**PHYS 631: Quantum Mechanics I (Fall 2020)**
**Homework 6**
**Assigned Monday, 9 November 2020**
**Due Monday, 16 November 2020**

**Problem 1.** When you're doing quantum mechanics, you're not *just* doing quantum mechanics. You're also doing, for example, *statistical* mechanics. The point of this problem is to explore this idea, from escaping random walks to geophysics, based on what we've covered so far.

(a) The free-particle Schrödinger equation

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\partial_x^2\psi, \tag{1}$$

under the imaginary-time replacement $t \longrightarrow -it$ (along with the replacement $\hbar \longrightarrow m$ to get rid of extra constants), becomes the **diffusion equation**

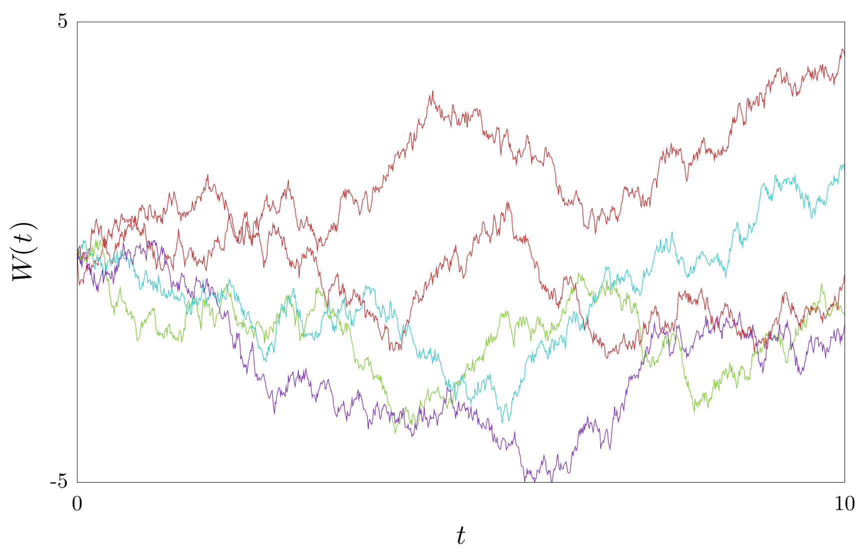
$$\partial_t\psi = \frac{1}{2}\partial_x^2\psi. \tag{2}$$

Make the same replacements in the free-particle propagator to show that the solution to the diffusion equation may be written

$$\psi(x,t) = \frac{1}{\sqrt{2\pi(t-t_0)}}\, e^{-(x-x_0)^2/2(t-t_0)}, \tag{3}$$

given the initial condition $\psi(x,t_0) = \delta(x-x_0)$. (Note that this solution only makes sense for $t \geq t_0$.)

(b) As the solution of the diffusion equation, the appropriately normalized $\psi(x,t)$ acts as a probability density for an ensemble of diffusing particles (*not* $|\psi(x,t)|^2$, as in quantum mechanics). The diffusing particles are said to undergo **Brownian motion**. We can take Eq. (3) to be a mathematical definition of Brownian motion, but more intuitively, you can think of a Brownian motion as a random walk, taking a random, independent step of variance $\Delta t$ during every time step $\Delta t$, but in the continuous limit $\Delta t \longrightarrow 0$. The resulting paths are a bit complicated to handle, because they turn out to be continuous but everywhere nondifferentiable functions of time. Thus, we'll only treat them mathematically via the diffusion equation, although it's good to have some underlying mental picture of what the individual, diffusing particles are up to. For illustration, five different realizations of Brownian motion are plotted below [here $W(t)$ is a standard notation for Brownian motion].



One nice application of the result of part (a) is to ask, given that a Brownian particle starts at some position $d > 0$, what is the probability that it will cross the origin, and how long does it take? To set this up, note that the Schrödinger equation with a potential

$$i\hbar\partial_t\psi = -\frac{\hbar^2}{2m}\partial_x^2\psi + V(x)\psi \tag{4}$$

goes to the damped diffusion equation

$$\partial_t\psi = \frac{1}{2}\partial_x^2\psi - \frac{1}{m}V(x)\psi \tag{5}$$

under the same imaginary-time replacements as before. This means that where $V(x) > 0$, particles are disappearing (or "decaying") exponentially at a rate $V(x)/m$ [note that this is particle *creation* if $V(x) < 0$].

A good way to set up this boundary-crossing problem is to make the region $x < 0$ completely absorbing—that is, $V(x) = \infty$ for $x < 0$, and $V(x) = 0$ for $x > 0$. Then any particles from the ensemble that cross the origin are removed from the ensemble, and we can track the crossing probability by computing the (decaying) norm of the probability distribution. This potential is equivalent to a single, infinite barrier in quantum mechanics, and the potential here similarly imposes a Dirichlet boundary condition on the probability distribution, $\psi(0,t) = 0$. It's easiest to satisfy this boundary condition by the method of images, which states that if $\psi(x,t)$ solves the diffusion equation (2), then

$$\check{\psi}(x,t) := \psi(x,t) - \psi(-x,t) \tag{6}$$

solves the diffusion equation with a Dirichlet boundary condition at $x = 0$. With the solution (3), starting at $x_0 = d$ at $t_0 = 0$, we have

$$\check{\psi}(x,t) = \frac{1}{\sqrt{2\pi t}}\left(e^{-(x-d)^2/2t} - e^{-(x+d)^2/2t}\right) \tag{7}$$

as the probability density for Brownian walkers starting at $x = d$ with a perfect absorber at $x = 0$.

Integrate this density over $x \in [0,\infty)$ to obtain the survival probability (i.e., the probability to *not* cross the origin) with time, then compute the crossing probability with time. Noting that the crossing probability $P_{\text{cross}}(t)$—which refers to the probability that, up to time $t$, the walker has *ever* touched the origin—and the probability density $f_{\tau_\text{d}}(x)$ for the *first*-crossing time $\tau_\text{d}$ are related by

$$P_{\text{cross}}(t) = \int_0^t d\tau\, f_{\tau_\text{d}}(\tau), \tag{8}$$

compute the first-crossing density $f_{\tau_\text{d}}(\tau)$.

In your solutions, you should find (i.e., show) that:

- The crossing probability converges to 1 as $t \longrightarrow \infty$ (that is, the Brownian walker will, with *certainty*, eventually hit the origin).
- The long-time tail of the first-crossing density scales as $\tau^{-3/2}$. This turns out to be universal behavior that is (mostly) independent of the details of the random walk.

(c) Lord Kelvin used a setup similar to that of (b) to estimate the age of the Earth. First, the **heat-conduction equation** is the same as the diffusion equation (2), but with the replacement $t \longrightarrow 2\alpha t$,

$$\partial_t\psi = \alpha\partial_x^2\psi, \tag{9}$$

where $\alpha$ is the **thermal diffusivity**. Here, $\psi(x,t)$ represents the space- and time-dependent temperature profile of a thermally conductive medium. Kelvin's model of the Earth is that it started as a ball of uniform temperature, which then cooled with time due to radiation at the surface. To model this, assume that we are looking at a relatively shallow depth near Earth's surface, so we can treat Earth's surface as flat, and let $\psi(x,t)$ denote the temperature profile at depth $x > 0$. We will also assume constant diffusivity $\alpha$ with depth.

The initial condition is

$$\psi(x,0) = \psi_0, \tag{10}$$

where $\psi_0$ is a "core temperature," as compared to the surface temperature (we'll reinterpret $\psi_0$ shortly). The temperature profile is subject to the Dirichlet boundary condition

$$\psi(0,t) = 0, \tag{11}$$

representing cooling at the surface (i.e., thermal contact with outer space). Now show that the solution

$$\psi(x,t) = \frac{\psi_0}{\sqrt{4\pi\alpha t}} \int_0^\infty dx' \left( e^{-(x-x')^2/4\alpha t} - e^{-(x+x')^2/4\alpha t} \right) \tag{12}$$

satisfies the initial condition and the boundary condition. Carry out the integration, and compute the temperature gradient at the surface

$$G := \left.\frac{\partial \psi}{\partial x}\right|_{x=0}. \tag{13}$$

Solving for $t$, you should find

$$t = \frac{\psi_0^2}{\pi \alpha G^2}. \tag{14}$$

The Earth's temperature gradient and thermal diffusivity can both be measured. For $\psi_0$, this can be taken to be the melting point of the Earth's crust (note that, handily, no *distance* appears, so the temperature at the edge of the region where $\alpha$ is constant will work nicely here). Lord Kelvin, using the measurements available at the time, gave an estimate of $10^8$ years for the age of the Earth, which is not too bad compared to the current estimate of $4.5 \times 10^9$ years.

(d) An interesting problem related to the boundary-crossing problem is that of a Brownian particle escaping from an interval $[0, L]$ in $x$. And, because we need to set up perfect absorbers at $x = 0$ and $x = L$, it's just the same as the infinite square well!

In Problem 1 of Homework 5, you showed that, given a solution $\psi(x,t)$ to the free-particle problem, the image-laden version

$$\check{\psi}(x,t) := \sum_{j=-\infty}^{\infty} \Big[ \psi(x + 2jL, t) - \psi(2jL - x, t) \Big] \tag{15}$$

is a solution to the infinite square well on $x \in [0, L]$ (note that we're skipping the normalization factor now, because we *want* the solution to become unnormalized).

Adapt this solution to the case of a Brownian walker starting at $x_0 \in [0, L]$, and show that probability of (first) escaping the interval $[0, L]$ before time $t$ is

$$P_{\text{escape}}(t) = 1 - \sum_{j=-\infty}^{\infty} \left[ \text{erf}\left( \frac{x_0 - 2jL}{\sqrt{2t}} \right) - \text{erf}\left( \frac{x_0 - 2(j - 1/2)L}{\sqrt{2t}} \right) \right]. \tag{16}$$

Note that the terms here have the same form as in the crossing probability in part (b).

(e) The expression (16) is a bit complicated to read, but it is useful for obtaining the short-time escape behavior. Assume the centered initial condition $x_0 = L/2$, and then compute the probability density of first-escape times $f_{\text{escape}}(\tau)$, which is related to $P_{\text{escape}}(\tau)$ in the same way as in Eq. (8). At this point it should be clear that the short-time behavior is dominated by the $j = 0$ term, and thus given by

$$f_{\text{escape}}(\tau) \sim \frac{L}{\sqrt{2\pi\tau^3}}\, e^{-L^2/8\tau}. \tag{17}$$

Reconcile this solution with your result from part (b).

(f) Using the eigenstates of the infinite square well, we can even get an expression for the evolving probability density for the escaping ensemble of Brownian walkers in part (d). Using the quantum eigenfunctions

$$\psi_n(x) = \sqrt{\frac{2}{L}}\, \sin\frac{n\pi x}{L}, \tag{18}$$

recall that the time dependence is of the form $e^{-iE_n t/\hbar}$, where

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}. \tag{19}$$

With the imaginary-time replacements, we have

$$\frac{E_n}{\hbar} \longrightarrow \frac{n^2\pi^2}{2L^2}, \tag{20}$$

and a time-dependence factor of $e^{-iE_n t/\hbar} \longrightarrow e^{-n^2\pi^2 t/2L^2}$, or that is,

$$\psi_n(x,t) = \sqrt{\frac{2}{L}}\, \sin\!\left(\frac{n\pi x}{L}\right) e^{-n^2\pi^2 t/2L^2}. \tag{21}$$

Now starting with the initial condition

$$\psi(x,0) = \delta(x - x_0), \tag{22}$$

write this as a superposition of eigenstates to derive an expression for the decaying (unescaped) density $\psi(x,t)$. Use your result to derive the expression

$$P_{\text{escape}}(t) = 1 - \frac{2}{\pi}\sum_{n=1}^{\infty} \frac{[1 - (-1)^n]}{n}\, \sin\!\left(\frac{n\pi x_0}{L}\right) e^{-n^2\pi^2 t/2L^2} \tag{23}$$

as an alternative to Eq. (16).

(g) Equation (23) is not obviously equivalent to Eq. (16); but the latter is useful for short-time asymptotics, while the former is better for long-time behavior. In this case the long-time behavior is dominated by the term with the smallest (i.e., ground-state) eigenvalue. Thus compute the long-time tail of the probability distribution of first-escape times, and show that the long-time decay is exponential.

This is much faster than the power-law decay of part (b). Essentially, the slow decay of the tail in (b) is due to diffusive trajectories that wander far away from the boundary before crossing it. In part (f), these trajectories don't happen because of the presence of a boundary on either side of the starting point.

**Problem 2.** This problem is a follow-up to Problem 5 Homework 3, which asked you to think about what something like a half of a derivative could be defined. Here we'll work through an example of an important class of fractional derivatives—specifically, the fractional Laplacian operator.

The Laplacian operator $\triangle \equiv \nabla^2$ is diagonal in the momentum representation, owing to the expression

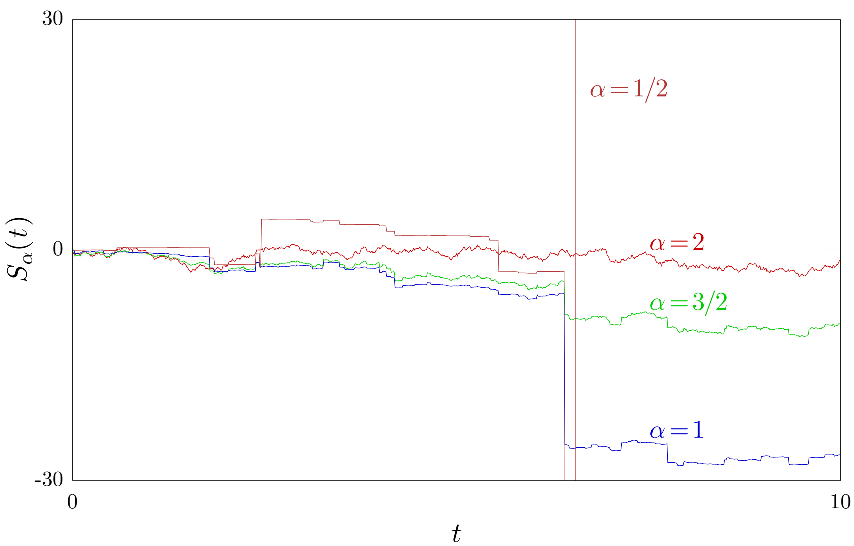
$$\triangle\, e^{i\mathbf{k}\cdot\mathbf{r}} = -k^2\, e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{24}$$

where $k = p/\hbar$. Then it is useful to define a fraction $\alpha/2$ of the Laplacian by

$$\frac{\partial^\alpha}{\partial|r|^\alpha}\, e^{i\mathbf{k}\cdot\mathbf{r}} \equiv -(-\triangle)^{\alpha/2}\, e^{i\mathbf{k}\cdot\mathbf{r}} := \left(-|k|^\alpha\right) e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{25}$$

for $\alpha \in (0,2]$. Note that this operator is defined in terms of a power of $-\triangle$ because it is positive definite. In this form, $\partial^\alpha/\partial|r|^\alpha$ is often called the **Riesz–Feller derivative**). The case $\alpha = 2$ recovers the standard Laplacian, and fractional derivatives outside this range can be defined by the recursion $\partial^{\alpha+2}/\partial|r|^{\alpha+2} = (\partial^\alpha/\partial|r|^\alpha)\triangle$.

So what good is it? Well, one can generalize quantum mechanics to "fractional quantum mechanics"[1] by changing $\nabla^2$ to $D_\alpha \partial^\alpha/\partial|r|^\alpha$ in the Schrödinger equation in the position representation ($D_\alpha$ is just a coefficient introduced to make the units work out). Unfortunately, it isn't clear if this generalization is at very useful. (Note, however, that the Hamiltonian for a relativistic particle may be written $\sqrt{p^2c^2 - m^2c^4}$, which in the massless limit has the form of the $\alpha = 1$ derivative.) The analogous replacement in the diffusion equation is an important generalization to model **anomalous diffusion**. Recalling that the position variance of a solution to the diffusion equation grows linearly with time, the solution to the fractional diffusion equation with the same initial condition but with $\alpha \in (0,2)$ would grow *more quickly* than $t$ (in fact the *slope* of $V_\mathbf{r}(t)$ grows without bound). In modeling the aggregate behavior of an ensemble of random walkers, roughly speaking, anomalous diffusion allows for the possibility of large steps, called **Lévy flights** or **extreme events**, with a power-law tail in the frequency distribution. Some example paths illustrating Lévy flights for different $\alpha$ are shown below (notice the jumps in the $\alpha < 2$ cases).




Anomalous diffusion models a wide range of phenomena from the dynamics of laser-cooled atoms to stock-market prices on short time scales to the foraging behavior of albatrosses. If you recall the colloquium from a couple of weeks ago, this fractional derivative also arises in "fractional electromagnetism" in cuprate semiconductors.[2]

[1] Nikolai Laskin, "Fractional quantum mechanics and Lévy path integrals," *Physics Letters A* **268**, 298 (2000) (doi: 10.1016/S0375-9601(00)00201-2); Nick Laskin, "Fractional Schrödinger equation," *Physical Review E* **66**, 056108 (2002) (doi: 10.1103/physreve.66.056108).

[2] Gabriele La Nave, Kridsanaphong Limtragool, and Philip W. Phillips "*Colloquium*: Fractional electromagnetism in quantum matter and high-energy physics," *Reviews of Modern Physics* **91**, 021003 (2019) (doi: 10.1103/RevModPhys.91.021003).

The goal of this problem is to use what you know about Fourier analysis to develop an expression for the fractional derivative—which turns out to be an integral! First, let's set up some Fourier basics. Suppose we assume a Fourier-transform convention

$$\tilde{f}(\mathbf{k}) = \frac{1}{(2\pi)^{d/2}} \int d^d r\, f(\mathbf{r})\, e^{-i\mathbf{k}\cdot\mathbf{r}}, \qquad f(\mathbf{r}) = \frac{1}{(2\pi)^{d/2}} \int d^d k\, \tilde{f}(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{26}$$

This is the usual convention in quantum mechanics, but setting $\hbar = 1$, and generalized to $d$ spatial dimensions. You have already proved the convolution theorem (in last week's homework), which in this convention reads

$$g(\mathbf{r}) := (f * K)(\mathbf{r}) := \int d^d r'\, K(\mathbf{r} - \mathbf{r}')\, f(\mathbf{r}') \qquad \Longleftrightarrow \qquad \tilde{g}(\mathbf{k}) = (2\pi)^{d/2} \tilde{K}(\mathbf{k})\, \tilde{f}(\mathbf{k}) \tag{27}$$

for some kernel $K(\mathbf{r})$.

Now the action of the fractional derivative on a general function $f(\mathbf{r})$ is given by completing the Fourier transform implicit in Eq. (25):

$$\frac{\partial^\alpha}{\partial |r|^\alpha} f(\mathbf{r}) := \frac{1}{(2\pi)^{d/2}} \int d^d k\, \tilde{f}(\mathbf{k})\, \frac{\partial^\alpha}{\partial |r|^\alpha} e^{i\mathbf{k}\cdot\mathbf{r}} = \frac{1}{(2\pi)^{d/2}} \int d^d k\, \left(-|k|^\alpha\right) \tilde{f}(\mathbf{k})\, e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{28}$$

The aim is now to employ the convolution theorem to invert the Fourier integral on the right-hand side.

(a) To proceed, we will need to find the Fourier counterpart to $|k|^\alpha$. However, directly approaching the inverse transform in $d$ dimensions is not so easy, because $|k|^\alpha$ doesn't factorize into different dimensions (unless $\alpha = 2$), and the integration in spherical coordinates is cumbersome beyond $d = 3$. Happily, there is a nice trick to do this; we will use the trick to work out the *forward* transform of $r^{-\gamma}$. First, let's start with the integral representation of the gamma function:

$$\Gamma(z) = \int_0^\infty ds\, s^{z-1}\, e^{-s}. \tag{29}$$

Change the integration variable to $s = r^2\lambda^2$, and then set $z = \gamma/2$ to obtain the integral formula

$$\frac{1}{r^\gamma} = \frac{2}{\Gamma(\gamma/2)} \int_0^\infty d\lambda\, \lambda^{\gamma-1}\, e^{-\lambda^2 r^2}. \tag{30}$$

(b) The point of the transformation is that the dependence on $\mathbf{r}$ is Gaussian on the right-hand side, and is thus a separable function in $d$ dimensions. Compute the Fourier transform of this formula to show that the Fourier transform of $r^{-\gamma}$ may be written

$$\frac{1}{(2\pi)^{d/2}} \int d^d r\, \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{r^\gamma} = \frac{2^{d/2-\gamma}\Gamma[(d-\gamma)/2]}{\Gamma(\gamma/2)}\, k^{\gamma-d}. \tag{31}$$

Then invert the transform and change variables in the exponents to show that the inverse transform of $k^\alpha$ is given by

$$\frac{2^{d/2+\alpha}\Gamma[(\alpha+d)/2]}{|\Gamma(-\alpha/2)|}\, \frac{1}{r^{\alpha+d}} = \frac{1}{(2\pi)^{d/2}} \int d^d k\, k^\alpha\, e^{-i\mathbf{k}\cdot\mathbf{r}}. \tag{32}$$

What is the range of $\alpha$ for which this derivation is valid?

(c) Finally, apply the convolution theorem (28) to Eq. (28) to obtain the integral expression

$$\frac{\partial^\alpha}{\partial |r|^\alpha} f(\mathbf{r}) = -\frac{2^\alpha\Gamma[(\alpha+d)/2]}{\pi^{d/2}|\Gamma(-\alpha/2)|} \int d^d r'\, \frac{f(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^{\alpha+d}} \tag{33}$$

for the fractional Laplacian. (Note the modulus on $\Gamma(-\alpha/2)$, in order to extend the expression to positive $\alpha$.)

The integral here is divergent for the parameters of interest, $\alpha \in (0,2)$ and $d \geq 1$. The integral is commonly regularized as

$$\frac{\partial^\alpha}{\partial |r|^\alpha} f(\mathbf{r}) = -\frac{2^\alpha \Gamma[(\alpha+d)/2]}{\pi^{d/2}|\Gamma(-\alpha/2)|} \int d^d r' \, \frac{f(\mathbf{r}') - f(\mathbf{r})}{|\mathbf{r}-\mathbf{r}'|^{\alpha+d}}, \tag{34}$$

which is the **Hadamard finite part** of the original integral.

Equation (34) is the main result: The thing to notice here is that the fractional Laplacian is a *nonlocal* operator (convolution with a power-law-tailed function)—unless $\alpha$ is an even integer, in which case it's quite local, in the sense that $\nabla^2 f(\mathbf{r})$ only depends on $f$ at points arbitrarily close to $\mathbf{r}$. This makes the fractional Laplacian tricky to handle, and a number of erroneous results have appeared in the literature, especially regarding how the fractional Laplacian works with Dirichlet boundary conditions (i.e., the infinite square well in fractional quantum mechanics).