One integral in three ways: Moments of a quantum distribution

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(Received 2005)

December 7, 2005

Abstract

Very recently, an exponential probability distribution with parameter has been used to calculate the decoherence factors for quantum states. We derive all moments of this distribution systematically in three different ways, presenting the results in terms of binomial coefficients or Pochhammer symbols, and Stirling numbers of the first and second kinds. We show how generalized harmonic numbers or polygamma functions provide another representation for the moments. Extensions of the approach are briefly mentioned.

Key words and phrases

decoherence factor, Stirling numbers, probability distribution, moments, polygamma function, generalized harmonic numbers, generating function

Introduction

Very recently, the integral

$$\bar{d^p} = \int_0^\infty d^p p(d)\mathrm{d}d = 2(D_\mathcal{E} - 1)\int_0^\infty d^p e^{-2d}(1 - e^{-2d})^{D_\mathcal{E}-2}\mathrm{d}d, \tag{1}$$

for $p = 1$ and 2 was used to approximately calculate the decoherence factors for $D_\mathcal{E}$ dimensional quantum states ([4], Appendix D). The mean $\bar{d}$ and standard deviation Δd were determined for a single subenvironment and then, using a biased random walk model, the results were extended to a collection of m subsystems by putting $\bar{d}_m = m\bar{d}$ and $\Delta d_m = \sqrt{m}\Delta d$. For an environment made up of qubits (quantum bits), $D_\mathcal{E} = 2$, the probability distribution $p(d)$ is a first order Poisson distribution, and $p_m(d)$ is the mth order Poisson distribution [3] (more precisely, an Erlang distribution.). In effect, the authors of Ref. [4] appeal to the central limit theorem in applying their random walk model. This approximation may be avoided by calculating the exact probability distribution function for a sum of independent random variables drawn from the distribution $p(d)$. Very recently, we found a Fourier inversion representation of this distribution, and it provides a formal integral representation of the mean value $\bar{d}_m$ and other moments [8].

Our calculation of all the moments of the quantum probability distribution $p(d)$ is related more broadly to the subject of the transition between classical and quantum physics. A paradigm for understanding decoherence uses the idea that environments decohere a system by measuring it, and that in measuring the system the environments come to have information about the system [3, 4]. The measure used by Blume-

Kohout and Zurek [4] as to how much information an environment $\mathcal{E}$ has about the system S is the quantum mutual information (QMI). The QMI is the amount of entropy produced by destroying correlations between S and $\mathcal{E}$: $I_{S\mathcal{E}} \equiv H(S) + H(\mathcal{E}) - H(S\mathcal{E})$, where the Von Neumann entropy $H = -\text{Tr}(\rho \log \rho)$, and ρ is the density matrix. The QMI has useful mathematical properties that make it convenient to employ in calculations.

Initially for their discussion Blume-Kohout and Zurek let the universe be an $(N+1)$-qubit Hilbert space $H = H_S \otimes \otimes_{i=1}^N H_{\mathcal{E}_i}$, where both H_S and all the $H_{\mathcal{E}_i}$ are single qubits (spin 1/2 particles). They then extend to environments of general dimension $D_\mathcal{E}$, with again $D_\mathcal{E} = 2$ being the qubit case. Among the tools they use is a formula conjectured (by Page, and later proved by others [19]) for the mean entropy $H(m, n)$ of an m-dimensional subsystem of an mn-dimensional system. When it comes to approximately calculating the decoherence factors for $D_\mathcal{E}$ dimensional quantum states, the first and second moments of the distribution $p(d)$ are required. The moments of interest take the form of Eq. (1), with the initial $p = 0, 1$, and 2 cases having been done before [18].

In this paper, we calculate the moment integral (1) in multiple fashion for general p. We encounter an interesting combination of special functions and special numbers, including the Stirling and generalized harmonic numbers, and the polygamma functions. We describe the connections of the moments $\bar{d^p}$ to sums of generalized harmonic numbers from different perspectives, and describe ready extensions of our results. Our work permits other statistics of the distribution $p(d)$ to be easily determined, as well as the asymptotic form of the moments or other quantities.

Evaluation of Eq. (1) in terms of special numbers

We will conveniently restrict p in Eq. (1) to be a nonnegative integer, but much of what we do does not require this condition. Of course, the case $p=0$ is just the normalization of the distribution $p(d)$. Similarly, we take $D_{\mathcal{E}} \geq 2$ to be an integer. As a first, benchmark result we have

Proposition 1

$$\bar{d^p} = (D_{\mathcal{E}}-1)\frac{\Gamma(p+1)}{2^p}\sum_{k=0}^{D_{\mathcal{E}}-2}(-1)^k\binom{D_{\mathcal{E}}-2}{k}\frac{1}{(k+1)^{p+1}} \tag{2a}$$

$$= (D_{\mathcal{E}}-1)\frac{\Gamma(p+1)}{2^p}\sum_{k=0}^{D_{\mathcal{E}}-2}\frac{(-1)^k}{k!}\frac{1}{(k+1)^{p+1}}\sum_{\ell=0}^{k}s(k,\ell)(D_{\mathcal{E}}-2)^\ell, \tag{2b}$$

where $s(n,m)$ are Stirling numbers of the first kind [1, 11, 15, 6, 20]. Equation (2a) follows by straightforwardly binomially expanding the right-most factor in the integrand of Eq. (1). This was the method of Ref. [4] and those results are recovered when $p=0$, 1, or 2. The cases of $p=0$, 1, and 2 were also treated in Ref. [18] by means of binomial expansion. In addition, those authors developed recursion relations based upon integration by parts. For Eq. (2b) we note that $\binom{x}{n} = (-1)^n(-x)_n/n!$, where $(a)_n = \Gamma(a+n)/\Gamma(a)$ is the Pochhammer symbol and Γ is the Gamma function, and use

$$(z)_n = \prod_{k=1}^{n}(z+k-1) = \sum_{k=0}^{n}(-1)^{n-k}s(n,k)z^k. \tag{3}$$

An alternative route to Eq. (2a) is afforded by writing Eq. (1) as

$$\bar{d^p} = 2^{D_\mathcal{E}-1}(D_\mathcal{E}-1)\int_0^\infty d^p e^{-D_\mathcal{E} d}\sinh^{D_\mathcal{E}-2} d\mathrm{d}d, \tag{4}$$

and then using a tabulated integral [14]. Yet again, depending upon whether $D_\mathcal{E}$ is an even or odd integer, one may expand $\sinh^{2n} x$ or $\sinh^{2n-1} x$ in Eq. (4) as a binomial series in cosh or sinh functions [14]. Then the application of other known integrals [14] returns Eq. (2a).

Instead, we may apply the exponential generating functions of the Stirling numbers of the first and second kinds, giving a series of expressions. We have

Proposition 2

$$\bar{d^p} = \frac{(D_\mathcal{E}-2)!}{2^p}\sum_{n=D_\mathcal{E}-2}^{\infty}\frac{S(n,D_\mathcal{E}-2)}{n!}\frac{\Gamma(p+n+1)}{(D_\mathcal{E}-1)^{p+n}}, \tag{5}$$

where $S(n,m)$ are Stirling numbers of the second kind [1, 11, 15, 6, 20], and

Proposition 3 (a)

$$\bar{d^p} = \left(-\frac{1}{2}\right)^p (D_\mathcal{E}-1)p!\sum_{n=p}^{\infty} s(n,p)\frac{(-1)^n}{n!}\frac{1}{(n+D_\mathcal{E}-1)}, \tag{6a}$$

(b)

$$\bar{d^p} = \frac{p}{2^p}\sum_{n=p}^{\infty} w(n,p-1)\frac{1}{n}\frac{(D_\mathcal{E}-1)}{(n+D_\mathcal{E}-1)}, \tag{6b}$$

where [2]

$$w(x,m) = \frac{1}{\Gamma(x)}\lim_{q\to x-1}\left(\frac{d}{dx}\right)^m (x-q)_q. \tag{7}$$

The quantities $w(n,m)$ are essentially sums of generalized harmonic numbers and are further described below.

For the proof of Eq. (4) we simply write Eq. (1) as

$$\bar{d^p} = 2(D_{\mathcal{E}} - 1) \int_0^\infty d^p e^{-2d(D_{\mathcal{E}}-1)} (e^{2d} - 1)^{D_{\mathcal{E}}-2} \mathrm{d}d, \tag{8}$$

use the generating function of $S(\ell, n)$ [1, 11, 15, 6], and carry out the resulting integration in terms of the Gamma function.

Remarks. (i) The use of the closed form [1, 6]

$$S(n, m) = \frac{1}{m!} \sum_{k=0}^{m} (-1)^{m-k} \binom{m}{k} k^n \tag{9}$$

returns Proposition 1. This is done by inserting Eq. (9) into Eq. (5), interchanging the two sums, and applying the binomial expansion. (ii) The Stirling numbers of the second kind are connected with the Poisson distribution in the following way. If X is a random variable with Poisson distribution with mean λ, then its jth moment is given by $E(X^j) = \sum_{k=1}^{j} S(j,k)\lambda^k$. Given this fact, the appearance of the numbers $S(n, k)$ in some way in the moments $\bar{d^p}$ could be anticipated.

In order to obtain Eq. (6a), we first make a change of variable in Eq. (1) so that

$$\bar{d^p} = \left(-\frac{1}{2}\right)^p (D_{\mathcal{E}} - 1) \int_0^1 \ln^p(1 - v) v^{D_{\mathcal{E}}-1} dv. \tag{10}$$

We then use the generating function of $s(n, m)$ [1, 11, 15, 6] and evaluate the resulting elementary integral. In order to obtain Eq. (6b) we use in Eq. (6a) the relation [2]

$$\left[{n \atop m}\right] = \frac{(n-1)!}{(m-1)!} w(n, m-1) = (-1)^{n-m} s(n, m). \tag{11}$$

The numbers $w(n,m)$ may be found recursively in terms of the generalized harmonic numbers [9]

$$H_n^{(r)} = \sum_{k=1}^n \frac{1}{k^r} = \frac{(-1)^{r-1}}{(r-1)!}\left[\psi^{(r-1)}(n+1) - \psi^{(r-1)}(1)\right], \tag{12}$$

where $\psi^{(j)}$ is the polygamma function, as $w(n,0)=1$ and

$$w(n,m) = \sum_{k=0}^{m-1}(1-m)_k H_{n-1}^{(k+1)} w(n,m-1-k), \tag{13}$$

or written in terms of a m-fold multiple sum [2]. The recursion (13) of Adamchik [2] is equivalent to one for $s(n,k)$ found by Shen [21], $(k-1)s(n,k) = -\sum_{m=1}^{k-1} s(n,k-m)H_{n-1}^{(m)}$. The w's are also given by [2]

$$w(n,m) = \frac{1}{(n-1)!}\sum_{i=m+1}^n s(n,i)(i-m)_m n^{i-m-1}. \tag{14}$$

In terms of the Stirling polynomials $\sigma_n(x)$ [15] we have [2] $\sigma_n(m) = w(m,m-n-1)/m$.

Asymptotic forms of the Stirling numbers and functions are known [7, 17, 16, 22], so that Eq. (11) gives asymptotic forms of the numbers $w(n,m)$. As examples, we apply two results of Ref. [16]. Put $r=(m-1)/\ln n$, let $2 \le m \le \eta \ln n$ for $\eta > 0$, and let μ be a fixed positive integer such that $2 \le \mu \le m$. Let $g(w) = 1/\Gamma(w+1)$ and L_n^α denote the associated Laguerre polynomial. Then Theorem 2 of Ref. [16] with error term Z_μ gives

$$w(n,m-1) = (-1)^{n-m}\ln^{m-1} n\left[\frac{1}{\Gamma(1+r)} + \sum_{k=2}^{\mu}\frac{g^{(k)}(r)}{\ln^k n}L_k^{m-k-1}(m-1) + Z_\mu(m,n)\right], \quad n\to\infty, \tag{15}$$

uniformly in m. The asymptotic form may be obtained alternatively, putting $q = [m-1+\sqrt{m-1}]/\ln n$, and then by Remark 1 of Ref. [16] we have

$$w(n,m-1) = (-1)^{n-m} \ln^{m-1} n \left[\frac{1}{\Gamma(1+q)} + \frac{\psi(1+q)}{\Gamma(1+q)} \frac{\sqrt{m-1}}{\ln n} + O\left(K_3 \frac{(m-1)^{3/2}}{\ln^3 n} e^{-\sqrt{m}} + \frac{\ln^m n}{nm!} \right) \right],$$

$$n \to \infty, \tag{16}$$

where K_3 is a constant.

Special case of the mean, $p = 1$

In order to further elucidate some of the underlying relations, we consider here in detail the special case for $\bar{d} = [\psi(D_\mathcal{E}) + \gamma]/2$, where $\gamma = -\psi(1)$ is the Euler constant. Since $w(n, 0) = 1$, Eq. (6b) immediately gives this result due to the partial fraction form of the digamma function [1]:

$$2\bar{d} = \sum_{n=1}^{\infty} \frac{1}{n} \frac{D_\mathcal{E} - 1}{(n + D_\mathcal{E} - 1)}. \tag{17}$$

Similarly, since $s(n, 1) = (-1)^{n-1}(n-1)!$, Eq. (6a) returns the result for the same reason.

From Eq. (2a) when $p = 1$ we have

$$2\bar{d} = \sum_{k=0}^{D_\mathcal{E}-2} \frac{(-1)^k}{(k+1)} \frac{(D_\mathcal{E}-1)!}{(k+1)!(D_\mathcal{E}-k-2)!} = \sum_{k=0}^{D_\mathcal{E}-2} \frac{(-1)^k}{(k+1)} \binom{D_\mathcal{E}-1}{k+1} = \psi(D_\mathcal{E}) + \gamma. \tag{18}$$

The last relation may be obtained in various ways. From [2]

$$\psi(t+1) + \gamma = -\sum_{k=1}^{\infty} \frac{(-t)_k}{kk!}, \tag{19}$$

by using $(-t)_k = (-1)^k k! \binom{t}{k}$, we have

$$\psi(t+1) + \gamma = \sum_{k=0}^{\infty} \frac{(-1)^k}{(k+1)} \binom{t}{k+1}, \tag{20}$$

recovering the Newtonian series for the digamma function [12]. When t is a positive integer in this series, it truncates at $k = t$, due to a property of the binomial coefficients. Yet another form of $2\bar{d}$ results from

$$\psi(t+1) + \gamma = -\sum_{p=1}^{\infty} (-1)^p \zeta(p+1) t^p, \tag{21}$$

where ζ is the Riemann zeta function. Together with [2, 5]

$$\zeta(p+1) = \sum_{k=1}^{\infty} (-1)^{k-p} \frac{s(k,p)}{kk!}, \tag{22}$$

we obtain other equivalences with Eqs. (2), (18), (19), or (20). Equation (21) follows immediately by inserting an integral representation for the zeta function, interchanging summation and integration, and applying a standard integral form of the digamma function [1]:

$$\sum_{p=1}^{\infty} t^p \zeta(p+1) = -\int_0^{\infty} \frac{[e^{-x} - e^{-(1-t)x}]}{(1-e^{-x})} dx = -\psi(1-t) - \gamma. \tag{23}$$

Various identities for special numbers can be developed by equating our different expressions for the moments of $d(p)$ or related quantities, but we hardly pursue this here. As a very simple example, we have from Eq. (4) at $p = 1$

$$\bar{d} = \frac{(D_{\mathcal{E}}-2)!}{2} \sum_{n=D_{\mathcal{E}}-2}^{\infty} (n+1) \frac{S(n, D_{\mathcal{E}}-2)}{(D_{\mathcal{E}}-1)^{n+1}} = \frac{1}{2}[\psi(D_{\mathcal{E}}) + \gamma]. \tag{24}$$

Surely this identity is not new, but we have yet to find it in the literature. Presumably Eq. (24) is independently verifiable by substituting an integral representation for the Stirling numbers of the second kind.

Extensions

We just briefly mention extensions of our work to other integrals. For instance, we find that

$$\frac{1}{2^{D_\mathcal{E}}}\int_0^\infty d^p e^{-2(D_\mathcal{E}-1)d}\frac{(e^{2d}-1)^{D_\mathcal{E}-2}}{d^{D_\mathcal{E}-2}}\mathrm{d}d = \frac{1}{2^{p+1}}\frac{1}{(D_\mathcal{E}-1)^{p+1}}\sum_{n=0}^\infty \frac{\Gamma(p+n+1)}{(m+1)_n}\frac{S(n+m,n)}{(D_\mathcal{E}-1)^n}. \tag{25}$$

Rather than simply apply Eq. (4), we have proceeded in a different manner by first performing a shift of index in the series corresponding to the exponential generating function for the Stirling numbers of the second kind, giving a series expansion in powers of x of the function $(e^x-1)^m/x^m$. Alternatively, the integral of Eq. (25) could be evaluated by means of binomial expansion, or by a change of variable and introduction of the Stirling numbers of the first kind.

Finally, we note that our Propositions enable the explicit determination of integrals of the form

$$\left(\frac{\partial}{\partial p}\right)^j\left(\frac{\partial}{\partial D_\mathcal{E}}\right)^m\int_0^\infty d^p p(d)\mathrm{d}d = 2(D_\mathcal{E}-1)\int_0^\infty d^p \ln^j d e^{-2d}(1-e^{-2d})^{D_\mathcal{E}-1}\ln^m[(1-e^{-2d})]\mathrm{d}d. \tag{26}$$

In this case, we treat p and $D_\mathcal{E}$ as continuous parameters and perform logarithmic differentiation. In particular, such results for $m=1$ are expected to have relevance in the calculation of quantum and semiclassical entropies and quantum mutual information [3, 4, 10]. For instance, the differential entropy of position is given by [10] $S^{(x)} = -\int P(x)\ln P(x)dx$. In the classical or semiclassical cases, $P(x)$ is the probability distribution in space and the integral is taken between the turning points of the motion, while quantum mechanically $P(x) = |\psi(x)|^2$, where ψ is the wave function and the integral is taken over all space.

Acknowledgement

This work was partially supported by Air Force contract number FA8750-04-1-0298.

References

[1] M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions, Washington, National Bureau of Standards (1964).

[2] V. Adamchik, On Stirling numbers and Euler sums, J. Comp. Appl. Math. **79**, 119-130 (1997).

[3] R. Blume-Kohout and W. H. Zurek, A simple example of "quantum Darwinism": redundant information storage in many-spin environments, arXiv:quant-ph/0408147 (2004), to appear in Found. Phys. (2005).

[4] R. Blume-Kohout and W. H. Zurek, Quantum Darwinism: entanglement, branches, and the emergent classicality of redundantly stored quantum information, arXiv:quant-ph/0505031 (2005), to appear in Phys. Rev. A.

[5] P. L. Butzer and M. Hauss, Stirling numbers of first and second kind, in: Approximation, Interpolation, and Summability, Israel Math. Conf. Proc., **4**, 89-108 (1991).

[6] C. A. Charalambides, Enumerative combinatorics, Chapman & Hall/CRC (2002).

[7] R. Chelluri, L. B. Richmond, and N. M.Temme, Asymptotic estimates for generalized Stirling numbers, Analysis **20**, 1-13 (2000); N. M. Temme, Asymptotic estimates of Stirling numbers, Stud. Appl. Math. **89**, 233-243 (1993).

[8] M. W. Coffey, unpublished (2005).

[9] M. W. Coffey, On one-dimensional digamma and polygamma series related to the evaluation of Feynman diagrams, J. Comput. Appl. Math. **183**, 84-100 (2005).

[10] M. W. Coffey, Semiclassical position entropy for hydrogen-like atoms, J. Phys. A **36**, 7441 (2003).

[11] L. Comtet, Advanced Combinatorics, Reichel (1974).

[12] H. T. Davis, Tables of the higher mathematical functions, Vol. 1, Principia Press, Bloomington, IN (1933).

[13] H. M. Edwards, Riemann's Zeta Function, Academic Press, New York (1974).

[14] I. S. Gradshteyn and I. M. Ryzhik, Table of Integrals, Series, and Products, Academic Press, New York (1980).

[15] R. L. Graham, D. E. Knuth, and O. Patashnik, Concrete Mathematics, 2nd ed., Addison Wesley (1994).

[16] H.-K. Hwang, Asymptotic expansions for the Stirling numbers of the first kind, J. Comb. Th., Series A, **71**, 343-351 (1995).

[17] G. Kemkes, C. F. Lee, D. Merlini, and B. Richmond, Stirling numbers for complex arguments: asymptotics and identities, SIAM J. Discrete Math. **16**, 179-191 (2003).

[18] P. J. Larcombe, E. J. Fennessey, and W. A. Koepf, Integral proofs of two alternating sign binomial coefficient identities, Util. Math. **66**, 93-103 (2004).

[19] D. N. Page, Average entropy of a subsystem, Phys. Rev. Lett. **71**, 1291-1294 (1993); S. Sen, Average entropy of a quantum subsystem, Phys. Rev. Lett. **77**, 1-3 (1996).

[20] J. Riordan, An introduction to combinatorial analysis, Wiley (1958); Combinatorial identities, Wiley (1968).

[21] L.-C. Shen, Remarks on some integrals and series involving the Stirling numbers and $\zeta(n)$, Trans. Amer. Math. Soc. **347**, 1391-1399 (1995).

[22] H. S. Wilf, The asymptotic behavior of the Stirling numbers of the first kind, J. Comb. Th., Series A **64**, 344-349 (1993).