Complete asymptotic expansion for integrals arising from one-dimensional diffusion with random traps

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The solution of various diffusion problems, in both continuous and discrete systems, can be expressed in terms of a Laplace transform of the exponential function of a fractional power. In this Brief Report the need for a complete asymptotic analysis of these functions is discussed in the context of one-dimensional diffusion with random trapping sites and the necessary asymptotic analysis is carried out.

Much attention[1–9] has been recently directed to the determination of the asymptotic behavior at long times of the survival probability and the probability of returning to the origin in the problem of diffusion with random traps. In the one-dimensional case,[6–9] these quantities can be written down as integrals, whose asymptotic behavior is easily determined by the saddle-point approximation. This approximation may often be very poor at finite times.[9] A complete asymptotic expansion is therefore desirable. This is possible since the above-mentioned integrals are of a type which admits such an expansion.[10]

In Ref. 8 the complete asymptotic expansion for the survival probability has been obtained as an approximation for the solution of the discrete random walk problem. Here we derive the asymptotic expansion for integrals arising as solutions of the continuous diffusion problem.[6,9] The solutions for both survival and return probabilities are special cases of a family of integrals which were encountered some 50 years ago in the problem of absorption of thermal neutrons.[11] Although the coefficients obtained in Ref. 11(a) are wrong, we will use the observation made there, that these integrals are a solution of a certain differential equation, to obtain a general recursion relation for the coefficients.

The integrals we wish to consider are of the type[11]

$$\phi_\nu(x) \equiv \int_0^\infty y^\nu \exp[-(y+x/\sqrt{y})]dy = 2\int_0^\infty w^{2\nu+1}\exp[-(w^2+x/w)]dw \;, \qquad (1)$$

where ν is real. This integral can also be written as

$$\phi_\nu(x) = 2x^{2(\nu+1)/3}\int_0^\infty u^{-(2\nu+3)} \times \exp[-x^{2/3}(u+1/u^2)]du \;, \qquad (2)$$

where $u \equiv x^{1/3}y^{-1/2}$. Since $u+1/u^2$ has a single minimum (at $u=2^{1/3}$), the above integral is of the type considered already by Laplace. It admits an asymptotic expansion[10]

$$\phi_\nu(x) \sim 2(\pi/3)^{1/2}(z/6)^{\nu+1/2}\exp(-z/2)\left[1+\sum_{k=1}^{\infty} a_k^{(\nu)} z^{-k}\right] \qquad (3)$$

with $z \equiv 3(2x^2)^{1/3}$. The first term in the expansion is the well-known steepest descent approximation.

To find a recursion relation for the coefficients $a_k^{(\nu)}$, we note that[11] $\phi_\nu(x)$ is a solution of the differential equation

$$\phi_\nu'''(x) - \frac{2\nu}{x}\phi_\nu''(x) + \frac{2}{x}\phi_\nu(x) = 0 \;. \qquad (4)$$

For $\nu = m/2$, m integer, it is possible to solve (4) for $\phi_0(x)$, and obtain the other integrals from[11(b)]

$$\phi_\nu'(x) = -\phi_{\nu-1/2}(x) \;. \qquad (5)$$

The same effort is required for obtaining the coefficients for an arbitrary real ν, as we show below. Define

$$g_\nu(x) \equiv z^{\nu+1/2}\left[1+\sum_{k=1}^{\infty} a_k^{(\nu)} z^{-k}\right] . \qquad (6)$$

By substituting Eqs. (3) and (6) in (4) we find that

$$x^3 g_\nu'''(x) - (2\nu+z)x^2 g_\nu''(x) + \frac{z}{3}(4\nu+1+z)x g_\nu'(x) - \frac{z}{9}[(2\nu+1)(1+z)+1/3]g_\nu(x) = 0 \;. \qquad (7)$$

Inserting the derivatives of $g(x)$,

$$x g_\nu'(x) = \tfrac{1}{3}z^{\nu+1/2}[(2\nu+1)+(2\nu-1)a_1^{(\nu)}z^{-1}+(2\nu-3)a_2^{(\nu)}z^{-2}+\cdots] \;, \qquad (8a)$$

$$x^2 g_\nu''(x) = \tfrac{1}{9}z^{\nu+1/2}[(2\nu+1)(2\nu-2)+(2\nu-1)(2\nu-4)a_1^{(\nu)}z^{-1}+(2\nu-3)(2\nu-6)a_2^{(\nu)}z^{-2}+\cdots] \;, \qquad (8b)$$

$$x^3 g_\nu'''(x) = \tfrac{1}{27}z^{\nu+1/2}[(2\nu+1)(2\nu-2)(2\nu-5)+(2\nu-1)(2\nu-4)(2\nu-7)a_1^{(\nu)}z^{-1}+(2\nu-3)(2\nu-6)(2\nu-9)a_2^{(\nu)}z^{-2}+\cdots] \;, \qquad (8c)$$

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in Eq. (7), which should hold for every power of z, we finally get

$$3(k+2)a_{k+2}^{(\nu)}=[6\nu^2+9\nu-6k(k+3)-\tfrac{19}{2}]a_{k+1}^{(\nu)}-[8\nu^3-6(2k-1)\nu^2-9(2k+1)\nu+4k^2(k+3)+3k-5]a_k^{(\nu)} . \tag{9}$$

With $a_0^{(\nu)}=1$ and $a_{-1}^{(\nu)}\equiv 0$, Eq. (9) is valid for $k\geq -1$.

We write down the first few coefficients explicitly:

$$6a_1^{(\nu)}=12\nu^2+18\nu+5 , \tag{10a}$$

$$72a_2^{(\nu)}=144\nu^4+336\nu^3+84\nu^2-144\nu-35 , \tag{10b}$$

$$1296a_3^{(\nu)}=1728\nu^6+4320\nu^5-4320\nu^4-13\,320\nu^3-288\nu^2+6210\nu+665 , \tag{10c}$$

$$31\,104a_4^{(\nu)}=20\,736\nu^8+41\,472\nu^7-217\,728\nu^6-411\,264\nu^5+577\,584\nu^4+993\,888\nu^3-341\,112\nu^2-488\,016\nu+9625 . \tag{10d}$$

In Ref. 11(a) the first two coefficients were calculated by a less direct route (which did not yield a recursion formula). Unfortunately, the second coefficient there is incorrect.

It should be pointed out that $\phi_\nu(x)$ is in fact a known special function. By taking the Mellin transform of (1) and applying the Mellin inversion formula, we obtain the Barnes integral representation for a Meijer G function,[12]

$$\phi_\nu(x)=\pi^{-1/2}G_{0,3}^{3,0}\left[\frac{x^2}{4}\middle|0,\tfrac{1}{2},\nu+1\right] . \tag{11}$$

If ν is not an integer or $-\frac{1}{2}$, then this can be further simplified to an expression in terms of the hypergeometric function ${}_0F_2$. In its character, therefore, ϕ_ν is similar to the product of two Bessel functions. More than merely giving the integral another name this places at one's disposal the variety of functional relations known for the G function, including series expansions and asymptotic expansions. In this way we find

$$\phi_{-1/2}(x)=\sqrt{\pi}+\sqrt{\pi}\sum_{k=1}^{\infty}\frac{(-1)^k(\sqrt{2}x)^{2k}}{(2k-1)!!(2k)!}+2\sum_{k=0}^{\infty}(-1)^k\frac{[\ln x-\psi(2k+2)-\frac{1}{2}\psi(k+1)]x^{2k+1}}{k!(2k+1)!} , \tag{12}$$

where $\psi(x)\equiv d[\ln\Gamma(x)]/dx$. The integer values of the psi (digamma) function are given by[12]

$$\psi(1)=-\gamma,\ \ \psi(m)=-\gamma+\sum_{k=1}^{m-1}k^{-1} , \tag{13}$$

γ being Euler's constant. This together with (5), extends the results in Ref. 11(b).

For the problem of one-dimensional diffusion with random traps of concentration c (and a diffusion constant of unity), the average (over all trap distributions) survival probability up to time t is[6,7,9]

$$\langle Q\rangle=\frac{8c^2}{\pi^2}\sum_{j=0}^{\infty}(2j+1)^{-2}\times\int_0^\infty \exp\left[-\frac{(2j+1)^2\pi^2 t}{l^2}-cl\right]l\,dl . \tag{14}$$

Its asymptotic behavior is determined by the $j=0$ term. By substituting $u=(c/\pi^2 t)^{1/3}l$, Eq. (14) is brought to the form of Eq. (2) with $\nu=-2$. The asymptotic expansion is therefore

$$\langle Q\rangle(t)\sim 16c(t/3\pi)^{1/2}\times\exp(-z/2)\left[1+\sum_{k=1}^{\infty}a_k^{(-2)}/z^k\right] , \tag{15}$$

where $z\equiv 3(2\pi^2c^2t)^{1/3}$ and $a_1^{(-2)}=\frac{17}{6}$, $a_2^{(-2)}=\frac{205}{72}$, $a_3^{(-2)}=-\frac{3115}{1296}$, $a_4^{(-2)}=\frac{137\,305}{31\,104},\ldots$. The improvement over the saddle-point approximation at a finite t, obtained by taking into account the first few terms in the expansion, is considerable. This is demonstrated in Fig. 1.

The expansion (15) has also been derived in Ref. 8 for a different integral, obtained as a solution for the discrete random walk problem. (Substitute $n/2$ there by t and $-\ln p$ there by c.) The fact that the two integrals have the same asymptotic expansion is physically clear. The continuous diffusion problem approximates the discrete case for small concentrations. But at long times the only random walkers to survive are those who were born on long trap-vacant intervals. The ensemble of all such segments corresponds to a small trap concentration.

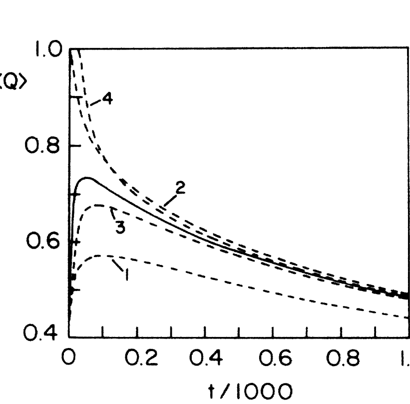

FIG. 1. Average survival probability for one-dimensional diffusion with random traps. Full solid line, exact value for the $j=0$ integral in Eq. (14). Dashed curves, partial sums up to $k=m$ in the asymptotic expansion, Eq. (15). m is denoted in the figure. Compare with Fig. 3(a) of Ref. 9.

Mathematically, it is seen that the integral (5) in Ref. 8 is proportional to $2\phi_1-\phi_0$, while the asymptotic expansion (15) is that of ϕ_{-2}. The recursion relation for ϕ_ν, which is easily obtained from integration by parts[11(b)]

$$\phi_\nu(x)=\nu\phi_{\nu-1}(x)+\tfrac{1}{2}x\phi_{\nu-3/2}(x)\ , \tag{16}$$

does not connect the indices 1, 0, and -2. It is therefore implied that there is another relation between the asymptotic expansions

$$g_1(x)-3g_0(x)=z^3g_{-2}(x)\ , \tag{17}$$

where g and z are defined as in (6). The coefficients must therefore obey

$$a_k^{(-2)}=a_k^{(1)}-3a_{k-1}^{(0)}\ . \tag{18}$$

That this is so can be verified directly from Eq. (10).

For the average probability of return to the origin one obtains[6,9]

$$\langle P\rangle=c^2\int_0^\infty \sum_{j=1}^{\infty}\exp(-j^2\pi^2t/l^2-cl)dl\ . \tag{19}$$

Taking the $j=1$ term and using the same substitution as in (14) brings Eq. (19) to the form (2) with $\nu=-\frac{3}{2}$. The asymptotic expansion is therefore

$$\langle P\rangle(t)\sim\tfrac{1}{3}c(2\pi z)^{1/2}\exp(-z/2)\left[1+\sum_{k=1}^{\infty}a_k^{(-3/2)}/z^k\right] \tag{20}$$

with z defined as above and $a_1^{(-3/2)}=\frac{5}{6}$, $a_2^{(-3/2)}=-\frac{35}{72}$, $a_3^{(-3/2)}=\frac{665}{1296}$, $a_4^{(-3/2)}=\frac{9625}{31\,104}, \ldots$.

We believe this demonstrates the convenience of using the continuous diffusion approach over the discrete random walk treatment[8] for discussing the asymptotic behavior. Firstly, both integrals (14) and (19) turn out to be special cases of the same integral (2). Secondly, the fact that this integral obeys the differential equation (4) makes it easy to derive the recursion relation (9) for the coefficients.

Finally, we note that the asymptotic expansion of the integral (1) may appear in many other physical situations. For example, the Schwartz, Slawsky, and Herzfeld (SSH) expression[13] for the probability of vibrational to translational energy transfer (in the collision of a Morse oscillator with gas molecules) contains the integral

$$f_2(x)=x^2\int_0^\infty e^{-y}\sinh^{-2}(xy^{-1/2})dy\ . \tag{21}$$

In the limit of large x this integral behaves as $4x^2\phi_0(2x)$. Therefore

$$f_2(x)=8(\pi/3)^{1/2}x^{7/3}\exp(-3x^{2/3})\left[1+\sum_{k=1}^{\infty}a_k^{(0)}/z^k\right]\ , \tag{22}$$

where $z\equiv 6x^{2/3}$ and $a_1^{(0)}=\frac{5}{6}$, $a_2^{(0)}=-\frac{35}{72}$, etc. This extends the results of Ref. 13, where only the steepest descent approximation is derived.

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