Partial differential equations. II
Physics 366
Lecture 23b–24

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1. INTRODUCTION

We are going to look at general solutions of the one-dimensional Schrödinger equation and the one-dimensional diffusion equation in terms of complete sets of eigenfunctions. The techniques illustrate how to solve such equations generally (i) by separation of variables, (ii) in terms of eigenfunctions, (iii) in terms of initial conditions, and (iv) in terms of a Green function.

2. ONE-DIMENSIONAL SCHRÖDINGER EQUATION WITH HARD BOUNDARIES

The Schrödinger equation for the wave function of a particle moving in one spatial dimension is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}+V(x)\psi(x,t)=i\hbar\frac{\partial\psi(x,t)}{\partial t}\ . \tag{2.1}$$

Let's consider the situation where the particle is moving freely within a "box" from which it cannot escape; this corresponds to a potential energy

$$V(x)=\begin{cases}0\ , & \text{for } 0<x<L,\\ \infty\ , & \text{for } x<0 \text{ or } x>L.\end{cases} \tag{2.2}$$

The result is the free-particle Schrödinger equation for $0<x<L$,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2}=i\hbar\frac{\partial\psi(x,t)}{\partial t}\ , \tag{2.3}$$

with the boundary conditions that the wave function vanishes at $x=0$ and $x=L$,

$$0=\psi(0,t)=\psi(L,t)\ . \tag{2.4}$$

We can solve the Schrödinger equation (2.3) by Fourier transforming:

$$\psi(x,t)=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\,\tilde\psi(x,\omega)e^{-i\omega t}\ ,\qquad \tilde\psi(x,\omega)=\int_0^L dt\,\psi(x,t)e^{i\omega t}\ . \tag{2.5}$$

The Fourier transform $\tilde\psi(x,\omega)$ satisfies the ordinary differential equation (remember the rule $\partial/\partial t\to -i\omega$),

$$-\frac{\hbar^2}{2m}\frac{d^2\tilde\psi(x,\omega)}{dx^2}=\hbar\omega\tilde\psi(x,\omega)\qquad\Longleftrightarrow\qquad \frac{d^2\tilde\psi(x,\omega)}{dx^2}+k^2\tilde\psi(x,\omega)=0\ ,\quad k^2=\frac{2m\omega}{\hbar}\ . \tag{2.6}$$

The solutions that meet the boundary conditions are

$$\tilde\psi(x,\omega_n)=a_n\sin(k_nx)\ ,\qquad \omega_n=\frac{\hbar k_n^2}{2m}\ ,\quad k_n=\frac{n\pi}{L}\ ,\quad n=1,2,\dots\ . \tag{2.7}$$

The general solution for $\tilde{\psi}(x,\omega)$ is the sum of all the possible solutions:

$$\tilde{\psi}(x,\omega) = \sum_{n=1}^{\infty} \tilde{\psi}(x,\omega_n) 2\pi\delta(\omega-\omega_n) = \sum_{n=1}^{\infty} 2\pi a_n \sin(k_n x)\delta(\omega-\omega_n) \; . \tag{2.8}$$

The corresponding general solution for $\psi(x,t)$ is

$$\psi(x,t) = \sum_{n=1}^{\infty} a_n \sin(k_n x) e^{-i\omega_n t} \; . \tag{2.9}$$

The spatial solutions $\sin(k_n x)$ are called the *stationary states* or *energy eigenstates*. Stationary states oscillate with a characteristic angular frequency $\omega_n = E_n/\hbar$, where E_n is the energy eigenvalue. The general solution for the wave function is a sum of products of the stationary-state wave functions, which depend on position, and the harmonic temporal oscillations at the eigenfrequencies.

The harmonic functions $\sin(k_n x)$ satisfy an orthogonality relation:

$$\begin{aligned}
\int_0^L dx \, \sin(k_n x)\sin(k_m x) &= \frac{1}{2}\int_0^L dx \, \cos[(k_n - k_m)x] - \frac{1}{2}\int_0^L dx \, \cos[(k_n + k_m)x] \\
&= \frac{1}{2}\underbrace{\frac{\sin[(n-m)\pi x/L]}{(n-m)\pi/L}\bigg|_{x=0}^{x=L}}_{=L\delta_{nm}} - \frac{1}{2}\underbrace{\frac{\sin[(n+m)\pi x/L]}{(n+m)\pi/L}\bigg|_{x=0}^{x=L}}_{=0} \\
&= \frac{L}{2}\delta_{nm} \; .
\end{aligned} \tag{2.10}$$

This allows us to invert the general solution (2.9) to find the expansion coefficients a_n:

$$a_n e^{-i\omega_n t} = \frac{2}{L}\int_0^L dx \, \sin(k_n x)\psi(x,t) \; . \tag{2.11}$$

We can find the expansion coefficients in terms of the initial ($t = 0$) wave function,

$$a_n = \frac{2}{L}\int_0^L dx \, \sin(k_n x)\psi(x,0) \; , \tag{2.12}$$

and if we plug this expression back into the general solution (2.9), we get

$$\psi(x,t) = \int_0^L dx' \, \psi(x',0) \underbrace{\frac{2}{L}\sum_{n=1}^{\infty} e^{-i\omega_n t}\sin(k_n x)\sin(k_n x')}_{=G(x,t;x',0)} \; . \tag{2.13}$$

Here $G(x,t;x',0)$ is the Green function or *propagator*; it allows us to express the wave function at time t in terms of the initial wave function. When $t = 0$, the Green function becomes the δ-function (at least it is so for x and x' in the interval $[0,L]$):

$$G(x,0;x',0) = \frac{2}{L}\sum_{n=1}^{\infty}\sin(k_n x)\sin(k_n x') = \delta(x-x') \; . \tag{2.14}$$

Now we're going to use what we've done up till now to call attention to a number of general points. We used the temporal Fourier transform to solve this problem because the quantum mechanics of isolated systems, like this single particle in a box, informs us that the general solution is a sum of products of spatial stationary states and temporal oscillations. If we didn't know anything about Fourier series or Fourier transforms, we would approach solving the Schrödinger equation (2.3) by using the technique of *separation of variables*, i.e., by looking for product solutions

$$\psi(x,t) = X(x)T(t) \; . \tag{2.15}$$

Plugging this assumption into the Schrödinger equation and dividing by XT, we get

$$-\frac{1}{X}\frac{d^2X}{dx^2} = i\frac{2m}{\hbar}\frac{1}{T}\frac{dT}{dt} = k^2 \; . \tag{2.16}$$

The left side of this equation is a function of x, and the right side is a function of t, so the only way the equation can be satisfied is if both sides are equal to the same constant, k^2, as indicated. The result is a pair of ordinary differential equations for $X(x)$ and $T(t)$,

$$\begin{aligned} \frac{d^2X}{dx^2} &= -k^2X \; , \\ \frac{dT}{dt} &= -i\omega T \; , \quad \omega = \frac{\hbar k^2}{2m} \; . \end{aligned} \tag{2.17}$$

The solution for $T(t)$ is a complex exponential $T(t) = T(0)e^{-i\omega t}$. In quantum-mechanical problems, we know from experience that there are product solutions with complex-exponential time dependence, so we typically start off by assuming that. The Fourier-transform method we used above is really the assumption that the general solution is a superposition of product solutions, each of which has a complex-exponential time dependence.

What we are left with is to find the solutions of the spatial equation. The solutions are called *stationary states* because the corresponding time dependence is the complex exponential, whose absolute square is always one, meaning that quantum probabilities don't change when the system is in a stationary state. They are also called *energy eigenstates* because the spatial equation can be regarded as an eigenvalue problem for a Hermitian operator, with the eigenvalues determining the allowed values of the energy.

In the case we are doing here, the equation for the stationary states is

$$\frac{d^2X}{dx^2} = -k^2X \; . \tag{2.18}$$

This is an eigenvalue problem for a Hermitian operator because the second-derivative operator, $H = d^2/dx^2$, is a Hermitian operator relative to the standard inner product for functions defined on the domain $[0, L]$ with the boundary condition that the functions vanish at $x = 0$ and $x = L$. The inner product is

$$(f, g) = \langle f|g\rangle = \int_0^L dx\, f^*(x)g(x) \; . \tag{2.19}$$

Recall that the way to go from a ket to the corresponding function is $f(x) = \langle x|f\rangle$; the function is called the position representation of the function.

To say that H is Hermitian means that $\langle f|H|g\rangle = (f, Hg) = (Hf, g) = \langle g|H|f\rangle^*$ for all functions f and g that satisfy the boundary conditions. We can easily show this by integrating twice by parts:

$$\begin{aligned} (f, Hg) &= \int_0^L dx\, f^*(x)\frac{d^2g(x)}{dx^2} \\ &= f^*(x)\frac{dg(x)}{dx}\bigg|_{x=0}^{x=L} - \int_0^L dx\, \frac{df^*(x)}{dx}\frac{dg(x)}{dx} \\ &= \left(f^*(x)\frac{dg(x)}{dx} - \frac{df^*(x)}{dx}g(x)\right)\bigg|_{x=0}^{x=L} + \int_0^L dx\, \frac{d^2f^*(x)}{dx^2}g(x) \\ &= \left(f^*(x)\frac{dg(x)}{dx} - \frac{df^*(x)}{dx}g(x)\right)\bigg|_{x=0}^{x=L} + (Hf, g) \; . \end{aligned} \tag{2.20}$$

For the boundary condition that the functions vanish at the endpoints, the boundary terms vanish, and we have the $H = d^2/dx^2$ is a Hermitian operator. It is easy to see that we could also use the boundary condition that the first derivative vanishes at the endpoints, and we will use that boundary condition when we study the diffusion equation below.

That H is Hermitian means that it has a complete set of orthonormal eigenstates, which we found above:

$$\begin{aligned}
\frac{d^2X_n(x)}{dx^2} &= -k_n^2 X_n(x)\ , \quad X_n(0) = X_n(L) = 0 \\
H|X_n\rangle &= -k_n^2|X_n\rangle\ , \quad \langle x=0|X_n\rangle = \langle x=L|X_n\rangle = 0 \\
\Longrightarrow \qquad X_n(x) &= \langle x|X_n\rangle = \sqrt{\frac{2}{L}}\sin(k_n x)\ , \quad k_n = \frac{n\pi}{L}\ , \quad n = 1, 2, \dots\ .
\end{aligned} \tag{2.21}$$

The eigenvalues k_n^2 give the allowed energies:

$$E_n = \hbar\omega_n = \frac{\hbar^2 k_n^2}{2m} = \frac{1}{2m}\left(\frac{n\pi\hbar}{L}\right)^2\ , \quad n = 1, 2, \dots\ . \tag{2.22}$$

We have chosen the stationary states to be normalized, and they are orthogonal:

$$\langle X_n|X_m\rangle = \int_0^L dx\, X_n^*(x)X_m(x) = \frac{2}{L}\int_0^L dx\, \sin(k_n x)\sin(k_m x) = \delta_{nm}\ . \tag{2.23}$$

Any wave function can be expanded in terms of these orthonormal eigenstates:

$$\begin{aligned}
\psi(x) &= \sum_{n=1}^{\infty} c_n X_n(x) = \sqrt{\frac{2}{L}}\sum_{n=1}^{\infty} c_n \sin(k_n x) &\Longleftrightarrow\qquad |\psi\rangle &= \sum_{n=1}^{\infty} c_n|X_n\rangle\ , \\
c_n &= \int_0^L dx\, X_n^*(x)\psi(x) = \sqrt{\frac{2}{L}}\int_0^L dx\, \sin(k_n x)\psi(x) &\Longleftrightarrow\qquad c_n &= \langle X_n|\psi\rangle\ .
\end{aligned} \tag{2.24}$$

The expansions in Eq. (2.24) are a species of Fourier series, but different from the Fourier series that we considered previously. In our previous considerations, the Fourier series were defined for functions on a domain of length L, just as here, but they used *periodic boundary conditions*. Periodic boundary conditions mean that the functions are periodic on the interval of length L; in the terms of our discussion of Hermiticity in Eq. (2.20), this implies that a function and its first derivative have the same value at the two endpoints. For the Fourier series that arise naturally here, where we require that the functions vanish at the endpoints, the Fourier functions are all sine functions—this is thus called a *Fourier sine series*—but we have, in some sense, twice as many wave numbers as for periodic boundary conditions, and this makes up for the absence of cosine functions in the Fourier series. It pays not to get too addicted to a particular kind of Fourier series, because different problems lead to different kinds of Fourier series.

The time evolution of the wave function can now be written as

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n X_n(x)e^{-i\omega_n t} = \sqrt{\frac{2}{L}}\sum_{n=1}^{\infty} c_n \sin(k_n x)e^{-i\omega_n t} \qquad\Longleftrightarrow\qquad |\psi(t)\rangle = \sum_{n=1}^{\infty} c_n|X_n\rangle e^{-i\omega_n t}\ . \tag{2.25}$$

If we plug the Fourier coefficients of Eq. (2.24), evaluated using the initial wave function, back into these expansions, we recover Eq. (2.13):

$$\psi(x,t) = \int_0^L dx'\, \psi(x',0)\, \underbrace{\frac{2}{L}\sum_{n=1}^{\infty} e^{-i\omega_n t}\sin(k_n x)\sin(k_n x')}_{=\,G(x,t;x',0)} \qquad\Longleftrightarrow\qquad |\psi(t)\rangle = \underbrace{\sum_{n=1}^{\infty} e^{-i\omega_n t}|X_n\rangle\langle X_n|}_{=\,U(t,0))}\psi(0)\rangle\ . \tag{2.26}$$

Table 1. One-dimensional Schrödinger equation for a free particle in a box

1. *Wave function*: $\psi(x,t) = \langle x|\psi(t)\rangle \ , \quad 0 < x < L$

2. *Schrödinger equation*: $i\hbar\dfrac{\partial\psi(x,t)}{\partial t} = -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\psi(x,t)}{\partial x^2} \iff i\hbar\dfrac{d|\psi(t)\rangle}{dt} = -\dfrac{\hbar^2}{2m}H|\psi(t)\rangle$

3. *Boundary conditions*: $\psi(0,t) = \psi(L,t) = 0$

4. *General solution*: $\psi(x,t) = \displaystyle\sum_{n=1}^{\infty} c_n X_n(x) e^{-i\omega_n t} \iff |\psi(t)\rangle = \sum_{n=1}^{\infty} c_n e^{-i\omega_n t}|X_n\rangle$

5. *Stationary states*: $\dfrac{d^2X_n(x)}{dx^2} = -k_n^2 X_n(x) \iff H|X_n\rangle = -k_n^2|X_n\rangle$

$$X_n(0) = X_n(L) = 0$$

$$k_n = \frac{n\pi}{L} \ , \quad E_n = \hbar\omega_n = \frac{\hbar^2 k_n^2}{2m}$$

$$X_n(x) = \sqrt{\frac{2}{L}}\sin(k_n x)$$

6. *Orthonormality*: $\delta_{nm} = \displaystyle\int_0^L dx\, X_n^*(x) X_m(x) \iff \delta_{nm} = \langle X_n|X_m\rangle$

7. *Completeness*: $\underbrace{\delta(x-x')}_{=\langle x|x'\rangle} = \displaystyle\sum_{n=1}^{\infty} X_n(x) X_n^*(x') \iff I = \sum_{n=1}^{\infty} |X_n\rangle\langle X_n|$

8. *Fourier coefficients*: $c_n = \displaystyle\int_0^L dx\, X_n^*(x)\psi(x,0) \iff c_n = \langle X_n|\psi(0)\rangle$

9. *Green function*: $\underbrace{G(x,t;x',0)}_{=\langle x|U(t,0)|x'\rangle} = \displaystyle\sum_{n=1}^{\infty} e^{-i\omega_n t} X_n(x) X_n^*(x') \iff U(t,0) = \sum_{n=1}^{\infty} e^{-i\omega_n t}|X_n\rangle\langle X_n|$

$$i\hbar\frac{\partial G(x,t;x',t')}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 G(x,t;x',t')}{\partial x^2} \iff i\hbar\frac{dU(t,0)}{dt} = -\frac{\hbar^2}{2m}HU(t,0)$$

$$G(x,0;x',0) = \delta(x-x') \iff U(0,0) = I$$

$$\psi(x,t) = \int_0^L dx'\, G(x,t;x',0)\psi(x',0) \iff |\psi(t)\rangle = U(t,0)|\psi(0)\rangle$$

Here $U(t,0)$ is the unitary evolution operator; its position representation, $G(x,t;x',t') = \langle x|U(t,0)|x'\rangle$, is the temporal Green function or propagator. These two satisfy the differential equations

$$\begin{gathered} i\hbar\frac{\partial G(x,t;x',t')}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 G(x,t;x',t')}{\partial x^2} \ , \quad G(x,0;x',0) = \delta(x-x') \ , \\ \iff \qquad i\hbar\frac{dU(t,0)}{dt} = -\frac{\hbar^2}{2m}HU(t,0) \ , \quad U(0,0) = I \ . \end{gathered} \tag{2.27}$$

The initial condition for the Green function is the completeness property of the stationary states:

$$\langle x|x'\rangle = \delta(x-x') = G(x,t;x',0) = \sum_{n=1}^{\infty} X_n(x) X_n^*(x') \qquad \iff \qquad I = U(0,0) = \sum_{n=1}^{\infty} |X_n\rangle\langle X_n| \ . \tag{2.28}$$

Table 1 summarizes the solution of the one-dimensional Schrödinger equation for a free particle in a box.

3. ONE-DIMENSIONAL DIFFUSION EQUATION WITH HARD BOUNDARIES

We now shift gears to consider the diffusion equation,

$$\frac{\partial^2 f}{\partial x^2} = \frac{1}{\alpha^2}\frac{\partial f}{\partial t} , \tag{3.1}$$

which resembles the Schrödinger equation, except that factor in front of the temporal derivative is real. We are going to consider the diffusion equation on the interval $0 < x < L$. Recall that the diffusion equation describes the flow of some quantity, e.g., concentration of some chemical or internal energy, under the influence of a gradient in that quantity. Let's assume that the quantity can't flow into the boundaries—the chemical is stuck in a flask, or the boundaries are thermal insulators—so the appropriate boundary conditions are that $\partial f/\partial x$ vanishes at the endpoints:

$$0 = \left.\frac{\partial f(x,t)}{\partial x}\right|_{x=0} = \left.\frac{\partial f(x,t)}{\partial x}\right|_{x=L} . \tag{3.2}$$

We expect the solutions of the diffusion equation to describe decay of derivatives to a final state where f is a constant. In particular, we do not expect the solutions to oscillate in time; this means that the Fourier transform is not an ideal tool for handling the diffusion equation (we could use the Fourier transform's first cousin, the Laplace transform, but won't do that here). Instead, we use the technique of separation of variables to inform us of the appropriate spatial and temporal dependences. Thus we begin by looking for solutions of the form

$$f(x,t) = X(x)T(t) . \tag{3.3}$$

Plugging this assumption into the diffusion equation and dividing by XT, we get

$$\frac{1}{X}\frac{d^2X}{dx^2} = \frac{1}{\alpha^2}\frac{1}{T}\frac{dT}{dt} = -k^2 . \tag{3.4}$$

The left side of this equation is a function of x, and the right side is a function of t, so the only way the equation can be satisfied is if both sides are equal to the same constant, $-k^2$, chosen here to be negative so that we get oscillatory solutions in x and exponentially decaying solutions in t. The result is a pair of ordinary differential equations for $X(x)$ and $T(t)$,

$$\begin{aligned} \frac{d^2X}{dx^2} &= -k^2 X , \\ \frac{dT}{dt} &= -\lambda T , \quad \lambda = \alpha^2 k^2 . \end{aligned} \tag{3.5}$$

The solution for $T(t)$ is a decaying exponential $T(t) = T(0)e^{-\lambda t}$.

What we are left with is to find the solutions of the spatial equation, which is identical to that for the Schrödinger equation, but with different boundary conditions, which change the allowed solutions from sines to cosines:

$$\begin{aligned} &\frac{d^2X_n(x)}{dx^2} = -k_n^2 X_n(x) , \quad \left.\frac{dX_n}{dx}\right|_{x=0} = \left.\frac{dX_n}{dx}\right|_{x=L} = 0 \\ &\Longrightarrow \qquad X_n(x) = \langle x|X_n\rangle = \sqrt{\frac{2-\delta_{n0}}{L}}\cos(k_n x) , \quad k_n = \frac{n\pi}{L} , \quad n = 0,1,2,\ldots . \end{aligned} \tag{3.6}$$

The boundary conditions are such as to make $H = d^2/dx^2$ a Hermitian operator, so the solutions are a complete, orthonormal set (the $-\delta_{n0}$ in the numerator of the square root is just a trick to make the $n = 0$ eigenfunction normalized without having to write it out as a separate case):

$$\langle X_n|X_m\rangle = \int_0^L dx\, X_n^*(x)X_m(x) = \frac{\sqrt{2-\delta_{n0}}\sqrt{2-\delta_{m0}}}{L}\int_0^L dx\, \cos(k_n x)\cos(k_m x) = \delta_{nm} . \tag{3.7}$$

The eigenvalues k_n^2 give the decay times for the modes:

$$\lambda_n = \alpha^2 k_n^2 = \left(\frac{n\pi\alpha}{L}\right)^2 , \quad n = 0,1,2,\ldots . \tag{3.8}$$

Table 2. One-dimensional diffusion equation with impenetrable boundaries

1. *Function*:	$f(x,t)=\langle x\|f(t)\rangle\ ,\quad 0<x<L$		
2. *Diffusion equation*:	$\frac{1}{\alpha^2}\frac{\partial f(x,t)}{\partial t}=\frac{\partial^2 f(x,t)}{\partial x^2}$	$\Longleftrightarrow$	$\frac{1}{\alpha^2}\frac{d\|f(t)\rangle}{dt}=H\|f(t)\rangle$
3. *Boundary conditions*:	$\left.\frac{\partial f(x,t)}{\partial x}\right\|_{x=0}=\left.\frac{\partial f(x,t)}{\partial x}\right\|_{x=L}=0$		
4. *General solution*:	$f(x,t)=\sum_{n=0}^{\infty}c_n X_n(x)e^{-\lambda_n t}$	$\Longleftrightarrow$	$\|f(t)\rangle=\sum_{n=0}^{\infty}c_n e^{-\lambda_n t}\|X_n\rangle$
5. *Spatial eigenfunctions*:	$\frac{d^2X_n(x)}{dx^2}=-k_n^2X_n(x)$	$\Longleftrightarrow$	$H\|X_n\rangle=-k_n^2\|X_n\rangle$
	$\left.\frac{dX_n(x)}{dx}\right\|_{x=0}=\left.\frac{dX_n(x)}{dx}\right\|_{x=L}=0$		
	$k_n=\frac{n\pi}{L}\ ,\quad \lambda_n=\alpha^2k_n^2$		
	$X_n(x)=\sqrt{\frac{2-\delta_{n0}}{L}}\cos(k_nx)$		
6. *Orthonormality*:	$\delta_{nm}=\int_0^L dx\, X_n^*(x)X_m(x)$	$\Longleftrightarrow$	$\delta_{nm}=\langle X_n\|X_m\rangle$
7. *Completeness*:	$\underbrace{\delta(x-x')}_{=\langle x\|x'\rangle}=\sum_{n=0}^{\infty}X_n(x)X_n^*(x')$	$\Longleftrightarrow$	$I=\sum_{n=0}^{\infty}\|X_n\rangle\langle X_n\|$
8. *Fourier coefficients*:	$c_n=\int_0^L dx\, X_n^*(x)\psi(x,0)$	$\Longleftrightarrow$	$c_n=\langle X_n\|\psi(0)\rangle$
9. *Green function*:	$\underbrace{G(x,t;x',0)}_{=\langle x\|K(t,0)\|x'\rangle}=\sum_{n=0}^{\infty}e^{-\lambda_n t}X_n(x)X_n^*(x')$	$\Longleftrightarrow$	$K(t,0)=\sum_{n=0}^{\infty}e^{-\lambda_n t}\|X_n\rangle\langle X_n\|$
	$\frac{1}{\alpha^2}\frac{\partial G(x,t;x',t')}{\partial t}=\frac{\partial^2 G(x,t;x',t')}{\partial x^2}$	$\Longleftrightarrow$	$\frac{1}{\alpha^2}\frac{dK(t,0)}{dt}=HK(t,0)$
	$G(x,0;x',0)=\delta(x-x')$	$\Longleftrightarrow$	$K(0,0)=I$
	$f(x,t)=\int_0^L dx'\, G(x,t;x',0)f(x',0)$	$\Longleftrightarrow$	$\|f(t)\rangle=K(t,0)\|f(0)\rangle$

The general time evolution of $f(x,t)$ can now be written as

$$f(x,t)=\sum_{n=1}^{\infty}c_nX_n(x)e^{-\lambda_n t}=\sqrt{\frac{1}{L}}\,c_0+\sqrt{\frac{2}{L}}\sum_{n=1}^{\infty}c_n\cos(k_nx)e^{-\lambda_n t}\ . \tag{3.9}$$

It should be clear that we are dealing here with yet another kind of Fourier series, called a *Fourier cosine series*, which is suited to the boundary conditions where the first derivative of functions vanishes at the endpoints. At late times the solution always approaches $c_0/\sqrt{L}$; notice that since the quantities we are dealing with must be positive, c_0 cannot be zero.

We summarize the remaining properties of solutions of the diffusion equation in Table 2. In contrast to the Schr̈dinger equation, the evolution operator is not unitary (it is Hermitian); it is denoted $K(t,0)$ and is called the *kernel*.

There is another thing we can do with the diffusion equation, and that is to add a source $s(x,t)$:

$$\frac{1}{\alpha^2}\frac{\partial f}{\partial t} - \frac{\partial^2 f}{\partial x^2} = s \ , \tag{3.10}$$

When $s(x,t)$ is positive, it describes the appearance of the quantity of interest at the position x and the time t, and when $s(x,t)$ is negative, it describes the corresponding disappearance.

It is useful to consider a source that is at a particle point x' in space and blinks on only for an instant at time t'; the solution for this source is the Green function since the source creates an initial condition immediately after t' for which the Green function is the solution. By integrating, we can then find the solution for any source. This way of getting the solution for the equation with source from the Green function for the equation with initial conditions is a standard one.

What we are proposing is that the following is the solution of the diffusion equation with source:

$$f(x,t) = \alpha^2 \int_{-\infty}^{t} dt' \int_0^L dx'\, G(x,t;x',t')s(x',t') = \alpha^2 \int_{-\infty}^{\infty} dt' \int_0^L dx'\, H(t-t')G(x,t;x',t')s(x',t') \tag{3.11}$$

In the first form we say that a source that blinks on at position x' and time t' creates an initial condition immediately after t', for which the Green function $G(x,t;x',t')$ is the solution at position x and time t; because the diffusion equation is linear, we get the full solution by integrating over all the different possible blinking sources at positions x' and at times t' before the time t we are interested in. The only real question in proposing this solution is what constant factor to put in front of $s(x',t')$ (this amounts to saying what initial condition the blinking source creates x' just after t'); not surprisingly, I have chosen the right constant. The second form in Eq. (3.11) extends the temporal integral to $+\infty$, but includes the unit (Heaviside) step function $H(t-t')$ so that sources at $t' > t$ do not contribute.

We proceed by showing that $H(t-t')G(x,t;x',t')$ satisfies the equation for a δ source:

$$\begin{aligned}
&\frac{1}{\alpha^2}\frac{\partial H(t-t')G(x,t;x',t')}{\partial t} - \frac{\partial^2 H(t-t')G(x,t;x',t')}{\partial x^2} \\
&\quad = \frac{1}{\alpha^2}\underbrace{\frac{dH(t-t')}{dt}}_{=\delta(t-t')} G(x,t;x',t') - H(t-t')\underbrace{\left(\frac{1}{\alpha^2}\frac{\partial G(x,t;x',t')}{\partial t} - \frac{\partial^2 G(x,t;x',t')}{\partial x^2}\right)}_{=0 \ \text{ for } t>t'} \\
&\quad = \frac{1}{\alpha^2}\delta(t-t')\underbrace{G(x,t;x',t)}_{=\delta(x-x')} \\
&\quad = \frac{1}{\alpha^2}\delta(t-t')\delta(x-x') \ .
\end{aligned} \tag{3.12}$$

Here we use the fact that the derivative of the unit step function is the δ-function, and we use

$$G(x,t;x',t') = \sum_{n=0}^{\infty} e^{-\lambda_n(t-t')}X_n(x)X_n^*(x') \qquad \Longrightarrow \qquad G(x,t;x',t) = \sum_{n=0}^{\infty} X_n(x)X_n^*(x') = \delta(x-x') \ . \tag{3.13}$$

In addition, we use the fact that $G(x,t;x',t')$ satisfies the diffusion equation without source for $t > t'$.

Now it is easy to show that the proposed solution (3.11) satisfies the diffusion equation with source,

$$\begin{aligned}
\frac{1}{\alpha^2}\frac{\partial f(x,t)}{\partial t} - \frac{\partial^2 f(x,t)}{\partial x^2} &= \alpha^2 \int_{-\infty}^{\infty} dt' \int_0^L dx' \underbrace{\left(\frac{1}{\alpha^2}\frac{\partial H(t-t')G(x,t;x',t')}{\partial t} - \frac{\partial^2 H(t-t')G(x,t;x',t')}{\partial x^2}\right)}_{=\frac{1}{\alpha^2}\delta(x-x')\delta(t-t')} s(x',t') \\
&= s(x,t) \ .
\end{aligned} \tag{3.14}$$

If you don't like the use of the step function, you can work directly with the first form in Eq. (3.11). The time derivative on the diffusion equation acts in two ways, first on the upper limit of the temporal integral by evaluating the integrand at $t' = t$ and second on the Green function itself. The result is

$$\begin{aligned}
\frac{1}{\alpha^2}\frac{\partial f(x,t)}{\partial t} - \frac{\partial^2 f(x,t)}{\partial x^2} &= \int_0^L dx' \, \underbrace{G(x,t;x',t)}_{=\delta(x-x')} s(x',t) \\
&\quad + \alpha^2 \int_{-\infty}^{t} dt' \int_0^L dx' \underbrace{\left(\frac{1}{\alpha^2}\frac{\partial G(x,t;x',t')}{\partial t} - \frac{\partial^2 G(x,t;x',t')}{\partial x^2}\right)}_{=0 \text{ for } t>t'} s(x',t') \\
&= s(x,t) \ .
\end{aligned} \tag{3.15}$$