Fundamental solution of the heat equation

For the heat equation:

$$u_t = ku_{xx}$$

on the whole line, we derived the "fundamental solution"

$$S(x,t) = \frac{1}{\sqrt{4\pi kt}} e^{-\frac{x^2}{4kt}}$$

by exploiting various symmetries of the equation. We then obtained the solution to the initial-value problem

$$u_t = ku_{xx} \qquad u(x,0) = \varphi(x)$$

as a "convolution" with the fundamental solution:

$$u(x,t) = \frac{1}{\sqrt{4\pi kt}} \int_{-\infty}^{\infty} e^{-\frac{(x-y)^2}{4kt}} \varphi(y)\, dy \tag{$*$}$$

The presence of the factors of t in the denominator of the fraction in front of the integral sign and in the fraction in the exponent under the integral sign begs the question: *In what sense are the initial conditions satisfied by this solution*?

We will explore this question by considering the limiting behavior of $(*)$ as t approaches zero from above (the solution is not defined for $t < 0$ because of the factor of $\sqrt{t}$). The limit is somewhat delicate to justify, so you'll have to bear with me through a somewhat complicated process. Here is what we are going to prove:

Theorem. *If $\varphi(x)$ is a bounded, continuous function, then*

$$u(x,t) = \frac{1}{\sqrt{4\pi kt}} \int_{-\infty}^{\infty} e^{-\frac{(x-y)^2}{4kt}} \varphi(y)\, dy$$

satisfies the heat equation $u_t = ku_{xx}$ for $t > 0$ and all $x \in \mathbb{R}$. Moreover,

$$\lim_{t\to 0+} u(x,t) = \varphi(x)$$

for all $x \in \mathbb{R}$.

The first step is to make what by now has become the standard change of variables in the integral: Let

$$p = \frac{x-y}{\sqrt{4kt}} \quad \text{so that} \quad dp = -\frac{dy}{\sqrt{4kt}}$$

Then $(*)$ becomes

$$u(x,t) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-p^2} \varphi(x - \sqrt{4kt}\, p)\, dp. \tag{$**$}$$

At this point, we might be tempted to declare victory — for a fixed value of x, if we put $t = 0$ in this last integral, we could then factor the $\varphi(x)$ out of the integral and write:

$$\begin{aligned}\lim_{t\to 0+} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-p^2} \varphi(x - \sqrt{4kt}\,p)\,dp &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-p^2} \lim_{t\to 0+} \varphi(x - \sqrt{4kt}\,p)\,dp \qquad \text{(Wrong!)} \\ &= \frac{1}{\sqrt{\pi}} \varphi(x) \int_{-\infty}^{\infty} e^{-p^2}\,dp = \varphi(x)\end{aligned}$$

but interchanging a limit and an (improper!) integral can be a tricky business.

Aside: For the record, here's a simple example where it doesn't work:

Let

$$f(s,y) = \begin{cases} 1 & \text{if } s < y < s+1 \\ 0 & \text{otherwise} \end{cases}$$

and consider

$$\lim_{s\to\infty} \int_0^{\infty} f(s,y)\,dy \qquad \text{and} \qquad \int_0^{\infty} \lim_{s\to\infty} f(s,y)\,dy.$$

Since

$$\int_0^{\infty} f(s,y)\,dy = 1$$

for any positive value of s (for a fixed positive value of s, the integral picks up the area of the square of side 1 below the graph), the first limit is clearly

$$\lim_{s\to\infty} \int_0^{\infty} f(s,y)\,dy = 1.$$

But for any fixed value of y, we have $f(s,y) = 0$ for $s > y$, and so

$$\lim_{s\to\infty} f(s,y) = 0 \quad \text{for all } y$$

and so the second limit is

$$\int_0^{\infty} \lim_{s\to\infty} f(s,y)\,dy = \int_0^{\infty} 0\,dy = 0.$$

So we have to be careful when interchanging limits. And now we'll be careful with our initial data limit.

Our goal is to show that

$$\lim_{t\to 0+} u(x,t) = \varphi(x)$$

in other words

$$\lim_{t\to 0+} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-p^2} \varphi(x - \sqrt{4kt}\,p)\,dp = \varphi(x).$$

To do this, we're going to break the integral up into two parts, based on the following observations:

- If t is very small, and p is not too large (so that $\sqrt{4kt}\,p$ is close to zero), we'll have that $\varphi(x - \sqrt{4kt}\,p)$ is very close to $\varphi(x)$, so the value of the part of the integral where "t is very small and p is not too large" should be close to $\varphi(x)$.

- If p is large, then e^{-p^2} is very small, so the value of the part of the integral where p is large should be close to zero.

The trick is going to be balancing the "t very small and p not too large" part with the "p is large" part to get the result. Here's how we're going to do it:

First, we're going to restate what we're trying to prove as

$$\lim_{t\to 0+} (u(x,t) - \varphi(x)) = 0$$

and rewrite the expression in parentheses in the limit on the left as:

$$u(x,t)-\varphi(x) = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-p^2}\varphi(x-\sqrt{4kt}\,p)\,dp - \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-p^2}\varphi(x)\,dp = \frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-p^2}\Big(\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big)\,dp$$

Aside: Let's take a moment to recall the precise definition of limit, since we're going to use it carefully here. When we say

$$\lim_{t\to 0} F(t) = L$$

we mean that for any "output tolerance" $\varepsilon > 0$, we can choose an "input tolerance" $\delta > 0$ and then guarantee that whenever the input t is within δ of 0 (in other words, if $|t| < \delta$), then the output $F(t)$ will be within ε of L (in other words $|F(t) - L| < \varepsilon$).

Limits as $t \to \infty$ are handled a little differently: For instance, when we say that

$$\int_0^{\infty} e^{-p^2}\,dp \quad \text{converges}$$

we mean that for any output tolerance ε there is a number M so that

$$\int_M^{\infty} e^{-p^2}\,dp < \varepsilon$$

which implies that the integral of e^{-p^2} from 0 to M is within the tolerance ε of the value of the improper integral (we can dispense with absolute value signs because e^{-p^2} is a positive function).

Our goal is to show that given $\varepsilon > 0$ we can find a $\delta > 0$ so that if $0 < t < \delta$ then

$$\left|\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-p^2}\Big(\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big)\,dp\right| < \varepsilon.$$

Our first step will use only that φ is a *bounded* function and that the improper integral

$$\int_{-\infty}^{\infty} e^{-p^2}\,dp \quad \text{converges}$$

The phrase "φ is bounded" means that there is a number B (the bound) so that $|\varphi(x)| < B$ for all $x \in \mathbb{R}$. The triangle inequality (or just common sense) then tells us that

$$\Big|\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big| < 2B$$

for all x, k, t and p. So we can estimate

$$\left|\frac{1}{\sqrt{\pi}}\int_M^\infty e^{-p^2}\Big(\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big)\,dp\right| \le \frac{1}{\sqrt{\pi}}\int_M^\infty e^{-p^2}\Big|\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big|\,dp \le \frac{2B}{\sqrt{\pi}}\int_M^\infty e^{-p^2}\,dp$$

and

$$\left|\frac{1}{\sqrt{\pi}}\int_{-\infty}^{-M} e^{-p^2}\Big(\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big)\,dp\right| \le \frac{1}{\sqrt{\pi}}\int_{-\infty}^{-M} e^{-p^2}\Big|\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big|\,dp \le \frac{2B}{\sqrt{\pi}}\int_{-\infty}^{-M} e^{-p^2}\,dp.$$

Because the integral of e^{-p^2} from $-\infty$ to ∞ converges, we can choose M large enough so that

$$\frac{2B}{\sqrt{\pi}}\int_M^\infty e^{-p^2}\,dp + \frac{2B}{\sqrt{\pi}}\int_{-\infty}^{-M} e^{-p^2}\,dp < \frac{\varepsilon}{2}$$

which in turn implies that

$$\left|\frac{1}{\sqrt{\pi}}\int_{|p|>M} e^{-p^2}\Big(\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big)\,dp\right| < \frac{\varepsilon}{2}. \tag{1}$$

Once M is chosen in this manner, we have to show that we can also make

$$\left|\frac{1}{\sqrt{\pi}}\int_{-M}^{M} e^{-p^2}\Big(\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big)\,dp\right| < \frac{\varepsilon}{2}. \tag{2}$$

Because φ is continuous at x, we know that we can choose a $\delta_1 > 0$ so that if $|x-y| < \delta_1$, then $|\varphi(y)-\varphi(x)| < \frac{1}{2}\varepsilon$. For the integral in (2), this means that we need to force t to be small enough so that $|\sqrt{4kt}\,p| < \delta_1$ for all p ranging from $-M$ to M. To do this, choose

$$\delta < \frac{\delta_1^2}{4kM^2}$$

Then we will have, for all $t < \delta$ and $-M < p < M$,

$$|\sqrt{4kt}\,p| < |\sqrt{4k\delta}\,p| < \sqrt{4k\frac{\delta_1^2}{4kM^2}}\,M = \delta_1,$$

so that in turn

$$\Big|\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big| < \frac{\varepsilon}{2} \quad \text{for all } p \text{ between } -M \text{ and } M.$$

Now we can prove estimate (2) above: If $t < \delta$ with δ given as above, then

$$\begin{aligned}\left|\frac{1}{\sqrt{\pi}}\int_{-M}^{M} e^{-p^2}\Big(\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big)\,dp\right| &\le \frac{1}{\sqrt{\pi}}\int_{-M}^{M} e^{-p^2}\Big|\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big|\,dp \\ &< \frac{1}{\sqrt{\pi}}\int_{-M}^{M} e^{-p^2}\frac{\varepsilon}{2}\,dp < \frac{\varepsilon}{2}\,\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-p^2}\,dp = \frac{\varepsilon}{2}\end{aligned}$$

Together, estimates (1) and (2) imply that if $0 < t < \delta$ then

$$\begin{aligned}|u(x,t)-\varphi(x)| &= \left|\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-p^2}\Big(\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big)\,dp\right| \\ &\le \left|\frac{1}{\sqrt{\pi}}\int_{|p|>M} e^{-p^2}\Big(\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big)\,dp\right| + \left|\frac{1}{\sqrt{\pi}}\int_{-M}^{M} e^{-p^2}\Big(\varphi(x-\sqrt{4kt}\,p)-\varphi(x)\Big)\,dp\right| \\ &< \frac{\varepsilon}{2}+\frac{\varepsilon}{2} = \varepsilon\end{aligned}$$

which is just what we need to conclude that

$$\lim_{t\to 0+} u(x,t) = \varphi(x).$$

Another phenomenon we can treat in a similar manner is what happens when the initial data $\varphi(x)$ as a "jump discontinuity" — this is a point x_0 where both the left-hand and right-hand limits of φ exist as $x \to x_0-$ or $x \to x_0+$, but they have different values. Our textbook uses the notation

$$\varphi(x_0+) = \lim_{x\to x_0+} \varphi(x) \qquad \text{and} \qquad \varphi(x_0-) = \lim_{x\to x_0-} \varphi(x)$$

for the right-hand and left-hand limits, respectively. The solution of the heat equation has an interesting limiting behavior at a point where the initial data φ has a jump:

Proposition. *If the initial data for the heat equation has a jump discontinuity at x_0, then the solution "splits the difference" between the left and right hand limits as $t \to 0+$, in other words:*

$$\lim_{t\to 0+} u(x,t) = \tfrac{1}{2}\Big(\varphi(x_0+) + \varphi(x_0-)\Big).$$

where u is defined by equation $(*)$ above.

To prove this, we rewrite the solution $u(x,t)$ using formula $(**)$, in other words

$$u(x,t) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-p^2} \varphi(x - \sqrt{4kt}\, p)\, dp. \qquad (**)$$

Then, for $x = x_0$, we break up the integral into the parts where $p > 0$ and $p < 0$, as follows:

$$u(x_0,t) = \frac{1}{\sqrt{\pi}} \left(\int_{-\infty}^{0} e^{-p^2} \varphi(x - \sqrt{4kt}\, p)\, dp + \int_{0}^{\infty} e^{-p^2} \varphi(x - \sqrt{4kt}\, p)\, dp \right)$$

We'll show that as $t \to 0+$, the second integral (times $1/\sqrt{\pi}$) approaches $\frac{1}{2}\varphi(x_0-)$ and leave the other integral to you.

Our goal is to show that

$$\lim_{t\to 0+} \frac{1}{\sqrt{\pi}} \int_{0}^{\infty} e^{-p^2} \varphi(x_0 - \sqrt{4kt}\, p)\, dp = \frac{1}{2}\varphi(x_0-).$$

As before, to do this, we're going to break the integral up into two parts, based on the following observations:

- If t is very small and positive, and p is not too large (so that $\sqrt{4kt}\, p$ is close to zero), we'll have that $\varphi(x_0 - \sqrt{4kt}\, p)$ is very close to $\varphi(x_0-)$, so the value of the part of the integral where "t is very small and p is not too large" should be close to $\varphi(x_0-)$.
- If p is large, then e^{-p^2} is very small, so the value of the part of the integral where p is large should be close to zero.

The trick is going to be balancing the "t very small and p not too large" part with the "p is large" part to get the result. And we do it the same was as before:

First, we're going to restate what we're trying to prove as

$$\lim_{t\to 0+}\left(\left[\frac{1}{\sqrt{\pi}}\int_0^\infty e^{-p^2}\varphi(x_0-\sqrt{4kt}\,p)\,dp\right]-\frac{1}{2}\varphi(x_0-)\right)=0$$

and rewrite the expression in parentheses in the limit on the left as:

$$\frac{1}{\sqrt{\pi}}\int_0^\infty e^{-p^2}\varphi(x_0-\sqrt{4kt}\,p)\,dp-\frac{1}{\sqrt{\pi}}\int_0^\infty e^{-p^2}\varphi(x_0-)\,dp=\frac{1}{\sqrt{\pi}}\int_0^\infty e^{-p^2}\Big(\varphi(x_0-\sqrt{4kt}\,p)-\varphi(x_0-)\Big)\,dp$$

As before, our goal is to show that given $\varepsilon>0$ we can find a $\delta>0$ so that if $0<t<\delta$ then

$$\left|\frac{1}{\sqrt{\pi}}\int_{-\infty}^\infty e^{-p^2}\Big(\varphi(x_0-\sqrt{4kt}\,p)-\varphi(x_0-)\Big)\,dp\right|<\varepsilon.$$

And as before, our first step will use only that φ is a *bounded* function and that the improper integral

$$\int_{-\infty}^\infty e^{-p^2}\,dp\quad\text{converges}$$

The phrase "φ is bounded" means that there is a number B (the bound) so that $|\varphi(x)|<B$ for all $x\in\mathbb{R}$. The triangle inequality (or just common sense) then tells us that

$$\Big|\varphi(x_0-\sqrt{4kt}\,p)-\varphi(x_0-)\Big|<2B$$

for all x_0, k, t and p. So we can estimate

$$\left|\frac{1}{\sqrt{\pi}}\int_M^\infty e^{-p^2}\Big(\varphi(x_0-\sqrt{4kt}\,p)-\varphi(x_0)\Big)\,dp\right|\le\frac{1}{\sqrt{\pi}}\int_M^\infty e^{-p^2}\Big|\varphi(x_0-\sqrt{4kt}\,p)-\varphi(x_0-)\Big|\,dp\le\frac{2B}{\sqrt{\pi}}\int_M^\infty e^{-p^2}\,dp$$

(we only need one of the two "tails" this time).

Because the integral of e^{-p^2} from 0 to ∞ converges, we can choose M large enough so that

$$\frac{2B}{\sqrt{\pi}}\int_M^\infty e^{-p^2}\,dp<\frac{\varepsilon}{2}$$

which in turn implies that

$$\left|\frac{1}{\sqrt{\pi}}\int_M^\infty e^{-p^2}\Big(\varphi(x_0-\sqrt{4kt}\,p)-\varphi(x_0-)\Big)\,dp\right|<\frac{\varepsilon}{2}. \tag{3}$$

Once M is chosen in this manner, we have to show that we can also make

$$\left|\frac{1}{\sqrt{\pi}}\int_0^M e^{-p^2}\Big(\varphi(x_0-\sqrt{4kt}\,p)-\varphi(x_0-)\Big)\,dp\right|<\frac{\varepsilon}{2}. \tag{4}$$

Because $\varphi(x_0-)$ is the limit of $\varphi(x)$ as $x\to x_0$ from the left, we know that we can choose a $\delta_1>0$ so that if $x_0-y<\delta_1$, then $|\varphi(y)-\varphi(x_0-)|<\frac{1}{2}\varepsilon$. For the integral in (4), this means that we need to force t to be small enough so that $|\sqrt{4kt}\,p|<\delta_1$ for all p ranging from 0 to M. To do this, choose

$$\delta<\frac{\delta_1^2}{4kM^2}$$

Then we will have, for all $t < \delta$ and $0 < p < M$,

$$\sqrt{4kt}\,p < \sqrt{4k\delta}\,p < \sqrt{4k\frac{\delta_1^2}{4kM^2}}\,M = \delta_1,$$

so that in turn

$$\left|\varphi(x_0 - \sqrt{4kt}\,p) - \varphi(x_0-)\right| < \frac{\varepsilon}{2} \quad \text{for all } p \text{ between } 0 \text{ and } M.$$

Now we can prove estimate (4) above: If $t < \delta$ with δ given as above, then

$$\left|\frac{1}{\sqrt{\pi}}\int_0^M e^{-p^2}\Big(\varphi(x_0 - \sqrt{4kt}\,p) - \varphi(x_0-)\Big)\,dp\right| \le \frac{1}{\sqrt{\pi}}\int_0^M e^{-p^2}\left|\varphi(x_0 - \sqrt{4kt}\,p) - \varphi(x_0-)\right|dp$$
$$< \frac{1}{\sqrt{\pi}}\int_0^M e^{-p^2}\frac{\varepsilon}{2}\,dp < \frac{\varepsilon}{2}\,\frac{1}{\sqrt{\pi}}\int_0^\infty e^{-p^2}\,dp < \frac{\varepsilon}{2}$$

Together, estimates (3) and (4) imply that if $0 < t < \delta$ then

$$\left|\left[\frac{1}{\sqrt{\pi}}\int_0^\infty e^{-p^2}\varphi(x_0 - \sqrt{4kt}\,p)\,dp\right] - \frac{1}{2}\varphi(x_0-)\right| = \left|\frac{1}{\sqrt{\pi}}\int_0^\infty e^{-p^2}\Big(\varphi(x_0 - \sqrt{4kt}\,p) - \varphi(x_0-)\Big)\,dp\right|$$
$$\le \left|\frac{1}{\sqrt{\pi}}\int_M^\infty e^{-p^2}\Big(\varphi(x_0 - \sqrt{4kt}\,p) - \varphi(x_0-)\Big)\,dp\right| + \left|\frac{1}{\sqrt{\pi}}\int_0^M e^{-p^2}\Big(\varphi(x_0 - \sqrt{4kt}\,p) - \varphi(x_0-)\Big)\,dp\right|$$
$$< \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon$$

which is just what we need to conclude that

$$\lim_{t\to 0+}\frac{1}{\sqrt{\pi}}\int_0^\infty e^{-p^2}\varphi(x_0 - \sqrt{4kt}\,p)\,dp = \frac{1}{2}\varphi(x_0-).$$

Together with

$$\lim_{t\to 0+}\frac{1}{\sqrt{\pi}}\int_{-\infty}^0 e^{-p^2}\varphi(x_0 - \sqrt{4kt}\,p)\,dp = \frac{1}{2}\varphi(x_0+).$$

(which you can prove by following what we just did for $\varphi(0-)$), we can conclude that

$$\lim_{t\to 0+} u(x_0,t) = \lim_{t\to 0+}\frac{1}{\sqrt{\pi}}\left(\int_0^\infty e^{-p^2}\varphi(x_0 - \sqrt{4kt}\,p)\,dp + \int_{-\infty}^0 e^{-p^2}\varphi(x_0 - \sqrt{4kt}\,p)\,dp\right) = \frac{1}{2}\Big(\varphi(x_0+)+\varphi(x_0-)\Big).$$

That's it.