:

\[
P(x, t + \Delta t) = \int_{-\infty}^{\infty} P(x - \Delta x, t) \phi_{\Delta t}(\Delta x) d(\Delta x)
\]

\[
= \int_{-\infty}^{\infty} \left[ P(x, t) - \Delta x \frac{\partial P(x, t)}{\partial x} + \frac{(\Delta x)^2}{2} \frac{\partial^2 P}{\partial x^2} \right. \\
\left. + \mathcal{O}((\Delta x)^3) \right] \phi_{\Delta t}(\Delta x) d(\Delta x) \Rightarrow 
\]

\[
P(x, t + \Delta t) = P(x, t) - \langle \Delta x \rangle \frac{\partial P}{\partial x} + \frac{1}{2} \left\langle (\Delta x)^2 \right\rangle \frac{\partial^2 P}{\partial x^2}
\]

and from here we write

\[
\frac{P(x, t + \Delta t) - P(x, t)}{\Delta t} = - \frac{\langle \Delta x \rangle}{\Delta t} \frac{\partial P}{\partial x} + \frac{1}{2} \frac{\left\langle (\Delta x)^2 \right\rangle}{\Delta t} \frac{\partial^2 P}{\partial x^2}
\]
Diffusion equation. Einstein’s derivation (two ways)

- Take the limit $\Delta t \to 0$:

$$
\frac{\partial P}{\partial t} = -\mu \frac{\partial P}{\partial x} + D \frac{\partial^2 P}{\partial x^2}
$$

- with $\mu$ is the drift and $D$ is the diffusion constant

$$
\mu = \lim_{\Delta t \to 0} \frac{\langle \Delta x \rangle}{\Delta t}, \quad 2D = \lim_{\Delta t \to 0} \frac{\langle (\Delta x)^2 \rangle}{\Delta t}
$$

- Recall that $P \leftrightarrow \rho$ so that we can write

$$
\frac{\partial \rho}{\partial t} = -\mu \frac{\partial \rho}{\partial x} + D \frac{\partial^2 \rho}{\partial x^2} = -\frac{\partial}{\partial x} \left[ \mu \rho - D \frac{\partial \rho}{\partial x} \right] = -\frac{\partial j}{\partial x}
$$

- $j$ is total current density.
Diffusion equation. Einstein’s derivation (two ways)

- Diffusion equation is a continuity equation with total current

\[ j = \mu \rho - D \frac{\partial \rho}{\partial x} \]

- First term: Drift
- Second term: Diffusion.

- Comparing the two results

\[ D = \lim_{\Delta t \to 0} \frac{\langle (\Delta x)^2 \rangle}{\Delta t}, \quad D = \frac{k_B T}{6\pi \eta a} \]

- Microscopic fluctuations of the trajectories are related to macroscopic parameters.
Wiener Process (Langevin approach)

- Diffusion equation: macroscopic/probabilistic description
- What about single trajectories?
- Microscopic approach to diffusion equation
- Notice that: $\frac{\Delta x}{\Delta t}$ is some sort of random object

$$\frac{\Delta x}{\Delta t} = \xi_{\Delta t}(t)$$
Wiener Process (Langevin approach)

- which are the properties $\xi_{\Delta t}(t)$ so that we obtain what we want? (no drift)

\[
\langle \xi_{\Delta t}(t) \rangle = \frac{\langle \Delta x \rangle}{\Delta t} = 0
\]

\[
\langle \xi^2_{\Delta t}(t) \rangle = \frac{\langle (\Delta x)^2 \rangle}{(\Delta t)^2} = \frac{2D}{\Delta t}
\]

- Magnitude of noise scales as $1/\sqrt{\Delta t}$
Wiener Process (Langevin approach)

- General correlation function

\[ \langle \xi_{\Delta t}(t)\xi_{\Delta t}(t') \rangle = \begin{cases} 0 & t \neq t' \\ \frac{2D}{\Delta t} & t = t' \end{cases} \]

- For \( \Delta t \to 0 \) (limiting noise)

\[ \lim_{\Delta t \to 0} \xi_{\Delta t}(t) = \xi(t) \]

- \( \xi(t) \): Gaussian white noise (no frequency dependence)

\[ \langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = 2D\delta(t - t') \]

- \( \delta(\Delta t) = 1/\Delta t \) (physicists interpretation of Dirac delta)

- so \( \Delta t \to 0 \) we have the Wiener Process (or Langevin equation)

\[ \frac{dx}{dt} = \eta(t) \]
Wiener Process (Langevin approach)

- Formal solution for a single trajectory
  \[ x(t) = x(t_0) + \int_{t_0}^{t} \xi(t') dt' \]

- Wiener Process is a Markov process: conditioned to \( x(t) \Rightarrow x(t + \Delta t) \)
  \[ x(t + \Delta t) = x(t) + \xi(t) \Delta t \]

- Two observations:
  - Important later on for statistical content of propagator
  - Numerics: More general problems: easier to simulate Langevin equation that solving numerically a general diffusion equation
Example: Diffusive particle on the real line

- Consider driftless case ($\mu = 0$)
- The solution is

$$\frac{\partial P}{\partial t} = D \frac{\partial^2 P}{\partial x^2} \Rightarrow$$

$$P(x, t) = \int_{-\infty}^{\infty} dx_0 \frac{e^{-(x-x_0)^2/4D(t-t_0)}}{\sqrt{4\pi D(t-t_0)}} P(x_0, t_0)$$

- For initial condition $P(x_0, t_0) = \delta(x_0 - \tilde{x}_0) \Rightarrow$ solution is the propagator (aka Green's function)

$$G(x, t|x_0, t_0) = \frac{e^{-(x-x_0)^2/4D(t-t_0)}}{\sqrt{4\pi D(t-t_0)}}$$

- Notice

$$P(x, t) = \int_{-\infty}^{\infty} dx_0 G(x, t|x_0, t_0) P(x_0, t_0)$$
Example: Diffusive particle on the semi-infinite line with reflecting boundary conditions at $x = 0$ (method of images)

- We want to solve diffusive particle in $\mathbb{R}^+ \cup \{0\}$ with BCs

$$\frac{\partial P(x, t)}{\partial x} \bigg|_{x=0} = 0$$

- Notice that this implies

$$\frac{\partial G(x, t|x_0, t_0)}{\partial x} \bigg|_{x=0} = 0$$

- This means no probability current at $x = 0$.
- Particles cannot escape from $\mathbb{R}^+ \cup \{0\}$
- Corresponding propagator is $G^{(R)}_+(x, t|x_0, t_0)$ is

$$G^{(R)}_+(x, t|x_0, t_0) = G(x, t|x_0, t_0) + G(x, t| - x_0, t_0)$$
Example: Diffusive particle on the semi-infinite line with reflecting boundary conditions at $x = 0$ (method of images)

- Graphically
Example: Diffusive particle on the semi-infinite line with absorbing boundary conditions at $x = 0$ (method of images)

- We want to solve diffusive particle in $\mathbb{R}^+ \cup \{0\}$ with BCs
  \[ P(x, t) \bigg|_{x=0} = 0 \]

- Notice that this implies
  \[ G(x, t | x_0, t_0) \bigg|_{x=0} = 0 \]

- This means probability is lost at $x = 0$.
- Particles escape from $\mathbb{R}^+ \cup \{0\}$
- Corresponding propagator is $G^{(A)}_+(x, t | x_0, t_0)$ is
  \[ G^{(A)}_+(x, t | x_0, t_0) = G(x, t | x_0, t_0) - G(x, t | -x_0, t_0) \]
Example: Diffusive particle on the semi-infinite line with absorbing boundary conditions at $x = 0$ (method of images)

▶ Graphically
Example: Diffusive particle in a box (method of images)

- Diffusive particle in a box $[0, L]$ with either $a \in \{ A(\text{absorbing}), R(\text{reflecting}) \}$ BCs

- Propagator is

$$G_{[0,L]}^{(a)}(x, t|x_0, t_0) = \sum_{n=-\infty}^{\infty} G_+^{(a)}(x, t|x_0 - 2nL, t_0)$$
Path integral approach (Derivation from discrete Wiener Process)

- Consider discretized Wiener Process with time step $\Delta t$

$$x(t + \Delta t) = x(t) + \sqrt{2D\Delta t}\zeta(t)$$

- Two states $x$ and $y$ are connected by transition matrix (Markov process)

$$W_{\Delta t}[y, t + \Delta | x, t] = \langle y - x - \sqrt{2D\Delta t}\zeta(t) \rangle_{\zeta(t)}$$

- For a larger path $\Rightarrow$ apply transition matrix several times
- Notation: $t_i = t_0 + i\Delta t$ for $i = 1, \ldots, M$
- Denote as $x(t_i) = x_i$ and $t_M = t$ $x_M = x$.
- We write

$$P(x, t) = \int_{-\infty}^{\infty} \prod_{i=0}^{M-1} dx_i \prod_{i=0}^{M-1} W_{\Delta t}(x_{i+1}, t_{i+1} | x_i, t_i) P(x_0, t_0)$$
Path integral approach (Derivation from discrete Wiener Process)

- or

\[
P(x, t) = \int_{-\infty}^{\infty} \left[ \prod_{i=0}^{M-1} dx_i \right] \left[ \prod_{i=0}^{M-1} \left\langle \delta \left( x_{i+1} - x_i - \sqrt{2D\Delta t} \zeta_i \right) \right\rangle \zeta_i \right] P(x_0, t_0)
\]

- The term in the integral is the well-known propagator:

\[
G(x, t|x_0, t_0) = \int \left[ \prod_{i=1}^{M-1} dx_i \right] \left[ \prod_{i=0}^{M-1} \left\langle \delta \left( x_{i+1} - x_i - \sqrt{2D\Delta t} \zeta_i \right) \right\rangle \zeta_i \right]
\]

- Express propagator in terms of Gaussian integrals:

\[
\prod_{i=0}^{M-1} \left\langle \delta \left( x_{i+1} - x_i - \sqrt{2D\Delta t} \zeta_i \right) \right\rangle \zeta_i = \prod_{i=0}^{M-1} \frac{1}{\sqrt{4\pi D\Delta t}} e^{-\frac{(x_{i+1} - x_i)^2}{4D\Delta t}}
\]
Path integral approach (Derivation from discrete Wiener Process)

- For small $\Delta t$ we have that $x_{i+1} - x_i = \Delta t \frac{dx(t_i)}{dt_i} + \mathcal{O}(\Delta t^2)$

- Argument of the exponential:

$$
\sum_{i=0}^{M-1} \frac{(x_{i+1} - x_i)^2}{4D\Delta t} = \frac{1}{4D} \Delta t \sum_{i=0}^{M-1} \left( \frac{dx(t_i)}{dt_i} \right)^2 \to \frac{1}{4D} \int_{t_0}^{t} d\tau \left( \frac{dx(\tau)}{d\tau} \right)^2
$$

- Finally

$$
P(x, t) = \int_{-\infty}^{\infty} dx_0 \int_{x_0}^{x} \mathcal{D}[x(t)] \exp \left[ - \frac{1}{4D} \int_{t_0}^{t} d\tau \left( \frac{dx(\tau)}{d\tau} \right)^2 \right] P(x_0, t_0),
$$

with

$$
\mathcal{D}[x(t)] = \lim_{M \to \infty} \frac{1}{\sqrt{4\pi D\Delta t}} \prod_{i=1}^{M-1} \frac{dx_i}{\sqrt{4\pi D\Delta t}}
$$
Path integral approach (Derivation from discrete Wiener Process)

Using the formalism of QM, it is possible to write the propagator as follows

$$\begin{align*}
G(x, t | x_0, t_0) &= \langle x \mid e^{-\hat{H}(t-t_0)} \mid x_0 \rangle \\
&= \int_{x(t_0)=x_0}^{x(t)=x} D[x(\tau)] \exp \left[ -\frac{1}{4D} \int_{t_0}^{t} d\tau \left( \frac{dx(\tau)}{d\tau} \right)^2 \right]
\end{align*}$$

with $\hat{H} = -D\nabla^2$ (space representation). From here we can write

$$P(x, t) = \int_{-\infty}^{\infty} dx_0 G(x, t | x_0, t_0) P(x_0, t_0)$$
Operator formalism

- Using bra and ket notation
  \[ \frac{\partial}{\partial t} P(x, t) = D \nabla^2 P(x, t) \Rightarrow |P(t)\rangle = e^{-DP^2(t-t_0)} |P(t_0)\rangle \]
  with \( P \) the momentum operator.

- In position representation \( \langle x | P(t) \rangle = P(x, t) \):
  \[ P(x, t) = \langle x | e^{-DP^2(t-t_0)} | P(t_0) \rangle \]
  \[ = \int dx_0 \langle x | e^{-DP^2(t-t_0)} | x_0 \rangle \langle x_0 | P(t_0) \rangle \]

- Solution of the diffusion equation in terms of propagator
  \[ P(x, t) = \int dx_0 G(x, t | x_0, t_0) P(x_0, t_0) \]
  where we have defined the propagator
  \[ G(x, t | x_0, t_0) = \langle x | e^{-\mathcal{H}(t-t_0)} | x_0 \rangle \]
  with \( \mathcal{H} = DP^2 \) is the Hamiltonian of a free particle.
Operator formalism

Summarising

- For 1d diffusion equation

\[ \frac{\partial}{\partial t} P(x, t) = D \nabla^2 P(x, t) \]

- Within (Wiener-Dirac-)Feynman path integral approach:

\[ G(x, t | x_0, t_0) = \int_{x(t_0) = x_0}^{x(t) = x} \mathcal{D}x(\tau) \exp \left[ -\frac{1}{4D} \int_{t_0}^{t} d\tau \left( \frac{dx(\tau)}{d\tau} \right)^2 \right] \]

- Propagator contains the statistical information of ALL paths of a Brownian motion starting at \( x(t_0) = x_0 \) and finishing at \( x(t) = x \)

- Using operators (QMf and notation)

\[ G(x, t | x_0, t_0) = \langle x | e^{-\mathcal{H}(t-t_0)} | x_0 \rangle \]
Propagator in terms of eigenfunctions and eigenvalues

To notice:

- Suppose \( \{|\psi_n\rangle\} \) a complete set of orthonormal eigenstates of \( \mathcal{H} \) with eigenvalues \( \{E_n\} \), that is \( \mathcal{H} |\psi_n\rangle = E_n |\psi_n\rangle \).

- Propagator can be written as follows

\[
G(x, t| x_0, t_0) = \langle x | e^{-\mathcal{H}(t-t_0)} | x_0 \rangle = \sum_n \langle x | \psi_n \rangle \langle \psi_n | e^{-\mathcal{H}(t-t_0)} | x_0 \rangle = \sum_n \psi_n(x) \psi^*_n(x_0) e^{-E_n(t-t_0)}
\]
Difussive particle in a box revisited and connection to the method of images

- Diffusion equation in a Box with BCs
  \[
  \frac{\partial P(x, t)}{\partial x} \bigg|_{x=0,L} = 0
  \]
  (no current at \(x = 0, L\))

- Hamiltonian: \(\mathcal{H} = -\frac{1}{2} \nabla^2 + V_{\text{box}}(x)\) with
  \[
  V_{\text{box}}(x) = \begin{cases} 
  0 & x \in (0, L) \\
  \infty & x = 0, L
  \end{cases}
  \]

- Eigenfunctions and eigenvalues
  \[
  \psi_0(x) = \frac{1}{L}, \quad \psi_n(x) = \sqrt{\frac{2}{L}} \cos \left( \frac{\pi nx}{L} \right), \quad n = 1, 2, \ldots
  \]
  \[
  E_n = D \frac{\pi^2 n^2}{L^2}
  \]
Difusssive particle in a box revisited and connection to the method of images

- Propagator

\[ G^{(R)}_{[0,L]}(x, t| x_0, t_0) = \frac{1}{L} + \frac{2}{L} \sum_{n=1}^{\infty} \cos \left( \frac{\pi nx}{L} \right) \cos \left( \frac{\pi n x_0}{L} \right) e^{-D \frac{\pi^2 n^2}{L^2} (t-t_0)} \]

- Note that \( \lim_{t \to \infty} G(x, t| x_0, t_0) = \frac{1}{L} \)
Example: Particle in a box with absorbing/reflecting boundary conditions

- Diffusion equation in a box with BCs
  \[ P(x, t) \bigg|_{x=0,L} = 0 \]

- Hamiltonian: \( \mathcal{H} = -\frac{1}{2} \nabla^2 + V_{\text{box}}(x) \)

- Eigenfunctions and eigenvalues
  \[ \psi_n(x) = \sqrt{\frac{2}{L}} \sin \left( \frac{\pi nx}{L} \right), \quad n = 1, 2, \ldots \]
  \[ E_n = D \frac{\pi^2 n^2}{L^2} \]

- Propagator
  \[ G^{(A)}_L(x, t|x_0, t_0) = \frac{2}{L} \sum_{n=1}^\infty \sin \left( \frac{\pi nx}{L} \right) \sin \left( \frac{\pi nx_0}{L} \right) e^{-D \frac{\pi^2 n^2 (t-t_0)}{L^2}} \]

- Notice that \( \lim_{t \to \infty} G_L(x, t|x_0, t_0) = 0 \).
Example: Particle in a box with absorbing/reflecting boundary conditions

Take absorbing case. Let us do some checks:

- Consider $L \to \infty$, and let us define

$$k_n = \frac{\pi n}{L} \Rightarrow \Delta k = k_{n+1} - k_n = \frac{\pi}{L}$$

Thus

$$\lim_{L \to \infty} G_{L}^{(A)}(x, t \mid x_0, t_0) = \lim_{L \to \infty} \frac{2}{L} \sum_{n=1}^{\infty} \sin \left( \frac{\pi n x}{L} \right) \sin \left( \frac{\pi n x_0}{L} \right) e^{-D \frac{\pi^2 n^2 (t-t_0)}{L^2}}$$

$$= \frac{2}{\pi} \lim_{L \to \infty, \Delta k \to 0} \Delta k \sum_{n=1}^{\infty} \sin (k_n x) \sin (k_n x_0) e^{-Dk_n^2(t-t_0)}$$

$$= \frac{2}{\pi} \int_{0}^{\infty} dk \sin (kx) \sin (kx_0) e^{-Dk^2(t-t_0)}$$

$$= \frac{1}{\pi} \int_{-\infty}^{\infty} dk \sin (kx) \sin (kx_0) e^{-Dk^2(t-t_0)}$$
Example: Particle in a box with absorbing/reflecting boundary conditions

But

\[
\sin (kx) \sin (kx_0) = \frac{1}{2} \left\{ \cos[k(x - x_0)] - \cos[k(x + x_0)] \right\}
\]

and

\[
\int_{-\infty}^{\infty} dk \cos[k(x \pm x_0)] e^{-Dk^2(t-t_0)} = \text{Re} \left[ \int_{-\infty}^{\infty} dk e^{ik(x \pm x_0)} e^{-Dk^2(t-t_0)} \right]
\]

\[
= \int_{-\infty}^{\infty} dk e^{ik(x \pm x_0)} e^{-Dk^2(t-t_0)}
\]

\[
= \sqrt{\frac{\pi}{D(t-t_0)}} e^{-\frac{(x \pm x_0)^2}{4D(t-t_0)}}
\]
Example: Particle in a box with absorbing/reflecting boundary conditions

This implies

\[ G_+^{(A)}(x, t|x_0, t_0) = \lim_{L \to \infty} G_L^{(A)}(x, t|x_0, t_0) = \frac{e^{-\frac{(x-x_0)^2}{4D(t-t_0)}}}{\sqrt{4\pi D(t-t_0)}} - \frac{e^{-\frac{(x+x_0)^2}{4D(t-t_0)}}}{\sqrt{4\pi D(t-t_0)}} = G(x, t|x_0, t_0) - G(x, t|-x_0, t_0) \]
Difussive particle in a box revisited and connection to the method of images

Finally

- Recall

\[ G_L^{(A)}(x, t| x_0, t_0) = \frac{2}{L} \sum_{n=1}^{\infty} \sin \left( \frac{\pi nx}{L} \right) \sin \left( \frac{\pi nx_0}{L} \right) e^{-D \frac{\pi^2 n^2 (t-t_0)}{L^2}} \]

\[ = \frac{1}{L} \sum_{n=-\infty}^{\infty} \sin \left( \frac{\pi nx}{L} \right) \sin \left( \frac{\pi nx_0}{L} \right) e^{-D \frac{\pi^2 n^2 (t-t_0)}{L^2}} \]

\[ = \frac{1}{2L} \sum_{n=-\infty}^{\infty} \left[ \cos \left( \frac{\pi n(x-x_0)}{L} \right) - \cos \left( \frac{\pi n(x+x_0)}{L} \right) \right] e^{-D \frac{\pi^2 n^2 (t-t_0)}{L^2}} \]

\[ = \frac{1}{2L} \sum_{n=-\infty}^{\infty} \left[ e^{i \left( \frac{\pi n(x-x_0)}{L} \right)} - e^{i \left( \frac{\pi n(x+x_0)}{L} \right)} \right] e^{-D \frac{\pi^2 n^2 (t-t_0)}{L^2}} \]
Difussive particle in a box revisited and connection to the method of images

- Focus on

\[ \frac{1}{2L} \sum_{n=-\infty}^{\infty} e^{i \left( \frac{\pi n (x-x_0)}{L} \right)} e^{-D \frac{\pi^2 n^2 (t-t_0)}{L^2}} \]

- Use Poisson’s summation formula

\[ \sum_{n=-\infty}^{\infty} f(n) = \sum_{k=-\infty}^{\infty} \int_{-\infty}^{\infty} f(x') e^{-i2\pi kx'} \, dx' \]

- In our case we have

\[ f(x') = \frac{1}{2L} e^{i \left( \frac{\pi x'(x-x_0)}{L} \right)} e^{-D \frac{\pi^2 (x')^2 (t-t_0)}{L^2}} \]
Difussive particle in a box revisited and connection to the method of images

So

\[
\int_{-\infty}^{\infty} f(x') e^{-i2\pi k x'} dx' \\
= \frac{1}{2L} \int_{-\infty}^{\infty} dx' e^{-i2\pi k x'} e^{i \left( \frac{\pi x' (x-x_0)}{L} \right)} e^{-D \frac{\pi^2 (x')^2(t-t_0)}{L^2}}
\]

\[
= \frac{1}{2L} \int_{-\infty}^{\infty} dx' \exp \left[ i \frac{x' \pi}{L} (-2kL + x - x_0) \right] e^{-D \frac{\pi^2 (x')^2(t-t_0)}{L^2}}
\]

\[
= \frac{1}{2\pi} \int_{-\infty}^{\infty} dy \exp [iy (-2kL + x - x_0)] e^{-Dy^2(t-t_0)}
\]

\[
= \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp \left[ -\frac{(x - x_0 - 2kL)^2}{4D(t-t_0)} \right]
\]
Difusive particle in a box revisited and connection to the method of images

This finally implies

\[ G_{L}^{(A)}(x, t|x_0, t_0) = \sum_{k=-\infty}^{\infty} \left[ e^{-\frac{(x-x_0-2kL)^2}{4D(t-t_0)}} \sqrt{4\pi D(t-t_0)} - e^{-\frac{(x+x_0-2kL)^2}{4D(t-t_0)}} \sqrt{4\pi D(t-t_0)} \right] \]

\[ = \sum_{k=-\infty}^{\infty} G_{+}^{(A)}(x, t|x_0 - 2kL, t_0) \]
Take Home Message

- QMf an alternative method to method of images (separation of variables, etc)

- In which situations will it become useful?
Recommended Reading

- S. Majumdar, Brownian functionals in physics and computer science, chap. legacy of A. Einstein, Current Science, 89, 2076 (2005)


- M. Yor, Some aspects of Brownian Motion, Lectures notes in Mathematics, 1992