A MATHEMATICAL ANALYSIS OF THE OPTIMAL EXERCISE BOUNDARY FOR AMERICAN PUT OPTIONS

XINFU CHEN AND JOHN CHADAM

Abstract. We study a free boundary problem arising from American put options. In particular we prove existence and uniqueness for this problem and we derive, and prove rigorously, high order asymptotic expansions for the early exercise boundary near expiry. We provide four approximations for the boundary: one is explicit and is valid near expiry (weeks); two others are implicit involving inverse functions and are accurate for longer time to expiry (months); the fourth is an ODE initial value problem which is very accurate for all times to expiry, is extremely stable, and hence can be solve instantaneously on any computer. We further provide an ode iterative scheme which can reach its numerical fixed point in five iterations for all time to expiry. We also provide a large time (equivalent to regular expiration times but large interest rate and/or volatility) behavior of the exercise boundary. To demonstrate the accuracy of our approximations, we present the results of a numerical simulation.

1. Introduction

With the Black-Scholes hypothesis of log-normal stock prices, the price $P(S,T)$ for an American put option on a share of price S at time T can be formulated as the solution to following free boundary problem (cf. Wilmott–Dewynne–Howison [27]):

$$(P)\quad \begin{cases} P_T + \frac{1}{2}\sigma^2 S^2 P_{SS} + r\,S\,P_s - r\,P = 0 & \text{for } T < T_F,\ S > S_f(T), \\ P(S,T) = E - S, \quad P_S(S,T) = -1 & \text{for } T < T_F,\ S \le S_f(T), \\ S_f(T_F) = E, \quad P(S,T_F) = \max\{0, E - S\} & \text{for } T = T_F,\ S > 0. \end{cases}$$

Here E is the exercise (strike) price, T_F the expiration time, σ the constant volatility, r the constant risk-free interest rate, and $S = S_f(T)$ the free boundary separating regions of optimally holding and exercising.

There is a considerable literature on the optimal exercise boundary, both analytical and numerical; see, for example, [1, 2, 3, 4, 6, 14, 15, 18, 20, 21, 24, 25, 26] and the references therein. A recent list of references, together with numerical approximations, can be found in [1, 8, 24].

For notational simplicity, we write problem (P) in a non-dimensional form. Let

$$k = 2r/\sigma^2, \quad S = E\,e^x, \quad T = T_F - 2t/\sigma^2\,, \quad P(S,T) = E\,p(x,t), \quad S_F(T) = E\,e^{s(t)}.$$

Then problem (P) becomes, for the transformed price $p(x,t)$ and the optimal exercise boundary $x = s(t)$,

$$(1.1)\quad \begin{cases} p_t - p_{xx} - (k-1)p_x + k\,p = 0 & \text{for } t > 0,\ x > s(t), \\ p(x,t) = 1 - e^x,\ p_x(x,t) = -e^x & \text{for } t > 0,\ x \le s(t), \\ s(0) = 0, \qquad p(x,0) = \max\{1 - e^x, 0\} & \text{for } t = 0,\ x \in \mathbb{R}, \\ p(x,t) > \max\{1 - e^x, 0\} & \text{for } t > 0,\ x > s(t). \end{cases}$$

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The last condition corresponds to the physical condition $P > E - S$ when $S > S_f(T)$. Though not necessary, we include this condition in (1.1) to make the definition of the free boundary clearer.

Unlike the American call option with dividend where $s(t) \sim -2\sqrt{t\alpha}$ with α being a constant [21], here for the put option, α becomes unbounded as $t \searrow 0$ (i.e. $T \nearrow T_F$), leading to difficulties in the theoretical analysis, numerical simulation, and accurate pricing and strategic trading during this extremely volatile period, i.e. the period where the relation between the asset and option prices is rapidly varying.

Although the analysis to be presented is quite technical, the high accuracy of the ensuing global estimates for the location of the early exercise boundary is quite important for practitioners. Knowing the location of the early exercise boundary a priori makes the pricing of American style financial derivatives amenable by Monte Carlo simulation which is the preferred systematic method of fund managers with thousands of instruments. In addition to the practical importance of these estimates, the technical methods to obtain them are also of theoretical interest. Since the methods do not use the convexity of the free boundary (we have proven the convexity of the free boundary for problem (P) in a separate paper [7]), they serve as a prototype for problems with non-convex free boundary problems. We expect this to be the most likely case in finance since even for the closely related problem (P) on a dividend–paying asset, numerical simulations by J. Detemple suggest (private communication) that the early exercise boundary may not be convex for all choices of the parameters.

In recent developments, Kuske and Keller [18], Bunch and Johnson [5], and Stamicar, Sevcovic and Chadam [25] derived independently the following similar asymptotic expansions for $\alpha(t) := s^2(t)/(4t)$:

$$\begin{array}{lrl} \text{(KK)} & 9\pi k^2\, t\, \alpha^2\, e^{2\alpha} & \sim 1\ , \\ \text{(BJ)} & 4k^2\, t\, \alpha\, e^{2\alpha} & \sim 1 - k^2/[2(1+k)^2]\ , \\ \text{(SSC)} & 4\pi k^2\, t\, e^{2\alpha} & \sim 1\ , \end{array}$$

for all sufficiently small positive t. Regardless of their differences, all these asymptotics capture the dominant behavior $\lim_{t\searrow 0} \frac{2\alpha(t)}{|\log t|} = 1$. Nevertheless, any two of the asymptotics (KK), (BJ) and (SSC) can not hold simultaneously. On the other hand, due to the singularity of problem (1.1) near the origin, numerical simulations are very difficult and typical methods such as the binomial or trinomial tree methods can hardly capture any asymptotic behavior of $\alpha(t)$ more accurately than the above approximations.

One purpose of this paper is to give a complete and rigorous mathematical justification to show that indeed (SSC) is the correct asymptotic behavior of $\alpha(t)$ as $t \searrow 0$. In addition, we shall prove rigorously that as $t \searrow 0$, $\alpha(t) = s^2(t)/(4t)$ has the more general asymptotic expansion

$$\alpha(t) = -\xi - \frac{1}{2\xi} + \frac{1}{8\xi^2} + \frac{17}{24\xi^3} - \frac{51}{64\xi^4} - \frac{287}{120\xi^5} + \frac{199}{32\xi^6} + O(\xi^{-7}), \quad \xi := \log\sqrt{4\pi k^2 t}. \tag{1.2}$$

Due to our particular choice of ξ, this expansion does not have a constant term, and also does not depend otherwise on any parameters.

Another purpose of this paper is to provide the following non–iterative approximations to $s(t)$ for both small and large t:

$$\text{(expl)} \qquad \alpha = -\xi - \frac{1}{2(\xi - a)} + \frac{1/8 + a/2}{(\xi - a)^2}, \qquad a = 0.96621...,$$

$$\text{(imp1)} \qquad \xi = -\alpha - \log\left\{1 - \frac{1}{2(\alpha+1)} - \frac{1}{2(\alpha+1)^2}\right\},$$

$$\text{(imp2)} \qquad \xi = -\alpha - \log\left\{\tfrac{2}{\sqrt{\pi}}\textstyle\int_0^{\sqrt{\alpha}} e^{-z^2} dz\right\} + \log\tfrac{e^{\alpha} + 2k\log(1+1/k)\, e^{1/\alpha}}{e^{\alpha} + e^{1/\alpha}},$$

$$\text{(ODE)} \qquad \tfrac{d}{dt} s(t) = \tfrac{s(t)}{2kt}\Gamma(s(t), t), \qquad \Gamma(z,t) := \tfrac{1}{2\sqrt{\pi t}} e^{-z^2/(4t) - (k-1)z/2 - (k+1)^2 t/4}.$$

There have been many contributions to the study of early exercise boundaries for American options with dividends; see, for example, Evans, Kuske and Keller [11] and Knessl [17]. An earlier theoretical work using a variational approach for Americam options with multiple assets, as well as a numerical algorithm for the pricing problem was supplied by Jaillet, Lamberton and Lapeyre [15]. By contrast, the main focus of this paper is to give a complete treatment, with particular attention on the singular behavior of the optimal exercise boundary near expiry, for the simplest non-trivial case of the American put without dividends. It is expected that analysis similar to ours can be carried over, with appropriate modifications, to the case with other payoffs, dividends and/or multiple assets. On the other hand, as mentioned earlier, even in the closely related case of problem (P) on a dividend–paying asset, the dependence of the near expiring behavior, and possibly the convexity, on the choice of parameters suggests that the necessary modifications may be subtle.

The explicit approximation (expl) and the first implicit approximation (imp1) are derived directly from the asymptotic expansion (1.2); they are fourth order in the sense that for small t, the α values calculated from (expl) or (imp1) have error of order $O(|\xi|^{-4})$. Our numerical simulation (cf.[8]) shows that both (expl) and (imp1) are far better than any straightforward truncations of (1.2) (assuming $T_F - T$ is larger than 1 second) both in accuracy and in the length of interval of validity of the formulas. For our running example (cf. Figure in §7) where $E = 1$, $r = 0.1$/year and $\sigma = 0.25/\sqrt{\text{year}}$, the approximation (expl) is accurate for $T_F - T$ less than several weeks and (imp1) is accurate for $T_F - T$ less than several months.

The second implicit approximation (imp2) is an interpolation of the small time behavior $\alpha \approx -\xi$ and large time behavior $s(t) \approx \log[(1 + k)/k]$ derived from Merton's solution for the infinite horizon problem for American put [22]. In general (imp2) is better than (imp1). For our running example, the error of the approximation (imp2) is less than 2×10^{-3} for $T_F - T$ up to three years.

The ode approximation (ODE) is to be solved with an initial condition compatible with the limit $\alpha + \xi \to 0$ as $\xi \to -\infty$. In numerical implementation, it is transformed to an equation for α in the $\xi = \log\sqrt{4\pi k^2 t}$ variable and the initial condition is approximated by $\alpha|_{\xi=\xi_0} = -\xi_0 - 1/(2\xi_0)$ where ξ_0 is a large negative number, say, $\xi_0 = -10$. Numerical simulation shows that this ode initial value problem is very stable, highly insensitive to any change of initial conditions, and hence can be solved instantaneously on any computer. The (ODE) approximation is better than any of the above three. For our running example, its error is less than 5×10^{-5} when $T_F - T$ is less than two months, 10^{-3} when $T_F - T$ less than one year, and 6×10^{-3} for all $T_F - T > 0$. We would like to point out that our (ODE) approximation has already surpassed those numerical approximations from the standard binomial or trinomial tree methods (with 1000 division points), which are typically used in literature as the "exact" solutions for comparisons; see the curve marked "Bino" in the Figure in §7.

The (ODE) approximation is derived from the following exact system:

$$\text{(1.3)}\qquad \begin{cases} \dot{s}(t) = \frac{s(t)}{2kt}\,\Gamma(s(t),t)\{1+m(t)\}, \\ m(t) = k\int_0^t \left\{\frac{s(t)-s(\tau)}{t-\tau}\,\frac{2t}{s(t)} - 1\right\}\frac{\Gamma(s(t)-s(\tau),t-\tau)}{\Gamma(s(t),t)}\,d\,s(\tau). \end{cases}$$

From this system, we obtain an iterative scheme: Starting with the ode approximation (corresponding to $m \equiv 0$), successively solve (1.3) with m evaluated at the previous iteration of s. As it turns out, this iteration converges very rapidly; a numerical fixed point (difference less than 10^{-7}) is obtained after only 5 iterations. The first iteration takes less than one minute and the total of five iterations takes less than 10 minutes (on a Sparc server). See Figure in §7 for the error estimate of the first three iterations.

Note that $t = \sigma^2(T_F - T)/2 = 2r(T_F - T)/k$ is large when σ and/or r are large. Hence, to include cases where r and/or σ are large, we also provide a long time behavior of s. For large t,

$$\text{(long)}\qquad \begin{aligned} s(t) &\sim s_\infty \exp\Big\{\hat{m}\int_{(k+1)^2t/4}^{\infty} \rho^{-3/2}e^{-\rho}\,d\rho\Big\}, \\ s_\infty &= s(\infty) = \log[k/(1+k)], \\ \hat{m} &= \frac{k+1}{4\sqrt{\pi}}\int_0^\infty \frac{s(\tau)}{s_\infty}\exp\Big\{\frac{k-1}{2}(s(\tau)-s_\infty) + \frac{(k+1)^2}{4}\tau\Big\}\,d\,s(\tau). \end{aligned}$$

Here $\hat{m}$ can be calculated approximately by using the (ODE) approximation for s, which is instantaneous since we can do so by solving (ODE). When (long) is incorporated with our non–iterative schemes such as (ODE), we can instantaneously obtain reliable approximate values of $s(t)$, for any t and any parameters r and σ; see Figure in §7 for $r = 0.1$/year and $\sigma = 0.25/\sqrt{\text{year}}$, and [8] for other values of the parameters.

This paper is organized as follows. In §2, we briefly establish, for mathematical completeness, the well–posedness of problem (1.1) via a classical variational approach [12]. We show that the solution (p, s) to (1.1) exists and is unique, that $s(t)$ is continuous and non–decreasing, and as $t \to \infty$, $(s(t), p(\cdot,t)) \to (s_\infty, p_\infty(\cdot))$, the solution to the infinite horizon problem [22]. During the review and revision of this manuscript, an alternative proof of the existence and uniqueness has appeared in the literature [23].

In §3 we derive several integral and integro–differential equations for s by using the fundamental solution Γ for the linear parabolic PDE for p; in particular we derive (1.3).

§§4–6 are devoted to showing that (1.3) has a solution $s(\cdot)$ with $\alpha := s^2(t)/(4t)$ satisfying the asymptotic behavior (1.2). In §4, we transform (1.3) into an equation of the form

$$\text{(1.4)}\qquad (\mathbf{I}+\mathbf{L})[u'] + G(u,\xi) = F[u]$$

where $u = u(\xi) = \alpha(t) = s^2(t)/(4t)$, $\xi = \log\sqrt{4\pi k^2 t}$, $\mathbf{I}$ is the identity operator, $\mathbf{L}$ a linear operator defined in (4.5), $F[u]$ a "small" non-linear operator, and G a function. In §5 we show that the operator $(\mathbf{I}+\mathbf{L})$ is invertible from C^0 to C^0 and that $\mathbf{L}[\phi]$ is always 1/2 more differentiable than ϕ, although $\|\phi - \mathbf{L}[\phi]\|_{C^0((-\infty,\xi])} \to 0$ as $\xi \to -\infty$ for any uniformly continuous function ϕ. In §6, we first establish the existence of a unique solution to (1.4), with $F[u]$ replaced by any known "small" function, in a finite interval $\xi \in (-j, \xi_0]$ for any j and some fixed negative large constant ξ_0. To take the limit $j \to \infty$, we show that (1.4), in a finite interval $[-j, \xi_0]$ or half finite interval $(-\infty, \xi_0]$, possesses a comparison principle, which allows us to construct sub and super solutions to sandwich the solutions. We let $j \to \infty$ to obtain solutions of (1.4) with given known F. A Schauder's fixed point theorem then can be used to establish the existence of a solution to (1.4). Uniqueness of the solution follows from the well–posedness result of §3. The asymptotic expansion (1.2) is proved by the comparison principle and construction of sub and super solutions.

Finally, in §7 we derive our approximation formula mentioned earlier, and for the purpose of illustration, provide a numerical simulation to support the advantages of our new approximations.

We repeat that recently we have shown [7] that the optimal boundary is convex; see also [10]. Using this property, many of the proofs here can be greatly simplified. Nevertheless, the method provided here is general enough to be extended to many similar option problems where the optimal exercise boundaries may not be convex.

2. Well-posedness of Problem (P)

In this section we briefly establish the well–posedness of the free boundary problem (1.1). For convenience, we denote by $\mathfrak{L}$ the operator

$$\mathfrak{L}[p] = p_{xx} + (k-1)p_x - k\,p.$$

Lemma 2.1. *Let $p(x,t)$, together with a free boundary $x = s(t)$, be a solution to (1.1). Then*

$$\begin{cases} \min\{p - p_0, p_t - \mathfrak{L}[p]\} = 0, & \text{in } \mathbb{R}\times(0,\infty), \\ p(x,0) = p_0(x) := \max\{1 - e^x, 0\} & \text{for all } x \in \mathbb{R}. \end{cases} \tag{2.1}$$

The proof follows from a straightforward verification and is omitted.

Theorem 2.2. *There exists a unique solution p to (2.1). In addition, if we define $s(t) = \sup\{x | p(x,t) = p_0(x)\}$ for all $t > 0$, then (i) $s(\cdot)$ is a strictly decreasing continuous function on $(0,\infty)$, (ii) $\lim_{t\searrow 0} s(t) = 0$, (iii) $p(x,t) > p_0(x)$ for all $x > s(t)$ and $t > 0$, and $p(x,t) = p_0(x)$ for all $x \le s(t)$ and $t \ge 0$, and (iv) (p,s) solves (1.1).*

Proof. The existence of a unique solution p follows from a well–developed parabolic theory for obstacle problems; see, for example, Friedman [12, Chpt. 1, Sec. 8]. Here for completeness and for the existence of $s(\cdot)$, we provide the main idea of the proof.

1. Uniqueness. Let p_1 and p_2 be arbitrary two solutions to (2.1). Denote $\gamma_i = (\partial_t - \mathfrak{L})p_i \ge 0$. Then

$$(p_1 - p_2)\{(p_1 - p_2)_t - \mathfrak{L}[(p_1 - p_2)]\} = (p_1 - p_2)(\gamma_1 - \gamma_2) \le 0 \quad \text{in } \mathbb{R}\times(0,\infty)$$

since $\gamma_1 = 0$ when $p_1 - p_2 > 0$ (as $p_1 > p_2 \ge p_0$) and $\gamma_2 = 0$ when $p_1 - p_2 < 0$. Integrating the above inequality over $x \in \mathbb{R}$ and using the Gronwall's inequality, one concludes that $p_1 \equiv p_2$.

2. Existence. For every $\varepsilon > 0$, let $q^\varepsilon(x,t)$ be the solution to the semi–linear parabolic Cauchy problem

$$\begin{cases} q^\varepsilon_t - \mathfrak{L}[q^\varepsilon] = \beta_\varepsilon(q^\varepsilon - p^\varepsilon_0) & \text{in } \mathbb{R}\times(0,\infty), \\ q^\varepsilon(\cdot,0) = p^\varepsilon_0(\cdot) := \rho^\varepsilon * p_0 & \text{on } \mathbb{R}\times\{0\}, \end{cases}$$

where $\rho^\varepsilon(z) := \varepsilon^{-1}\rho(\varepsilon^{-1}z)$ with $\rho(\cdot)$ being a smooth and non–negative mollifier of unit integral over $\mathbb{R}^1$, and $\beta_\varepsilon(\cdot)$ is any non-negative, bounded, and smooth function defined on $\mathbb{R}$ with the properties

$$\beta'_\varepsilon(z) \le 0 \ \text{ for all } \ z \in \mathbb{R}, \qquad \beta_\varepsilon(0) = k, \quad \text{and} \quad \beta_\varepsilon(z) = 0 \ \text{ for } \ z > \varepsilon.$$

Existence of a unique smooth solution q^ε follows from standard parabolic PDE theory; see, for example, [13]. To take the limit $\varepsilon \to 0$ to obtain a solution to (2.1), we need to establish a few ε–independent a priori estimates for q^ε.

Differentiating the differential equation with respect to t gives $(\partial_t - \mathfrak{L} - \beta'_\varepsilon)q^\varepsilon_t = 0$ in $\mathbb{R} \times (0,\infty)$. When $t = 0$, $q^\varepsilon_t(\cdot,0) = \mathfrak{L}[p^\varepsilon_0] + \beta_\varepsilon(0) \geq 0$ in $\mathbb{R}^1$ since $\beta_\varepsilon(0) = k$ and in the distributional sense $\mathfrak{L}[p_0] \geq -k$ which implies $\mathfrak{L}[p^\varepsilon_0] = \rho^\varepsilon * \mathfrak{L}[p_0] \geq -k$. Therefore, by comparison, $q^\varepsilon_t > 0$ on $\mathbb{R} \times [0,\infty)$.

Also one can show that p^ε_0 is a subsolution and **1** is a supsolutions so that $p^\varepsilon_0 < q^\varepsilon < 1$ in $\mathbb{R} \times (0,\infty)$.

Note that $p^\varepsilon_0 < q^\varepsilon$ implies $\beta^\varepsilon(q^\varepsilon - p^\varepsilon_0) \in [0,k)$ on $\mathbb{R} \times (0,\infty)$. Consequently, by local PDE regularity estimates, the set $\{q^\varepsilon\}_{0<\varepsilon<1}$ is bounded in $C^{\beta,\beta/2}(\mathbb{R} \times [0,\infty)) \cap W^{2,1}_r((-R,R) \times (0,R) \setminus (-\delta,\delta) \times (0,\delta))$ for every $\beta \in (0,1)$, $r > 1$, $\delta > 0$, and $R > \delta$. Hence, there exist $\gamma \in L^\infty(\mathbb{R}\times(0,\infty))$ and $p \in C^{\beta,\beta/2}(\mathbb{R}\times[0,\infty)) \cap W^{2,1}_{r,\text{loc}}(\mathbb{R}\times[0,\infty)\setminus(0,0))$ such that, along some sequence $\varepsilon \searrow 0$, $\beta_\varepsilon(q^\varepsilon - p^\varepsilon_0) \to \gamma$ weakly in $L^r(B_R(0)\times(0,R))$, and $q^\varepsilon \to p$ strongly in $C^{\beta,\beta/2}([-R,R] \times [0,R])$ and weakly in $W^{2,1}_r((-R,R) \times (0,R) \setminus ((-\delta,\delta) \times (0,\delta))$ for every $r > 1, \beta \in (0,1), \delta > 0$ and $R > \delta$. Taking the limit of the differential equation for q^ε along that convergent sequence, we conclude that $p(\cdot,0) = p_0(\cdot)$ and

$$p_t - \mathfrak{L}[p] = \gamma \in [0,k], \quad p \geq p_0, \quad p_t \geq 0 \qquad \text{in } \mathbb{R} \times (0,\infty).$$

Since $q^\varepsilon \to p$ locally uniformly, $p(x_0,t_0) - p_0(x_0) > 0$ implies $q^\varepsilon > p^\varepsilon_0 + \varepsilon$, i.e., $\beta^\varepsilon(q^\varepsilon - p^\varepsilon) = 0$, in a ε–independent neighborhood of (x_0,t_0) for all sufficiently small positive ε in the sequence, and therefore, $\gamma = 0$ in a neighborhood of (x_0,t_0). Thus p is a solution to (2.1).

3. The free boundary. Let $\mathbf{C} := \{(x,t) \in \mathbb{R} \times [0,\infty) \mid p(x,t) = p_0(x)\}$ be the contact set in the obstacle problem terminology. Since $p_t \geq 0$, there exists a (semi-continuous) function $T : \mathbb{R} \to [0,\infty) \cup \{\infty\}$, such that $\mathbf{C} = \{(x,t) \mid x \in \mathbb{R}^1, 0 \leq t \leq T(x)\}$.

Since $p_t - \mathfrak{L}[p] = \gamma \geq 0$ in $\mathbb{R} \times (0,\infty)$, a comparison principle implies that $p > 0$ in $\mathbb{R} \times (0,\infty)$. It then follows that $T(x) = 0$ for all $x > 0$ since $p_0(x) = 0$ for all $x \geq 0$.

Now we show that $T(\cdot)$ is non-increasing. Indeed, if $T(x_0) > 0$, then defining a new function $\tilde{p}$ by $\tilde{p} = p$ in $[x_0,\infty) \times [0,T(x_0)]$ and $\tilde{p} = p_0$ in $(-\infty,x_0] \times [0,T(x_0)]$, one can verify that $\tilde{p}$ is a solution to (2.1) in $\mathbb{R} \times [0,T(x_0)]$, so that, by uniqueness, $p = \tilde{p}$. Consequently, $(-\infty,x_0] \times [0,T(x_0)] \in \mathbf{C}$, and therefore $T(x) \geq T(x_0)$ for all $x \leq x_0$. Thus $T(\cdot)$ is non–increasing.

Next we show that $T(x)$ is strictly decreasing for $x \leq 0$. Suppose this is not true. Then for some $x_2 < x_1 \leq 0$, $T(x_2) = T(x_1) < \infty$. Consequently, $p(\cdot,t_0) = p_0(\cdot)$ in $[x_2,x_1]$ and $p > p_0$ in $(x_2,\infty) \times (T(x_2),\infty)$. It then follows that $p_t - \mathfrak{L}[p] = \gamma \equiv 0$ in $(x_2,\infty) \times (T(x_2),\infty)$. Since p_0 is smooth in (x_2,x_1), so is p in $(x_2,x_1) \times [T(x_2),\infty)$. Thus $p_t(\frac{x_1+x_2}{2}, T(x_2)) = \mathfrak{L}[p_0](\frac{x_1+x_2}{2}) = -k$, contradicting $p_t \geq 0$. Hence, $T(x)$ is strictly decreasing on $(-\infty,0]$.

It then follows that the function $t = T(x)$ for $x \leq 0$ admits an inverse $x = s(t)$ defined for all $t \geq 0$ and is non–decreasing. As inverse functions of strictly monotonic functions are continuous, $s(\cdot)$ is continuous. Note that $T(x) = 0$ for $x > 0$ and $T(x) > 0$ for $x < 0$ implies that $s(0) = 0$.

Finally we verify that $s(t)$ is strictly decreasing. In fact, if $s(t)$ is a constant over an interval $[t_1,t_2]$, then $p_t - \mathfrak{L}[p] = 0$ in $(s(t_1),\infty) \times (t_1,t_2)$ and $p(s(t_1),t) = p_0(s(t_1))$ for all $t \in [t_1,t_2]$, so that $p \in C^\infty([s(t_1),\infty) \times (t_1,t_2)$. As $p_t \geq (\not\equiv)0$ and $(\partial_t - \mathfrak{L})p_t = 0$ in $[s(t_1),\infty) \times (t_1,t_2)$, the Hopf Lemma then gives $p_{tx} > 0$ on

$\{s(t_1)+\} \times (t_1, t_2)$, which implies that $p_x(s(t)+, t)$ is strictly increasing for $t \in (t_1, t_2)$. On the other hand, $p \in W^{2,1}_{r,loc}(\mathbb{R} \times (0, \infty)$ for any $r > 1$ and the definition of $s(\cdot)$ implies that $p_x(s(t), t) = p_{0x}(s(t_1))$ is a constant for all $t \in (t_1, t_2)$, and we have a contradiction. Hence, $s(t)$ is strictly decreasing. This completes the proof. □

Theorem 2.3. *There exists a unique solution (p, s) to (1.1). In addition, $p \in W^{2,1}_{r,loc}(\mathbb{R} \times [0, \infty) \setminus (0, 0))$ for any $r > 1$, and $p > 0$, $p_t \geq 0$, and $p_x < 0$ in $\mathbb{R} \times (0, \infty)$. Furthermore, $s(\cdot)$ is continuous and strictly decreasing and as $t \to \infty$,*

$$s(t) \quad \to \quad s_\infty := \log(1 + 1/k), \tag{2.2}$$

$$p(x, t) \quad \to \quad p_\infty(x) := \begin{cases} 1 - e^x & \text{if } x \leq s_\infty, \\ (1 - e^{s_\infty})e^{-k(x - s_\infty)} & \text{if } x > s_\infty. \end{cases} \tag{2.3}$$

Proof. We need only show the assertions (2.2), (2.3), and $p_x < 0$ in $\mathbb{R} \times (0, \infty)$ since the rest follows from Lemma 2.1 and the proof of Theorem 2.2. As $\gamma = k$ for $x < s(t)$ and $= 0$ for $x > s(t)$, $(\partial_t - \mathfrak{L})[p_x] = \gamma_x \leq 0$ in the distributional sense. A strong maximum principle then implies that $p_x < 0$ in $\mathbb{R} \times (0, \infty)$. It remains to show (2.2) and (2.3).

First of all, we can use comparison to show that $p(\cdot, t) < p_\infty(\cdot)$ for all $t \geq 0$. This inequality implies, by the definition of s, that $s(t) > s_\infty$ for all $t > 0$.

Next, as we know that $p_t(\cdot, \cdot) \geq 0$ and $s(\cdot)$ is strictly decreasing, the existence of an upper bound $p_\infty(\cdot)$ for $p(\cdot, t)$ and a lower bound s_∞ for $s(\cdot)$ then implies that the limits $p^*(\cdot) = \lim_{t \to \infty} p(\cdot, t)$ and $s^* = \lim_{t \to \infty} s(t)$ exist. From the differential equation, we can derive that $\mathfrak{L}[p^*] = 0$ in (s^*, ∞), $p^* = p_0$ in $(-\infty, s^*]$, and $p^* \in W^2_{r,loc}(\mathbb{R})$ for any $r > 1$. Solving for (p^*, s^*) from these relations we find that $s^* = s_\infty$ and $p^*(\cdot) = p_\infty(\cdot)$. This completes the proof. □

Remark 2.1. The limit $(s_\infty, p_\infty(\cdot))$ is the classical solution of Merton [22] for the infinite horizon problem for American puts.

Remark 2.2. That $s(t)$ is not differentiable at $t = 0$ is due to the non–smoothness of the initial data $p(\cdot, 0) = p_0 = \max\{1 - e^x, 0\}$. To see this, consider the hodograph transformation: Let $x = X(z, t)$ be the inverse function of $z = p_x(x, t) + e^x$. Then $s(t) = X(0, t)$ and $X(z, t)$ solves the following initial Neumann boundary value problem for a quasi–linear parabolic PDE:

$$\begin{cases} X_t - \frac{1}{X_z^2} X_{zz} + (k - 1) - kzX_z = 0 \quad \text{for } z > 0, t > 0, \\ X_z(0, t) = 1/k \quad \text{for } \ t > 0, \\ X(\cdot, 0) = \max\{0, \log(z)\} \quad \forall z > 0. \end{cases} \tag{2.4}$$

This problem is highly singular since $X(z, 0) = 0$ for $z \in (0, 1)$, which is due to the fact that $-p_{0x}(0)$ has a jump from 0 to 1.

From (2.4), we see that if for some $\beta > 0$, $s(t)$ is $C^{1+\beta}$ near some $t = t_0 > 0$, then $s(\cdot) \in C^\infty((t_0, \infty))$. Indeed, s in $C^{1+\beta}$ near t_0 implies $p(x, t)$ in $C^{2+\beta, 1+\beta/2}$ in a neighborhood of $\mathbb{R} \times \{t_0\}$, so that $X(\cdot, t_0)$ is in $C^{1+\beta}([0, \delta])$ (and $X_z \neq 0$) for some $\delta > 0$. Local regularity theory for quasi-linear parabolic equation (see for example, [19]) then implies that $s(t) = X(0, t)$ is $C^\infty((t_0, \infty))$.

In the subsequent sections, we shall show (by a totally different method) that $s(\cdot) \in C^2((0,\delta))$ for some $\delta > 0$, so that $s \in C^\infty((0,\infty))$.

3. Integral representation for the free boundary $x = s(t)$

In this section, we use the Green's representation for solutions of the linear parabolic PDE in (1.1) to derive, for the free boundary $x = s(t)$, several integral and integro–differential equations including (1.3) which is to be solved later to establish the asymptotic behavior of $s(t)$ for small positive t.

We denote by $\Gamma(x,t)$ the fundamental solution to the operator $\partial_t - \mathfrak{L}$; more precisely,

$$\Gamma(x,t) = \frac{1}{2\sqrt{\pi t}} \exp\Big\{ - \frac{[x+(k-1)t]^2}{4t} - kt \Big\} = \frac{1}{2\sqrt{\pi t}} \exp\Big\{ - \frac{[x+(k+1)t]^2}{4t} + x \Big\}. \tag{3.1}$$

Since $(\partial_t - \mathfrak{L})[p] = \gamma$ in $L^r_{loc}(\mathbb{R}\times(0,\infty))$ for any $r > 1$ and $\gamma = k$ for $x < s(t)$ and $\gamma = 0$ for $x > s(t)$, the Green's identity gives, for the unique solution (p,s) of (1.1),

$$p(x,t) = \int_{-\infty}^0 (1-e^y)\Gamma(x-y,t)\,dy + k\int_0^t \int_{-\infty}^{s(t-\tau)} \Gamma(x-y,\tau)\,dyd\tau \quad x \in \mathbb{R}, t > 0. \tag{3.2}$$

It is worth mentioning that the first integral on the right–hand side is the price for the European put option because $e^{kt}\Gamma(x-y,t)dy$ is the probability that at expiry the stock price (after scaling) is y, for which the option has value $e^{-kt}\max\{1-e^y, 0\}$. Consequently, the second integral in (3.2) is the extra value (premium) of the American put option over the European put option, if the option is exercised optimally (i.e., exercise the option as soon as the (scaled) stock price s is below $s(t)$).

Lemma 3.1. *Let $s \in C^0([0,\infty)) \cap C^1((0,\infty)) \cap W^{1,1}((0,1))$ be any function and $p(x,t)$ be defined as in (3.2). Set $p_0(x) = \max\{1-e^x, 0\}$. Then for all $t > 0$ and $x \neq 0$ and $x \neq s(t)$,*

$$\begin{aligned}
p(x,t) &= p_0(x) + \int_0^t \Big\{\Gamma(x,\tau) - k\int_{s(t-\tau)}^0 \Gamma(x-y,\tau)dy\Big\}d\tau, \\
p_x(x,t) &= p_{0x}(x) + \int_0^t \Big\{\Gamma_x(x,\tau) + k\,\Gamma(x,\tau) - k\,\Gamma(x-s(t-\tau),\tau)\Big\}d\tau, \\
p_t(x,t) &= \Gamma(x,t) + k\int_0^t \Gamma(x-s(t-\tau),\tau)\dot{s}(t-\tau)\,d\tau, \\
p_{xx}(x,t) &= p_{0xx}(x) + \Gamma(x,t) + \int_0^t \Big\{\Gamma_x(x,\tau) + k\Gamma(x,\tau) - k\,\Gamma_x(x-s(t-\tau),\tau)\Big\}d\tau, \\
p_{xt}(x,t) &= \Gamma_x(x,t) + k\int_0^t \Gamma_x(x-s(t-\tau),\tau)\dot{s}(t-\tau)\,d\tau.
\end{aligned} \tag{3.3}$$

Consequently, (p, s) solves (1.1) if and only if s satisfies one of the following equations: for all $t > 0$,

$$\int_0^t \Gamma(s(t), \tau) d\tau = k \int_0^t \int_{s(t-\tau)}^0 \Gamma(s(t) - y, \tau) dy d\tau, \tag{3.4}$$

$$\int_0^t \Big\{\Gamma_x(s(t), \tau) + k\,\Gamma(s(t), \tau)\Big\} d\tau = k \int_0^t \Gamma(s(t) - s(t - \tau), \tau)\, d\tau, \tag{3.5}$$

$$\Gamma(s(t), t) = -k \int_0^t \Gamma(s(t) - s(t - \tau), \tau)\dot{s}(t - \tau)\, d\tau, \tag{3.6}$$

$$\Gamma(s(t), t) = \frac{k}{2} + k \int_0^t \Big\{\Gamma_x(s(t) - s(t - \tau), \tau) - \Gamma(s(t) - s(t - \tau), \tau)\Big\}\, d\tau, \tag{3.7}$$

$$\dot{s}(t) = -\frac{2\Gamma_x(s(t), t)}{k} - 2 \int_0^t \Gamma_x(s(t) - s(t - \tau), \tau)\dot{s}(t - \tau)\, d\tau. \tag{3.8}$$

Theorem 3.2. *Let $s \in C^1((0, \infty)) \cap C^0([0, \infty))$ and $\alpha(t) = s^2(t)/(4t)$. Assume that as $t \searrow 0$, $\alpha(t) = [-1 + o(1)] \log \sqrt{t}$ and $t\,\dot{\alpha}(t) = O(1)$. Then s, together with p defined in (3.2), solve (1.1) if and only if s satisfies the integro–differential equation, for all $t > 0$,*

$$\dot{s}(t) = \frac{s(t)\Gamma(s(t), t)}{2kt} + \int_0^t \Big\{\frac{s(t) - s(t - \tau)}{\tau} - \frac{s(t)}{2t}\Big\}\Gamma(s(t) - s(t - \tau), \tau)\dot{s}(t - \tau)\, d\tau. \tag{3.9}$$

One notices that (3.9) is exactly equivalent to (1.3).

Remark 3.1. Since $\Gamma_x(x, t) = -\frac{x+(k-1)t}{2t}\Gamma(x, t)$, adding (3.8) and (3.6) multiplied by $\frac{\lambda s(t)+2(k-1)t}{4t}$ gives

$$\dot{s}(t) = \frac{(2 - \lambda)s\Gamma(s, t)}{2kt} + \int_0^t \Big\{\frac{s(t) - s(t - \tau)}{\tau} - \frac{\lambda s(t)}{2t}\Big\}\Gamma(s(t) - s(t - \tau), \tau)\dot{s}(t - \tau)\, d\tau. \tag{3.10}$$

Setting $\lambda = 1$ gives (3.9) or (1.3). We choose the particular value $\lambda = 1$ is to make the integral as small as possible, because the most significant contribution of the integral comes from small τ and when τ is small, $\frac{s(t)-s(t-\tau)}{\tau} \approx s'(t) = \frac{s(t)}{2t}[1 + \frac{t\dot{\alpha}(t)}{\alpha}] \approx \frac{s(t)}{2t}$. Indeed, the cancellation is even stronger than this. A linear combination of equations (3.6)–(3.8) shows that the integral on the right–hand side of (3.9) is equal to

$$\int_0^t \Big\{\frac{\dot{s}(t) + \dot{s}(t - \tau)}{2}\,\frac{s(t) - s(t - \tau)}{\tau} - \dot{s}(t)\dot{s}(t - \tau) + \tfrac{k+1}{2}\dot{s}(t)\Big\}\Gamma(s(t) - s(t - \tau), \tau)\, d\tau.$$

Due to the strong cancellation of the first two terms in the integrand, the ratio $m(t)$ of the integral and the first term on the right–hand side of (3.9) can be expanded as $0 + 0\xi^{-1} + 0\xi^{-2} + \frac{1}{4}\xi^{-3} + O(\xi^{-4})$ where $\xi = \log[\sqrt{4\pi k^2 t}]$. Thus, we can drop the integral in (3.9) to obtain the (ODE) in §1 approximating $s(t)$ accurately for small as well as large t (when t is large, $\dot{s}(t) = O(t^{-3/2}e^{-(k+1)^2 t/4})$ is exponentially small).

Remark 3.2. From (3.4) one can immediately obtain a rough estimate for $s(t)$ for small t. In fact, since $\int_{-\infty}^0 \Gamma(y, t)\, dy = \frac{1}{2}e^{-kt}$, the double integral in (3.4) can be written as $\theta(t)\, kt$ with $\theta(t) \in (0, 1/2)$. Also since $\Gamma(s(t), t) = \frac{1+o(1)}{\sqrt{4\pi t}}e^{-s(t)^2/(4t)}$ for small t, $\int_0^t \Gamma(s(t), \tau)\, d\tau = \frac{[1+o(1)]\sqrt{t\,\alpha}}{\sqrt{\pi}} \int_{\sqrt{\alpha}}^\infty \eta^{-2}e^{-\eta^2}\, d\eta$ where $\alpha = s^2/(4t)$. Thus (3.4) gives $\lim_{t\searrow 0} \alpha(t) = \infty$. Consequently, $\int_{\sqrt{\alpha}}^\infty \eta^{-2}e^{-\eta^2} d\eta = \frac{1}{2}\alpha^{-3/2}e^{-\alpha}(1+O(\alpha^{-1}))$ and, from (3.4),

$$\alpha^{-1}e^{-\alpha}[1 + O(\alpha^{-1})] = \sqrt{4\pi k^2 t}\;\theta(t)\;.$$

Hence α is of order at least $O(|\log t|)$. One can further calculate, assuming $\alpha = [-1 + o(1)] \log \sqrt{t}$, that $\theta = \alpha^{-1}(1 + o(1))$. It then follows that $\alpha = |\log \sqrt{4\pi k^2 t}|(1 + o(1))$, a conjecture first made correctly in [25].

It is worth mentioning here that $\theta(t) \approx \alpha^{-1}$ eliminates any $\log|\log t|$ corrections (as suggested in [18] and [5]) to the leading order approximation $\alpha \approx -\log[\sqrt{t}]$ for small t.

The smallness of $\theta(t)$ results from the strong cancellation of the integral $k\int_0^t\int_{-\infty}^{s(t-\tau)}\Gamma(x-y,\tau)dyd\tau$ which represents the extra value of the American put over the European put, and the integral $-k\int_0^t\int_{-\infty}^{0}\Gamma(x-y,\tau)dyd\tau = p_0 * \Gamma(\cdot,t) - \{p_0 + \int_0^t\Gamma(x,\tau)d\tau\}$ which relates to that part of the premium added on to the European put to account for the possibility that the future stock price drops below x. It seems to us that this strong cancellation was not observed in [18], resulting in $\log|\log t|$ terms appearing in their expansion of α.

The asymptotic behavior $\alpha = -\log\sqrt{4\pi k^2 t} + o(1)$ for small t can also be similarly derived from (3.5).

Remark 3.3. Equation (3.6) or (3.7) can be used to derive an interesting and highly non-trivial limit: $\lim_{t\to 0}\Gamma(s(t),t) = k$. Indeed, using the change of variable $\eta = \frac{s(t-\tau)-s(t)}{2\sqrt{\tau}}$, one obtains from (3.6)

$$\Gamma(s(t),t) = k[\,1+o(1)\,]\int_0^{\sqrt{\alpha}}\frac{2e^{-\eta^2}}{\sqrt{\pi}}\Big(2-\frac{s(t)-s(t-\tau)}{\dot{s}(t-\tau)\tau}\Big)^{-1}d\eta = k+o(1)$$

since when τ/t is small, $\frac{s(t)-s(t-\tau)}{\dot{s}(t-\tau)\tau} \approx 1$, whereas when τ/t is not small, $\eta \gg 1$ so that $\frac{s(t)-s(t-\tau)}{\dot{s}(t-\tau)\tau}$ can be replaced by 1 as an approximation.

Remark 3.4. A system exactly equivalent to (3.7) was derived in [25] and was used to derive formally (SSC) in §1. The system was also used to obtain accurate approximations of s for small t, via an iteration scheme: starting with $s \equiv 0$, update s by solving (3.7) with the right–hand side evaluated at a previous s. Nevertheless, this scheme does not seem to converge, though its first several iterations converge rapidly (for small t); For more details, see [8, 25]. This is one of our reasons for deriving (3.9) and using it to analyze $s(t)$ theoretically and also numerically.

Proof of Lemma 3.1. Since $\Gamma(\cdot,0)$ is the Delta function,

$$\begin{aligned}\int_{-\infty}^{0}(1-e^y)\Gamma(x-y,t)\,dy &= p_0(x) + \int_0^t\int_{-\infty}^{0}p_0(y)\Gamma_\tau(x-y,\tau)dyd\tau\\ &= p_0(x) + \int_0^t\Big\{\Gamma(x,\tau) - k\int_{-\infty}^{0}\Gamma(x-y,\tau)\,dy\Big\}d\tau\end{aligned}$$

by using $\Gamma_\tau(x-y,\tau) = \Gamma_{xx}+(k-1)\Gamma_x - k\Gamma$ and integrating by parts. Substituting this identity into (3.2) we obtain (3.3). The rest of the equations, for p_x, p_t, p_{xx}, and p_{xt}, follow by differentiating (3.3) (A substitution $\Gamma_{xx}+k\Gamma_x = \Gamma_\tau+\Gamma_x+k\Gamma$ is needed for p_{xx}). We remark that all the integrals are convergent due to the regularity assumption we made on s. It remains to show the second part of the lemma.

First we assume that (p,s) solves (1.1). Then $p(x,t)-p_0(x)$, as well as all its derivatives, vanish when $x < s(t)$. Thus, letting $x \nearrow s(t)$ we obtain from the equations for $p, p_x, p_t, p_{xx}-p_x$, and p_{xt} the corresponding equations asserted. Here, in taking the limits for p_{xx} and p_{xt}, we need the following fact: for any continuous function f,

$$\lim_{x\to s(t)\pm}\int_0^t\Gamma_x(x-s(t-\tau),\tau)f(t-\tau)\,d\tau = \mp\frac{f(t)}{2} + \int_0^t\Gamma_x(s(t)-s(t-\tau),\tau)f(t-\tau)\,d\tau.$$

Next we assume that s satisfies one of the equations in the second part of the Lemma, and show that (p,s) solves (1.1). First we notice that p satisfies $p(\cdot,0)=p_0(\cdot)$ and for $t>0$, $p_t-\mathfrak{L}[p]=0$ for $x>s(t)$ and $=k$ for $x<s(t)$. In addition, $p\in W^{2,1}_{r,loc}(\mathbb{R}\times[0,\infty)\setminus\{(0,0)\})$ for any $r>0$. From the equations we derived for p,p_x,p_t,p_{xx}, and p_{xt}, we see that the equations in the second part of the lemma are, respectively, equivalent to the conditions $p=p_0$, $p_x=p_{0x}$, $p_t=0$, $p_{xx}-p_x=p_{0xx}-p_{0x}$, and $p_{xt}=0$ at $(s(t)–,t)$ for all $t>0$. Each of these conditions provides, by the uniqueness of solutions of the initial boundary value problem of the parabolic equation $p_t-\mathfrak{L}[p]=-k$ in the set $\{(x,t)\mid x\le s(t),t>0\}$, that $p\equiv p_0$ in the set, which implies that (p,s) solves (1.1). This completes the proof. ☐

Proof of Theorem 3.2. Assume that (p,s) solves (1.1). Then $p_{xt}=p_t=0$ at $(s(t)–,t)$ for all $t>0$. Equation (3.9) then follows from $p_{xt}+\frac{s(t)+2(k-1)t}{4t}p_t=0$ at $(s(t)–,t)$.

Now we assume that s satisfies (3.9) and show that (p,s) solves (1.1). We need only show that $p_t=0$ for all $x<s(t)$. Note that p defined in (3.2) is smooth (enough in our subsequent analysis) in the set $\{(x,t)\mid x\le s(t)–,t>0\}$, and (3.9) implies $p_{xt}+\frac{s(t)+2(k-1)t}{4t}p_t=0$ at $(s(t)–,t)$ for all $t>0$. Since $\frac{s(t)+2(k-1)t}{4t}$ is negative and p_t is singular near the origin, we cannot directly apply a standard parabolic PDE theory to conclude that $p_t=0$ for $x<s(t)$ and all $t\ge0$.

Differentiating the equation $p_t-\mathfrak{L}[p]=k$ with respect to t, multiplying the resulting equation by p_t and integrating over $(-\infty,s(t))$ we obtain, after integration by parts and the substitution $p_{xt}=-\frac{s(t)+2(k-1)t}{4t}p_t$ at the boundary $x=s(t)–$,

$$\frac{1}{2}\frac{d}{dt}\int_{-\infty}^{s(t)}p_t^2dx+\int_{-\infty}^{s(t)}(p_{xt}^2+k\,p_t^2)dx=\Big\{\frac{\dot s(t)}{2}-\frac{s(t)}{4t}\Big\}p_t^2(s(t)-,t)=-\frac{\sqrt{t}\,\dot\alpha(t)}{2\sqrt{\alpha(t)}}p_t^2(s(t)-,t)$$

by the definition $\alpha(t)=s^2/(4t)$. Using $p_t^2(s(t)-,t)=\int_{-\infty}^{s(t)}2p_tp_{xt}dx\le\int_{-\infty}^{s(t)}(\delta p_t^2+\delta^{-1}p_{xt}^2)dx$ with $\delta=|\frac{t\dot\alpha(t)}{2\sqrt{\alpha(\tau)}}|$ we then obtain

$$\frac{d}{dt}\int_{-\infty}^{s(t)}p_t^2(x,t)dx\le\frac{t(\dot\alpha(t))^2}{2\alpha(t)}\int_{-\infty}^{s(t)}p_t^2(x,t)dx\ .$$

Solving the differential inequality over (ε,t) $(0<\varepsilon<t)$ then gives

$$\int_{-\infty}^{s(t)}p_t^2(x,t)\,dx\le\exp\Big\{\int_\varepsilon^t\frac{\tau\dot\alpha^2(\tau)}{2\alpha(\tau)}\,d\tau\Big\}\int_{-\infty}^{s(\varepsilon)}p_t^2(x,\varepsilon)\,dx. \tag{3.11}$$

We now show that the right–hand side approaches zero as $\varepsilon\searrow0$.

First of all, using the assumptions on α we can calculate

$$\exp\Big\{\int_\varepsilon^t\frac{\tau\dot\alpha^2(\tau)}{2\alpha(\tau)}\,d\tau\Big\}\le|\log\varepsilon|^{O(1)}. \tag{3.12}$$

Next we estimate $\int_{-\infty}^{s(\varepsilon)}p_t^2(x,\varepsilon)dx$ by using the representation of p_t in Lemma 3.1. First we consider the integral in the representation of p_t. Observe that our assumption on α implies $\dot s(\varepsilon-\tau)<0$ and $[s(\varepsilon)-s(\varepsilon-\tau)+(k-1)\tau]<0$ for all small ε and $\tau\in(0,\varepsilon)$. Therefore, for all $x<s(\varepsilon)$, $\Gamma(x-s(\varepsilon-\tau),\tau)\le C\exp\{-\frac{[x-s(\varepsilon)]^2}{4\varepsilon}\}\tau^{-1/2}\exp\{-\frac{[s(\varepsilon)-s(\varepsilon-\tau)]^2}{4\tau}\}$ where C is independent of ε. Hence, with a change of variable

$\tau \to \eta$ via $\eta = [s(\varepsilon-\tau)-s(\varepsilon)]/(2\sqrt{\tau})$, we can estimate

$$\begin{aligned} 0 < -\int_0^\varepsilon \Gamma(x-s(\varepsilon-\tau),\tau)\dot s(\varepsilon-\tau)\,d\tau &\le C\exp\{-\tfrac{[x-s(\varepsilon)]^2}{4\varepsilon}\}\int_0^{\sqrt{\alpha(\varepsilon)}} \frac{e^{-\eta^2}}{1-\frac{s(\varepsilon)-s(\varepsilon-\tau)}{2\tau\dot s(\varepsilon-\tau)}}\,d\eta \\ &\le C\exp\{-\tfrac{[x-s(\varepsilon)]^2}{4\varepsilon}\} \end{aligned}$$

since the assumption on α implies that $0 < \frac{s(\varepsilon)-s(\varepsilon-\tau)}{2\tau\dot s(\varepsilon-\tau)} < \frac{3}{4}$ for all small ε and $\tau \in (0,\varepsilon)$. It then follows from the representation for p_t in Lemma 3.1 that

$$\int_{-\infty}^{s(\varepsilon)} p_t(x,\varepsilon)^2 dx \le \int_{-\infty}^{s(\varepsilon)} \Big\{\Gamma^2(x,\varepsilon)+C\exp\{-\tfrac{[x-s(\varepsilon)]^2}{2\varepsilon}\}\Big\} \le C\Big\{\varepsilon^{-1/2}\int_{\sqrt{\alpha(\varepsilon)}}^\infty e^{-2\eta^2}d\eta+\sqrt{\varepsilon}\Big\}$$

by using $\Gamma(x,\varepsilon) \le C\varepsilon^{-1}\exp\{-\frac{x^2}{4\varepsilon}\}$ and a change of variable $x = -2\sqrt{\varepsilon}\eta$. Since $\alpha(\varepsilon) = -\frac{1}{2}\log\varepsilon + O(1)$ for small ε, $\int_{\sqrt{\alpha(\varepsilon)}}^\infty e^{-2\eta^2}\,d\eta = [1+O(\alpha(\varepsilon)^{-1})]e^{-2\alpha(\varepsilon)}/(4\sqrt{\alpha(\varepsilon)}) = O(\varepsilon)$. Hence, $\int_{-\infty}^{s(\varepsilon)} p_t^2(x,\varepsilon) = O(\sqrt{\varepsilon})$. Substituting this last estimate and (3.12) into (3.11) and sending $\varepsilon \searrow 0$ we then conclude that $\int_{-\infty}^{s(t)} p_t^2(x,t) = 0$ for any $t > 0$. This implies that $p_t = 0$ for all $x < s(t)$ thereby completing the proof of the theorem. ☐

4. Asymptotic behavior of $s(t)$.

In this section, we study the integro–differential equation (3.9) for small t.

4.1. **Reformulation of the Problem.** To study (3.9), it is convenient to study the function $s^2(t)/(4t)$ in the $\log(t)$ scale. For this purpose, we change variables from (s,t) to (u,ξ) by

$$\begin{cases} t = \frac{1}{4\pi k^2}e^{2\xi}, \\ s(t) = -2\sqrt{t\,u(\xi)} \end{cases} \quad\Leftrightarrow\quad \begin{cases} \xi = \log\sqrt{t}+\log\sqrt{4\pi k^2}, \\ u(\xi) = s^2(t)/(4t)\ (=\alpha(t)). \end{cases}$$

To transform the integro–differential equation (3.9) into the new unknown $u(\xi)$, we bear in mind that we are interested in small t, i.e., large negative ξ. Also, $u(\xi) = -\xi - O(\xi^{-1})$ and $u'(\xi) = -1 + O(\xi^{-2})$. The absence of a constant term in the expansion of $u(\xi)$ is due to the presence of the particularly chosen constant $4\pi k^2$ in the definition of ξ.

In the sequel, $' = \frac{d}{d\xi}$ and $F[u](\xi)$ denotes the value at ξ of the function $F[u]$ when F is an operator.

Now we transform (3.9) into the new variables (u,ξ). Simple substitution yields

$$\begin{aligned} s(t)\Big\{\dot s(t) - \tfrac{s(t)}{2kt}\,\Gamma(s(t),t)\Big\} &= u'(\xi) + G(u(\xi),\xi), \\ G(u,\xi) &:= 2u\Big(1-\exp\{-u-\xi+\tfrac{(k-1)\sqrt{u}e^\xi}{2k\sqrt{\pi}}+\tfrac{(k+1)^2e^{2\xi}}{16k^2\pi}\}\Big). \end{aligned} \tag{4.1}$$

To convert the integral in (3.9), we change the variable τ to z via $\tau = \frac{4zt}{(1+z)^2}$. Then

$$z = \frac{\tau}{(\sqrt{t}+\sqrt{t-\tau})^2} = \frac{(\sqrt{t}-\sqrt{t-\tau})^2}{\tau}, \qquad \eta := \log\sqrt{4\pi k^2(t-\tau)} = \xi + \log\frac{1-z}{1+z}.$$

For notational simplicity, we write $u = u(\xi)$, $\hat u = u(\eta)$, and $\hat u' = u'(\eta)$. Then $s(t) = -2\sqrt{tu}$, $s(t-\tau) = -2\sqrt{(t-\tau)\hat u}$, $\dot s(t-\tau) = \frac{\sqrt{\hat u}}{\sqrt{t-\tau}}[1+\hat u'/(2\hat u)]$, and

$$\begin{aligned} &s(t)\int_0^t \Big(\frac{s(t)}{2t} - \frac{s(t)-s(t-\tau)}{\tau}\Big)\,\dot s(t-\tau)\,\Gamma(s(t)-s(t-\tau),\tau)\,d\tau \\ = &\int_0^1 \Big\{\frac{1+z^2}{z}\sqrt{u} - \frac{1-z^2}{z}\sqrt{\hat u}\Big\}\Big\{1+\frac{\hat u'}{2\hat u}\Big\}\frac{\sqrt{\hat u}\sqrt{-\xi}\,e^{\xi z-b}}{\sqrt{\pi z}}dz \end{aligned}$$

where

$$
\begin{aligned}
b \;=\;& \log\sqrt{-\xi/u}+(u+\xi)z+\log[1+z]+ \\
& \tfrac{1-z}{2}\{u-\hat u\}+\tfrac{1-z^2}{4z}\{\sqrt{u}-\sqrt{\hat u}\}^2-\tfrac{(k-1)e^{\xi}}{2k\sqrt{\pi}}\{\sqrt{u}-\tfrac{1-z}{1+z}\sqrt{\hat u}\}+\tfrac{(k+1)^2ze^{2\xi}}{4k^2\pi(1+z)^2}.
\end{aligned} \tag{4.2}
$$

Writing $(\frac{1+z^2}{z}\sqrt{u}-\frac{1-z^2}{z}\sqrt{\hat u})\sqrt{\hat u}$ as $\frac{u-u(\xi-2z)}{2z}+\frac{u(\xi-2z)-\hat u}{2z}-\frac{(\sqrt{u}-\sqrt{\hat u})^2}{2z}+z(\sqrt{u\hat u}+\hat u)$, we can transform equation (3.9) (multiplied by $s(t)$) to

$$
u'(\xi)+\int_0^1 \frac{u(\xi)-u(\xi-2z)}{2z}\,\frac{\sqrt{-\xi}e^{\xi z}}{\pi z}\,dz+G(u(\xi),\xi)=F[u](\xi) \tag{4.3}
$$

where $G(u,\xi)$ is as in (4.1) and the operator F is defined by

$$
\begin{aligned}
F[u](\xi) &= -\int_0^1 \Big\{f_1+f_2+\hat u' f_3\Big\}\,dz\,, \qquad (4.4)\\
f_1 &= \Big\{\tfrac{u-u(\xi-2z)}{2z}(e^{-b}-1)+\tfrac{u(\xi-2z)-\hat u}{2z}e^{-b}-\tfrac{(\sqrt{u}-\sqrt{\hat u})^2}{2z}e^{-b}\Big\}\,\tfrac{\sqrt{-\xi}e^{\xi z}}{\sqrt{\pi z}},\\
f_2 &= z(\sqrt{u\hat u}+\hat u)\,\tfrac{\sqrt{-\xi}e^{\xi z-b}}{\sqrt{\pi z}},\\
f_3 &= \Big\{\tfrac{1+z^2}{z}\sqrt{\tfrac{u}{\hat u}}-\tfrac{1-z^2}{z}\Big\}\tfrac{\sqrt{-\xi}e^{\xi z-b}}{\sqrt{\pi z}}.
\end{aligned}
$$

Now we introduce a Linear operator $\mathbf{L}:\phi\to\mathbf{L}[\phi]$ by

$$
\begin{aligned}
\mathbf{L}[\phi](\xi) &= \int_0^1\Big(\frac{1}{z}\int_0^z \phi(\xi-2\zeta)d\zeta\Big)\frac{\sqrt{-\xi}e^{\xi z}}{\sqrt{\pi z}}\,dz\,.\\
&= \int_0^1 \phi(\xi-2\zeta)\varrho(\xi,\zeta)\,d\zeta,\quad \varrho(\xi,\zeta):=\int_\zeta^1\frac{\sqrt{-\xi}e^{\xi z}}{z\sqrt{\pi z}}\,dz\,.
\end{aligned} \tag{4.5}
$$

Then equation (3.9) or (4.3) can be written as, for $\xi<0$ (i.e., $t<1/(4\pi k^2)$),

$$
(\mathbf{I}+\mathbf{L})[u'](\xi)+G(u(\xi),\xi)=F[u](\xi), \tag{4.6}
$$

where $\mathbf{I}$ represents the identity operator.

Theorem 4.1. *Assume that $k>0$. Then there exists a constant $\xi_0<0$ such that (4.6) admits a unique positive solution $u(\cdot)\in C^2((-\infty,\xi_0])$ having the asymptotic expansion, as $\xi\to-\infty$,*

$$
u(\xi)\;=\;u_0(\xi)+O(\xi^{-4}),\quad u_0:=-\xi-\frac{1}{2\xi}+\frac{1}{8\xi^2}+\frac{17}{24\xi^3}. \tag{4.7}
$$

4.2. **Proof of Theorem 4.1.** We use the following Schauder's fixed point theorem:

> *A continuous map* $\mathbf{T}$ *from a compact and convex subset* $\mathbf{D}$ *of a Banach space* $\mathbf{X}$ *to* $\mathbf{D}$ *possesses at least a fixed point.*

To apply this theorem, we define, for some negative constant ξ_0 to be chosen later,

$$
\begin{aligned}
\mathbf{X} &= C^1((-\infty,\xi_0])\,,\qquad \|v\|_{\mathbf{X}}:=\sup_{\xi\in(-\infty,\xi_0]}\{|v(\xi)|+|v'(\xi)|\,\}\,,\\
\mathbf{D} &= \{v\in\mathbf{X}\ |\ |v(\xi)|+|v'(\xi)|+|v''(\xi)|\le|\xi|^{-1}\ \ \forall\,\xi\in(-\infty,\xi_0]\}\,.
\end{aligned}
$$

The uniform decay of derivatives of functions in $\mathbf{D}$ ensures that $\mathbf{D}$ is compact and convex in $\mathbf{X}$. We also need two technical lemmas.

Lemma 4.2. *Let u_0 be as in (4.7). There exists a positive constant C_0, depending only on k, such that for every $\xi_0 \le -2$ and every $u \in \{u_0\} + \mathbf{D}$, the function $F[u](\cdot)$ defined in (4.4) is continuous differentiable on $(-\infty, \xi_0]$ and*

$$\Big|F[u](\xi) + 1\Big| + \Big|\frac{d}{d\xi}F[u](\xi)\Big| \quad \le \quad C_0|\xi|^{-2} \qquad \forall\, \xi \in (\infty, \xi_0]\,. \tag{4.8}$$

Lemma 4.3. *Let C_0 be as in the previous Lemma. There exist a positive constant $M(C_0)$ and a negative constant $\Xi(C_0) \le -2$ such that if $\xi_0 \le \Xi[C_0]$ and $f \in C^1((-\infty, \xi_0])$ satisfies*

$$|f(\xi) + 1| + |f'(\xi)| \le C_0|\xi|^{-2} \qquad \forall \xi \in (-\infty, \xi_0],$$

then there exists a unique solution $w \in C^2((-\infty, \xi_0])$ to

$$(P1) \quad \begin{cases} (\mathbf{I} + \mathbf{L})[w'](\xi) + G(w(\xi), \xi) = f(\xi) & \forall\, \xi \in (-\infty, \xi_0], \\ \lim_{\xi \to -\infty}(w(\xi) + \xi) = 0\,. \end{cases} \tag{4.9}$$

In addition, the solution satisfies, for u_0 defined as in (4.7),

$$|w(\xi) - u_0(\xi)| + |w'(\xi) - u_0'(\xi)| + |\xi|^{-1}\,|w''(\xi) - u_0''(\xi)| \quad \le \quad M(C_0)|\xi|^{-3} \quad \forall\, \xi \le \xi_0.$$

Proof of Theorem 4.1. We choose $\xi_0 = \min\{\Xi[C_0], -M(C_0)\}$ where $C_0, M(C_0)$ and $\Xi[C_0]$, depending only on k, are as in the previous two lemmas.

For every $v \in \mathbf{D}$, we define $\mathbf{T}[v] = w - u_0$ where w is the solution to (4.9) with $f := F[u_0 + v]$. By Lemma 4.2 and Lemma 4.3, $\mathbf{T}$ is well-defined. In addition, from the estimates for w and the definition of ξ_0, $\mathbf{T}[v] \in \mathbf{D}$; i.e., $\mathbf{T}$ maps $\mathbf{D}$ into itself.

Now we show that $\mathbf{T} : \mathbf{D} \subset \mathbf{X} \to \mathbf{X}$ is continuous. For this purpose, let v_j, $j = 1, 2, \cdots, \infty$, be functions in $\mathbf{D}$ such that $v_j \to v_\infty$ in $\mathbf{X} = C^1((-\infty, \xi_0])$ as $j \to \infty$. We want to show that $\mathbf{T}[v_j] \to \mathbf{T}[v_\infty]$ in $\mathbf{X}$. As every member of $\{\mathbf{T}[v_j]\}_{j=1}^{\infty}$ is in $\mathbf{D}$, which is compact in $\mathbf{X}$, any subsequence of $\{\mathbf{T}[v_j]\}$ has a subsubsequence convergent to a limit, say $\tilde v$, in $\mathbf{X}$. Since along that subsubsequence, $F[u_0 + v_j] \to F[u_0 + v_\infty]$, $(\mathbf{T}[v_j])' \to \tilde v'$, and $\mathbf{L}[(u_0 + \mathbf{T}[v_j])'\,] \to \mathbf{L}[(u_0 + \tilde v)']$ in $C^0((-\infty, \xi_0])$, we conclude by taking the limit of the integro–differential equation satisfied by $\mathbf{T}[v_j]$ that $u_0 + \tilde v$ is a solution to (4.9) with $f = F[u_0 + v_\infty]$. It then follows by uniqueness of (4.9) that $\tilde v = \mathbf{T}[v_\infty]$. Consequently, the whole sequence $\{\mathbf{T}[v_j]\}$ converges to $\mathbf{T}[v_\infty]$ in $\mathbf{X}$. Thus, $\mathbf{T}$ is continuous. The Schauder fixed point theorem then shows that $\mathbf{T}$ has at least one fixed point, which, after adding u_0, gives a solution to (4.3).

Finally, by Theorem 3.2, such a solution u is unique. This proves Theorem 4.1. ☐

4.3. **Proof of Lemma 4.2.** For notational simplicity, in the sequel, $O(f)$ stands for a quantity satisfying $|O(f)| \le C|f|$, where C is a positive constant depending only on k.

Since $u - u_0 \in \mathbf{D}$, $|u'(\xi) + 1| \le 2/|\xi|$, so that, by the mean value theorem and the definition $\eta = \xi + \log\frac{1-z}{1+z}$,

$$u - \hat u = u(\xi) - u(\eta) \quad = \quad u'(\xi - \theta)\{\xi - \eta\} = [1 + O(|\xi|^{-1})]\log\tfrac{1-z}{1+z}.$$

It then follows from the Lebesgue's dominated convergence theorem that $F \in C^1((-\infty, \xi_0])$. It remains to estimate $F[u]$ and its derivative.

First we estimate f_1. Note that b, defined in (4.2), is uniformly bounded in $z \in (0, 1)$ and $\xi \in (-\infty, \xi_0]$. In addition, that $u - u_0 \in \mathbf{D}$ and $\eta - \xi = \log\frac{1-z}{1+z} = -2z + (z^2)$ implies that $b = O(z^2 + z|\xi|^{-1} + \xi^{-2})$ so that

$|f_1| = O(z^2 + z|\xi|^{-1} + \xi^{-2})\frac{\sqrt{-\xi}e^{\xi z}}{\sqrt{\pi z}}$. Note that for every $\xi < 0$ and $i > -1/2$,

$$\int_0^1 z^i \frac{\sqrt{-\xi}e^{\xi z}}{\sqrt{\pi z}}\,dz \le \frac{|\xi|^{-i}}{\sqrt{\pi}} \int_0^\infty z^{i-1/2}e^{-z}\,dz = O(|\xi|^{-i}).$$

It then follows that $\int_0^1 |f_1|dz = O(\xi^{-2})$. A direct differentiation also shows that $\int_0^1 |\frac{d}{d\xi} f_1|\,dz = O(\xi^{-2})$ since $u'' = O(|\xi|^{-1})$.

Similarly, we can show that $\int_0^1 (|\hat{u}' f_3| + |\frac{d}{d\xi}\hat{u}' f_3|)dz = O(\xi^{-2})$.

For the integral involving f_2, we write $\sqrt{u\hat{u}} + \hat{u} = 2u - \frac{1}{2}(\sqrt{u} - \sqrt{\hat{u}})^2 - \frac{3}{2}(u - \hat{u}) = -2\xi + O(|\xi|^{-1} + |\xi|^{-1}\log^2\frac{1+z}{1-z} + \log\frac{1+z}{1-z})$. Hence, $\int_0^1 f_2\,dz = \int_0^1 \frac{-2z\xi\sqrt{-\xi}e^{\xi z}}{\sqrt{\pi z}}\,dz + O(|\xi|^{-2}) = -1 + O(\xi^{-2})$. A differentiation also gives $|\int_0^1 \frac{d}{d\xi} f_2\,dz| = O(\xi^{-2})$. This completes the proof. □

Remark 4.1. The integral in (3.10) is of size $|\xi|/s(t)$ if $\lambda \neq 1$. When $\lambda = 1$, this integral is of size $(\mathbf{L}[u'] - F[u])/s(t) = O(\xi^{-2})/s(t)$ since $u' = -1 + O(\xi^{-2})$ and $\mathbf{L}[u'] = -1 + O(\xi^{-2})$. Hence, the ratio of the integral and the first term on the right–hand side of (3.9) is of size $O(\xi^{-3})$; see Remark 3.1.

4.4. **Idea for the proof of Lemma 4.3.** To complete the proof of Theorem 4.1, it remains to prove Lemma 4.3, which will be done in the next two sections. Here we provide the main idea of the proof.

We first investigate in §5 the linear operator $\mathbf{L}$. In particular, we show that the inverse operator $(\mathbf{I}+\mathbf{L})^{-1}$ is a bounded operator from C^0 to C^0. Also, we show that $\mathfrak{L}[\phi]$ is always 1/2 more differentiable than ϕ.

Then in §6, we study, for any large integer j, an initial value problem $(\mathrm{P1})_j$ of the integro–differential equation in (P1) in the interval $[-j, \xi_0]$ with "initial value" $w = u_0$ in $(-\infty, -j]$. The existence of a solution follows from a standard Picard iteration technique.

To obtain certain desired behavior of the solution of $(\mathrm{P1})_j$, we find that $(\mathrm{P1})_j$, as well as (P1), satisfy a comparison principle: larger initial data and larger source term produce larger solutions. Because of the large positive derivative $\frac{\partial}{\partial u}G(u_0, \xi) \sim 2|\xi|$, this comparison principle allows us to construct sub and super solutions of the form $u_0 \pm M|\xi|^{-3}$ to sandwich the solution to $(\mathrm{P1})_j$. Thus, we can take the limit $j \to \infty$ to obtain a solution to (P1) with the desired asymptotic behavior. Uniqueness of solutions to (P1) also follows from the comparison principle.

5. The operator $\mathbf{L}$.

In this section we study the operator $\mathbf{L}$ defined in (4.5).

Lemma 5.1. *There exists a universal positive constant c_0 such that for every $\xi_0 \le -2$,*

$$c_0\|\phi\|_{C^0(-\infty,\xi_0])} \le \|(\mathbf{I}+\mathbf{L})[\phi]\|_{C^0(-\infty,\xi_0])} \le 2\|\phi\|_{C^0((-\infty,\xi_0])} \quad \forall\,\phi \in C^0((-\infty,\xi_0])\,. \tag{5.1}$$

Consequently, $\mathbf{I}+\mathbf{L}$ admits a bounded inverse $(\mathbf{I}+\mathbf{L})^{-1}$ from $C^0((-\infty,\xi_0])$ to itself and

$$\tfrac{1}{2} \le \|\,(\mathbf{I}+\mathbf{L})^{-1}\,\|_{C^0((-\infty,\xi_0]\to C^0((-\infty,\xi_0])} \le \tfrac{1}{c_0}. \tag{5.2}$$

Proof. From (4.5) and a change of variables $z \to Z/|\xi|$ and $\zeta \to \theta/|\xi|$, we can write $\mathbf{L}[\phi]$ as

$$\mathbf{L}[\phi](\xi) = \int_0^{-\xi} \phi(\xi + 2\theta/\xi)\varrho_1(\xi,\theta)\,d\theta, \quad \varrho_1(\xi,\theta) = \int_\theta^{-\xi} \frac{e^{-Z}}{Z\sqrt{\pi Z}}\,dZ.$$

Using $\sup_{\xi<0}\int_0^{-\xi} \varrho_1(\xi,\theta)\,d\theta = 1$, we obtain the second inequality in (5.1).

To prove the first inequality in (5.1), we notice that $\mathbf{L}$ is linear, so that we can without loss of generality assume $\|\phi\|_{C^0} = 1 = \sup_{\xi<\xi_0}\phi(\xi)$.

Let $j \ge 2$ be any integer, and let $\xi_j \in (-\infty, \xi_0]$ be a point such that $\phi(\xi_j) \ge 1 - 1/j$. Since $\int_0^{-\xi_j} \varrho_1(\xi_j, \theta) < 1$, for any $m \in (0, 1/2)$,

$$(\mathbf{I}+\mathbf{L})[\phi](\xi_j) \ge \int_0^{-\xi_j} \Big\{1 + \phi(\xi_j + 2\theta/\xi_j)\Big\}\varrho_1(\xi_j,\theta)\,d\theta - \frac{1}{j} \ge m\varrho_1(\xi_j, 1)\{1 - A(\xi_j, m)\} - \frac{1}{j}$$

where $A(\xi, m) = \text{measure}\{\theta \in [0,1] \mid \phi(\xi + 2\theta/\xi) + 1 < m\}$. Suppose $A(\xi_j, m) > 0$. Then there is a unique $\hat{\xi}_j \in (\xi_j + 2/\xi_j, \xi_j)$ such that $\phi(\xi) + 1 > m$ in $(\hat{\xi}_j, \xi_j]$ and $\phi(\hat{\xi}_j) + 1 = m$. Since $\hat{\xi}_j + 2/\hat{\xi}_j < \xi_j + 2/\xi_j$, $A(\hat{\xi}_j, m) \ge \frac{\xi_j}{\hat{\xi}_j} A(\xi_j, m) \ge \frac{\xi_j}{\xi_j + 2/\xi_j} A(\xi_j, m) > \frac{1}{2} A(\xi_j, m)$. Hence

$$\begin{aligned} -(\mathbf{I}+\mathbf{L})[\phi](\hat{\xi}_j) &= 1 - m - \mathbf{L}[\phi](\hat{\xi}_j) \ge -m + \int_0^{-\hat{\xi}_j} \{1 - \phi(\hat{\xi}_j + 2\theta/\hat{\xi}_j)\}\varrho_1(\hat{\xi}_j, \theta)\,d\theta \\ &\ge -m + (2 - m)A(\hat{\xi}_j, m)\varrho_1(\hat{\xi}_j, 1) \ge -m + (1 - \tfrac{m}{2})A(\xi_j, m)\varrho_1(\xi_j, 1). \end{aligned}$$

It then follows that, regardless of the size of $A(\xi_j, m)$,

$$\|(\mathbf{I}+\mathbf{L})[\phi]\|_{C^0} + \tfrac{1}{j} \ge \varrho_1(\xi_j, 1)\max\Big\{m[1 - A(\xi_j, m)], -m + (1 - \tfrac{m}{2})A(\xi_j, m)\Big\} \ge \varrho_1(-2, 1)\tfrac{m(2-3m)}{2+m}.$$

Sending $j \to \infty$ and taking $m = 1/3$ we then conclude that (5.1) holds with $c_0 = \varrho_1(-2, 1)/7$.

The invertibility of $\mathbf{I} + \mathbf{L}$ and the estimate (5.2) follow from (5.1) and the Hahn–Banach theorem. □

Next, we show that $\mathbf{L}[\phi]$ is 1/2 more differentiable than ϕ.

Lemma 5.2. *For every $\beta \in [0, 1]$, there exists a positive constant $C(\beta)$ such that*

$$\|\phi\|_{C^0([a-2,b])} + C(\beta)\sqrt{|a|}\,[\phi]_{\beta,[a-2,b]} \ge \begin{cases} [\,\mathbf{L}[\phi]\,]_{\beta+1/2,[a,b]} & \text{if } \beta \in [0, 1/2), \\ [\mathbf{L}[\phi]\,]^*_{1,[a,b]} & \text{if } \beta = 1/2, \\ [(\mathbf{L}[\phi])'\,]_{\beta-1/2,[a,b]} & \text{if } \alpha \in (1/2, 1] \end{cases} \tag{5.3}$$

where $[\psi]^*_{1,[a,b]} := \sup_{a\le\xi_2<\xi_1\le b} \frac{|\psi(\xi_2)-\psi(\xi_1)|}{|\xi_2-\xi_1|\,\max\{1,|\log(\xi_1-\xi_2)|\}}$ *and*

$$[\psi]_{\beta,[c,d]} = \sup_{c\le\xi_2<\xi_1\le d} \frac{|\psi(\xi_2) - \psi(\xi_1)|}{|\xi_2 - \xi_1|^\beta} \quad \forall \beta \in [0, 1]. \tag{5.4}$$

We remark that $\mathbf{L}[\phi](\xi)$ depends only on values of ϕ in $[\xi - 2, \xi]$. Also the factor $\sqrt{|a|}$ on the left–hand side of (5.3) is necessary since $\lim_{\xi\to\infty}\{\mathbf{L}[\phi](\xi) - \phi(\xi)\} = 0$ for any bounded and uniformly continuous function ϕ.

Proof. Let ξ_1 and ξ_2 be any numbers such that $a \le \xi_2 < \xi_1 \le b$. Set $h = \xi_1 - \xi_2$. Since $\|\mathbf{L}\|_{C^0\to C^0} \le 2$, we need only consider the case $h < 1/4$. Also, $\mathbf{L}[\mathbf{1}](\xi) = \int_0^{-\xi} \varrho(\xi,\theta)d\theta = \int_0^{-\xi} \frac{e^{-z}}{\sqrt{\pi z}}\,dz$, so that $\|\mathbf{L}[\mathbf{1}]\|_{C^1} \le 1$. Hence, by considering the function $\phi(\xi) - \phi(\xi_2)\mathbf{1}$ if necessary, we can assume that $\phi(\xi_2) = 0$.

First, we consider the case $\beta \in [0, 1/2]$. Using (4.5) we have

$$\begin{aligned} \mathbf{L}[\phi](\xi_2) - \mathbf{L}[\phi](\xi_1) &= \int_0^{1-h/2} \phi(\xi_2 - 2\zeta)\Big\{\varrho(\xi_2, \zeta) - \varrho(\xi_1, \zeta + h/2)\Big\}\,d\zeta \\ &\quad + \int_{1-h/2}^{1} \phi(\xi_2 - 2\zeta)\varrho(\xi_2, \zeta)\,d\zeta - \int_0^{h/2} \phi(\xi_1 - 2\zeta)\varrho(\xi_1, \zeta)\,d\zeta\,. \end{aligned}$$

Now $\phi(\xi_2)=0$ implies $|\phi(\xi_2-2\zeta)|\le[\phi]_\beta|2\zeta|^\beta$ for all $\zeta\in[0,1]$ and $|\phi(\xi_1-2\zeta)|\le h^\beta[\phi]_\beta$ for all $\zeta\in[0,h/2]$. Hence, $|\mathbf{L}[\phi](\xi_2)-\mathbf{L}[\phi](\xi_1)|$ is bounded by

$$[\phi]_\beta\Big\{\int_0^{1-h/2}(2\zeta)^\beta\Big|\varrho(\xi_1-h,\zeta)-\varrho(\xi_1,\zeta+h/2)\Big|\,d\zeta+\int_{1-h/2}^1\varrho(\xi_2,\zeta)\,d\zeta+\int_0^{h/2}h^\beta\varrho(\xi_1,\zeta)\,d\zeta\Big\}.$$

Direct integration shows that this quantity is bounded by $C(\beta)\sqrt{|\xi_2|}[\phi]_\beta h^{\beta+1/2}$ if $\beta\in[0,1/2)$ and by $C(\beta)\sqrt{|\xi_2|}[\phi]_\beta h\,|\log h|$ if $\beta=1/2$. This proves (5.3) for the case $\beta\in[0,1/2]$.

Next we consider $\beta\in(1/2,1]$. Set $\Phi(\xi)=\int_{\xi_2}^\xi\phi(\eta)\,d\eta$. Then $\mathbf{L}[\phi]=\int_0^1\frac{\Phi(\xi)-\Phi(\xi-2z)}{2z}\frac{\sqrt{-\xi}e^{\xi z}}{\sqrt{\pi z}}$, and

$$\begin{aligned}\frac{d}{d\xi}\mathbf{L}[\phi](\xi) &= \int_0^1\frac{\phi(\xi)-\phi(\xi-2z)}{2z}\frac{\sqrt{-\xi}e^{\xi z}}{\sqrt{\pi z}}\,dz\\ &\quad+\frac{1}{2\xi}\int_0^1\frac{\Phi(\xi)-\Phi(\xi-2z)}{2z}\frac{(1+\xi z)\sqrt{-\xi}e^{\xi z}}{\sqrt{\pi z}}\,dz=:I(\xi)+II(\xi)\ .\end{aligned}$$

Note that $\frac{d}{d\xi}II(\xi)$ is bounded by $[\phi]_\beta$ since $\Phi'=\phi$ and $|\phi(\xi)-\phi(\xi-2z)|\le[\phi](2z)^\beta$ and $\beta>1/2$. It remains to consider $I(\cdot)$. We write

$$\begin{aligned}I(\xi_1)-I(\xi_2) &= \int_0^1\frac{\phi(\xi_1)-\phi(\xi_1-2z)-\phi(\xi_2)+\phi(\xi_2-2z)}{2z}\frac{\sqrt{-\xi_1}e^{\xi_1 z}}{\sqrt{\pi z}}\,dz+\\ &\quad\int_0^1\frac{\phi(\xi_2)-\phi(\xi_2-2z))}{2z}\ \frac{\sqrt{-\xi_1}e^{\xi_1 z}-\sqrt{-\xi_2}e^{\xi_2 z}}{\sqrt{\pi z}}\,dz.\end{aligned}$$

Since $|\phi(\xi_2)-\phi(\xi_2-2z)|\le[\phi]_\beta(2z)^\beta$ with $\beta>1/2$, the second integral is bounded by $h[\phi]_\beta|\xi_1|^{-\beta}\int_0^\infty(1+Z)Z^{\beta-3/2}e^{-Z}\,dZ\le Ch[\phi]_\beta|\xi_1|^{-\beta}$. To estimate the first integral, we use

$$|\phi(\xi)-\phi(\xi-2z)-\phi(\xi_2)+\phi(\xi_2-2z)|\le 2[\phi]_\beta\min\{h^\beta,(2z)^\beta\}$$

so that the first integral is bounded by

$$2[\phi]_\beta\int_0^\infty\frac{\min\{(2z)^\beta,h^\beta\}}{2z}\frac{\sqrt{-\xi_2}e^{\xi_2 z}}{\sqrt{\pi z}}\,dz\le C\sqrt{-\xi_2}[\phi]_\beta h^{\beta-1/2}.$$

In summary, we have $|\frac{d}{d\xi}\mathbf{L}[\phi](\xi_1)-\frac{d}{d\xi}\mathbf{L}[\phi](\xi_2)|\le C[\phi]_\beta\sqrt{-\xi_2}h^{\beta-1/2}$. This completes the proof. ☐

Remark 5.1. With the same technique, one can show that, for any positive non-integer β, $\mathbf{L}[\phi]\in C^\beta$ if $\phi\in C^{\beta-1/2}$. Also we can show that $F[u]$ defined in (4.4) is always $1/2$ more differentiable that u', assuming that $u\sim-\xi+o(1/\xi)$. We omit the details.

6. Proof of Lemma 4.3

6.1. **The Truncated Problem.** We first study problem (P1) in a finite interval $[-j,\xi_0]$:

$$(6.1)\qquad (\mathrm{P1})_j\quad\begin{cases}(\mathbf{I}+\mathbf{L})[w'](\xi)+G(w(\xi),\xi)=f(\xi) & \forall\,\xi\in(-j,\xi_0],\\ w(\xi)=u_0(\xi), & \forall\xi\in(-\infty,-j]\ .\end{cases}$$

Since we aim for positive solutions, we extend $G(w,\xi)$ for negative w by 0.

Lemma 6.1. *Let $-j<\xi_0\le-2$, $f(\cdot)$ be any continuous function on $[-j,\xi_0]$, and u_0 be any differentiable function on $(-\infty,\xi_0]$. Then (P1)$_j$ admits a unique solution $w\in C^1([-j+,\xi_0])$.*

Proof. We first note that $\mathbf{L}[w'] = \int_0^1 \frac{w(\xi)-w(\xi-2z)}{2z}\frac{\sqrt{-\xi}e^{\xi z}}{\sqrt{\pi z}}\,dz$, so that $\|\mathbf{L}[w']\|_{C^0([-j,\xi])} \le C_j[w]_{3/4,[-j-2,\xi]}$ for all $\xi\in[-j,\xi_0]$, where $C_j = j^{1/4}\int_0^\infty Z^{-3/4}e^{-Z}dZ$ and $[\phi]_{\beta,[a,b]}$ is as in (5.4). We remark that if $\phi(a)=0$, then $[\phi]_{0,[a,b]} \ge \|\phi\|_{C^0([a,b])} := \sup_{\xi\in[a,b]}|\phi(\xi)|$.

Next we note that the function $G(w,\xi)$, after extension by 0 for negative w, is uniformly bounded, and $L_j = \sup_{\xi\in[-j,0],w\ge 0}|G_w(w,\xi)| < \infty$.

We now use Picard iteration to establish the existence and uniqueness. Starting with $w_0 \equiv u_0$, we successively define w_i, $i=1,2,\cdots$, by $w_i = u_0$ in $(-\infty,-j]$ and

$$w_i(\xi) = u_0(-j) + \int_{-j}^{\xi}\Big\{f(\hat\xi) - G(w_{i-1}(\hat\xi),\hat\xi) - \mathbf{L}[w'_{i-1}](\hat\xi)\Big\}d\hat\xi, \quad \xi\in[-j,\xi_0].$$

Taking the difference of the equations (and also their derivative) for w_{i+1} and w_i we obtain, for all $i\ge 1$ and all $\xi\in(-j,\xi_0]$,

$$\begin{aligned}[][w_{i+1}-w_i]_{0,[-j,\xi]} &\le L\int_{-j}^{\xi}\Big\{[w_i-w_{i-1}]_{0,[-j,\hat\xi]} + [w_i-w_{i-1}]_{3/4,[-j,\hat\xi]}\Big\}d\hat\xi,\\ [w_{i+1}-w_i]_{1,[-j,\xi]} &\le L\Big\{[w_i-w_{i-1}]_{0,[-j,\xi]} + [w_i-w_{i-1}]_{3/4,[-j,\xi]}\Big\}\end{aligned}$$

where $L=\max\{C_j,L_j\}$. Since $[\phi]_{3/4,[a,b]} \le ([\phi]_{1,[a,b]})^{3/4}([\phi]_{0,[a,b]})^{1/4}$ for any ϕ and any interval $[a,b]$, mathematical induction then gives, for $\beta=0,3/4,1$ and all $i\ge 2$,

$$[w_{i+1}-w_i]_{\beta,[-j,\xi]} \le \frac{M^i(\xi+j)^{i/4}}{(i\,!)^{1/4}}\Big(\frac{i}{4(\xi+j)}\Big)^{\beta} \qquad \forall \xi\in(-j,\xi_0]$$

for some sufficiently large constant M depending only on j and u_0. Following the rest steps of the Picard iteration method (see, for example, [9]) we then complete the proof. □

To take the limit $j\to\infty$ for solutions of $(P1)_j$, we need certain estimates. This will be done via a comparison principle and construction of sub and super solutions.

6.2. **The Comparison Principle.** For convenience, we introduce a non-linear operator $\mathbf{N}$ defined by

$$\mathbf{N}[w](\xi) = (\mathbf{I}+\mathbf{L})[w'](\xi) + G(w(\xi),\xi)\,. \tag{6.2}$$

Lemma 6.2. (Comparison Principle) *Let $\xi_0 \le -2$ be any number and w_1 and w_2 be two (piecewise) continuous differentiable functions on $(-\infty,\xi_0]$ satisfying the following:*

(i) $\min\{w_1,w_2\}\ge 3/2$ *in* $(-\infty,\xi_0]$;

(ii) There exists $j\in\{\infty\}\cup(-\xi_0,\infty)$ *such that*

$$\mathbf{N}[w_1](\xi) \ge \mathbf{N}[w_2](\xi) \quad \forall\,\xi\in(-j,\xi_0]$$

and $\liminf_{\xi\to-\infty}\{w_1(\xi)-w_2(\xi)\}\ge 0$ *if* $j=\infty$, *and* $w_1(\xi)\ge w_2(\xi)$ *on* $(-\infty,-j]$ *if* $j<\infty$.

Then $w_1(\xi)\ge w_2(\xi)$ *for all* $\xi\in(-\infty,\xi_0]$.

Proof. Let $\varepsilon\in(0,1/4)$ be any constant. We define

$$\xi_\varepsilon = \sup\{\xi\le\xi_0 \mid w_1+\varepsilon > w_2 \ \text{ in } \ (-\infty,\xi)\}.$$

The "initial condition" in assumption (ii) implies that ξ_ε is well–defined and $\xi_\varepsilon > -j$. We claim that $\xi_\varepsilon=\xi_0$. In fact, if this is not true, then $w_2 < w_1+\varepsilon$ in $(-\infty,\xi_\varepsilon)$, and at $\xi=\xi_\varepsilon$, $w_2 = w_1+\varepsilon$ and $w_2'\ge w_1'$. In addition, $G(w_2(\xi_\varepsilon),\xi_\varepsilon) = G_2(w_1(\xi_\varepsilon)+\varepsilon,\xi_\varepsilon) > G(w_1(\xi_\varepsilon),\xi_\varepsilon)$ since $w_1(\xi_\varepsilon) = -\varepsilon + \max\{w_1(\xi_\varepsilon), w_2(\xi_\varepsilon)\} > 5/4$ and $G_w(w,\xi) > 0$ when $w > 5/4$. Hence

$$\begin{aligned}\mathbf{N}[w_1](\xi_\varepsilon) &= w_1'(\xi_\varepsilon) + \int_0^1 \frac{\{w_1(\xi_\varepsilon)+\varepsilon\} - \{w_1(\xi_\varepsilon - 2z)+\varepsilon\}}{2z}\frac{\sqrt{-\xi_\varepsilon}e^{\xi_\varepsilon z}}{\sqrt{\pi z}}dz + G(w_1(\xi_\varepsilon),\xi_\varepsilon)\\ &< w_2'(\xi_\varepsilon) + \int_0^1 \frac{w_2(\xi_\varepsilon) - w_2(\xi_\varepsilon - 2z)}{2z}\frac{\sqrt{-\xi_\varepsilon}e^{\xi_\varepsilon z}}{\sqrt{\pi z}}dz + G(w_2(\xi_\varepsilon),\xi_\varepsilon) = \mathbf{N}[w_2](\xi_\varepsilon),\end{aligned}$$

which contradicts the assumption that $\mathbf{N}[w_1] \geq \mathbf{N}[w_2]$ in $(-j,\xi_0]$. This contradiction shows that $\xi_\varepsilon = \xi_0$; namely $w_1(\xi) + \varepsilon \geq w_2(\xi)$ in $(-\infty,\xi_0]$. Sending ε to 0 we then obtain the assertion of the lemma. □

One notices that the condition (i) is used only to ensure that $G_w(w,\xi) > 0$ for any $w \geq \max\{w_1, w_2\}$.

For later applications, we also provide the following maximum principle.

Lemma 6.3. (Maximum Principle) *Let $L(\cdot)$ be a continuous and uniformly positive function on $(-\infty,\xi_0]$ and W be a Lipschitz continuous functions on $(-\infty,\xi_0]$ satisfying*

$$(\mathbf{I}+\mathbf{L})[W'](\xi) + L(\xi)W(\xi) \geq 0 \quad \forall \xi \in (-\infty,\xi_0], \qquad \inf_{\xi\leq\xi_0} W(\xi) > -\infty.$$

Then $W \geq 0$ on $(-\infty,\xi_0]$.

The proof follows closely the proof for the previous lemma and is omitted.

6.3. **Estimates for Solutions of $(\mathbf{P1})_j$.** Let C_0 be the constant in Lemma 4.2.

Lemma 6.4. *There exists a large negative constant $\Xi_1(C_0)$ such that if $\xi_0 \leq \Xi_1(C_0)$ and $f(\cdot) \in C^0((-\infty,\xi_0]$ satisfying*

$$|f(\xi)+1| \leq C_0\xi^{-2}, \tag{6.3}$$

then the unique solution w to $(P1)_j$ with $u_0 = -\xi - \frac{1}{2}\xi^{-1} + \frac{3}{8}\xi^{-2} + \frac{17}{24}\xi^{-3}$ satisfies

$$|w(\xi) - u_0| \leq (1 + \tfrac{1}{2}C_0)|\xi|^{-3}, \qquad \forall \xi \in (-\infty,\xi_0], \tag{6.4}$$

$$|w'(\xi) - u_0'| \leq \tfrac{2C_0+2}{c_0}\xi^{-2} \qquad \forall \xi \in (-\infty,\xi_0]. \tag{6.5}$$

Proof. Let $w_\pm = u_0 \mp M\xi^{-3}$ where $M > 0$ is to be determined. Then $\frac{w_\pm(\xi)-w_\pm(\xi-2z)}{2z} = w_\pm'(\xi) + z\,O(|\xi|^{-3})$. It then follows that $\mathbf{L}[w_\pm'] = \int_0^1 \frac{w_\pm(\xi)-w_\pm(\xi-2z)}{2z}\frac{\sqrt{-\xi}e^{\xi z}}{\sqrt{\pi z}}dz = w_\pm'(\xi) + O(|\xi|^{-4})$. Consequently,

$$\begin{aligned}&\mathbf{N}[w_\pm] - f(\xi) = (\mathbf{I}+\mathbf{L})[w_\pm'] + G(w_\pm,\xi) - f(\xi)\\ =\ & 2w_\pm'(\xi) + 2w_\pm(1 - e^{-w_\pm - \xi}) - f(\xi) + O(|\xi|^{-4})\\ =\ & -1 - f(\xi) \pm 2M\xi^{-2} + O(|\xi|^{-3}).\end{aligned}$$

Hence, taking $M = C_0/2 + 1$ and $\Xi_1[C_0]$ large enough, we have $\pm\mathbf{N}[w_\pm] > 0$ in $(-\infty,\xi_0]$. The comparison principle then gives $w_- \leq w \leq w_+$ in $(-\infty,\xi_0]$ and therefore also (6.4). In addition,

$$(\mathbf{I}+\mathbf{L})[w' - u_0'](\xi) \;=\; f(\xi) - G(w(\xi),\xi) - 2u_0' + O(|\xi|^{-4}) = O(\xi^{-2}).$$

The estimate (6.5) then follows from the boundedness of $\|(\mathbf{I}+\mathbf{L})^{-1}\|_{C^0\to C^0}$. □

Now we are ready to prove Lemma 4.3.

6.4. **Proof of Lemma 4.3.** Let C_0 and $\Xi_1(C_0)$ be as in Lemmas 4.2 and 6.4 respectively. Let $\xi_0 \le \Xi_1(C_0)$.

For each integer $j > |\xi_0|$, let w_j be the solution to $(P1)_j$. From Lemma 6.4, we know that we can extract a subsequence from $\{w_j\}_{j>|\xi_0|}$, which converges to w in $C^\beta((-\infty,\xi_0])$ for any $\beta \in (0,1)$ and some Lipschitz continuous function w satisfying the estimates (6.4) and (6.5). Consequently, $G(w_j(\cdot),\cdot) \to G(w(\cdot),\cdot)$ in $C^0((-\infty,\xi_0])$. Also, from the expression $\mathbf{L}[w_j'](\xi) = \int_0^1 \frac{w_j(\xi)-w_j(\xi-2z)}{2z} \frac{\sqrt{-\xi}e^{\xi z}}{\sqrt{\pi z}}\,dz$ we see that $\mathbf{L}[w_j'] \to \mathbf{L}[w']$ uniformly in $(-\infty,\xi_0]$. Hence, from $w_j' = f - \mathbf{L}[w_j'] - G(w_j,\cdot)$, we conclude that $w_j(\cdot)' \to w'(\cdot)$ in $C^0((-\infty,\xi_0])$ and w is a $C^1((-\infty,\xi_0])$ solution to (P1). Uniqueness of the solution to (P1) follows from the comparison principle, i.e., Lemma 6.2 with $j=\infty$.

It remains to show that $w \in C^2$ and to estimate w'' and w' (better than (6.5)).

First of all, $f(\cdot)+G(w(\cdot),\cdot)$ is differentiable. Also, that $w' \in C^0$ and Lemma 5.2 implies that $\mathbf{L}[w'] \in C^{1/2}$ so that $w' = f - G(w,\cdot) - \mathbf{L}[w'] \in C^{1/2}$. Repeating this process we then conclude that $w \in C^2$.

Once we know that w is C^2, we can differentiate the equation for w to obtain

$$(\mathbf{I}+\mathbf{L})[w''] + L(\xi)w' = f_\xi - G_\xi(w,\xi) - \psi$$

where $L(\xi) = G_w(w(\xi),\xi))$ and $\psi = \int_0^1 \frac{w(\xi)-w(\xi-2z)}{2z} \frac{\sqrt{-\xi}e^{\xi z}}{\sqrt{\pi z}} \left\{\frac{1}{\xi} + z\right\} dz = O(\xi^{-2})$ since $w' = -1 + O(|\xi|^{-1})$.

Using the estimate (6.4) and the definition of G in (4.1) we see that $L(\xi) = G_w(w,\xi) = -2\xi - 1 - 2\xi^{-1} + O(|\xi|^{-2})$ and $G_\xi = -2\xi - 1 - \xi^{-1} + O(\xi^{-2})$. Since $(\mathbf{I}+\mathbf{L})[u_0''] = O(|\xi|^{-3})$ we have $(\mathbf{I}+\mathbf{L})[(w-u_0)''] + L(\xi)(w-u_0)' = f_\xi - G_\xi - \psi - L(\xi)u_0' + O(|\xi|^{-3}) = O(\xi^{-2})$ by the assumption on f_ξ.

Now we can use the maximum principle (Lemma 6.3) to estimate $(u-u_0)'$ and $(u-u_0)''$. For large constant M to be determined, set $W_\pm = -M\xi^{-3} \pm (u-u_0)'$. Then $(\mathbf{I}+\mathbf{L})[W'] + L(\xi)W = 2M\xi^{-2} + O(1)|\xi|^{-2} + O(|\xi|^{-3})$ where $O(1)$ depends only on C_0. Hence, taking M large (depending only on C_0) such that $M + O(1) = 1$ and then taking $\Xi(C_0)$ large enough negative, we have, when $\xi_0 \le \Xi(C_0)$, that $W_\pm > 0$ in $(-\infty,\xi_0]$, i.e., $|(w-u_0)'| \le M|\xi|^{-3}$. (Note the improvement over (6.5)). In addition, from $(\mathbf{I}-\mathbf{L})[(w-u_0)''] = O(|\xi|^{-2}) - L(w-u_0)' = O(|\xi|^{-2})$ and the boundedness of $(\mathbf{I}+\mathbf{L})^{-1}$ we conclude that $(w-u_0)'' = O(\xi^{-2})$. This completes the proof of Lemma 4.3, and also of Theorem 4.1. ☐

Remark 6.1. Using the same argument as in problem $(P1)_j$ (the Picard iteration), one can extend the solution u of (4.3) to $\xi \in (-\infty,\infty)$.

Remark 6.2. With the preceding argument for the C^2 differentiability of w, one can actually show that solution u to (4.3) is C^∞. To do this, one writes the equation as

$$u' + \mathbf{L}[u'] + \mathbf{L}_1^u[u'] = (F[u] + \mathbf{L}_1^u[u']) - G(u,\cdot)$$

where $\mathbf{L}_1^u[\phi'] = \int_0^1 \phi'(\eta) f_3\,dz$ is the part of $F[u]$ involving the integral of $u'(\eta)f_3$. Then the right–hand side of the equation is always 1/2 more differentiable than that of u'. As the operator norm from $C^0((\infty,\xi])$ to $C^0((-\infty,\xi])$ of $\mathbf{L}_1^u$ is of order $|\xi|^{-1}$, one sees that $(\mathbf{I}+\mathbf{L}+\mathbf{L}_1^u)^{-1}$ is bounded from C^0 to C^0. It then follows from a boot strap argument that $u \in C^\infty$. See also Remark 2.2.

6.5. **Higher order expansions.**

Theorem 6.5. *There exist constants $c_1, c_2, c_3, \cdots$ such that as $\xi \to -\infty$, the unique solution to* (P1) *has the asymptotic expansion $u \sim -\xi + \sum_{i=1}^\infty c_i\xi^{-i}$; in particular, (1.2) holds (with $\alpha(t)$ replaced by $u(\xi)$).*

Proof. **1. Construction of the asymptotic expansion.** First of all, we can replace $G(u,\xi)$ defined in (4.1) by $2u(1-e^{-u-\xi})$ since the terms dropped are of order $O(|\xi|e^{\xi})$. Similarly, we can drop the exponentially small terms in b defined in (4.2) (These are equivalent to replacing the fundamental solution $\Gamma(x,t)$ in (3.1) by $\frac{1}{2\sqrt{\pi t}}e^{-x^2/(4t)}$). Writing the equation (4.6) as $G(u,\xi)=F[u]-(\mathbf{I}+\mathbf{L})[u]$, and solving for u we obtain

$$u(\xi)=-\xi-\log\Big\{1+\frac{(\mathbf{I}+\mathbf{L})[u']-F[u]}{2u(\xi)}\Big\}.$$

Starting with $u=\xi+O(1)$ and successively replacing u on the right–hand side by its previous expansion, we then obtain expansions of all order. The key here is that the right–hand side produces a unique $n+1^{th}$ order expansion, if an n^{th} order expansion of u is given, because of the denominator $2u(\xi)$.

With the help of *Mathematica*'s symbolic package, we obtain, in particular, the expansion (1.2); see the *Mathematica* program in www.math.pitt.edu/˜xfc.

2. Rigorous verification of the expansion.

For every $n\geq 2$, set $u_n=-\xi+\sum_{i=1}^{n}c_i\xi^{-i}$ and define

$$\mathbf{X}_n=\Big\{w\in C^1((-\infty,\xi_n])\ \Big|\ |(w-u_n)(\xi)|+\tfrac{1}{|\xi|}|(w-u_n)'(\xi)|\leq M_n|\xi|^{-n-1}\ \text{ for all }\ \xi\leq\xi_n\Big\}.$$

We shall use mathematical induction to show that, for every integer $n\geq 2$, $u\in\mathbf{X}_n$ provided that we take ξ_n and M_n large enough.

Suppose $u\in\mathbf{X}_n$. Then one can verify that $F[u]-F[u_n]=O(|\xi|^{-n-1})$. In deriving this, we need

$$u(\xi)-u(\eta)\;=\;\int_\xi^\eta u'(\hat\xi)\,d\hat\xi=\int_\xi^\eta(u_n'+O(|\xi|^{-n})\,d\hat\xi=u_n(\xi)-u_n(\eta)+|\xi-\eta|O(|\xi|^{-n}).$$

Now define $w_\pm=u_{n+1}\pm M|\xi|^{-n-2}$ where M is to be determined. We can calculate $\mathbf{N}[w_\pm]:=(\mathbf{I}+\mathbf{L})[w_\pm']+G(w_\pm,\xi)=\mathbf{N}[u_{n+1}]\pm 2M|\xi|^{-n-1}+O(|\xi|^{-n-2})$ since $L(\xi):=G_w(u,\xi)=2|\xi|+O(1)$.

From the construction of u_{n+1}, we have $\mathbf{N}[u_{n+1}]=F[u_n]+O(|\xi|^{-n-1})$, and we then conclude that $\mathbf{N}[w_\pm]-\mathbf{N}[u]=F[u_n]-F[u]\pm 2M|\xi|^{-n-1}+O(1)|\xi|^{-n-1}=2\pm M|\xi|^{-n-1}+O(1)|\xi|^{-n-1}$ where $O(1)$ is independent of M if ξ is large enough. Hence, there exist a large constant M_{n+1} and large negative constant ξ_{n+1} such that for $M=M_{n+1}$, $\pm(\mathbf{N}[u]-\mathbf{N}[w_\pm])>0$ in $(-\infty,\xi_{n+1})]$. Therefore, by comparison, $w_-<u<w_+$, i.e., $|u-u_{n+1}|\leq M_{n+1}|\xi|^{-n-2}$ for all $\xi\leq\xi_{n+1}$. We take M large enough. With this estimate, we also obtain $(\mathbf{I}+\mathbf{L})[(u-u_{n+1})']=\{\mathbf{N}[u]-\mathbf{N}[u_{n+1}]\}-\{G(u,\xi)-G(u_{n+1},\xi)\}=O(|\xi|^{-n-1})$. Consequently, by the boundedness of $(\mathbf{I}+\mathbf{L})^{-1}$, $|u'-u_{n+1}|=O(|\xi|^{-n-1})$. Thus, $u\in\mathbf{X}_{n+1}$. This completes the proof. ☐

Remark 6.3. We did not include the second order derivative of u in the definition of $\mathbf{X}_n$ since we do not intend to establish the estimate for u''. On the other hand, we do need to include the second order derivative of u in $\mathbf{X}$ in the proof of Theorem 4.1 to make the set $\mathbf{D}$ compact in $\mathbf{X}$.

7. Approximations of the Early Exercise Boundary

In applications, one needs to find quickly the early exercise boundary

$$S_f(T)=Ee^{s(t)},\quad s(t)=-2\sqrt{t\,\alpha(t)},\quad \alpha(t)=u(\xi),\quad \xi=\log\sqrt{4\pi k^2t},\ k=2r\sigma^{-2},\quad t=\tfrac12\sigma^2(T_F-T)$$

of the American put option. There have been a number of theoretical approximations, see, for example, Stamicar–Sevcovic–Chadam [25], Kuske–Keller [18], Bunch–Johnson [5], and MacMillan–Barone-Adesi–Whaley [14, Appendix 14A]. In this section we derive our new approximations mentioned in §1. The advantages of our new approximations will be presented in our companion paper [8] where detailed numerical comparisons among our new proposed approximations and those in [25, 18, 5, 14] for a variety of parameter ranges and expiration times are given. For the purpose of demonstration, we provide one example here; see the attached Figure. In the sequel, σ^2 and r are measured in annualized units, i.e. have units 1/year.

7.1. **An Explicit Approximation Near Expiry.** One notices that expansions such as (1.2) cannot be used for $\xi \geq 0$ (equivalent to $t \geq 1/(4\pi k^2)$ or $T_F - T > \sigma^2/(8\pi r^2)$). Indeed, our numerical evidence [8] shows that approximations based on the truncations of (1.2) break down much earlier, and higher order expansions approximate $s(t)$ better than the second order only if $T_F - T$ is shorter than a few minutes, and therefore, are of no practical use. In this aspect, the best choice for practical estimation of $S_F(T)$ near expiry is the second order approximation $u(\xi) \approx -\xi - \frac{1}{2\xi}$. It is good for $T_F - T$ less than a week when $\sigma = 0.25/\sqrt{\text{year}}, r = 0.1/\text{year}$. Nevertheless, we still want to use (1.2) to obtain better approximations.

We recall that the particular choice of the constant $4\pi k^2$ in the definition of $\xi = \log\sqrt{t} + \log\sqrt{4\pi k^2}$ is to eliminate the constant term in the expansion of $u(\xi)$. If we use another variable such as $\hat{\xi} = \log\sqrt{Bt}$ and expand u in terms of $1/\hat{\xi}$, then the corresponding expansions make sense for all $t < 1/B$. Based on this idea, for any $a > 0$, we expand $u(\xi)$ as $u = -\xi - \frac{1}{2(\xi-a)} + \frac{1/8+a/2}{(\xi-a)^2} + \frac{17/24-a/4-a^2/2}{(\xi-a)^3} + \cdots$. Being equivalent to (1.2) as $\xi \to -\infty$, this new expansion, however, can be evaluated for all $t < e^a/(4\pi k^2)$. In particular, taking $a = 0.96621$ to be the positive root to $17/24 - a/4 - a^2/2 = 0$ and truncating the expansion at the fourth order, we obtain (expl) in §1. Numerical evidence shows that this new approximation (expl) is better than any of the straightforward truncations of (1.2), both in accuracy and in the length of the interval of validity. For $\sigma = 0.25/\sqrt{\text{year}}$ and $r = 0.1/\text{year}$, the approximation is very accurate for $T_F - T$ less than one month.)

7.2. **An Implicit/Series Approximation.** We can extend further the above idea. We seek approximations which meet two requirements: (i) they are valid asymptotic expansions as $\xi \to -\infty$, and (ii) they are analytic for all $\xi \in \mathbb{R}$. We find that such approximations can be easily obtained if we regard ξ as function of u, i.e., the inverse function of $\xi = \xi(u)$.

For every $a > 0$, we convert (1.2) into its equivalent form $\xi = -u - \log\{1 - \frac{1}{2(u+a)} - \frac{a}{2(u+a)^2} + \frac{1-a^2}{2(u+a)^2} + \cdots\}$. Hence, taking $a = 1$ and truncating the expansion at the fourth order, we obtain the implicit formula (imp1) in §1. As a special advantage, this expansion is meaningful for all time since for every $\xi \in \mathbb{R}$, there is a unique u solving (imp1) and $\xi \to \infty$ as $u \to 0$, which is compatible with the fact that $u = \frac{s(t)^2}{4t} \to 0$ as $\xi = \log\sqrt{4\pi k^2 t} \to \infty$. Our numerical experiments in [8] show that (imp1) is much better than (expl). It is reasonably good for $T_F - T$ as long as one year when $\sigma = 0.25$ and $r = 0.1$. See the attached Figure.

7.3. **Implicit/Interpolation Approximation.** The approximation (imp1) is based on the asymptotic expansion (1.2) which concerns *only* the behavior of $s(t)$ near expiry. We now derive an approximation which incorporates as well the asymptotic behavior of u for large $t = e^{2\xi}/(4\pi k^2)$.

Using (3.6) and the change of variable $\tau \to z$ via $z = (s(t) - s(t-\tau))/(2\sqrt{\tau})$ we obtain

$$e^{-u-\xi} = \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{u}} e^{-z^2} \theta_1(t,z)\theta_2(t,z)\, dz =: \frac{2\theta(t)}{\sqrt{\pi}} \int_0^{\sqrt{u}} e^{-z^2}\, dz \tag{7.1}$$

where

$$\theta_1(t,z) = \Big\{2 - \frac{s(t) - s(t-\tau)}{\tau\, s'(t-\tau)}\Big\}^{-1}, \qquad \theta_2(t,z) = \exp\{\tfrac{(k-1)s(t-\tau)}{2} + \tfrac{(k+1)^2(t-\tau)}{4}\}.$$

Note that $\theta_1(t,0) = 1$ and $\theta(t,\sqrt{u}) = 1/2$. Also, $\lim_{t\to 0}\theta_2(t,z) = 1$ uniformly in z and $\lim_{t\to 0}\theta_1(t,z) = 1$ for any fixed finite z. Hence $\lim_{t\to 0}\theta(t) = 1$; Cf. Remark 3.3.

Now we consider $\theta(t)$ for large t. From Theorem 2.3, we obtain $u = s^2(t)/(4t) \approx \log^2[1+1/k]/(4t)$, and $1/\theta(t) = \frac{2}{\sqrt{\pi}} e^{u+\xi} \int_0^{\sqrt{u}} e^{-z^2} dz \approx 2k\log[1+1/k]$ for large t (or ξ). Once we know the behavior of $\theta(t)$ for small and large t, we can approximate $\theta(t)$ for any t by interpolation. Without considering any more detailed behavior of θ for intermediate sizes of t, we choose, for simplicity, the approximation

$$\frac{1}{\theta(t)} \approx \frac{\theta(0)e^u + \theta(\infty)e^{1/u}}{e^u + e^{1/u}} = \frac{e^u + 2k\log(1+1/k)e^{1/u}}{e^u + e^{1/u}}.$$

Substituting this approximation into (7.1) and taking the log of both sides, we then obtain (imp2) in §1. The attached Figure shows that (imp2) is better than (imp1) when $T_F - T$ is larger than one month (for $r = 0.1$ and $\sigma = 0.25$). When $T_F - T$ is less than month, (imp1) is better than (imp2) since for small t, (imp1) is a fourth order approximation whereas (imp2) is only first order.

We remark that (imp1) can be revised to provide approximations which has higher order (as $t \to 0$) than (imp2), yet still capture the asymptotic behavior $s(t) \sim s_\infty$ for large t.

7.4. **An ODE Approximation.** The (ODE) approximation in §1 is obtained by neglecting the integral in (3.10). In the (u,ξ) variable, it can be written as

$$\begin{cases} \dfrac{1}{2u}\dfrac{du}{d\xi} = \exp\Big\{ -u - \xi + \frac{(k-1)\sqrt{u}e^{\xi}}{2k\sqrt{\pi}} - \frac{(k+1)^2e^{2\xi}}{16k^2\pi}e^{2\xi}\Big\} - 1 \quad \text{for} \quad \xi \in \mathbb{R}^1, \\ \lim_{\xi\to-\infty}\{u(\xi) + \xi\} = 0. \end{cases} \tag{7.2}$$

In numerically solving this ode problem, the initial condition can be taken as $u|_{\xi=\xi_0} = -\xi_0 - \frac{1}{2\xi_0}$ for large negative ξ_0, say $\xi_0 = -7$. This initial value problem is extremely stable with respect to the initial condition. Indeed, solutions with initial conditions $u|_{\xi=-7} = 1, 7, 10$ are indistinguishable when $\xi = -6$, since the initial difference decays with a speed $e^{-(\xi-\xi_0)G_w(u_0,\xi)} \approx e^{-2|\xi_0|(\xi-\xi_0)}$. Also, the computing time is almost instantaneous. Our numerical simulations indicate that this (ODE) approximation is better than any of the previous three algebraic approximations, and is very accurate for a variety of parameter ranges of σ and r and almost all time $t > 0$.

7.5. **An ODE Iterative scheme.** For the purpose of numerical comparison of the accuracy of theoretical approximations, highly accurate solutions for $s(t)$ are needed. Such solutions can be obtain by an iteration based on (3.10). We write (3.10) as (1.3). Asymptotic expansion gives, for small t, $m(t) = 0 + 0\xi^{-1} + 0\,\xi^{-2} + \frac{1}{4}\xi^{-3} + O(\xi^{-4}) \approx \frac{1}{4}\xi^{-3}$ and for large t,

$$m(t) \approx m(\infty) = k\int_0^\infty \Big\{1 - \frac{2s(\tau)}{s(\infty)}\Big\} \exp\Big\{\frac{(k-1)}{2}s(\tau) + \frac{(k+1)^2}{4}\tau\Big\}\dot{s}(\tau)\, d\tau.$$

We remark that the integral is finite since letting t in (3.6) approach ∞ gives the identity

$$1 = -k\int_0^\infty \exp\Big\{\frac{(k-1)}{2}s(\tau) + \frac{(k+1)^2}{4}\tau\Big\}\dot{s}(\tau)\,d\tau.$$

Hence, $|m(\infty)| < 1$. Our numerical simulation shows that $m(t)$ changes sign exactly once, and this occurs near $\xi = 0$; for $r = 0.1$ and $\sigma = 0.25$, the minimum of $m(t)$ is $-0.003...$ which occurs near $\xi = -5$, and the maximum is $0.17...$ which is attained at $\xi = \infty$. From here, we can see why the ODE approximation (approximating m by 0) is very accurate for all $t > 0$.

The ode iterative scheme that we propose is as follows: update s by solving (1.3) for s with $m(t)$ evaluated at a previous s; more precisely, $m^{(0)}(t) \equiv 0$, and for $n = 0, 1, \cdots$, $s^{(n)}(t) = -2\sqrt{t\,u^{(n)}(t)}$ where

$$(7.3)\quad \begin{cases} \dfrac{du^{(n)}}{d\log\sqrt{4\pi k^2 t}} &= 2u^{(n)}\Big\{\frac{1+m^{(n)}}{\sqrt{4\pi k^2 t}}\exp\Big[\frac{k-1}{2}\sqrt{t\,u^{(n)}} - u^{(n)} - \frac{(k+1)^2}{4}t\Big] - 1\Big\}, \quad t \ge \delta, \\ u^{(n)}(\delta) &= -\frac{1}{2}\log[4\pi k^2\delta] - \frac{1}{2}\log^{-1}[4\pi k^2\delta]), \end{cases}$$

$$m^{(n+1)}(t) = \begin{cases} ks^{(n)}(\delta) + \int_\delta^t \Big\{\frac{s^{(n)}(t)-s^{(n)}(\tau)}{t-\tau}\frac{2t}{s^{(n)}(t)} - 1\Big\}\frac{k\Gamma(s^{(n)}(t)-s^{(n)}(\tau),t-\tau)}{\Gamma(s^{(n)}(t),t)}\dot{s}^{(n)}(\tau)\,d\tau, & t \ge \delta_1, \\ \frac{1}{4}\log^{-3}\sqrt{4\pi k^2 t}, & t \in [\delta, \delta_1], \end{cases}$$

where δ and δ_1 are small numbers, say, $\delta = e^{-27}$ and $\delta_1 = e^{-18}$. The ode for u is solved in the $\xi = \log\sqrt{4\pi k^2 t}$ variable, and a change of variable $\tau = t\eta^2$ is used in evaluating the integral for m. For $t \in [\delta_1, t_{\max}]$ ($t_{\max} = e^5$ will make $s(t_{\max})$ within 0.1% of s_∞), an increasing number, say $32, 48, 72, 108, \cdots$, of points evenly distributed on the $\log t$ scale can be used to interpolate the function $m^{(1)}(t), m^{(2)}(t), m^{(3)}(t), \cdots$. In general, three iterations will provide a solution of relative error less than 10^{-5}, for all t, and five iterations will produce a numerical fixed point, which costs a total of less than 10 minutes computing time on a Sparc server.

7.6. **An Approximation for Large Time.** Although options with very long expiry rarely exist in practice, it is still useful to find the long time behavior (more precise than $S_f \approx Ek/(1+k)$) of the optimal exercise boundary since the scaling $t = \frac{\sigma^2}{2}(T_F - T) = \frac{2r}{k}(T_F - T)$ tells us that short time expiration can be considered as long if r or σ is large. For this reason, we provide an approximation for large time, so that when incorporated with our ode and/or implicit approximations, it will provide instantaneously a reliable approximation valid for all t and consequently for all ranges of σ and r.

Approximating $\Gamma(s(t),t)\{1 + m(t)\}$ on the right–hand side of (1.3) by $\frac{1+m(\infty)}{2\sqrt{\pi t}}e^{-\frac{(1-k)}{2}s(\infty)-\frac{(k+1)^2}{4}t}$ and integrating the resulting approximation from t to ∞ we obtain (long) in §1. As the ode solution is a good approximation, $\hat{m}$ in (long) can be approximately calculated by using the ode approximation for $s^{(0)}(\tau)$ in the integral; the computing time for this approximation is almost instantaneous since we can do so for $s^{(0)}$.

7.7. **A Numerical Example.** To give the reader an idea of the accuracy of our approximations, we provide in the following Figure the results of a numerical simulation with typical parameters $E = 1$ (dollar), $r = 0.1$ (1/year), $\sigma = 0.25$ ($1/\sqrt{\text{year}}$) and $k = 2r/\sigma^2 = 3.2$. For other parameters, see [8].

In the Figure, the vertical axis is $\log_{10}$ (errors) (with labelling being the actual size of the errors) of the various approximations for the optimal exercise boundary $S_f(T)$, whereas the horizontal axis is the time to

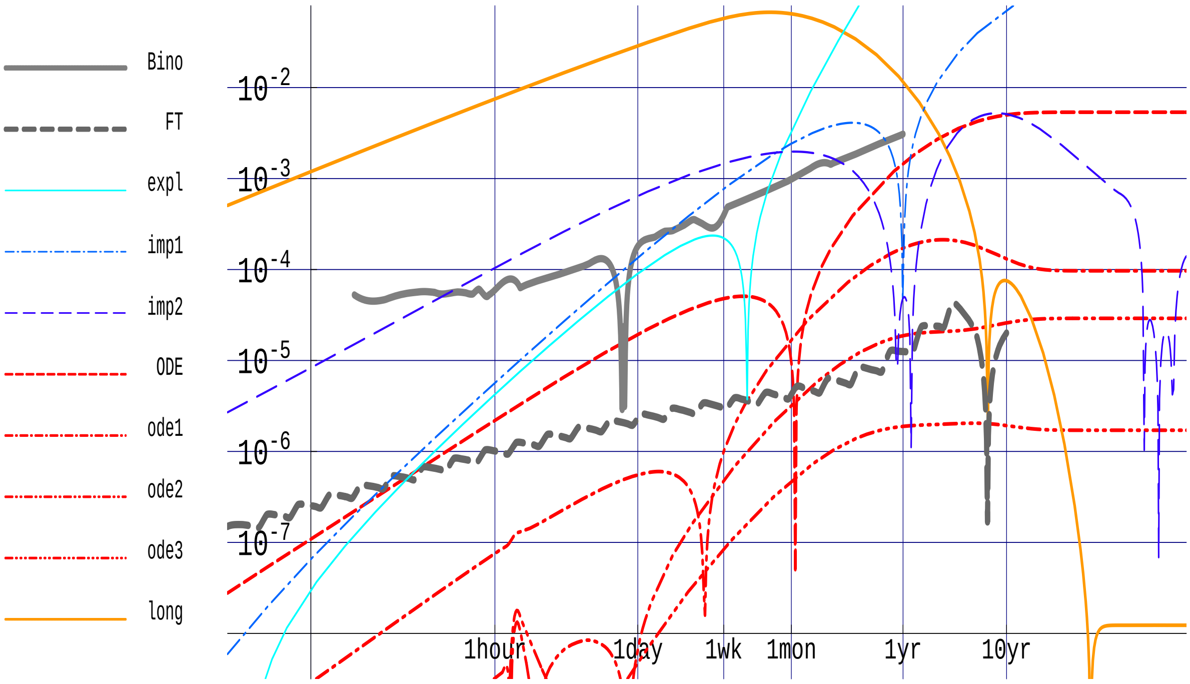

FIGURE Error (in $\log_{10}$) of Approximations for $r = 0.1$ and $\sigma = 0.25$

expiry $((T_F - T))$ in the log scale. In calculating the errors, the "exact" solution to which all the approximations are compared is actually the fifth iteration of (7.3), which is a numerical fixed point to equation (3.9). The labels "Bino", "FT", "expl", "imp1", "imp2", "ODE", "ode1", "ode2", "ode3", and "long" stand for the Binomial tree method, the front tracking and extrapolation method (www.math.pitt.edu/˜xfc), the explicit approximation (expl), the implicit/series approximation (omp1), the implicit/interpolation approximation (imp2), the ode approximation (ODE), the iterative ode approximation (7.3) of the first, second, and third iterations, and the large time approximation (long), respectively. All the cusps (except those near the right and lower edges of the Figure) are the points where errors change sign (since $\log_{10}(\text{error}) = -\infty$ at these points). The non–smoothness of the curve marked "imp2" near the right edge of the Figure is due the inefficiency of our Newton's method in finding the roots u of (imp2) for large t. The bumps of "ode2" and "ode3" at the lower edge of the Figure are numerical round-off errors.

The classical binomial and/or trinomial tree methods are typically used in the literature to find solutions to serve as the "exact" solutions with which approximations are to be compared. In calculating the optimal boundary $S_F(T)$, the point where the functions $P(S,T)$ and $E - S$ depart (tangentially), these tree methods are computing time extensive. Depending on the initial guess of S_F, for each given T, it takes, with the number of division points $n = 1000$, about 5-20 minutes to find $S_f(T)$. The complexity of the method is $O(n^2)$ and the error is of order $O(\frac{\log n}{n})$. The solution used in the Figure contains 50 different sample Ts so that it takes about 10 hours of computing time.

The front tracking method that one of the authors designed has the same complexity $O(n^2)$ and error $O(\frac{\ln n}{n})$ as that of the binomial tree method. However, one can use solutions obtained with divisions $n, n/2$, and $n/4$ respectively to extrapolate a much more accurate solution, as one can see from the significant difference between the curves marked "Bio" and "FT". Given a fixed time $T_{\max}$, it takes, with $n = 2000$, about 15 minutes to find $S_F(T)$ for all $(T_F - T) \leq T_{\max}$. The solution used in the Figure is actually the union of solutions for $T_F - T$ in the interval $(\frac{1}{2}T_{\max}, T_{\max}]$ with $T_{\max} = 10/2^i$ (year) for $i = 0, 1, \cdots, 25$, and therefore, it takes a total of 10 computing hours.

As mentioned earlier, the ODE approximation is almost instantaneous. From the Figure, one can see that the (ODE) approximation has already surpassed that obtained from the binomial method (with 1000 division). For the ode iterative scheme, the computing time for the first iteration takes about 1 minute. To finish the fifth iteration, it takes a total of about 10 minutes.

We shall leave it to the reader to draw conclusions on the accuracy of the approximations given in the Figure.

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Department of Mathematics, University of Pittsburgh, Pittsburgh, PA 15260, USA, e-mail:xinfu+@pitt.edu

Department of Mathematics, University of Pittsburgh, Pittsburgh, PA 15260, USA, e-mail:chadam+@pitt.edu