THE FUNDAMENTAL SOLUTION TO THE WRIGHT–FISHER EQUATION*

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Abstract. The Wright–Fisher equation, which was introduced as a model to study demography in the presence of diffusion, has had a renaissance as a model for the migration of alleles in the genome. Our goal in this paper is to give a careful analysis of the fundamental solution to the Wright–Fisher equation, with particular emphasis on its behavior for a short time near the boundary.

Key words. Wright–Fisher equation, estimates on the fundamental solution

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Introduction. The aim of this article is to study the fundamental solution $p(x,y,t)$ to the Cauchy initial value problem for the Wright–Fisher equation, that is, the fundamental solution for the equation

\[
\frac{\partial}{\partial t}u(x,t) = x(1-x)\frac{\partial^2}{\partial x^2}u(x,t) \text{ in } (0,1) \times (0,\infty) \quad \text{with boundary values}
\]

\[
\lim_{t \downarrow 0} u(x,t) = \varphi(x) \text{ for } x \in (0,1) \text{ and } u(0,t) = 0 = u(1,t) \text{ for } t \in (0,\infty).
\]

Our interest in this equation is the outgrowth of questions asked by Nick Patterson, who uses it to model the distribution and migration of genes in his work at the Broad Institute. Patterson initially sought help from Charles Fefferman, and it was Fefferman who relayed Patterson’s questions to the second author. Using much more purely analytic technology, the same questions have been addressed by Charles Epstein and Rafe Mazzeo, who are preparing a paper (cf. [2]) on the topic. Earlier work on the same equation can be found in [8] and [5].

The challenge here comes from the degeneracy of the elliptic operator $x(1-x)\frac{\partial^2}{\partial x^2}$ at the boundary $\{0,1\}$. In order to analyze $p(x,y,t)$ for $x$ and $y$ near the boundary, we will compare it to the fundamental solution to the Cauchy initial value problem

\[
\frac{\partial}{\partial t}u(x,t) = x^2\frac{\partial^2}{\partial x^2}u(x,t) \text{ in } (0,\infty) \times (0,\infty) \quad \text{with boundary values}
\]

\[
u(0,t) = 0 \text{ and } \lim_{t \downarrow 0} u(x,t) = \varphi(x) \text{ for } x \in (0,\infty),
\]

and in order to provide a context for this problem, we will devote the rest of this introduction to an examination of some easier but related equations.

First consider the Cauchy initial value problem:

\[
\frac{\partial}{\partial t}u(x,t) = x^2\frac{\partial^2}{\partial x^2}u(x,t) \text{ in } (0,\infty) \times (0,\infty) \quad \text{with boundary values}
\]

\[
u(0,t) = 0 \text{ and } \lim_{t \downarrow 0} u(x,t) = \varphi(x) \text{ for } x \in (0,\infty).
\]

The fundamental solution for this problem is the density for the distribution of the solution to the Itô stochastic differential equation:

\[dX(t,x) = \sqrt{2}X(t,x)dB(t) \text{ with } X(0,x) = x,\]

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where \( \{B(t) : t \geq 0\} \) is a standard, \( \mathbb{R} \)-valued Brownian motion. As is well known, the solution is \( X(t, x) = x \exp(\sqrt{2}B(t) - t) \), and so
\[
\mathbb{P}(X(t, x) \leq y) = \mathbb{P}\left( B(t) \leq 2^{-1/2} \left( \log \frac{x}{y} + t \right) \right) = \frac{1}{\sqrt{2\pi t}} \int_{-\infty}^{2^{-1/2}(\log \frac{x}{y} + t)} e^{-\frac{\xi^2}{2}} d\xi.
\]
Hence, the fundamental solution to (0.3) is
\[
p(x, y, t) = y^{-2/3} \bar{p}(x, y, t) \quad \text{where} \quad \bar{p}(x, y, t) = \frac{\sqrt{xy}}{4\pi t} \exp\left( -\frac{1}{4t} \left[ \left( \log \frac{y}{x} \right)^2 + t^2 \right] \right).
\]
Isolating the factor \( y^{-2} \) is natural since the operator \( x^2 \partial_x^2 \) is formally self-adjoint with respect to \( \frac{dy}{y^2} \), and therefore one should expect that \( y^2 \bar{p}(x, y, t) \) is symmetric, which indeed it is. Furthermore, it should be noted that the spacial boundary condition is invisible here since \( X(t, 0) \equiv 0 \) and \( X(t, x) > 0 \) \( \forall t \geq 0 \) if \( x > 0 \). Finally, elementary calculus shows that although \( \bar{p}(x, y, t) \) is smooth on \((0, \infty)^2\), spatial derivatives of \( \bar{p}(x, y, t) \) become unbounded as \( x = y \to 0 \).

Next, consider the Cauchy initial value problem:
\[
\partial_t u(x, t) = x \partial_x^2 u(x, t) + \frac{1}{2} \partial_x u(x, t) \quad \text{in} \quad (0, \infty) \times (0, \infty) \quad \text{with boundary values}
\]
\[u(0, t) = 0 \quad \text{and} \quad \lim_{\tau \to 0} u(x, t) = \varphi(x) \quad \text{for} \quad x \in (0, \infty),\]
\[
(0.4)
\]
When one ignores the spacial boundary condition, the fundamental solution to this problem is the density for the distribution of the solution to
\[dX(t, x) = \sqrt{2|X(t, x)|} dB(t) + \frac{1}{2} dt \quad \text{with} \quad X(0, x) = x.
\]
Although the coefficient of \( dB(t) \) is not Lipschitz continuous at 0, a theorem of Watanabe and Yamada (cf. Chapter 10 in [7]) says that this equation has an almost surely unique solution and that this solution stays nonnegative if \( x \geq 0 \). Further, using Itô’s formula, one can check that the distribution of this solution is the same as the distribution of \( \left(x^2 + 2^{-1/2}B(t)\right)^2 \). Thus, when one ignores the spacial boundary condition, the fundamental solution is
\[
y^{-1/2}(\pi t)^{-1/2} e^{-\frac{x^2}{4t}} \cosh 2 \sqrt{\frac{xy}{t^2}},
\]
where again we have isolated the factor which is the Radon-Nikodým derivative of the measure \( \frac{dy}{y^2} \) with respect to which the diffusion operator is formally self-adjoint. Obviously, apart from this factor, the fundamental solution is smooth, in fact, analytic, all the way to the boundary. On the other hand, if we impose the spacial boundary condition, then the fundamental solution is the density of
\[
y \sim \mathbb{P}\left( B(t) \leq 2^{1/2} \left( y^{1/2} - x^{1/2} \right) \quad \text{and} \quad B(\tau) > -\sqrt{2x} \quad \text{for} \quad \tau \in [0, t] \right),
\]
and an application of the reflection principle shows that this density is
\[
y^{-1/2} \bar{p}(x, y, t) \quad \text{where} \quad \bar{p}(x, y, t) = (\pi t)^{-1/2} e^{-\frac{x^2}{2t}} \sinh 2 \sqrt{\frac{xy}{t^2}},
\]
which is smooth but has derivatives which become unbounded as \( x = y \) tends to 0.
So far as we know, there is no general theory which predicts the behavior displayed by these two examples. Indeed, past experience with degenerate parabolic equations inclined us to believe that, because $x^2$ has a smooth, nonnegative extension to $\mathbb{R}$, whereas $x$ does not, the heat equation for $x^2 \partial_x^2$ should have smoother solutions than the one for $x \partial_x^2 + \frac{1}{2} \partial_x$. Be that as it may, as we will see in the next section, the fundamental solution to (0.2) has regularity properties which resemble those of the fundamental solution to (0.4) when one ignores the spatial boundary condition, and the reason for this is easy to understand. Namely, because the diffusion corresponding to (0.2) gets absorbed when it hits 0, the density of its distribution is the same on $(0, \infty)$ as the density of the diffusion when the spatial boundary condition is ignored. For potentially practical applications, the most useful results in this article are likely to be the small time estimates for the Wright–Fisher fundamental solution in Corollaries 4.4 and 4.5 (as well as the slight refinement in Theorem 6.4) and the expansion procedure, described in Theorem 6.2, for measures evolving under the Wright–Fisher forward equation. Although the derivative estimates in section 5 may have some mathematical interest, their practical value is probably not significant.

1. **The model equation.** Following a suggestion made by Charles Fefferman, in this section we will study the one-point analogue of the Wright–Fisher equation. Specifically, we write down that fundamental solution $q(x, y, t)$ for the Cauchy initial value problem:

$$
\partial_t u = x \partial_x^2 u \quad \text{in} \ (0, \infty) \times (0, \infty)
$$

(1.1)

with $u(0, t) = 0$ and $\lim_{t \to 0} u(x, t) = \varphi(x)$ for $(x, t) \in (0, \infty) \times (0, \infty)$.

Actually, prior to our own work on this topic, Fefferman wrote down an expression for this fundamental solution as a Fourier transform, and Noam Elkies recognized that Fefferman’s Fourier expression could be inverted to yield the formula at which we will arrive by non-Fourier techniques. See the discussion following (6.2).

Because $x \partial_x^2$ is formally self-adjoint with respect to $y^{-1} dy$, it is reasonable to write $q(x, y, t) = y^{-1} \tilde{q}(x, y, t)$ and to expect $\tilde{q}(x, y, t)$ to be symmetric with respect to $x$ and $y$. In addition, an elementary scaling argument shows that $\tilde{q}(x, y, t) = \tilde{q}(\frac{x}{t}, \frac{y}{t}, 1)$. Taking a hint from the second example in the introduction, we seek $\tilde{q}(x, y, 1)$ in the form

$$
\tilde{q}(x, y, 1) = e^{-x-y} q(xy).
$$

If we do, then in order that $q$ be a solution to our evolution equation, we find that it is necessary and sufficient that

$$
\xi q''(\xi) - q(\xi) = 0, \quad \xi \in (0, \infty),
$$

(1.2)

and we will show that the solution to (1.2) which makes

$$
q(x, y, t) \equiv y^{-1} \tilde{q}(x, y, t), \quad \text{where} \quad \tilde{q}(x, y, t) = e^{-\frac{x+y}{t^2}} q \left( \frac{xy}{t^2} \right)
$$

(1.3)

into a fundamental solution is the one satisfying

$$
\lim_{\xi \to 0} q(\xi) = 0 \quad \text{and} \quad \lim_{\xi \to 0} q'(\xi) = 1.
$$

(1.4)

Before proceeding, it will be useful to have the following simple version of the minimum principle. Namely, if $\xi w''(\xi) - w(\xi) \geq 0$, $w(0) = 0$, and $w' > 0$ in an
interval $(0, \delta)$ for some $\delta > 0$, then $w > 0$ on $(0, \infty)$. Indeed, if not, then there would exist a $\xi_0 > 0$ such that $w > 0$ on $(0, \xi_0)$ and $w(\xi_0) = 0$. In particular, this would mean that $w$ achieves a strictly positive, maximum value at some $\xi \in (0, \xi_0)$, and this would lead to the contradiction $w''(\xi) \leq 0 < w(\xi) \leq \xi w''(\xi)$.

Now suppose that $q$ satisfies (1.2) and (1.4). Then

$$0 < q(\xi) \leq \xi e^{2\xi^2}$$

for $\xi \in (0, \infty)$.

To see this, apply the preceding to $w = q$ and $w = (1 + \epsilon)\xi e^{2\xi^2} - q(\xi)$ for $\epsilon > 0$.

Given the estimate above, we know that the Laplace transform

$$f(\lambda) = \int_{(0, \infty)} e^{-\lambda \xi} q(\xi) \, d\xi$$

exists for all $\lambda > 0$. Moreover, by (1.2) and (1.4),

$$\int_{(\lambda, \infty)} f(\mu) \, d\mu = \int_{(0, \infty)} e^{-\lambda \xi} q(\xi) \frac{d\xi}{\xi} = \int_{(0, \infty)} e^{-\lambda \xi} q''(\xi) \, d\xi = \lambda^2 f(\lambda) - 1,$$

and so $-f(\lambda) = \lambda^2 f'(\lambda) + 2\lambda f(\lambda)$, or, equivalently, $f(\lambda) = A \lambda^{-2} e^{\lambda}$ for some $A$. Plugging this back into (1.5), we see that $A = 1$. That is, we now know that

$$\int_{(0, \infty)} e^{-\lambda \xi} q(\xi) \, d\xi = \frac{e^{\frac{1}{\lambda^2}}}{\lambda^2}$$

and

$$\int_{(0, \infty)} e^{-\lambda \xi} q''(\xi) \, d\xi = \frac{e^{\frac{1}{\lambda^2}}}{\lambda^2} - 1.$$ 

In particular, this proves that there is at most one $q$ which satisfies both (1.2) and (1.4).

As is easily verified,

$$q(\xi) = \sum_{n=1}^{\infty} \frac{\xi^n}{n!(n-1)!}$$

satisfies (1.2) and (1.4), and it is therefore the one and only function which does. In particular, this means that

$$\frac{\cosh(2\xi^2) - 1}{2} \leq q(\xi) \leq \xi e^{2\xi^2}$$

for $\xi \in (0, \infty)$.

We now define $\tilde{q}(x, y, t)$ and $q(x, y, t)$ as in (1.3) for the $q(\xi)$ given by (1.7). On the basis of (1.2), it is easy to check that $q(x, y, t)$ satisfies the Kolmogorov backward and forward equations:

$$\partial_t q(x, y, t) = x \partial_x^2 q(x, y, t) \quad \text{and} \quad \partial_y q(x, y, t) = \partial_y^2(y q(x, y, t)).$$

Also, from (1.6) we know that

$$\int_{(0, \infty)} e^{-\lambda y} q(x, y, t) \, dy = e^{-\frac{\xi}{1 - \xi^2}} - e^{-\frac{\xi}{\xi^2}} \quad \text{for } \Re \lambda > -\frac{1}{t}.$$ 

Thus, as $t \searrow 0$, $\int_{(0, \infty)} q(x, y, t) \, dy$ tends to 1 uniformly for $x \in [\delta, \infty)$ for each $\delta > 0$. At the same time, from (1.8), we know that

$$e^{-\frac{\xi}{1 - \xi^2}} \cosh \left(\frac{2\sqrt{-t}}{t}\right) - 1 \leq q(x, y, t) \leq \frac{x}{t^2} e^{-\frac{\xi}{1 - \xi^2}}.$$
from which it is clear that, as \( t \searrow 0 \),
\[
\int_{(0,\infty)\setminus(x-\delta,x+\delta)} q(x, y, t) \, dy \longrightarrow 0 \quad \text{for each } \delta > 0
\]
uniformly fast for \( x \) in bounded subsets of \((0, \infty)\). Hence, for each \( \varphi \in C_0((0, \infty); \mathbb{R}) \),
\[
(1.11) \quad u_\varphi(x, t) = \int_{(0,\infty)} \varphi(y)q(x, y; t) \, dy \longrightarrow \varphi(x) \quad \text{uniformly on compacts in } (0, \infty).
\]
At the same time, from (1.10), it is clear that, as \( x \searrow 0 \), \( u_\varphi(x, t) \longrightarrow 0 \) uniformly for \( t \in [\delta, \infty) \) for every \( \delta > 0 \). Summarizing, we have now shown that \( q(x, y, t) \) is a fundamental solution to (1.1).

It will be important for us to know that the estimate in (1.10) can be improved when \( xy \geq t^2 \). Namely, there exists an \( \delta_0 \in (0, 1) \) such that
\[
(1.12) \quad \delta_0 \frac{(xy)^{\frac{1}{2}}}{t^{\frac{1}{2}}} e^{-\frac{\alpha \tau - \sigma^2}{2 t}} \leq \bar{q}(x, y, t) \leq \frac{(xy)^{\frac{1}{2}}}{\delta_0 t^{\frac{1}{2}}} e^{-\frac{\alpha \tau - \sigma^2}{2 t}} \quad \text{when } xy \geq t^2.
\]
Clearly (1.12) comes down to showing that
\[
\delta_0 \xi^{\frac{1}{2}} e^{2\frac{\xi}{4}} \leq q(\xi) \leq \delta_0^{-1} \xi^{\frac{1}{2}} e^{2\frac{\xi}{4}} \quad \text{for } \xi \geq 1.
\]
To prove this, one can either use the relationship (cf. (7.4) and (7.6)) between \( q(\xi) \) and Bessel functions or standard estimates for solutions to parabolic equations. The latter approach entails using the fact that, by standard estimates for solutions to parabolic equations (e.g., section 5.2.2 in [6]), there is an \( \alpha_0 \in (0, 1) \) such that
\[
\frac{\alpha_0}{t^{\frac{1}{2}}} \leq q(1, 1, t) \leq \frac{1}{\alpha_0 t^{\frac{1}{2}}} \quad \text{for } t \in (0, 1),
\]
which, because \( q(1, 1, t) = e^{-\frac{2}{t^2}} q(t^{-2}) \), gives (1.12).

We close this section with a discussion of the diffusion process associated with (1.1) and show that \( q(x, y, t) \) is the density for its transition probability function. Perhaps the simplest way to describe this process is to consider the Itô stochastic integral equation:
\[
(1.13) \quad Y(t, x) = x + \int_0^t \sqrt{2Y(\tau, x)} \, dB(\tau), \quad (t, x) \in [0, \infty) \times (0, \infty),
\]
where \( \{B(\tau) : \tau \geq 0\} \) is an \( \mathbb{R} \)-valued Brownian motion on some probability space \((\Omega, \mathcal{F}, \mathbb{P})\). Using the Watanabe–Yamada theorem alluded to in the introduction, one can show that, for each \( x \in [0, \infty) \), there is an almost surely unique solution to (1.13). Further, if \( \zeta_0^Y(x) = \inf\{t \geq 0 : Y(t, x) = 0\} \), then \( t \geq \zeta_0^Y(x) \Rightarrow Y(t, x) = 0 \). To describe the relationship between (1.1) and \( Y(t, x) \), we introduce the \( \sigma \)-algebra \( \mathcal{F}_t \) which is generated by \( \{B(\tau) : [0, t]\} \). Then \( Y(t, x) \) is \( \mathcal{F}_t \)-measurable. In addition, by Itô’s formula, if \( w \) is an element of \( C^{2,1}([0, \infty) \times (0, t)) \cap C_0([0, \infty) \times [0, t]) \) and \( f = \partial_t w + x \partial_x^2 w \) is bounded, then
\[
\left( w(Y(t \land t \land \zeta_0^Y(x), x), t \land t \land \zeta_0^Y(x)) - \int_0^{t \land t \land \zeta_0^Y(x)} f(Y(s, x)) \, ds, \mathcal{F}_t, \mathbb{P} \right)
\]
is a martingale. In particular, if \( \varphi \in C_b((0, \infty); \mathbb{R}) \) and \( u_\varphi \) is given by (1.11), then, by taking \( w(x, \tau) = u_\varphi(x, t - \tau) \) and applying Doob’s stopping time theorem, one sees that

\[
(1.14) \quad u_\varphi(x, t) = \int_{(0, \infty)} \varphi(y)q(x, y, t) \, dy = \mathbb{E}[\varphi(Y(t, x)), \zeta^Y_t(x) > t].
\]

This proves that \( u_\varphi \) is the one and only solution to (1.1) and that \( q(x, \cdot, t) \) is the density for the distribution of \( Y(t, x) \) on \( \{\zeta^Y_t(x) > t\} \). As a consequence of uniqueness, we know that \( q(x, y, t) \) satisfies the Chapman–Kolmogorov equation,

\[
(1.15) \quad q(x, y, s + t) = \int_{(0, \infty)} q(x, \xi, s)q(\xi, y, t) \, d\xi,
\]

a fact which could have been also deduced from (1.9).

2. The Wright–Fisher equation. In this section we will lay out our strategy for analyzing the Wright–Fisher equation:

\[
(2.1) \quad \frac{\partial_t u(x, t)}{u(x, t)} = x(1 - x)\frac{\partial^2_x u(x, t)}{u(x, t)} \text{ on } (0, 1) \times (0, \infty)
\]

\[
\text{with } u(0, t) = 0 = u(1, t) \text{ and } \lim_{t \searrow 0} u(\cdot, t) = \varphi
\]

for \( \varphi \in C_b((0, 1); \mathbb{R}) \). Specifically, we want to explain how we plan to transfer to its fundamental solution \( p(x, y, t) \) the properties of \( q(x, y, t) \).

Because we cannot simply write it down, proving that \( p(x, y, t) \) even exists requires some thought. Using the separation of variables and taking advantage of the facts that the operator \( x(1 - x)\partial^2_x \) is formally self-adjoint in the \( L^2 \) space for the measure \( \frac{dy}{y(1 - y)} \) and that, for each \( n \geq 1 \), the space of polynomials of degree \( n \) is invariant for this operator, Kimura [1] constructed a fundamental solution as an expansion in terms of the eigenvalues and eigenfunctions. Like all such constructions, his expression for \( p(x, y, t) \) is very useful as \( t \to \infty \), when only one term in eigenfunction expansion dominates, but it gives very little information about \( p(x, y, t) \) for small \( t \). In addition, his approach relies so heavily on the particular equation that it would be difficult to apply his methods to even slightly different equations. For this reason, we will not use his analysis.

To get started, we will begin with the diffusion corresponding to (2.1). Thus, for \( x \in [0, 1] \), let \( \{X(t, x) : t \geq 0\} \) be the stochastic process determined by the Itô stochastic integral equation:

\[
(2.2) \quad X(t, x) = x + \int_0^t \sqrt{2X(\tau, x)(1 - X(\tau, x))} \, dB(\tau).
\]

Once again, one can show that, for each \( x \in [0, 1] \), (2.2) has a solution which is almost surely unique. Further, if \( \zeta^X_\xi(x) = \inf\{t \geq 0 : X(t, x) = \xi\} \) for \( \xi \in [0, 1] \) and \( \zeta^X = \zeta^X_0(X) \wedge \zeta^X_1(X) \), then \( X(t, x) = X(\zeta^X_t(x), x) \) for \( t \geq \zeta^X_t(x) \).

From the preceding existence and uniqueness results, one can show (cf. Chapters 6 and 8 in [7]) that if

\[
P(t, x, \Gamma) = \mathbb{P}(X(t, x) \in \Gamma \text{ and } \zeta^X(x) > t),
\]

then \( P(t, x, \cdot) \) satisfies the Chapman–Kolmogorov equation:

\[
(2.3) \quad P(s + t, x, \Gamma) = \int_{(0, 1)} P(t, y, \Gamma) P(s, x, dy) \quad \text{for } x \in (0, 1) \text{ and } \Gamma \in \mathcal{B}_{(0, 1)}.
\]
In addition, by the same sort of argument with which we derived (1.14), one has
\[
\int_{(0,1)} \varphi(y) P(t, x, dy) = \varphi(x) + \int_0^t \left( \int_{(0,1)} y(1-y) \varphi''(y) P(\tau, x, dy) \right) d\tau
\]
for any \( \varphi \in C_c^1((0,1); \mathbb{R}) \). Hence, for each \( x \in (0,1) \), \( P(t, x, \cdot) \) tends weakly to the unit point mass at \( x \) as \( t \searrow 0 \), and, in the sense of Schwartz distributions \( \partial_t u = \partial_y^2 (y(1-y)u) \)
and therefore, by standard hypoellipticity results for parabolic operators (e.g., section 3.4.2 in [6]), is smooth with respect to \( (y,t) \in (0,1) \times (0,\infty) \). In particular, we now know that, for each \( x \in (0,1) \), \( P(t, x, dy) = p(x, y,t) dy \) where \( (y,t) \rightarrow p(x, y, t) \) is smooth and satisfies
\[
\partial_t p(x, y, t) = \partial_y^2 (y(1-y)p(x, y, t)) \quad \text{in} \quad (0,1) \times (0,\infty) \quad \text{with} \quad \lim_{t \searrow 0} p(x, \cdot, t) = \delta_x.
\]
Furthermore, another application of the uniqueness statement for solutions to (2.2) shows that \( (t, x) \in (0,\infty)\times(0,1) \mapsto P(t, x, \cdot) \) is weakly continuous, and so \( (t, x, y) \mapsto p(t, x, y) \) is measurable. Hence, from (2.3), we know that
\[
p(x, y, s+t) = \int_{(0,1)} p(\xi, y, t)p(\xi, x, s) d\xi, \quad s, t \in (0,\infty), \text{ and } x, y \in (0,1).
\]
In addition, because, by uniqueness, the distribution of \( 1 - X(t, x) \) is the same as that of \( X(t, 1-x) \), it is clear that
\[
p(x, y, t) = p(1-x, 1-y, t).
\]
Finally, as we will show below,
\[
y(1-y)p(x, y, t) = x(1-x)p(y, x, t).
\]
Actually, if one uses Kimura’s results, (2.7) is clear. However, for the reasons given earlier, we will give an alternative proof.

In order to focus attention on what is happening at one endpoint, let \( \beta \in (0,1) \) be given, and consider the fundamental solution \( p_\beta(x, \xi, t) \) to
\[
\dot{u} = x(1-x)u'' \quad \text{on} \quad (0, \beta) \quad \text{with} \quad u(0,t) = 0 = u(\beta, t) \quad \text{and} \quad u(\cdot, 0) = \varphi
\]
for \( \varphi \in C_c((0,\beta); \mathbb{R}) \). Next, given \( 0 < \alpha < \beta < 1 \), define \( \eta_0^{X,\alpha,\beta}(x) = 0 \),
\[
\eta_{2n-1,\alpha,\beta}^X(x) = \inf \{ t \geq \eta_{2(n-1),\alpha,\beta}^X(x) : X(t,x) = \beta \} \quad \text{and} \quad
\eta_{2n,\alpha,\beta}^X(x) = \inf \{ t \geq \eta_{2n-1,\alpha,\beta}^X(x) : X(t,x) = \alpha \}
\]
for \( n \geq 1 \). Then (cf. Theorem 4.3 below), for \( x \in (0,\alpha] \) and \( \varphi \in C_c((0,\alpha); \mathbb{R}) \),
\[
\int_{(0,1)} p(x, t, \varphi) d\xi = \sum_{n=0}^{\infty} E[\varphi(X(t,x)), \eta_{2n,\alpha,\beta}^X(x) < t < \eta_{2n+1,\alpha,\beta}^X(x)]
\]
\[
= \int_{(0,\infty)} p_\beta(x, \xi, t) \varphi(\xi) d\xi
\]
\[
+ \sum_{n=1}^{\infty} E \left[ \int_{(0,\alpha)} p_\beta(\alpha, \xi, t - \eta_{2n,\alpha,\beta}^X(x)) \varphi(\xi) d\xi, \eta_{2n,\alpha,\beta}^X(x) < t \right].
\]
Hence, for $x, y \in (0, \alpha]$,

$$
(2.9) \quad p(x, y, t) = p_\beta(x, y, t) + \sum_{n=1}^{\infty} \mathbb{E}[p_\beta(\alpha, y, t - \eta_{2n,[\alpha, \beta]}(x)), \eta_{2n,[\alpha, \beta]}(x) < t],
$$

where the convergence of the series of the right can be controlled by the fact (cf. Lemma 4.2 below) that $\mathbb{P}(\eta_{2n,[\alpha, \beta]}(x) < t)$ decreases very rapidly as $n \to \infty$. In view of (2.9), analysis of $p(x, \xi, t)$ on $(0, \alpha]^2 \times (0, \infty)$ comes down to that of $p_\beta(x, \xi, t)$ on $(0, \alpha]^2 \times (0, \infty)$.

3. A change of variables. With the goal of applying the results in section 1, we will make a change of variables, one which was used also by Feller (see [3] and [4]). Namely, we want to choose a $\psi : [0, 1] \to [0, \infty)$ so that $\psi(0) = 0$ and the process $X^\psi(t, x) \equiv \psi \circ X(t, x)$ satisfies a stochastic integral equation of the form

$$
(3.1) \quad X^\psi(t, x) = \psi(x) + \int_0^t \sqrt{2X^\psi(\tau, x)} dB(\tau) + \int_0^t b(X^\psi(\tau, x)) d\tau
$$

for $t < \zeta^\psi(x) = \inf\{\tau \geq 0 : X^\psi(\tau, x) = \psi(1)\}$. As an application of Itô’s formula, we see that $\psi$ will have to be the solution to

$$
(3.2) \quad x(1 - x) \psi'(x)^2 = \psi(x) \quad \text{with} \quad \psi(0) = 0,
$$

which means that

$$
(3.3) \quad \psi(x) = (\arcsin \sqrt{x})^2, \quad \psi(1) = \frac{\pi^2}{4}, \quad \text{and} \quad \psi^{-1}(x) = (\sin \sqrt{x})^2.
$$

In addition, his formula tells us that

$$
(3.4) \quad b(x) = \psi^{-1}(x) \left(1 - \psi^{-1}(x)\right) \psi'' \circ \psi^{-1}(x) = \frac{\psi \psi''}{\left(\psi'\right)^2} \circ \psi^{-1}
$$

$$
= \frac{\sin(2\sqrt{x}) - 2\sqrt{x} \cos(2\sqrt{x})}{\sin(2\sqrt{x})}.
$$

Note that, although it goes to $\infty$ at the right-hand endpoint $\frac{\pi^2}{4}$, $b$ admits an extension to $\left(-\frac{\pi^2}{4}, \frac{\pi^2}{4}\right)$ as a real analytic function which vanishes at 0.

Our strategy should be clear now. We want to apply the results in section 1 to analyze the fundamental solution $r(x, y, t)$ to the heat equation $\partial_t u(x, t) = x^2 \partial_x^2 u(x, t) + b(x) \partial_x u(x, t)$ associated with $X^\psi(t, x)$ and then transfer our conclusions to $p(x, y, t)$ via $p(x, y, t) = \psi'(y) r(\psi(x), \psi(y), t)$. However, because $b$ becomes infinite at $\frac{\pi^2}{4}$, $x^2 \partial_x^2 + b(x) \partial_x$ is a nontrivial perturbation of $x^2 \partial_x^2$. Thus it is fortunate that, by the considerations in section 2, we have to analyze only the fundamental solution $r_\theta(x, y, t)$ to

$$
(3.5) \quad \partial_t u(x, t) = x^2 \partial_x^2 u(x, t) + b(x) \partial_x u(x, t) \quad \text{on} \quad (0, \theta) \quad \text{with} \quad u(0, t) = 0 = u(\theta, t)
$$

for $\theta \in (0, \frac{\pi^2}{4})$. Indeed, because $r_\theta(x, y, t)$ does not “feel” $b$ off of $(0, \theta)$, when analyzing it we can replace $b$ by any smooth, compactly supported function $b_\theta$ on $\mathbb{R}$ which coincides with $b$ on $(0, \theta)$.

With the preceding in mind, we now look at equations of the form

$$
(3.6) \quad \partial_t u(x, t) = x^2 \partial_x^2 u(x, t) + xc(x) \partial_x u(x, t) \quad \text{on} \quad (0, \infty) \quad \text{with} \quad u(0, t) = 0,
$$

where $c \in C^\infty_c(\mathbb{R}; \mathbb{R})$. 

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LEMMA 3.1. Set

\[ C(x) = \frac{1}{2} \int_0^\infty c(\xi) \, d\xi \quad \text{and} \quad V_c(x) = -x \left( \frac{c'(x)}{2} + \frac{c(x)^2}{4} \right). \]

Then \( u \) is a solution to \( \partial_t u(x, t) = x \partial_x^2 u(x, t) + xc(x) \partial_x u(x, t) \) if and only if \( u(x, t) = e^{-C(x)}w(x, t) \), where \( w \) is a solution to

\[ \partial_t w(x, t) = x \partial_x^2 w(x, t) + V_c(x)w(x, t). \]

Proof. The easiest way to check it is by direct computation.

As Lemma 3.1 shows, the analysis of solutions to (3.6) reduces to that of solutions to (3.8). Thus, we look at equations of the form

\[ \partial_t w(x, t) = x \partial_x^2 w(x, t) + V(x)w(x, t) \quad \text{on} \quad (0, \infty)^2 \]

where \( V \) is a smooth, compactly supported function. Using the time-honored perturbation equation of Duhamel, we look for the fundamental solution

\[ \text{q}\ V(x, y, t) = q(x, y, t) + \int_0^t \int_{(0, \infty)} q(x, \xi, t - \tau)V(\xi)q(\xi, y, \tau) \, d\xi d\tau. \]

To solve (3.10), set \( q_0^V = q \) and

\[ q_n^V(x, y, t) = \int_0^t \int_{(0, \infty)} q(x, \xi, t - \tau)V(\xi)q_{n-1}^V(\xi, y, \tau) \, d\xi d\tau \quad \text{for} \quad n \geq 1. \]

Proceeding by induction and using the Chapman–Kolmogorov equation of (1.15) satisfied by \( q \), one sees that

\[ |q_n^V(x, y, t)| \leq \frac{(||V||_\infty t)^n}{n!}q(x, y, t). \]

At the same time, by the estimate in (1.12) and induction, it is clear that \( q_n^V \) is continuous on \((0, \infty)^3\) for each \( n \geq 0 \), and from these one can easily check that

\[ q^V(x, y, t) = \sum_{n=0}^\infty q_n^V(x, y, t) \]

is a continuous function of \((x, y, t) \in (0, \infty)^3\) which solves (3.10). In addition, because (by another inductive argument)

\[ q_n^V(x, y, t) = \int_0^t \int_{(0, \infty)} q_{n-1}^V(x, \xi, t - \tau)V(\xi)q(\xi, y, \tau) \, d\xi d\tau, \]

one can use (1.3) and induction to see that

\[ yq_n^V(x, y, t) = \int_0^t \int_{(0, \infty)} \tilde{q}(x, \xi, t - \tau)\xi^{-1}V(\xi)q_{n-1}^V(\xi, y, \tau) \, d\xi d\tau \]

\[ = \int_0^t \int_{(0, \infty)} \tilde{q}(\xi, x, t - \tau)\xi^{-1}V(\xi)q_{n-1}^V(y, \xi, \tau) \, d\xi d\tau = xq_n^V(y, x, t). \]
Hence,

\[(3.14) \quad \bar{q}^V(x, y, t) = \bar{q}^V(y, x, t) \quad \text{where} \quad \bar{q}^V(x, y, t) \equiv yq^V(x, y, t).\]

We next verify that \(q^V\) is the fundamental solution to (3.9). That is, we want to show that if \(\varphi \in C_0([0, \infty); \mathbb{R})\) vanishes at 0 and

\[
w^V(\varphi)(x, t) = \int_{(0, \infty)} \varphi(y)q^V(x, y, t) \, dy,
\]

then \(w^V(\varphi)\) is a smooth solution to (3.9) with initial data \(\varphi\). Since it is clear that \(w^V(\varphi)(0, t) = 0\) and that \(w^V(\varphi)(\cdot, t) \rightarrow \varphi\) uniformly on compacts as \(t \downarrow 0\), what remains is to show that \(w^V(\varphi)\) is smooth and satisfies the differential equation in (3.9). For this purpose, set (cf. (1.11))

\[
w^\epsilon(\varphi)(x, t) \equiv \int_{(0, \infty)} q(x, y, \epsilon)w^V(\varphi)(y, t) \, dy
= u^\epsilon(\varphi)(x, t + \epsilon) + \int_0^t \int_{(0, \infty)} q(x, \xi, t + \epsilon - \tau)V(\xi)w^V(\varphi)(\xi, \tau) \, d\xi d\tau.
\]

Then, as \(\epsilon \downarrow 0\), \(w^\epsilon \rightarrow w^V(\varphi)\) and

\[
(x\partial_x^2 + V - \partial_t)w^\epsilon(\varphi)(x, t) = \int_{(0, \infty)} q(x, \xi, \epsilon)(V(x) - V(\xi))w^V(\varphi)(\xi, t) \, d\xi \rightarrow 0
\]

uniformly on compacts. Hence, \(w^V(\varphi)\) satisfies \(\partial_t w^V(\varphi)(x, t) = x\partial_x^2 w^V(\varphi)(x, t) + V(x)w^V(\varphi)(x, t)\)

on \((0, \infty)^2\) in the sense of distributions and is therefore a smooth, classical solution.

**Theorem 3.2.** Set (cf. (1.14))

\[
Q^V(t, x, \Gamma) = \mathbb{E} \left[ e^{\int_0^t V(Y(\tau, x)) \, d\tau}, Y(t, x) \in \Gamma \right], \quad \Gamma \in \mathcal{B}(0, \infty).
\]

Then

\[
Q^V(t, x, \Gamma) = \int_{\Gamma} q^V(x, y, t) \, dy.
\]

In particular,

\[(3.15) \quad 0 \leq q^V(x, y, t) \leq e^\epsilon\|V^+\|u q(x, y, t)\]

and

\[(3.16) \quad q^V(x, y, s + t) = \int_{(0, \infty)} q^V(x, \xi, s)q^V(\xi, y, t) \, d\xi.
\]

**Proof.** Given \(\varphi \in C_0([0, \infty); \mathbb{R})\) which vanishes at 0, one can apply Itô’s formula and the fact that \(w^V(\varphi)\) is a smooth solution to (3.9) which is bounded on \((0, \infty) \times [0, t]\), to check that, for each \(t > 0\),

\[
\left( e^{\int_0^t V(Y(\tau, x)) \, d\tau} w^V(\varphi)(Y(s, x), t - s), \mathcal{F}_s, \mathbb{P} \right)
\]
is a martingale for \( s \in [0, t] \). Hence, the first assertion follows from the equality of the expectation values of this martingale at times \( s = 0 \) and \( s = t \).

Given the first assertion, it is clear that \( q^V \geq 0 \). In addition, the right-hand side of (3.15) follows from the initial expression for \( q^V(t, x, \cdot) \), and (3.16) is a consequence of

\[
Q^V(s + t, x, \Gamma) = \int_{(0, \infty)} Q^V(t, \xi, \Gamma) Q^V(s, x, d\xi) \quad \text{for } \Gamma \in \mathcal{B}(0, \infty),
\]

which is an elementary application of the Markov property for the process \( \{Y(t, x) : (t, x) \in (0, \infty)^2\} \).

Given \( \theta \in (0, \infty) \), the next step is to produce from \( q^V(x, y, t) \) the fundamental solution \( q^V_\theta(x, y, t) \) to

\[
\partial_t w(x, t) = x \partial_x^2 w(x, t) + V(x)w(x, t) \quad \text{on } (0, \theta) \times (0, \infty)
\]

with \( w(0, t) = 0 = w(\theta, t) \) and \( \lim_{t \downarrow 0} w(\cdot, t) = \varphi \).

**Lemma 3.3.** Set \( \zeta^V_\theta(x) = \inf\{t \geq 0 : Y(t, x) = \theta\} \), and define

\[
q^V_\theta(x, y, t) = q^V(x, y, t) - \mathbb{E} \left[ e^{\int_0^{\zeta^V_\theta(x)} V(Y(\tau, x)) d\tau} q^V(\theta, y, t - \zeta^V_\theta(x)), \zeta^V_\theta(x) \leq t \right]
\]

for \( (x, y, t) \in (0, \theta)^2 \times (0, \infty) \). Then \( q^V_\theta(x, y, t) \) is a nonnegative, smooth function which is dominated by \( e^{\|V\|_{u,0}(\theta)} q(x, y, t) \) and satisfies

\[
q^V_\theta(x, y, s + t) = \int_{(0, \theta)} q^V_\theta(x, \xi, s) q^V_\theta(\xi, y, t) d\xi \quad \text{and} \quad y q^V_\theta(x, y, t) = x q^V_\theta(y, x, t).
\]

Finally, for each \( y \in (0, \theta) \), \( (x, t) \mapsto q^V_\theta(x, y, t) \) is a solution to (3.17) with \( \varphi = \delta_y \).

**Proof.** We begin by showing that \( q^V_\theta(x, y, t) \) is continuous, and clearly this comes down to checking that

\[
w_0(x, y, t) = \mathbb{E} \left[ e^{\int_0^{\zeta^V_\theta(x)} V(Y(\tau, x)) d\tau} q^V(\theta, y, t - \zeta^V_\theta(x)), \zeta^V_\theta(x) \leq t \right]
\]

is continuous. To this end, set

\[
w_s(x, y, t) = \mathbb{E} \left[ e^{\int_0^{\zeta^V_\theta(x)} V(Y(\tau, x)) d\tau} q^V(\theta, y, t - \zeta^V_\theta(x)_s), \zeta^V_\theta(x)_s \leq t \right],
\]

where \( \zeta^V_\theta(x)_s = \inf\{t \geq s : Y(t, x) = \theta\} \). Because

\[
|w_s(x, y, t) - w_0(x, y, t)| \leq 2 \sup_{\tau \in (0, t]} q^V(\theta, y, \tau) e^{\|V\|_{u,0}(\theta)} \mathbb{P}(\zeta^V_\theta(x) \leq s),
\]

we know that, as \( s \searrow 0 \), \( w_s \to w_0 \) uniformly on compact subsets of \( (0, \theta)^2 \times (0, \infty) \),

\[
w_s(x, y, t) = \int_{(0, \infty)} w_0(\xi, y, t - s) q^V(x, \xi, s) d\xi,
\]
and it is clear that the right-hand side is a continuous function of \((x,y,t) \in (0,\theta)^2 \times (0,\infty)\).

We next note that

\[
\int_{(0,\theta)} \varphi(y)q^Y_\theta(x,y,t)\,dy = \mathbb{E}
\left[e^{\int_0^t V(Y(\tau,x))\,d\tau} \varphi(Y(t,x)), \zeta_\theta^Y(x) > t\right]
\]

for bounded, Borel measurable \(\varphi\) on \([0,\theta]\) which vanishes on \([0,\theta]\). Indeed, simply write the right-hand side of (3.19) as the difference between the expectation of the integrand without any restriction on \(\zeta_\theta^Y(x)\) and the one over \(\{\zeta_\theta^Y(x) \leq t\}\). As a consequence of (3.19) it is obvious that \(q^Y_\theta(x,y,t)\) is a nonnegative function which satisfies the asserted upper bound. In addition, the first equality in (3.18) also follows from (3.19) combined with the Markov property. Namely,

\[
\begin{align*}
\int_{(0,\theta)} \varphi(y)q^Y_\theta(x,y,s+t)\,dy &= \mathbb{E}
\left[e^{\int_0^{s+t} V(Y(\tau,x))\,d\tau} \varphi(Y(s+t,x)), \zeta_\theta^Y(x) > s+t\right] \\
&= \mathbb{E}
\left[e^{\int_0^s V(Y(\tau,x))\,d\tau} \int_{(0,\theta)} \varphi(y)q^Y_\theta(Y(s,x),y,t)\,dy, \zeta_\theta^Y(x) > s\right] \\
&= \int_{(0,\theta)} \varphi(y) \left(\int_{(0,\theta)} q^Y_\theta(\xi,y,t)q^Y_\theta(x,\xi,s)\,d\xi\right)\,dy.
\end{align*}
\]

To prove the second equality in (3.18), we will again apply (3.19). However, before doing so, note that (1.3) plus the Markov property for \(\{Y(t,x) : (t,x) \in (0,\infty)^2\}\) implies that, for any \(t > 0\) and nonnegative, Borel measurable \(F\) on \(C([0,t];[0,\infty])\),

\[
\int_{(0,\infty)} \mathbb{E}[F \circ (Y(\cdot,x)\mid [0,t]), \zeta_\theta^Y(x) > t] \frac{dx}{x} = \int_{(0,\infty)} \mathbb{E}[F \circ (\tilde{Y}(\cdot,y)\mid [0,t]), \zeta_\theta^Y(y) > t] \frac{dy}{y},
\]

where \(\tilde{Y}(\tau,y) = Y((t-\tau)^+,y)\). To see this, note that it suffices to check it for \(F\)'s of the form \(F(\omega) = \prod_{m=0}^n \varphi_m(\omega(\tau_m))\) for some \(n \geq 1\), \(0 = \tau_0 < \cdots < \tau_n = t\), \(\omega \in C([0,t];[0,\infty])\), and \(\{\varphi_m : 0 \leq m \leq n\} \subseteq C_c((0,\infty);[0,\infty])\), in which case it is an easy application of the Markov property and (1.3). Returning to the second equality in (3.18), take

\[
F(\omega) = \varphi_0(\omega(0))e^{\int_0^t V(\omega(\tau))\,d\tau} \varphi_1(\omega(t))1_A(\omega),
\]

where \(A = \{\omega : \omega(\tau) \neq \theta\text{ for }\tau \in [0,t]\}\). Then

\[
F \circ (\tilde{Y}(\cdot,y)\mid [0,t]) = \varphi_0(Y(t,x))e^{\int_0^t V(Y(\tau,x))\,d\tau} \varphi_1(Y(0,x))1_{(t,\infty)}(\zeta_\theta^Y(x)),
\]

and so, by \((*)\),

\[
\int\int_{(0,\theta)^2} \varphi_0(x)q^Y_\theta(x,y,t)\varphi_1(y)\frac{dxdy}{x} = \int\int_{(0,\theta)^2} \varphi_0(x)q^Y_\theta(y,x,t)\varphi_1(y)\frac{dxdy}{x}
\]

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for all nonnegative, Borel measurable \( \phi_0 \) and \( \phi_1 \) which vanish at 0. Together with the continuity already proved, this shows that \( q^V_0(x, y, t) \) satisfies the second part of (3.18).

Because it is clear that, for each \( (y, t) \in (0, \theta) \times (0, \infty) \), \( q^V_0(x, y, t) \to 0 \) as \( x \to \{0, \theta\} \) and that, by (3.19), \( q^V_0(\cdot, y, t) \to \delta_y \) as \( t \to \infty \), all that remains to be shown is that, for each \( y \in (0, \theta) \), \( (x, t) \in (0, \theta) \times (0, \infty) \to q^V_0(x, y, t) \) is smooth and satisfies \( \partial_t w(x, t) = x\partial_x^2 w(x, t) + V(x)w(x, t) \). But, by the second equality in (3.18), this is equivalent to showing that \( (y, t) \to q^V_0(x, y, t) \) is smooth and satisfies \( \partial_t w(y, t) = \partial_x^2 (y\tilde{w}(y, t)) + V(y)\tilde{w}(y, t) \). Moreover, by standard regularity theory for solutions to parabolic equations, we will know that it is a smooth solution to this equation as soon as we show that it is a solution in the sense of Schwartz distributions. Finally, by an elementary application of Itô’s formula and Doob’s stopping time theorem, we know from (3.19) that

\[
\int_{(0, \theta)} \varphi(y)q^V_0(x, y, t) \, dy - \varphi(x) = \mathbb{E} \left[ \int_0^{t \wedge \tau} \exp \left( \int_0^\tau V(Y(\sigma, x)) \, d\sigma \right) \left( Y(\tau, x)\partial_y^2 \varphi(Y(\tau, x)) + V(Y(\tau, x))\varphi(Y(\tau, x)) \right) \, d\tau \right]
\]

for any \( \varphi \in C_c^\infty((0, \theta); \mathbb{R}) \).

\section{4. Back to Wright–Fisher.}

We are now ready to return to the Wright–Fisher equation. To be precise, let \( \psi \) and \( b \) be the functions defined in (3.3) and (3.4), and set \( c(x) = \frac{b(x)}{x} \). Given \( \beta \in (0, 1) \), let \( c_\beta \) be a smooth, compactly supported function which coincides with \( c \) on \( (0, \psi(\beta)) \), and define

\[
\begin{align*}
(4.1) \quad p_\beta(x, y, t) &= \frac{1}{y(1 - y)} \frac{\psi(y)\psi(x)^{V_\beta}(\psi(x), \psi(y), t)}{\sqrt{\psi(x)^\psi(y)}} \quad \text{for } (x, y, t) \in (0, \beta)^2 \times (0, \infty), \\
\text{where } V_\beta(x) &= -x \left( \frac{c_\beta(x)}{2} + \frac{c_\beta(x)^2}{4} \right).
\end{align*}
\]

By (3.2) and (3.18),

\[
(4.2) \quad p_\beta(x, y, s + t) = \int_{(0, \beta)} p_\beta(\xi, y, t) p_\beta(x, \xi, s) \, d\xi
\]

and

\[
y(1 - y)p_\beta(x, y, t) = x(1 - x)p_\beta(y, x, t).
\]

\begin{lemma}
For each \( \beta \in (0, 1) \) and \( \varphi \in C_c((0, \beta); \mathbb{R}) \),
\[
(4.3) \quad \mathbb{E} \left[ \varphi(X(t, x)), \zeta_\beta^X(x) > t \right] = \int_{(0, \beta)} \varphi(y)p_\beta(x, y, t) \, dy \quad \text{for } (x, t) \in (0, \beta) \times (0, \infty).
\]

Furthermore, if \( 0 < \alpha < \beta < \gamma < 1 \) and \( \{\eta_{n, \alpha, \beta}^X(x) : n \geq 0\} \) is defined as in (2.8), then
\[
(4.4) \quad p_\gamma(x, y, t) = p_\alpha(x, y, t) + \sum_{n=1}^{\infty} \mathbb{E} \left[ p_\beta(\alpha, y, t - \eta_{2n, \alpha, \beta}^X(x)), \eta_{2n, \alpha, \beta}^X(x) < t \wedge \zeta_\gamma^X(x) \right]
\]

for \( (x, y, t) \in (0, \alpha)^2 \times (0, \infty) \).
Proof. To prove (4.3), let \( u(x,t) \) denote the right-hand side, and set \( w(x,t) = u(\psi^{-1}(x),t) \). Then, using the second equality in (3.4), one can easily check that

\[
w(x,t) = e^{-C_\beta(x)} \int_{(0,\psi(\beta))} \eta^\alpha_{\psi(\beta)}(x,\xi,t) \tilde{\varphi}(\xi) \, d\xi,
\]

where \( C_\beta(x) = \frac{1}{\beta} \int_0^x c_\beta(\xi) \, d\xi \) and \( \tilde{\varphi} = e^{C_\beta \varphi} \circ \psi^{-1} \). Hence, by Lemmas 3.1 and 3.3, \( w \) is smooth and satisfies \( \partial_t w(x,t) = x \partial_x^2 w(x,t) + xc(x) \partial_x w(x,t) \) in \((0,\psi(\beta)) \times (0,\infty)\) with boundary conditions \( w(0,t) = 0 = w(\psi(\beta),t) \) and \( \lim_{t \to 0} w(\cdot,t) = \varphi \circ \psi^{-1} \).

Thus, using (3.2), one can check that \( u \) is smooth on \((0,\beta) \times (0,\infty)\) and satisfies \( \partial_t u(x,t) = x(1-x) \partial_x^2 u(x,t) \) there with boundary conditions \( u(0,t) = 0 = u(\beta,t) \) and \( \lim_{t \to 0} u(\cdot,t) = \varphi \). In particular, one can use Itô’s formula and Doob’s stopping time theorem to conclude from this that \( u(x,t) \) equals the left-hand side of (4.3).

Given (4.3), the proof of (4.4) is essentially the same as that of (2.9). The only change is that one has to take into account the condition \( \zeta^X(\cdot,t) > t \), but this causes no serious difficulty. \( \square \)

Before going further, we will need the estimates contained in the following lemma.

**Lemma 4.2.** Let \( 0 < x < \alpha < \beta < 1 \) and \( t \in [0,1] \). Then

\[
P(\zeta^Y_{\psi(\alpha)}(\psi(x)) \leq t) \leq \frac{\psi(x)}{\psi(\alpha)} e^{-\left(\frac{\Psi(\beta)-\Psi(\alpha)}{4\Psi(\beta)t}\right)^2}
\]

and

\[
P(\eta^X_{2n,[\alpha,\beta]}(x) \leq t) \leq \frac{x}{\alpha} e^{-4n^2(\alpha-x)^2} \quad \text{for } n \geq 1.
\]

**Proof.** Because \( Y(\cdot,\psi(x)) \) and \( X(\cdot,x) \) get absorbed at 0 and, up to the time they hit \( \{0,1\} \), are random time changes of Brownian motion, one has

\[
P(\zeta^Y_{\psi(\alpha)}(\psi(x)) < \infty) = \frac{\psi(x)}{\psi(\alpha)} \quad \text{and} \quad P(\zeta^X_{\psi(\alpha)}(\psi(x)) < \infty) = \frac{x}{\alpha}.
\]

Further, because, by the Markov property, given that \( \zeta^Y_{\psi(\alpha)}(\psi(x)) \leq \infty \), \( \zeta^Y_{\psi(\alpha)}(\psi(x)) - \zeta^Y_{\psi(\alpha)}(\psi(x)) \) is independent of \( \zeta^Y_{\psi(\alpha)}(\psi(x)) \) and has the same distribution as \( \zeta^Y_{\psi(\alpha)}(\psi(x)) \):

\[
P(\zeta^Y_{\psi(\alpha)}(\psi(x)) \leq t) \leq \frac{\psi(x)}{\psi(\alpha)} P(\zeta^Y_{\psi(\alpha)}(\psi(x)) \leq t).
\]

Similarly,

\[
P(\eta^X_{2n,[\alpha,\beta]}(x) \leq t) \leq \frac{2n}{\alpha} P(\eta^X_{2n,[\alpha,\beta]}(x) \leq t).
\]

To complete the first estimate, use Itô’s formula, Doob’s stopping time theorem, and Fatou’s lemma to see that \( e^{\lambda \psi(\beta) \int [e^{-\lambda^2 \psi(\beta) \zeta^Y_{\psi(\alpha)}(\psi(x))}] \, d\tau} \) is dominated by

\[
\lim_{t \to \infty} E \left[ \exp \left( \lambda Y(t \wedge \zeta^Y_{\psi(\beta)}(\psi(\alpha)),\psi(\alpha)) - \lambda^2 \int_0^{t \wedge \zeta^Y_{\psi(\beta)}(\psi(\alpha))} Y(\tau,\psi(\alpha)) \, d\tau \right) \right] = e^{\lambda \psi(\alpha)}
\]

\( \forall \lambda \in \mathbb{R} \). Hence,

\[
P(\zeta^Y_{\psi(\alpha)}(\psi(\alpha)) \leq t) \leq \exp \left( \lambda^2 \psi(\beta) t - \lambda (\psi(\beta) - \psi(\alpha)) \right) \quad \forall \lambda \in \mathbb{R},
\]

and so the asserted estimate follows when one takes \( \lambda = \frac{\psi(\beta) - \psi(\alpha)}{2\psi(\beta) t} \).
The argument for the second estimate is similar. Namely, for any \( n \geq 0 \), given that \( \eta_{n, [\alpha, \beta]}^X (\alpha) < \infty \), \( \eta_{n+1, [\alpha, \beta]}^X (\alpha) - \eta_{n, [\alpha, \beta]}^X (\alpha) \) is independent of \( \eta_{n, [\alpha, \beta]}^X (\alpha) \) and has the same distribution as, depending on whether \( n \) is even or odd, \( \zeta_\beta (\alpha) \) or \( \zeta_\alpha (\beta) \). Hence, for \( n \geq 1 \) and \( \lambda \in \mathbb{R} \),

\[
E[e^{-\lambda^2 \eta_{2n, [\alpha, \beta]}^X (\alpha)}] = E[e^{-\lambda^2 \zeta_{\beta}^X (\beta)}]^n E[e^{-\lambda^2 \zeta_{\alpha}^X (\alpha)}]^n.
\]

Finally, one takes into account the fact that \( x(1-x) \leq \frac{1}{4} \) for \( x \in [0, 1] \), the same distribution as, depending on whether \( n \) is even or odd, \( \zeta_\beta (\alpha) \) or \( \zeta_\alpha (\beta) \). Hence, for \( n \geq 1 \) and \( \lambda \in \mathbb{R} \),

\[
E[e^{-\lambda^2 \zeta_{\beta}^X (\beta)} \vee E[e^{-\lambda^2 \zeta_{\alpha}^X (\alpha)}] \leq e^{-\lambda (\beta - \alpha)} \text{ for all } \lambda > 0
\]

and therefore that

\[
\mathbb{P}(\eta_{2n, [\alpha, \beta]}^X (\alpha) \leq t) \leq \exp \left( -\frac{4n^2(\beta - \alpha)^2}{t} \right).
\]

**Theorem 4.3.** There is a unique continuous function \( (x, y, t) \in (0, 1)^2 \times (0, \infty) \mapsto p(x, y, t) \in (0, \infty) \) such that

\[
\int_{(0,1)} \varphi(y)p(x, y, t) \, dy = E[\varphi(X(t, x))] \text{ for } (x, t) \in (0, 1) \times (0, \infty)
\]

and all bounded, Borel measurable functions \( \varphi \) on \([0, 1]\) which vanish on \( \{0, 1\} \). Moreover, \( p(x, y, t) \) satisfies (2.5), (2.6), (2.7), and, for each \( 0 < \alpha < \beta < 1 \),

\[
p(x, y, t) = p_\beta(x, y, t) + \sum_{n=1}^{\infty} E[p_\beta(\alpha, y, t - \eta_{2n, [\alpha, \beta]}^X (x)), \eta_{2n, [\alpha, \beta]}^X (x) < t]
\]

\( \forall (x, y, t) \in (0, \alpha]^2 \times (0, \infty) \). Finally, \( p(x, y, t) \) is smooth and, for each \( y \in (0, 1) \), satisfies

\[
\partial_t p(x, y, t) = x(1-x)\partial_y^2 p(x, y, t) \text{ on } (0, 1) \times (0, \infty)
\]

with \( p(0, y, t) = 0 = p(1, y, t) \) and \( \lim_{t \to 0} p(\cdot, y, t) = \delta_y \).

**Proof.** Let \( 0 < \alpha < \beta < 1 \) and \( (x, t) \in (0, \alpha] \times (0, \infty) \) be given. From (4.4) and Lemma 4.2, it is clear that the family \( \{p_\gamma(x, \cdot, t) \mid (0, \alpha] : \gamma \in (\beta, 1)\} \) is equicontinuous and, by (4.4), \( \gamma \rightsquigarrow p_\gamma(x, \cdot, t) \) is nondecreasing. Hence, there is a unique continuous function \( y \in (0, 1) \mapsto p(x, y, t) \in (0, \infty) \) such that \( p(x, y, t) = \lim_{\gamma \searrow 1} p_\gamma(x, y, t) \). Furthermore, from (4.3) and (4.4), one knows that (4.5) and (4.6) hold. In addition, (2.5) and (2.7) follow from (4.2), and (2.6) follows from (4.5) together with the observation that \( 1 - X(t, x) \) has the same distribution as \( X(t, 1-x) \).

Knowing (2.5), (2.7), and (4.5) and that \( p(x, \cdot, t) \) is continuous, one can easily check that \( (x, y, t) \rightsquigarrow p(x, y, t) \) is continuous. Finally, the proof that \( p(x, y, t) \) is smooth and satisfies (4.6) is a repeat of the sort of reasoning which we used in the final part of the proof of Lemma 3.3.

**Corollary 4.4.** Set \( \bar{p}(x, y, t) = y(1-y)p(x, y, t) \) and, for \( \beta \in (0, 1) \),

\[
\bar{q}^\beta_x(\xi, \eta, t) = \eta q^\beta_x(\xi, \eta, t).
\]
Then, for each $0 < \alpha < \beta$ and $\theta \in (0,1)$,
\[
\left| \sqrt{\psi'(x) \psi'(y)} \bar{p}(x,y,t) - q^V_{\psi}(\psi(x), \psi(y), t) \right| \\
\leq K(\alpha, \beta, \theta) e^{U_\beta(\theta) \beta - \alpha} \exp \left[ - \frac{\mu_\beta(\beta - \alpha)^2}{t} \right]
\]
for all $(x, y, t) \in (0, \theta \alpha)^2 \times (0, 1]$, where (cf. (4.1))
\[
U_\beta = \sup_{\xi \in (0, \psi(\beta))] \nu_\beta(\psi(\beta)) \wedge 4\psi'(\beta) + 1, \text{ and } K(\alpha, \beta, \theta) = \frac{2\pi^2 \beta^3}{\psi(\alpha) \alpha^4 (1 - \theta)^2}.
\]
In particular, if
\[
O_\beta = \sup \{ V_\beta(\eta) - V_\beta(\xi) : (\xi, \eta) \in (0, \psi(\beta))] \} \text{ and } \nu_\beta = \frac{1}{4\psi'(\beta)} \wedge 3,
\]
then (cf. (1.12))
\[
\left| \sqrt{\psi'(x) \psi'(y)} \bar{p}(x,y,t) - 1 \right| \leq K(\alpha, \beta, \theta) e^{O_\beta(\beta - \alpha) \psi(y) \psi(x))} \exp \left[ - \frac{\nu_\beta(\beta - \alpha)^2}{t} \right]
\]
for all $(x, y, t) \in (0, \theta \alpha) \times (0, 1]$ with $\sqrt{\psi(y)} - \sqrt{\psi(x)} \leq \beta - \alpha$.

Proof. Because
\[
\bar{p}(x,y,t) = \bar{p}(x,y,t) + \sum_{n=1}^{\infty} E[\bar{p}(\alpha, \psi(x,y,t) - \eta_{2n, [\alpha, \beta]}(x), \eta_{2n, [\alpha, \beta]}(x) < t)],
\]
we know that $\sqrt{\psi'(x) \psi'(y)} \bar{p}(x,y,t)$ equals
\[
\bar{q}^V_{\psi(\beta)}(\psi(x), \psi(y), t) + \sqrt{\psi'(x)} \sum_{n=1}^{\infty} E[\bar{q}^V_{\psi(\beta)}(\psi(x), \psi(y), t - \eta_{2n, [\alpha, \beta]}(x), \eta_{2n, [\alpha, \beta]}(x) < t)].
\]
Thus, $\sqrt{\psi'(x) \psi'(y)} \bar{p}(x,y,t)$ is dominated by
\[
\bar{q}^V_{\psi(\beta)}(\psi(x), \psi(y), t) + \sqrt{\psi'(x) \psi'(y)} \sup_{\tau \in (0, t)} \bar{q}^V_{\psi(\beta)}(\psi(x), \psi(y), t) \sum_{n=1}^{\infty} E(\eta_{2n, [\alpha, \beta]}(x) < t)
\]
and $\sqrt{\psi'(x) \psi'(y)} \bar{p}(x,y,t)$ dominates $\sqrt{\psi'(x) \psi'(y)} \bar{p}(x,y,t) = \bar{q}^V_{\psi(\beta)}(\psi(x), \psi(y), t)$, which, by Lemma 3.3, is equal to
\[
\bar{q}^V_{\psi(\beta)}(\psi(x), \psi(y), t) - \mathbb{E} \left[ e^{\int_{\xi}^{\psi(\beta)}(\psi(x)) dt} \right] \bar{q}^Y_{\psi(\beta)}(\psi(x), \psi(y), t - \gamma_{\psi(\beta)}(\psi(x)), \gamma_{\psi(\beta)}(\psi(x)) < t) \right].
\]
Since $(1 - \xi) \frac{1}{2} \psi'(\xi) \in [1, \frac{1}{2}]$ for $\xi \in [0, 1]$ and, by the second part of Lemma 4.2,
\[
(4.8) \sum_{n=1}^{\infty} E(\eta_{2n, [\alpha, \beta]}(x) < t) \leq \frac{x}{\alpha} \left( 1 + \frac{\sqrt{\pi t}}{4(\beta - \alpha)} \right) e^{-\frac{4(\beta - \alpha)^2}{\pi t}} \leq \frac{2x}{\alpha(\beta - \alpha)} e^{-\frac{4(\beta - \alpha)^2}{\pi t}},
\]
the right-hand side of the upper bound can be replaced by
\[ \bar{q}^{V_\beta}(\psi(x), \psi(y), t) \geq \frac{\tau}{2} \sup_{\tau \in (0,t]} \bar{q}^{V_\beta}(\psi(x), \psi(y), \tau) \frac{2e}{\alpha(\beta - \alpha)} e^{-\frac{4(\beta - \alpha)^2}{t}}. \]

At the same time, because the derivative of \( \sqrt{\psi} \) dominates 1 and \( y \leq \theta \alpha \), the upper bound in (1.10) leads to
\[
\bar{q}^{V_\beta}(\psi(\alpha), \psi(y), \tau) \leq e^{U_\beta} \sup_{\tau \in (0,t]} \frac{\psi(\alpha)\psi(y)}{\tau^2} e^{-\frac{(\sqrt{\psi(y)} - \sqrt{\psi(\alpha)})^2}{\tau}} \leq e^{U_\beta} \sup_{\tau \in (0,t]} \frac{\psi(\alpha)\psi(y)}{\tau^2} e^{-\frac{\alpha^2(1-\theta)^2}{\tau}} \leq e^{U_\beta} \frac{\psi(\alpha)\psi(y)}{\alpha^4(1-\theta)^4}
\]
for \( \tau \in (0,t] \). Thus, after combining this with the preceding, we find that
\[
\sqrt{\psi'(x)\psi'(y)}\bar{p}(x, y, t) \leq \bar{q}^{V_\beta}(\psi(x), \psi(y), t) + \frac{\sqrt{2\pi}x\psi'(\psi(y))e^{U_\beta}}{\alpha^4(1-\theta)^4(\beta - \alpha)} e^{-\frac{4(\beta - \alpha)^2}{t}},
\]
which, because \( \xi \leq \psi(\xi) \leq \pi \xi \), means that
\[
(4.9) \quad \sqrt{\psi'(x)\psi'(y)}\bar{p}(x, y, t) \leq \bar{q}^{V_\beta}(\psi(x), \psi(y), t) + \frac{\sqrt{2\pi}x\psi'(\psi(y))e^{U_\beta}}{\alpha^4(1-\theta)^4(\beta - \alpha)} e^{-\frac{4(\beta - \alpha)^2}{t}}.
\]

In view of the lower bound in the first paragraph of the proof, to prove the complementary lower bound, we need to estimate the term on the right which is preceded by a minus sign. But by the first part of Lemma 4.2 and (1.10), it is clear that this term is dominated by
\[
\mathbb{E}[e^{\psi(\alpha)\psi(x)U_\beta} \bar{q}^{V_\beta}(\psi(\beta), \psi(y), t - \zeta^{\psi(\beta)}(\psi(x))) \zeta^{\psi(\beta)}(\psi(x)) < t)] \leq \frac{\psi(x)e^{U_\beta}}{\psi(\alpha)} e^{-\frac{\psi(y)\psi(x)(\beta - \alpha)^2}{4\psi(\beta)}} \sup_{\tau \in (0,t]} \bar{q}(\psi(\beta), \psi(y), \tau) \leq e^{U_\beta} e^{-\frac{\psi(y)\psi(x)(\beta - \alpha)^2}{4\psi(\beta)}} \sup_{\tau \in (0,t]} \frac{\psi(\alpha)}{\psi(y)} e^{\frac{(\sqrt{\psi(y)} - \sqrt{\psi(\alpha)})^2}{\tau}} \leq \frac{\psi(x)\psi(y)\psi(\beta)e^{U_\beta}}{\psi(\alpha)\alpha^4(1-\theta)^4} \exp \left( -\frac{(1+4\psi(\beta))(\beta - \alpha)^2}{4\psi(\beta)t} \right),
\]
since \( (\sqrt{\psi(\beta)} - \sqrt{\psi(y)})^2 \geq \alpha^2(1-\theta)^2 + (\beta - \alpha)^2 \). Hence, we now know that
\[
(4.10) \quad \sqrt{\psi'(x)\psi'(y)}\bar{p}(x, y, t) \geq \bar{q}^{V_\beta}(\psi(x), \psi(y), t) - \frac{\psi(x)\psi(y)\psi(\beta)e^{U_\beta}}{\psi(\alpha)\alpha^4(1-\theta)^4} \exp \left( -\frac{(1+4\psi(\beta))(\beta - \alpha)^2}{4\psi(\beta)t} \right).
\]

Given (4.9) and (4.10), the initial assertion follows immediately. To prove the second estimate, note that
\[
\bar{q}(\psi(x), \psi(y), t) \geq \begin{cases} \frac{\psi(x)\psi(y)}{t^2} e^{-\frac{1}{t^2}} & \text{if } \psi(x)\psi(y) \leq t^2, \\ \frac{\psi(x)\psi(y)^2}{t^2} e^{-\frac{1}{t^2}} & \text{if } \psi(x)\psi(y) \geq t^2. \end{cases}
\]
Hence, since \( \psi(x) + \psi(y) \geq (\sqrt{\psi(y)} - \sqrt{\psi(x)})^2 \), the second estimate is an easy consequence of the first when one takes into account the condition that \( |\sqrt{\psi(y)} - \sqrt{\psi(x)}| \leq \beta - \alpha \).

**Corollary 4.5.** For each \( 0 < \alpha < \beta < 1 \) and \( \theta \in (0, 1) \),

\[
|\sqrt{\psi(x)}\psi'(y)\tilde{p}(x,y,t) - \tilde{q}(\psi(x), \psi(y), t)| \\
\leq te^\alpha \|V_{\beta}\|_u \left[ \|V_{\beta}\|_u \tilde{q}(\psi(x), \psi(y), t) + \frac{\pi^2 K(\alpha, \beta, \theta)}{e(\beta - \alpha)^3} \psi(x)\psi(y)e^{-(\alpha - \beta)^2} \right]
\]

\( \forall (x, y, t) \in (0, \theta\alpha]^2 \times (0, 1) \) and

\[
\leq te^\alpha \|V_{\beta}\|_u \left[ \|V_{\beta}\|_u + \frac{\pi^2 K(\alpha, \beta, \theta)}{e(\beta - \alpha)^3} \left( t^2 \vee (\psi(x)\psi(y)) \right) \right]
\]

\( \forall (x, y, t) \in (0, \theta\alpha]^2 \times (0, 1) \) satisfying \( |\sqrt{\psi(y)} - \sqrt{\psi(x)}| \leq \beta - \alpha \).

**Proof.** Just as in the proof of Corollary 4.4, the second inequality is a consequence of the first. Furthermore, given the first inequality in Corollary 4.4, the first inequality here comes down to the estimate

\[
|\tilde{q}^{V_{\beta}}(\xi, \eta, t) - \tilde{q}(\xi, \eta, t)| \leq \left( \sum_{n=1}^{\infty} \left( \frac{t\|V_{\beta}\|_u}{n!} \right)^n \right) \tilde{q}(\xi, \eta, t),
\]

which is a trivial consequence of (3.12) and (3.13).

**5. Derivatives.** In order to get regularity estimates, it will be important to know how to represent derivatives of the solutions to (1.1) in terms to derivatives of the initial data. For this purpose, observe that if \( u \) is a smooth solution to (1.1) and \( u^{(m)} \) is its \( m \)th derivative with respect to \( x \), then \( u^{(m)} \) satisfies

\[
(5.1) \quad \partial_t w(x, t) = x\partial_x^2 w(x, t) + m\partial_x w(x, t).
\]

Thus, we should expect that

\[
u^{(m)}(x, t) = \int_{(0, \infty)} \varphi^{(m)}(y)q^{(m)}(x, y, t) \, dy,
\]

where \( \varphi^{(m)} \) is the \( m \)th derivative of the initial data \( \varphi \) and \( q^{(m)}(x, y, t) \) is the fundamental solution to (5.1).

In order to verify this suspicion, we need to know something about \( q^{(m)}(x, y, t) \) when \( m \geq 1 \), and there are two ways of going about this. The first is to notice that if \( w \) satisfies (5.1) and \( v(x, t) = w(x^2, t) \), then \( v \) satisfies

\[
\partial_t v(x, t) = \frac{1}{4} \left( \partial_x^2 v(x, t) + \frac{2m - 1}{x} \partial_x v(x, t) \right).
\]

Since, apart from the factor of \( \frac{1}{4} \), the operator on the right-hand side is the radial part of the Laplacian in \( \mathbb{R}^{2m} \), one sees that

\[
(5.2) \quad q^{(m)}(x, y, t) = \frac{y^{m-1} e^{-\frac{xy}{t}}}{t^m} q^{(m)} \left( \frac{xy}{t^2} \right), \quad \text{where} \quad q^{(m)}(\xi) = \frac{1}{2\pi^m} \int_{S^{2m-1}} e^{\frac{i}{2} \xi \cdot \omega} d\omega,
\]
\(\omega_0\) being any reference point on the \(2m-1\) unit sphere \(S^{2m-1}\) in \(\mathbb{R}^{2m}\) and \(d\omega\) denoting integration with respect to the surface measure for \(S^{2m-1}\). Starting from here, one can use elementary facts about Bessel functions to see that \(q^{(m)}\) is given by the series

\[
q^{(m)}(\xi) = \sum_{n=0}^{\infty} \frac{\xi^n}{n!(n+m-1)!}.
\]

Alternatively, knowing that \((5.2)\) holds, one can proceed as in section 1 to show \(q^{(m)}\) must solve

\[
\xi \partial^2_{\xi} q^{(m)}(\xi) + m \partial_{\xi} q^{(m)}(\xi) - q^{(m)}(\xi) = 0
\]

and therefore that

\[
q^{(m)}(\xi) = q^{(m)}(0)(m-1)! \sum_{n=0}^{\infty} \frac{\xi^n}{n!(n+m-1)!}.
\]

Hence, since, by the expression for \(q^{(m)}\) in \((5.2)\), \(q^{(m)}(0)\) must be the area of \(S^{2m-1}\) divided by \(2\pi^m\), \((5.3)\) follows.

Observe that, as distinguished from \(q(x,y,t)\), \(q^{(m)}(x,\cdot,t)\) has a total integral 1 for all \(m \geq 1\) and \((x,t) \in (0,\infty)^2\). To understand the behavior of \(q^{(m)}(x,y,t)\) for small \(t > 0\), one can use (cf. (7.4) and (7.6)) the expression in \((5.2)\). Alternatively, proceeding as in the second derivation of \((1.12)\), one knows that there is an \(\delta_m \in (0,1)\) such that \(t^{\frac{m}{2}}q^{(m)}(1,1,t) \in (\delta_m,\delta_m^{-1})\) for \(t \in (0,1]\). Thus,

\[
\delta_m \xi^{\frac{m}{2}} e^{2\xi} \leq q^{(m)}(\xi) \leq \delta_m^{-1} \xi^{\frac{m}{2}} e^{2\xi} \quad \text{for } \xi \geq 1,
\]

and so

\[
(5.4) \quad \delta_m \frac{y^{m-1}(xy)^{\frac{1}{2}}}{t^{\frac{m}{2}}} e^{-\frac{(\frac{m}{2}-\frac{1}{2})^2}{t}} \leq q^{(m)}(x,y,t) \leq \delta_m^{-1} \frac{y^{m-1}(xy)^{\frac{1}{2}}}{t^{\frac{m}{2}}} e^{-\frac{(\frac{m}{2}-\frac{1}{2})^2}{t}}
\]

for \(xy \geq t^2\). On the other hand, by \((5.3)\), after readjusting \(\delta_m\), one has

\[
(5.5) \quad \delta_m \frac{y^{m-1}}{t^m} e^{-\frac{ru}{t}} \leq q^{(m)}(x,y,t) \leq \delta_m^{-1} \frac{y^{m-1}}{t^m} e^{-\frac{ru}{t}} \quad \text{when } xy \leq t^2.
\]

Finally, set \(q(0)(x,y,t) = q(x,y,t)\). Then, because \(q^{(m)}(\xi) = \partial_{\xi}^m q(\xi)\), it is easy to check that

\[
\partial_x q^{(m)}(x,y,t) = \frac{1}{t} \left( q^{(m+1)}(x,y,t) - q^{(m)}(x,y,t) \right) \quad \forall m \geq 0
\]

and therefore that

\[
(5.6) \quad \partial_x^m q^{(k)}(x,y,t) = \frac{1}{t^m} \sum_{\ell=0}^{m} (-1)^\ell \binom{m}{\ell} q^{(m-k+\ell)}(x,y,t) \quad \forall k, m \in \mathbb{N}.
\]

**Theorem 5.1.** Suppose that \(\varphi \in C^m((0,\infty) ; \mathbb{R})\), set \(\varphi^{(\ell)} = \partial_\xi^\ell \varphi\), and assume that \(\varphi^{(\ell)}\) is bounded on \((0,1)\) and has subexponential growth at \(\infty\) for each \(0 \leq \ell \leq m\). If \(\varphi\) tends to \(0\) at \(0\), then

\[
(5.7) \quad \partial_x^m \int_{(0,\infty)} \varphi(y) q(x,y,t) \, dy = \int_{(0,\infty)} \varphi^{(m)}(y) q^{(m)}(x,y,t) \, dy.
\]
Moreover, for any \( \ell \geq 1 \),

\[
(5.8) \quad \partial_x^\ell \int_{(0, \infty)} \varphi(y) q^{(\ell)}(x, y, t) \, dy = \int_{(0, \infty)} \varphi^{(m)}(y) q^{(m+\ell)}(x, y, t) \, dy
\]
even if \( \varphi \) does not vanish at 0.

**Proof.** Since every \( \varphi \) satisfying our hypotheses can be written as the \( \ell \)th derivative of one which vanishes at 0, it is clear that (5.8) is an immediate corollary of (5.7).

In proving (5.7), first observe that, by an obvious cutoff argument and the estimates in (5.4) and (5.5), it suffices to handle \( \varphi \)'s which vanish off of a compact subset of \([0, \infty)\). Second, suppose that we knew (5.7) when \( \varphi \in C^\infty_c((0, \infty); \mathbb{R}) \). Given a \( \varphi \in C^m((0, \infty); \mathbb{R}) \) which vanishes at 0 and to the right of some point in \((0, \infty)\), set \( \varphi_\epsilon(y) = 1_{(2\epsilon, \infty)}(y) \varphi(y-2\epsilon) \) for \( \epsilon > 0 \). Next, choose \( \rho \in C^\infty_c((-1, 1); [0, \infty)) \) with a total integral 1, and set \( \tilde{\varphi}_\epsilon(y) = \rho_\epsilon * \varphi_\epsilon \), where \( \rho_\epsilon(y) = \epsilon^{-1} \rho(\epsilon^{-1} y) \). Then \( \tilde{\varphi}_\epsilon \in C^\infty_c((0, \infty); \mathbb{R}) \), and so we would know that

\[
\partial_x^m \int_{(0, \infty)} \tilde{\varphi}_\epsilon(y) q(x, y, t) \, dy = \int_{(0, \infty)} \tilde{\varphi}_\epsilon^{(m)}(y) q^{(m)}(x, y, t) \, dy.
\]

For each \( (t, x) \in (0, \infty)^2 \), it is clear that the left-hand side of the preceding tends to the left-hand side of (5.7) as \( \epsilon \downarrow 0 \). To handle the right-hand side, write it as the sum of

\[
\int_{(0, 3\epsilon)} \rho_\epsilon^{(m)} * \varphi_\epsilon(y) q^{(m)}(x, y, t) \, dy \quad \text{and} \quad \int_{(3\epsilon, \infty)} \rho_\epsilon * \varphi_\epsilon^{(m)}(y) q^{(m)}(x, y, t) \, dy.
\]

As \( \epsilon \downarrow 0 \), the second of these tends to the right-hand side of (5.7). At the same time, by (5.6), we know that, for each \( (t, x) \in (0, \infty)^2 \), for sufficiently small \( \epsilon > 0 \), the first of these is dominated by a constant times

\[
\int_{(0, 3\epsilon)} y^{m-1} \left( \int_{(0, \infty)} |\rho_\epsilon^{(m)}(\xi)| |\varphi_\epsilon(y - \xi)| \, d\xi \right) \, dy
\]

\[
= \int_{[2\epsilon, 3\epsilon]} |\rho_\epsilon^{(m)}(\xi - 2\epsilon)| \left( \int_{[\xi, 3\epsilon]} y^{m-1} |\varphi(y - \xi)| \, dy \right) \, d\xi
\]

\[
\leq (3\epsilon)^m \left( \int_{(0, 3\epsilon)} |\rho_\epsilon^{(m)}(\xi)| \, d\xi \right) \int_{(0, 3\epsilon)} \frac{|\varphi(y)|}{y} \, dy \to 0 \quad \text{as} \quad \epsilon \downarrow 0.
\]

Hence, it suffices to treat \( \varphi \in C^\infty_c((0, \infty); \mathbb{R}) \).

To prove (5.7) for \( \varphi \in C^\infty_c((0, \infty); \mathbb{R}) \), assume that \( \varphi \) vanishes off of \((a, b)\), and set

\[
u(x, t) = \int_{(0, \infty)} \varphi(y) q(x, y, t) \, dy.
\]

Because

\[
(x\partial_x^\ell)^t \int_{(0, \infty)} \varphi(y) q(x, y, t) \, dy = \int_{(0, \infty)} (y\partial_y^\ell)^t \varphi(y) q(x, y, t) \, dy,
\]

it is obvious that \( \partial_x^\ell \nu(x, t) \) is bounded on \( \frac{1}{2} \times (0, \infty) \) \( \forall \ell \geq 0 \). At the same time, from (5.6) and the estimates in (5.4) and (5.5), we know that, for each \( \ell \geq 0 \) and \( T > 0 \),
\( \partial_x^\ell q(x, y, t) \) is uniformly bounded on \((0, T] \times (a, \infty) \times (0, T]\). Hence, for all \( \ell \geq 0 \) and \( T > 0 \), \( \partial_x^\ell u(x, t) \) is uniformly bounded on \((0, \infty) \times (0, T]\), and so it is now easy to check that \( u^{(m)}(x, t) \equiv \partial_x^m u(x, t) \) is the unique solution to \( \partial_t w(x, t) = x \partial_x^2 w + m \partial_x w(x, t) \) which is bounded on finite time intervals and has an initial value \( \varphi^{(m)} \). Since this means that \( u^{(m)}(x, t) \) is given by the right-hand side of (5.7), we are done. \( \Box \)

**Corollary 5.2.** For \( 0 \leq k \leq m \) and \((s, x, t, y) \in (0, \infty)^2\), set

\[
q^{(m,k)}(x, y, s, t) = \int_{(0, \infty)} q^{(m)}(x, \xi, s) q^{(k)}(\xi, y, t) d\xi.
\]

Then

\[
q^{(m,k)}(x, y, s, t) = \frac{1}{(s + t)^{m-k}} \sum_{j=0}^{m-k} \binom{m-k}{j} s^j t^{m-k-j} q^{(k+j)}(x, y, s + t).
\]

**Proof.** By the Chapman–Kolmogorov equation, (5.9) is obvious when \( k = m \). To prove it in general, assume that it holds for some \( m \) and \( 0 \leq k \leq m \). Then, by (5.6) and the induction hypothesis, for \( 0 \leq k \leq m \),

\[
\begin{align*}
\frac{1}{s} q^{(m+1,k)}(x, y, s, t) - \frac{1}{s} q^{(m,k)}(x, y, s, t) &= \partial_x q^{(m,k)}(x, y, s, t) \\
&= \frac{1}{(s + t)^{m+1-k}} \sum_{j=1}^{m-k} \binom{m-k}{j-1} s^j t^{m+1-k-j} q^{(k+j)}(x, y, s + t) \\
&\quad - \frac{1}{(s + t)^{m+1-k}} \sum_{j=0}^{m-k} \binom{m-k}{j} s^j t^{m+1-k-j} q^{(k+j)}(x, y, s + t),
\end{align*}
\]

and so, again by the induction hypothesis, \( q^{(m+1,k)}(x, y, s, t) \) equals

\[
\begin{align*}
\frac{1}{(s + t)^{m+1-k}} \sum_{j=1}^{m+1-k} \binom{m+1-k}{j-1} s^j t^{m+1-k-j} q^{(k+j)}(x, y, s + t) \\
&\quad + \sum_{j=0}^{m-k} \binom{m-k}{j} s^j t^{m+1-k-j} q^{(k+j)}(x, y, s + t)
\end{align*}
\]

\[
= \frac{1}{(s + t)^{m+1-k}} \sum_{j=0}^{m+1-k} \binom{m+1-k}{j} s^j t^{m+1-k-j} q^{(k+j)}(x, y, s + t). \quad \Box
\]

The reason for our interest in the preceding results is that they allow us to produce rather sharp estimates on the derivatives of \( q^V(x, y, t) \).

**Lemma 5.3.** Set

\[
C_m(V) = \frac{5^m}{2} \max\{ \| \partial^\ell V \|_u : 0 \leq \ell \leq m \}
\]

and

\[
S_m(x, y, t) = \sum_{\ell=0}^{m} \binom{m}{\ell} q^{(\ell)}(x, y, t).
\]
Then
\[
\left| \partial_x^n q (x, y, t) \right| \leq \frac{1 + (tC_m(V))^m \left( e^{t^2 \|V\|_u} - 1 \right) S_m(x, y, t)}{1 - tC_m(V)} t^m
\]
for \((x, y, t) \in (0, \infty)^2 \times (0, 1)\).

Proof. Clearly (cf. (3.11) and (3.13)) it suffices to prove that, for each \(n \in \mathbb{N}\),
\[
\left| \partial_x^m q_n (x, y, t) \right| \leq C_m(V)^{m+n} (2^n \|V\|_u)^{(n-m)^+} \frac{t^n}{(n-m)!} S_m(x, y, t)
\]
for \((x, y, t) \in (0, \infty)^2 \times (0, 1)\). When \(n = 0\) this is obvious from (5.6) with \(k = 0\), and when \(m = 0\) there is nothing to do. Since (5.6) already explains how to proceed for general \(m \geq 1\), we will concentrate on the case when \(m = 1\).

Using (3.11) and Theorem 5.1, one can write \(\partial_x q_1^Y (x, y, t)\) as the sum of
\[
\int_0^\tau \left( \int_{(0, \infty)} \partial_x q(x, \xi, t - \tau) V(\xi) q(\xi, y, \tau) \, d\xi \right) \, d\tau
\]
and
\[
\int_0^\tau \left( \int_{(0, \infty)} q^{(1)}(x, \xi, \tau) \partial_\xi (V(\xi) q(\xi, y, t - \tau)) \, d\xi \right) \, d\tau.
\]

By (5.6) and (5.9), the first of these is dominated by \(\|V\|_u\) times
\[
\int_0^\tau (t - \tau)^{-1} \left( \int_{(0, \infty)} (q(x, \xi, t - \tau) + q^{(1)}(x, \xi, t - \tau)) q(\xi, y, \tau) \, d\xi \right) \, d\tau
= \frac{1}{2} q^{(1)}(x, y, t) + \frac{q(x, y, t)}{t} \int_0^\tau \frac{t + \tau}{t - \tau} \, d\tau \leq \frac{1}{2} q^{(1)}(x, y, t) + \frac{1}{2} q(x, y, t).
\]

As for the second, it can be dominated by
\[
\int_0^\tau \left( \|V'\|_u + \|V\|_u (t - \tau)^{-1} \right) q^{(1,0)}(x, y, \tau, t - \tau) \, d\tau + \log 2 \|V\|_u q^{(1)}(x, y, t)
\leq \left( \frac{1}{2} \|V\|_u + \frac{3t}{8} \|V'\|_u \right) q(x, y, t) + \left( \frac{t}{8} \|V'\|_u + \frac{3}{2} \|V\|_u \right) q^{(1)}(x, y, t).
\]

After combining these, one gets that \(\partial_x q_1^Y (x, y, t) \leq C_1(V) S_1(x, y, t)\) for \(t \in (0, 1]\).

Given the preceding, the argument for \(n \geq 2\) is easy. Namely, by (3.11'),
\[
\partial_x q_n^{Y+1} (x, y, t) = \int_0^t \left( \int_{(0, \infty)} \partial_x q_n^{Y} (x, \xi, t - \tau) V(\xi) q(\xi, y, \tau) \, d\xi \right) \, d\tau.
\]

Thus, one can use the preceding and induction on \(n \geq 1\) to get the asserted estimate.

For general \(m \geq 1\), the strategy is the same. One has to apply the argument just given to estimate \(\partial_x q_Y (x, y, t)\) not only once but \(m\) times. At the end of the \(m\)th repetition, one arrives at the estimate \(\left| \partial_x^m q_n^Y (x, y, t) \right| \leq C_m(V)^n t^n - m S_m(x, y, t)\) for \(0 \leq n \leq m\). After the \(m\)th repetition, one switches from (3.11) to (3.11') and proceeds inductively as above. \(\square\)
Theorem 5.4. Set \( \bar{p}(x,y,t) = y(1-y)p(x,y,t) \). For each \( 0 < \alpha < \beta < 1, \theta \in (0,1), \) and \( m \in \mathbb{Z}^+ \), there exists a \( K_m(\alpha, \beta, \theta) < \infty \) such that

\[
\left| \partial_x^m \bar{p}(x,y,t) \right| \leq K_m(\alpha, \beta, \theta) \psi(y) \left( \frac{q(\psi(x), \psi(y), t) \vee q^{(m)}(\psi(x), \psi(y), t)}{\tau^m} + e^{-4(\beta - \alpha)^2} \right)
\]

\( \forall (x,y,t) \in (0,\theta\alpha] \times (0,1] \). In particular, for each \( \epsilon > 0 \), \( \bar{p}(x,y,t) \) has bounded derivatives of all orders on \( (0,1)^2 \times [\epsilon, \infty) \).

Proof. Given the first assertion, the second assertion is an easy application of the symmetry properties of \( \bar{p}(x,y,t) \), the equation \( \partial_t \bar{p}(x,y,t) = x(1-x)\partial_x^2 \bar{p}(x,y,t) \), and the fact that

\[
\bar{p}(x,y,s+t) = \int_{(0,1)} p(x,\xi,s) \bar{p}(y,\xi,t) d\xi,
\]

which is a consequence of symmetry and the Chapman–Kolmogorov equation for \( p(x,y,t) \).

Next set \( \bar{p}_\beta(x,y,t) = y(1-y)\bar{p}_\beta(x,y,t) \), note that, by (4.2), \( \bar{p}_\beta(x,y,t) = \bar{p}_\beta(y,x,t) \), and observe that, by symmetry,

\[
\partial_x^m \bar{p}(x,y,t) = \partial_x^m \bar{p}_\beta(x,y,t) + \sum_{n=1}^{\infty} E \left[ \partial_x^m \bar{p}_\beta(x,\alpha,t - \eta^{X}_{2n,\alpha,\beta}(y)), \eta^{X}_{2n,\alpha,\beta}(y) < t \right]
\]

and therefore, by (4.8), that

\[
\left| \partial_x^m \bar{p}(x,y,t) \right| \leq \left| \partial_x^m \bar{p}_\beta(x,y,t) \right| + \frac{y}{\alpha} \left( 1 + \frac{\sqrt{\pi t}}{4(\beta - \alpha)} \right) \sup_{\tau \in (0,t)} \left| \partial_x^m \bar{p}_\beta(x,\alpha,\tau) \right| e^{-4(\beta - \alpha)^2}.
\]

In addition, if \( \tilde{q}^{V_\beta}(\xi,\eta,t) = \eta^{V_\beta}(\xi,\eta,t) \), because both \( \bar{p}_\beta \) and \( \tilde{q}^{V_\beta} \) are symmetric, (4.1) implies that \( \bar{p}_\beta(x,y,t) \) equals

\[
\tilde{q}^{V_\beta}(\psi(x), \psi(y), t) = \sqrt{\psi'(x)\psi'(y)} \left[ e^{\int_0^t \zeta_{\psi(\beta)}(\psi(\psi))) d\tau} \right] \frac{\tilde{q}^{V_\beta}(\psi(x), \psi(\beta), t - \zeta_{\psi(\beta)}(\psi(y)))}{\sqrt{\psi'(x)\psi'(y)}}, \quad \zeta_{\psi(\beta)}(\psi(y)) < t.
\]

Thus, there is a \( C_m(\beta) < \infty \) such that

\[
\left| \partial_x^m \bar{p}_\beta(x,y,t) \right| \leq C_m(\beta) \left[ \max_{0 \leq \ell \leq m} \left| (\partial_x^\ell q^{V_\beta})(\psi(x), \psi(y), t) \right| \right]
\]

\[
+ \frac{\psi(y)}{\psi(\alpha)} e^{-\frac{(\psi(\alpha) - \psi(y))^2}{4\psi(\alpha)}} \sup_{\tau \in (0,t)} \max_{0 \leq \ell \leq m} \left| (\partial_x^\ell q^{V_\beta})(\psi(x), \psi(\beta), \tau) \right|.
\]

Finally, by combining these with the estimates in (5.4), (5.5), and Lemma 5.3, using \( (\psi(\beta) - \psi(\alpha))^2 \geq (\psi(\beta) - \psi(\alpha))^2 \), one gets the desired result. \( \square \)

6. Two concluding results. In this section we will present two results which might be of computational interest. The first answers one of the questions which Nick Patterson originally asked. Namely, he wanted to know whether one can justify a Taylor’s approximation for solutions to the Wright–Fisher equation (1.1).
In the following, $L = x(1 - x)\partial_x^2$ is the Wright–Fisher operator, $X(t, x)$ is the Wright–Fisher diffusion given by (2.2), and $\zeta^X(x) = \inf\{t \geq 0 : X(t, x) \notin (0, 1)\}$. By Itô’s formula,
\[
\mathbb{E}[\varphi(X(t, x))] = \varphi(x) + \int_0^t \mathbb{E}[L\varphi(X(\tau, x))] \, d\tau
\]
for any $\varphi \in C^2([0, 1]; \mathbb{R})$. In addition, since $\xi(1 - \xi) \leq \frac{1}{4}$ for $\xi \in [0, 1]$,
\[
(6.1) \quad \mathbb{P}(\zeta^X(x) \leq t) \leq 2e^{-\frac{2(\varphi(x) - t)^2}{L^m(0)}}.
\]

**Lemma 6.1.** Assume that $\varphi \in C^{2(n+1)}((0, 1); \mathbb{R})$ for some $n \geq 0$ and that $L^m \varphi$ admits a continuous extension to $[0, 1]$ for each $0 \leq m \leq n + 1$. Then, for each $(x, t) \in (0, 1) \times (0, \infty)$,
\[
\left| \mathbb{E}[\varphi(X(t, x)), \zeta^X(x) > t] - \sum_{m=0}^{n} \frac{t^m}{m!} L^m \varphi(x) \right|
\]
\[
- \frac{1}{n!} \int_0^t (t - \tau)^n \mathbb{E}[L^{n+1} \varphi(X(\tau, x)), \zeta^X(x) > \tau] \, d\tau \leq 2e^{-\frac{2(\varphi(x) - t)^2}{L^m(0)}} \sum_{m=0}^{n} \frac{t^m}{m!} (|L^m \varphi(0)| + |L^m \varphi(1)|).
\]

**Proof.** Set $\zeta^X_r(x) = \inf\{t \geq 0 : |X(t, x)| \wedge |1 - X(t, x)| \leq r\}$ for $r \in (0, 1)$. By Itô’s formula and Doob’s stopping time theorem,
\[
\mathbb{E}[\varphi(X(t \wedge \zeta^X_r(x), x))] = \varphi(x) + \mathbb{E} \left[ \int_0^{t \wedge \zeta^X_r(x)} L\varphi(X(\tau, x)) \, d\tau \right]
\]
for each $r \in (0, 1)$. Thus, after letting $r \searrow 0$, we know first that
\[
\mathbb{E}[\varphi(X(t \wedge \zeta^X(x), x))] = \varphi(x) + \int_0^t \mathbb{E}[L\varphi(X(\tau, x)), \zeta^X(x) > \tau] \, d\tau
\]
and then, by (6.1), that the result holds for $n = 0$.

Next, assume the result for $n$. By applying the result for $n = 0$ to $L^{n+1} \varphi$, we see that
\[
\left| \int_0^t (t - \tau)^n \mathbb{E}[L^{n+1} \varphi(X(\tau, x)), \zeta^X(x) > \tau] \, d\tau - \frac{t^{n+1}}{n+1} L^{n+1} \varphi(x) \right|
\]
\[
- \frac{1}{n+1} \int_0^t (t - \tau)^{n+1} \mathbb{E}[L^{n+2} \varphi(X(\tau, x)), \zeta^X(x) > \tau] \, d\tau \leq 2e^{-\frac{2(\varphi(x) - t)^2}{L^m(0)}} \sum_{m=0}^{n} \frac{t^m}{m!} (|L^m \varphi(0)| + |L^m \varphi(1)|) \int_0^t (t - \tau)^n \, d\tau
\]
\[
\leq 2e^{-\frac{2(\varphi(x) - t)^2}{L^m(0)}} \sum_{m=0}^{n} \frac{t^m}{m!} (|L^m \varphi(0)| + |L^m \varphi(1)|) \frac{t^{n+1}}{n+1}.
\]
Thus, by induction, the result follows for general $n$’s. \qed

Given $f \in C((0, 1); \mathbb{R})$, set $f(x) = x(1 - x)f(x)$. 

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Theorem 6.2. Assume that $f \in C^\infty((0,1]; \mathbb{R})$ and that, for each $n \geq 0$, $L^n \bar{f}$ extends to $[0,1]$ as a continuous function. Then, for each $n \geq 0$ and $(y,t) \in (0,1) \times (0,\infty)$,

$$
\left| \int_{(0,1)} f(x)p(x,y,t) \, dx - \sum_{m=0}^{n} \frac{t^m}{m!} f_m(y) - \frac{1}{y(1-y)n!} \int_{0}^{t} (t-\tau)^n E[L^{n+1} \bar{f}(X(\tau,y))], \zeta^X(y) > \tau] \, d\tau \right| \leq e^{-2n^2(1-y)^2} \sum_{m=0}^{n} \frac{t^m}{m!} (|f_m(0)| \vee |f_m(1)|),
$$

where $f_m(y) = \frac{L^m \bar{f}}{y(1-y)^m}$ for $m \geq 0$.

Proof. Because $y(1-y)p(x,y,t) = x(1-x)p(y,x,t)$,

$$
y(1-y) \int_{(0,1)} f(x)p(x,y,t) \, dx = \int_{(0,1)} \bar{f}(x)p(y,x,t) \, dx = E[\bar{f}(X(t,y)), \zeta^X(y) > \tau].
$$

Hence, the desired result follows from Lemma 6.1 with $\varphi = \bar{f}$. \qed

The second topic deals with possible improving of the first estimate in Corollary 4.5. A look at the argument there reveals that the weak link is the replacement of $\bar{q}^{V_{\beta}}$ by $\bar{q}$ in the first estimate in Corollary 4.4. Of course, the problem with $\bar{q}^{V_{\beta}}$ is that we can only estimate it but cannot give an explicit expression for it in terms of familiar quantities. Nonetheless, if one is interested in $\bar{p}(x,y,t)$ when all the variables are small, one can make a modest improvement by using a Taylor approximation for $V_{\beta}$.

In order to carry this out, we will need the following computation, which is of some independent interest on its own.

Lemma 6.3. For each $m \geq 1$, define $\{C_{k,j}^{(m)} : k \in \mathbb{N} & 0 \leq j \leq k\}$ so that

$$
C_{k,0}^{(m)} = \frac{(m+k-1)!}{(m-1)!}, \quad C_{k,k}^{(m)} = 1, \quad \text{and} \quad C_{k+1,j}^{(m)} = (m+k+j)C_{k,j}^{(m)} + C_{k,j-1}^{(m)}, \quad 1 \leq j \leq k.
$$

Next, set $C_{1,1} = 1$ and $C_{k,j} = C_{k-1,j-1}^{(2)}$ for $k \geq 2$ and $1 \leq j \leq k$. Then

$$
q^{(m)}(x,y,t)y^k = \sum_{j=0}^{k} C_{k,j}^{(m)} t^{k-j} x^j q^{(m+k+j)}(x,y,t) \quad \text{for} \quad m \geq 1 \text{ and } k \geq 1,
$$

and

$$
q(x,y,t)y^k = \sum_{j=1}^{k} C_{k,j} t^{k-j} x^j q^{(k+j)}(x,y,t) \quad \text{for} \quad k \geq 1.
$$

In particular, for $k \geq 1$,

$$
\int_{0}^{t} \left( \int_{(0,\infty)} q(x,\xi,t-\tau)\xi^k q(\xi,y,\tau) \, d\xi \right) \, d\tau = tx \sum_{j=1}^{k} Q^{(k,j)}(x,y,t),
$$
where
\[ Q^{(k,j)}(x, y, t) = \frac{(k + j)!}{(2k + 1)!} C_{k,j} t^{k-j} x^j \sum_{i=0}^{k+j} \frac{(k-j+i)!}{i!} q^{(i)}(x, y, t). \]

**Proof.** Starting from the expression for \( q^{(m)}(x, y, t) \) in (5.2) and remembering that \( q^{(m)}(x, y, t) \) satisfies (5.1), one sees that
\[ x \partial_x^2 q^{(m)}(x, y, t) + m \partial_x q^{(m)}(x, y, t) = \left( \frac{x + y}{t^2} - \frac{m}{t} \right) q^{(m)}(x, y, t) - \frac{2x}{t^2} q^{(m+1)}(x, y, t). \]

At the same time, by (5.6),
\[ x \partial_x^2 q^{(m)}(x, y, t) + m \partial_x q^{(m)}(x, y, t) = \frac{x}{t^2} q^{(m+2)}(x, y, t) + \left( \frac{m}{t^2} - \frac{m}{t} \right) q^{(m)}(x, y, t). \]
Hence,
\[ \frac{x}{t^2} q^{(m+2)}(x, y, t) + \left( \frac{m}{t^2} - \frac{m}{t} \right) q^{(m)}(x, y, t) = 0 \text{ for all } m \geq 0. \]

Given (6.2), an easy inductive argument proves the first equation, and given the first equation, the second one follows immediately from \( q(x, y, t)y = x q^{(2)}(x, y, t) \), which is (6.2) when \( m = 0 \) and \( k = 1 \).

Finally, from the second equation, we know that (cf. Corollary 5.2 and (5.9))
\[ \int_0^t \left( \int_{(0, \infty)} q(x, \xi, t - \tau) \xi^k q(\xi, y, \tau) d\xi \right) d\tau \]
\[ = \sum_{j=1}^k C_{k,j} x^j \int_0^t (t - \tau)^{k-j} q^{(k-j,0)}(x, y, t - \tau, \tau) d\tau \]
\[ = \sum_{j=1}^k C_{k,j} t^{k-j} x^j \sum_{i=0}^{k+j} \frac{(k + j)!}{i!} \int_0^t (t - \tau)^{k-j+i} \tau^{k-j-i} d\tau q^{(i)}(x, y, t) \]
\[ = t \sum_{j=1}^k C_{k,j} t^{k-j} x^j \sum_{i=0}^{k+j} \frac{(k + j)!}{i!(2k + 1)!} q^{(i)}(x, y, t), \]
which is easy to recognize as the expression we want. □

It is amusing to note that the numbers \( \{C_{k,j} : 1 \leq j \leq k\} \) are the coefficients for the polynomial which gives the \( k \)th moment of \( q(x, \cdot, t) \). That is,
\[ \int_{(0, \infty)} y^k q(x, y, t) dy = \sum_{j=1}^k C_{k,j} t^{k-j} x^j. \]
To see this, simply start with the equation for \( y^m q(x, y, t) \) in Lemma 6.3 and, remembering that the integral of \( q^{(m)}(x, \cdot, t) \) is 1 for all \( m \geq 1 \), integrate both sides with respect to \( y \in (0, \infty) \).

With Lemma 6.3 we can implement the idea mentioned above. To this end, first use (3.12) to check that
\[ \left| q^{\frac{V_2^{1/2}}{a}}(x, y, t) - q(x, y, t) - \int_0^t \left( \int_{(0, \infty)} q(x, \xi, t - \tau) V_2(\xi) q(\xi, y, \tau) d\xi \right) d\tau \right| \]
\[ \leq \frac{(t\|V_2\|_u)^{2} e^{t\|V_2\|_u}}{2} q(x, y, t). \]
Second, use Taylor’s theorem and the fact that \( V_2^q(0) = 0 \) to see that

\[
\left| \int_0^t \left( \int_{(0,\infty)} q(x,\xi,t-\tau) V_2^q(\xi) q(\xi,y,\tau) \, d\xi \right) \, d\tau \right|
- V_2^q(0) \int_0^t \left( \int_{(0,\infty)} q(x,\xi,t-\tau) q(\xi,y,\tau) \, d\xi \right) \, d\tau
\leq \frac{\|V''_q\|_u}{2} \int_0^t \left( \int_{(0,\infty)} q(x,\xi,t-\tau) \xi^2 q(\xi,y,\tau) \, d\xi \right) \, d\tau.
\]

Third, use elementary calculus to show that \( V_2^q(0) = -\frac{28}{135} \), and combine this with the preceding and the second equation in Lemma 6.3 to conclude that

\[
(6.4) \quad q^\frac{1}{3}(x,y,t) - q(x,y,t) + \frac{28tx}{135} \sum_{j=0}^3 j q^{(j)}(x,y,t)
\leq \frac{\|V''_u\|_u}{2} e^{\|V''_u\|_u} l^2 q(x,y,t) + \frac{\|V''_u\|_u}{10} t \psi(x,y) \left[ \sum_{j=0}^3 j q^{(j)}(\psi(x),\psi(y),t) + 2 \psi(x) \sum_{j=0}^4 q^{(j)}(\psi(x),\psi(y),t) \right]
\]

After putting (6.4) together with the first estimate in Corollary 4.4, we arrive at the following theorem.

**Theorem 6.4.** For \((x,y,t) \in (0,\frac{1}{4}]^2 \times (0,1] \),

\[
\left| \sqrt{\psi'(x)\psi'(y)} p(x,y,t) - \psi(x,y,t) + \frac{28t\psi(x)\psi(y)}{135} \sum_{j=0}^3 j q^{(j)}(\psi(x),\psi(y),t) \right|
\leq K e^{U} (1 + \sqrt{\pi}t) \psi(x,y) e^{-\frac{\pi t}{4}} + \frac{\|V''_u\|_u}{2} e^{\|V''_u\|_u} l^2 \bar{q}(\psi(x),\psi(y),t)
+ \frac{\|V''_u\|_u}{10} t \psi(x,y) \left[ \sum_{j=0}^3 j q^{(j)}(\psi(x),\psi(y),t) + 2 \psi(x) \sum_{j=0}^4 q^{(j)}(\psi(x),\psi(y),t) \right],
\]

where \( U = U_2^q \), \( K = K(\frac{1}{2}, \frac{3}{4}, \frac{1}{2}) \), and \( \mu = \mu_2^q \) are the constants determined by the prescription given in Corollary 4.4.

It should be evident that the preceding line of reasoning can be iterated to obtain better and better approximations to \( p(x,y,t) \). However, even the next step is dauntingly messy, since it requires one to deal with integrals of the form

\[
\iint_{0 \leq \tau_1 < \tau_2 \leq t} \left( \int_{(0,\infty)^2} q(x,\xi_2,\tau_2-\tau_1) \xi_2 q(\xi_2,\xi_1,\tau_2-\tau_1) q(\xi_1,y,\tau_1) d\xi_1 d\xi_2 \right) d\tau_1 d\tau_2,
\]

a task which is possible but probably not worth the effort.

**7. Appendix.** In this appendix we discuss a few important facts about the functions \( q^{(m)}(\xi) \) which appear in this article. The function \( q^{(0)}(\xi) \) is the same as the function \( q(\xi) \) which was introduced as the solution to (1.2) satisfying the boundary conditions in (1.4). As we saw, one representation of \( q(\xi) \) is as the power series in

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(1.7). By comparing this expression with the power series in (5.3) for $q^{(2)}(\xi)$, one finds that

\begin{equation}
q(\xi) = \xi q^{(2)}(\xi).
\end{equation}

We now want to show how to estimate the numbers $\delta_m$ which occur in (1.12) and (5.4). Isolating the polar angle corresponding to $\omega_0$ and using the fact that the $2m-2$ sphere has an area $\frac{2\pi^{m-\frac{1}{2}}}{\Gamma(m-\frac{1}{2})}$, one can pass from the integral representation of $q^{(m)}(\xi)$ in (5.2) to

\begin{equation}
q^{(m)}(\xi) = \frac{1}{\sqrt{\pi} \Gamma (m - \frac{1}{2})} \int_{0}^{\pi} e^{2\sqrt{\xi} \cos \theta} \sin^{2m-1} \theta \, d\theta \quad \text{for } m \geq 1.
\end{equation}

Afinadores of Bessel functions will recognize that (7.2) says that, when $m \geq 1$, $q^{(m)}(\xi) = \xi \frac{I_{m-1}(2\sqrt{\xi})}{I_m(2\sqrt{\xi})}$, where $I_{m-1}$ is the $(m-1)$st Bessel function with a purely imaginary argument. In conjunction with (7.1), this means that $q(\xi) = \sqrt{\xi} I_1(2\sqrt{\xi})$, which is the route which Elkies took when he inverted Fefferman’s Fourier expression.

Turning to the estimation of the $\delta_m$, set

\[ g_m(\eta) = e^{-\eta} \int_{0}^{\pi} e^{\eta \cos \theta} \sin^{2m-2} \theta \, d\theta \quad \text{for } \eta \in [0, \infty). \]

By (7.2),

\[ q^{(m)}(\xi) = \frac{1}{\sqrt{\pi} \Gamma (m - \frac{1}{2})} e^{2\sqrt{\xi}} g_m(2\sqrt{\xi}). \]

Because $1 - \cos \theta \geq 8^{-\frac{1}{2}} \theta^2$ for $\theta \in \left[0, \frac{\pi}{4}\right]$, $\cos \theta \leq 2^{-\frac{1}{2}}$ for $\theta \in \left[\frac{\pi}{4}, \pi\right]$, and $\sin \theta \leq \theta$ for $\theta \in [0, \pi]$, $g_m(\eta)$ is bounded above by

\begin{align*}
\int_{0}^{\frac{\pi}{4}} e^{-8^{-\frac{1}{2}} \eta \theta^2 \theta^{2m-2}} \, d\theta + e^{-(1-2^{-\frac{1}{2}})\eta} \frac{\pi^{2m-1}}{2m-1} \\
\leq 2^{2m-\frac{1}{2} - m} \int_{0}^{\infty} e^{-t \left( m - \frac{1}{2} \right)} \, dt + e^{-(1-2^{-\frac{1}{2}})\eta} \frac{\pi^{2m-1}}{2m-1} \\
= \left[ 2^{2m-\frac{1}{2} - m} \Gamma(m - \frac{1}{2}) + \frac{1}{2m-1} \left( \frac{(m - \frac{1}{2}) \pi^2}{e \left( 1 - 2^{-\frac{1}{2}} \right)} \right)^{m-\frac{1}{2}} \right] e^{2\eta^{\frac{1}{2}}} \eta^{\frac{1}{2} - m}.
\end{align*}

Hence, for $m \geq 1$,

\begin{equation}
q^{(m)}(\xi) \leq \left[ 2^{2m-\frac{5}{2}} \pi^{-\frac{1}{2}} + \frac{1}{(2m-1)\pi^{\frac{1}{2}} \Gamma(m - \frac{1}{2})} \left( \frac{(m - \frac{1}{2}) \pi^2}{e \left( 1 - 2^{-\frac{1}{2}} \right)} \right)^{m-\frac{1}{2}} \right] \xi^{\frac{1}{2} - m} e^{2\sqrt{\xi}},
\end{equation}

and so

\begin{equation}
q(\xi) \leq \left[ 2^{-\frac{1}{4}} \pi^{-\frac{1}{4}} + \frac{3^{\frac{1}{2}}}{2^{\frac{1}{2}} e^{\frac{3}{2}} \left( 1 - 2^{-\frac{1}{2}} \right)^{\frac{3}{2}}} \right] \xi^{\frac{1}{4}} e^{2\sqrt{\xi}}.
\end{equation}

$\forall \xi \in (0, \infty)$, although neither of these estimates is close to optimal unless $\xi \in [1, \infty)$.
The corresponding lower bound is easy, although it holds only when \( \eta \geq 1 \). Namely, when \( \eta \geq 1 \),

\[
g_m(\eta) \geq \int_{0}^{\frac{\pi}{4}} e^{-(1-\cos \theta)\eta} \sin^{2m-2} \theta \, d\theta \geq \int_{0}^{\frac{\pi}{4}} e^{-\frac{4\theta}{\pi}} \left( \frac{2\pi \theta}{\eta} \right)^{2m-2} d\theta
\]

\[
\geq \frac{2^{3m-3}}{\pi^{2m-2} \eta^{\frac{3}{2}}} \int_{0}^{\frac{\pi}{4}} e^{-\frac{4\theta}{\pi}} \theta^{2m-2} d\theta \geq \frac{\pi}{2^{m+1}(2m-1)e^{\frac{2\pi}{\eta}}} \eta^{\frac{1}{2} - m},
\]

and so

\[
q^{(m)}(\xi) \geq \frac{\sqrt{\pi}}{(2m-1)2^{2m+\frac{1}{2}}e^{\frac{2\pi}{\eta}} \Gamma(m - \frac{1}{2})} \xi^{\frac{1}{2} - m} e^{2\sqrt{\xi}}
\]

and

\[
q(\xi) \geq (2^{\frac{1}{2}}3e^{\frac{2\pi}{\eta}})^{-1} \xi^{\frac{1}{2}} e^{2\sqrt{\xi}}
\]

for \( \xi \in [1, \infty) \).

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