Logarithmic potential of Hermite polynomials and information entropies of the harmonic oscillator eigenstates[a]

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The problem of calculating the information entropy in both position and momentum spaces for the nth stationary state of the one-dimensional quantum harmonic oscillator reduces to the evaluation of the logarithmic potential $V_n(t) = -\int_{-\infty}^{\infty}(H_n(x))^2 \ln|x-t|e^{-x^2}\,dx$ at the zeros of the Hermite polynomial $H_n(x)$. Here, a closed analytical expression for $V_n(t)$ is obtained, which in turn yields an exact analytical expression for the entropies when the exact location of the zeros of $H_n(x)$ is known. An inequality for the values of $V_n(t)$ at the zeros of $H_n(x)$ is conjectured, which leads to a new, nonvariational, upper bound for the entropies. Finally, the exact formula for $V_n(t)$ is written in an alternative way, which allows the entropies to be expressed in terms of the even-order spectral moments of the Hermite polynomials. The asymptotic ($n \gg 1$) limit of this alternative expression for the entropies is discussed, and the conjectured upper bound for the entropies is proved to be asymptotically valid. © *1997 American Institute of Physics.* [S0022-2488(97)00709-3]

I. INTRODUCTION

In the framework of the modern density functional theory,[1–5] the physical and chemical properties of a many fermion system may be completely described by means of the single-particle probability density, which is to be denoted by $\rho(\mathbf{r})$ in position space and $\gamma(\mathbf{p})$ in momentum space. The spread or extent of these quantum-mechanical probability densities is measured by the Boltzmann–Shannon information entropy, which for one-dimensional systems is defined as

$$S_\rho = -\int_{-\infty}^{\infty} \rho(x) \ln \rho(x)\, dx, \tag{1}$$

in position space, and

$$S_\gamma = -\int_{-\infty}^{\infty} \gamma(p) \ln \gamma(p)\, dp, \tag{2}$$

in momentum space. These entropies are closely related to fundamental and/or experimentally measurable quantities, such as, e.g., the kinetic energy and the magnetic susceptibility, which makes them useful in the study of the structure and dynamics of atomic and molecular systems.[6–10] Moreover, they have been applied to a wide range of quantum-mechanical problems, such as the mathematical formulation of the position-momentum uncertainty principle[11–13] and spreading of wave packets,[14,15] approximate calculations of energy eigenvalues and eigenstates by means of the maximum-entropy principle,[16,17] and time evolution of chemical reactions.[18]

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[a]Expanded version of a talk presented at the International Workshop on Orthogonal Polynomials in Mathematical Physics (Madrid, June 1996).

The calculation of position and momentum entropies for physically interesting quantum states has been the subject of considerable effort in recent years. It has been shown[19,20] that, for the stationary states of many important systems, such as D-dimensional harmonic oscillator and hydrogen atom, the entropies can be expressed in terms of the integrals

$$E_n \equiv -\int_{-\infty}^{\infty} (p_n(x))^2 \ln(p_n(x))^2 w(x)\, dx,$$

where $p_n(x)$ are orthogonal polynomials with respect to the weight function $w(x)$. These integrals are called ''entropies of the orthogonal polynomials $p_n(x)$,'' and they are closely related to the L^p-norms, whose study is of independent interest in the theory of general orthogonal and extremal polynomials.[21]

Asymptotic formulas for E_n in the $n\to\infty$ limit have been obtained in the case when $p_n(x)$ are general orthogonal polynomials on a finite interval,[22] or Freud orthogonal polynomials $[w(x)=\exp(-|x|^m),\ m>0]$ on the whole real axis.[21,23,24] However, the analytical value of these entropies is only known for Chebyshev polynomials of the first and second kinds, in an exact form, and for Gegenbauer polynomials in an approximate way.[19] The problem of determining the entropies of general orthogonal polynomials remains open.

For the nth eigenstate of the one-dimensional harmonic oscillator Hamiltonian,

$$H=\frac{p^2}{2m}+\frac{1}{2}\, m\omega^2 x^2,$$

the probability densities for position and momentum are expressed in terms of the Hermite polynomial $H_n(x)$,

$$\rho(x)=\frac{\alpha}{2^n n!\sqrt{\pi}}\,(H_n(\alpha x))^2 e^{-\alpha^2x^2},\qquad \gamma(p)=\frac{1}{2^n n!\sqrt{\pi}\alpha}\,(H_n(p/\alpha))^2 e^{-p^2/\alpha^2},$$

where $\alpha\equiv(m\omega)^{1/2}$ (we choose units such that $\hbar=1$). The corresponding entropies of position and momentum can be written as

$$S_\rho=-\ln\,\alpha+S_n\,,\quad S_\gamma=\ln\,\alpha+S_n\,, \tag{3}$$

where

$$S_n=\ln(2^n n!\sqrt{\pi})+n+\frac{1}{2}+\frac{1}{2^n n!\sqrt{\pi}}\,E_n(H) \tag{4}$$

is given in terms of $E_n(H)$, the so-called entropy of Hermite polynomials, whose expression is

$$E_n(H)=-\int_{-\infty}^{\infty}(H_n(x))^2 \ln(H_n(x))^2 e^{-x^2}\, dx. \tag{5}$$

The values of S_n have been numerically calculated up to $n=500$,[19] while for $n\gg 1$ they are approximately given by the asymptotic formula

$$S_n \sim \ln(\pi\sqrt{2n})-1, \tag{6}$$

which has been rigorously proved by means of the theory of strong asymptotics of Freud polynomials,[23] and can also be derived from the semiclassical (Wentzel–Kramers–Brillouin) approximation for one-dimensional quantum systems.[25,26] On the other hand, the variational inequality relating entropy and standard deviation for arbitrary one-dimensional random variables,[12]

$$S_A \leqslant \tfrac{1}{2} + \ln(\sqrt{2\pi}\Delta A),$$

together with Eq. (3) and the well-known values of ΔX and ΔP for the harmonic oscillator eigenstates,

$$(\Delta X)^2 = \left(n+\frac{1}{2}\right)\frac{1}{\alpha^2}, \quad (\Delta P)^2 = \left(n+\frac{1}{2}\right)\alpha^2,$$

yields the upper bound

$$S_n \leqslant \tfrac{1}{2} + \ln \sqrt{(2n+1)\pi}. \tag{7}$$

However, the exact analytical value of S_n has been calculated only in the simplest cases $n=0$ and $n=1$.[19] For the ground state $(n=0)$ we have

$$S_0 = \ln(\sqrt{\pi}) + \tfrac{1}{2}, \tag{8}$$

so that in this case the equality sign holds in (7) and the entropy sum $S_\rho + S_\gamma = 2S_n$ attains the lower bound in the optimal entropic uncertainty relation for one-dimensional position and momentum,[11,12]

$$S_\rho + S_\gamma \geqslant 1 + \ln \pi,$$

while in the first excited state $(n=1)$ we have

$$S_1 = \ln(2\sqrt{\pi}) - \tfrac{1}{2} + \gamma, \tag{9}$$

where γ is Euler's constant. The main aim of the present work is to find the generalization of these results to arbitrary values of n.

The Hermite polynomial $H_n(x)$ has n real and simple zeros, and is of the form $H_n(x) = 2^n x^n + O(x^{n-1})$ (see, e.g., Ref. 27), so that it can be factorized as

$$H_n(x) = 2^n \prod_{i=1}^{n} (x - x_{n,i}),$$

where $x_{n,i}$ $(i=1,2,...,n)$ is the ith root of $H_n(x)$. Introducing this expression into the logarithmic function in (5), and taking into account the normalization integral for Hermite polynomials,

$$\int_{-\infty}^{\infty} (H_n(x))^2 e^{-x^2}\, dx = 2^n n! \sqrt{\pi},$$

we see that $E_n(H)$ can be written in the form[20]

$$E_n(H) = -2^n n! \sqrt{\pi} \ln(2^{2n}) + 2\sum_{i=1}^{n} V_n(x_{n,i}), \tag{10}$$

where $V_n(t)$ is the logarithmic potential of the Hermite polynomial $H_n(x)$, defined as

$$V_n(t) = -\int_{-\infty}^{\infty} (H_n(x))^2 \ln|x-t| e^{-x^2}\, dx. \tag{11}$$

The n (real and simple) zeros of $H_n(x)$ are symmetrically distributed around the origin, since $H_n(-x)=(-1)^n H_n(x)$.[27] Therefore, it is readily seen that $V_n(-t)=V_n(t)$, and Eq. (10) can also be written as

$$E_n(H)=-2^n n!\sqrt{\pi}\,\ln(2^{2n})+2\epsilon V_n(0)+4\sum_{i=1}^{m} V_n(x_{n,i}), \tag{12}$$

where $x_{n,i}$ $(i=1,2,...,m)$ is the ith *positive* root of $H_n(x)$, and we have introduced the convenient notations

$$m\equiv\left[\frac{n}{2}\right],\quad \epsilon\equiv n-2m. \tag{13}$$

In the latter equation, the square brackets denote integer part of the expression within, so that ϵ is equal to 0 or 1 according to whether n is even or odd.

Equations (10) and (12) show that the problem of calculating $E_n(H)$, and hence S_n, reduces to the evaluation of $V_n(t)$ at the zeros of $H_n(x)$. In Sec. II below we obtain a closed analytical expression for $V_n(t)$ in terms of ${}_1F_1$ and ${}_2F_2$ hypergeometric functions, which, unlike the recursive formula derived in Ref. 20, provides us with analytical expressions for $E_n(H)$ and S_n when the exact location of the zeros of $H_n(x)$ is known. An inequality for the values of $V_n(t)$ at the zeros of $H_n(x)$ is conjectured, which leads to a new upper bound for S_n, stronger than that in Eq. (7) for n odd. Finally, in Sec. III, it is shown that the exact formula for $V_n(t)$ can be written as an infinite series involving the Gauss ${}_2F_1$ hypergeometric function, which enables us to express $E_n(H)$ and S_n in terms of the even–order spectral moments $\mu_{2k}(n)$ of the Hermite polynomials. Comparison of the asymptotic $(n\gg 1)$ limit of this alternative expression with Eq. (6) proves the asymptotic validity of the conjectured upper bound for S_n.

II. CALCULATION OF THE LOGARITHMIC POTENTIAL AND THE ENTROPIES

To calculate $V_n(t)$, we first make use of the multiplication formula for Hermite polynomials (see, e.g., Ref. 28),

$$H_m(x)H_n(x)=\sum_{j=0}^{\min(m,n)}\frac{m!\,n!\,2^j}{(m-j)!\,(n-j)!\,j!}\,H_{m+n-2j}(x),$$

which in the particular case $m=n$ gives, writing $j=n-k$,

$$(H_n(x))^2=2^n n!\sum_{k=0}^{n}\binom{n}{k}\frac{H_{2k}(x)}{2^k k!}.$$

Substituting this equation in the expression (11) of the logarithmic potential $V_n(t)$, we find

$$V_n(t)=2^n n!\sum_{k=0}^{n}\binom{n}{k}\frac{W_{2k}(t)}{2^k k!},\quad W_{2k}(t)=-\int_{-\infty}^{\infty}H_{2k}(x)\ln|x-t|e^{-x^2}\,dx. \tag{14}$$

Now we are faced with the problem of calculating the integrals $W_{2k}(t)$, which can also be considered as logarithmic potentials for Hermite polynomials and thus have independent interest. To achieve this goal, we consider the Taylor series expansion

$$W_{2k}(t)=\sum_{r=0}^{\infty}\frac{W_{2k}^{(r)}(0)}{r!}\,t^r. \tag{15}$$

Making the change of variables $x=y+t$ in Eq. (14), we have

$$W_{2k}(t)=-\int_{-\infty}^{\infty}H_{2k}(y+t)\ln|y|e^{-(y+t)^2}\,dy.$$

By repeated application of Leibniz's rule for differentiating under the integral sign, and taking into account that, from Rodrigues' formula for Hermite polynomials,

$$\frac{d^r}{dz^r}\,(e^{-z^2}H_n(z))=(-1)^r e^{-z^2}H_{n+r}(z),$$

we obtain

$$W_{2k}^{(r)}(t)=(-1)^r W_{2k+r}(t),$$

so that Eq. (15) reads

$$W_{2k}(t)=\sum_{r=0}^{\infty}\frac{(-1)^r W_{2k+r}(0)}{r!}\,t^r. \tag{16}$$

The parity property $H_n(-x)=(-1)^n H_n(x)$ implies that $W_{2k+r}(0)=0$ if r is odd, and Eq. (16) simplifies to

$$W_{2k}(t)=\sum_{r=0}^{\infty}\frac{W_{2k+2r}(0)}{(2r)!}\,t^{2r},\quad W_{2k+2r}(0)=-2\int_0^{\infty}H_{2k+2r}(x)e^{-x^2}\ln x\,dx. \tag{17}$$

The integrals $W_{2k+2r}(0)$ may be evaluated by means of the following result,[27]

$$\int_0^{\infty}H_{2n}(x)x^{\nu}e^{-2\alpha x^2}\,dx=(-1)^n\frac{2^{2n-(\nu+3)/2}}{\sqrt{\pi}\alpha^{(\nu+1)/2}}\,\Gamma\left(\frac{\nu+1}{2}\right)\Gamma\left(n+\frac{1}{2}\right)F\left(-n,\,\frac{\nu+1}{2};\,\frac{1}{2};\,\frac{1}{2\alpha}\right),$$

where $F(a,b;c;z)={}_2F_1(a,b;c;z)$ is the Gauss hypergeometric function, which is valid for Re $\alpha>0$, Re $\nu>-1$. In our case, with $\alpha=\frac{1}{2}$ and $n=k+r$, we obtain

$$\int_0^{\infty}H_{2k+2r}(x)x^{\nu}e^{-x^2}\,dx=(-1)^{k+r}\frac{2^{2k+2r-1}}{\sqrt{\pi}}\,\Gamma\left(\frac{\nu+1}{2}\right)\Gamma\left(k+r+\frac{1}{2}\right)F\left(-k-r,\,\frac{\nu+1}{2};\,\frac{1}{2};1\right). \tag{18}$$

The hypergeometric function of unit argument on the right-hand side can be simplified using the property[29]

$$F(-n,b;c;1)=\frac{(c-b)_n}{(c)_n},$$

where n is a positive integer or zero, c is not a negative integer or zero, and $(z)_n$ is Pochhammer's symbol,

$$(z)_n=\frac{\Gamma(z+n)}{\Gamma(z)}=(-1)^n\,\frac{\Gamma(1-z)}{\Gamma(1-z-n)}. \tag{19}$$

We thus have

$$F\left(-k-r,\ \frac{\nu+1}{2};\frac{1}{2};1\right)=\frac{(-\nu/2)_{k+r}}{(\frac{1}{2})_{k+r}}=\frac{\Gamma(\frac{1}{2})\Gamma(k+r-\nu/2)}{\Gamma(k+r+\frac{1}{2})\Gamma(-\nu/2)},$$

and Eq. (18) then reads

$$\int_0^\infty H_{2k+2r}(x)x^\nu e^{-x^2}\,dx=(-1)^{k+r}2^{2k+2r-1}\Gamma\left(\frac{\nu+1}{2}\right)\frac{\Gamma(k+r-\nu/2)}{\Gamma(-\nu/2)}.$$

Differentiating this equation with respect to ν, we obtain

$$\int_0^\infty H_{2k+2r}(x)x^\nu e^{-x^2}\ln x\,dx=(-1)^{k+r}2^{2k+2r-1}\Gamma\left(\frac{\nu+1}{2}\right)\frac{\Gamma(k+r-\nu/2)}{\Gamma(-\nu/2)}$$
$$\times\frac{1}{2}\left(\psi\left(\frac{\nu+1}{2}\right)-\psi\left(k+r-\frac{\nu}{2}\right)+\psi\left(-\frac{\nu}{2}\right)\right),\qquad(20)$$

where $\psi(z)=\Gamma'(z)/\Gamma(z)$ is the logarithmic derivative of the gamma function. In the case when $k+r=0$, this formula reduces to

$$\int_0^\infty H_0(x)x^\nu e^{-x^2}\ln x\,dx=\frac{1}{4}\Gamma\left(\frac{\nu+1}{2}\right)\psi\left(\frac{\nu+1}{2}\right),$$

so that we readily get

$$W_0(0)=-\frac{1}{2}\Gamma\left(\frac{1}{2}\right)\psi\left(\frac{1}{2}\right)=\frac{\sqrt{\pi}}{2}(\gamma+2\ln 2).\qquad(21)$$

On the other hand, both $\Gamma(z)$ and $\psi(z)$ have simple poles for $z=0$, with residues 1 and -1, respectively. Therefore, when $k+r>0$, we can take the limit $\nu\to 0$ in Eq. (20) to obtain

$$\int_0^\infty H_{2k+2r}(x)e^{-x^2}\ln x\,dx=-\frac{\sqrt{\pi}}{4}(-1)^{k+r}2^{2k+2r}\Gamma(k+r),\quad k+r>0,$$

which in turn leads to

$$W_{2k+2r}(0)=\frac{\sqrt{\pi}}{2}(-1)^{k+r}2^{2k+2r}\Gamma(k+r),\quad k+r>0.\qquad(22)$$

We can evaluate $W_{2k}(t)$ by substituting Eqs. (21) and (22) into (17). In the case $k=0$, we have

$$W_0(t)=W_0(0)+\sum_{r=1}^\infty\frac{W_{2r}(0)}{(2r)!}t^{2r}=\frac{\sqrt{\pi}}{2}\left(\gamma+2\ln 2+\sum_{r=1}^\infty\frac{(-1)^r2^{2r}\Gamma(r)}{\Gamma(2r+1)}t^{2r}\right).\qquad(23)$$

Using the recurrence and duplication formulas for the gamma function,[27,29]

$$\Gamma(z+1)=z\Gamma(z),\quad\Gamma(2z)=2^{2z-1}(\tfrac{1}{2})_z\Gamma(z),$$

together with (19), and shifting the summation index to $s=r-1$, Eq. (23) can be written in terms of a ${}_2F_2$ hypergeometric function,

$$W_0(t)=\frac{\sqrt{\pi}}{2}\left(\gamma+2\ln 2-2t^2\ {}_2F_2\left(1,1;\ \frac{3}{2},2;-t^2\right)\right). \tag{24}$$

On the other hand, for $k>0$ we have

$$W_{2k}(t)=\sum_{r=0}^{\infty}\frac{W_{2k+2r}(0)}{(2r)!}\,t^{2r}=\frac{\sqrt{\pi}}{2}(-1)^k 2^{2k}\sum_{r=0}^{\infty}\frac{(-1)^r 2^{2r}\Gamma(k+r)}{\Gamma(2r+1)}\,t^{2r}, \tag{25}$$

and use of the duplication formula for the gamma function and Eq. (19) leads to

$$W_{2k}(t)=\frac{\sqrt{\pi}}{2}(-1)^k 2^{2k}(k-1)!\,M\left(k,\ \frac{1}{2},-t^2\right), \tag{26}$$

where $M(a,c,z)={}_1F_1(a;c;z)$ is Kummer's confluent hypergeometric function. Substituting Eqs. (24) and (26) into (14), we finally obtain

$$V_n(t)=2^n n!\sqrt{\pi}\left(\frac{\gamma}{2}+\ln 2-t^2\ {}_2F_2\left(1,1;\ \frac{3}{2},2;-t^2\right)+\frac{1}{2}\sum_{k=1}^{n}\binom{n}{k}\frac{(-1)^k 2^k}{k}\,M\left(k,\ \frac{1}{2},-t^2\right)\right), \tag{27}$$

which is the sought for closed analytical expression for the logarithmic potential $V_n(t)$ defined by Eq. (11).

In the particular case $t=0$, using the identity

$$\gamma+2\ln 2+\sum_{k=1}^{n}\binom{n}{k}\frac{(-1)^k 2^k}{k}=-\psi\left(m+\epsilon+\frac{1}{2}\right), \tag{28}$$

whose proof can be found in the Appendix, Eq. (27) reduces to

$$V_n(0)=-2^{n-1}n!\sqrt{\pi}\,\psi(m+\epsilon+\tfrac{1}{2}). \tag{29}$$

The function $V_n(t)$ in Eq. (27) is plotted against t for $0\leqslant n\leqslant 5$ in Fig. 1. Therefrom we see that $V_n(t)$ has n local minima, which are located at the zeros of $H_n(x)$,[20] and the value of $V_n(t)$ at these minima decreases monotonically as $|x_{n,i}|$ increases. We also observe that it holds the inequality

$$V_n(x_{n,i})\leqslant V_n(0), \tag{30}$$

which is strict for $x_{n,i}\neq 0$. We conjecture Eq. (30) to be valid for all n, although we have not been able to prove it analytically. On the other hand, $V_n(0)<0$ for all $n\geqslant 1$, since then[27,29]

$$\psi\left(m+\epsilon+\frac{1}{2}\right)=-\gamma-2\ln 2+2\sum_{k=1}^{m+\epsilon}\frac{1}{2k-1}>0, \tag{31}$$

so that the absolute value of $V_n(x_{n,i})$ increases monotonically with $|x_{n,i}|$. This implies, in view of Eqs. (10) and (12), that the contribution of the zeros of $H_n(x)$ to the entropy S_n increases as so does their absolute value.

A closed formula for the entropy of Hermite polynomials $E_n(H)$ can be obtained by combining Eqs. (10) and (27),

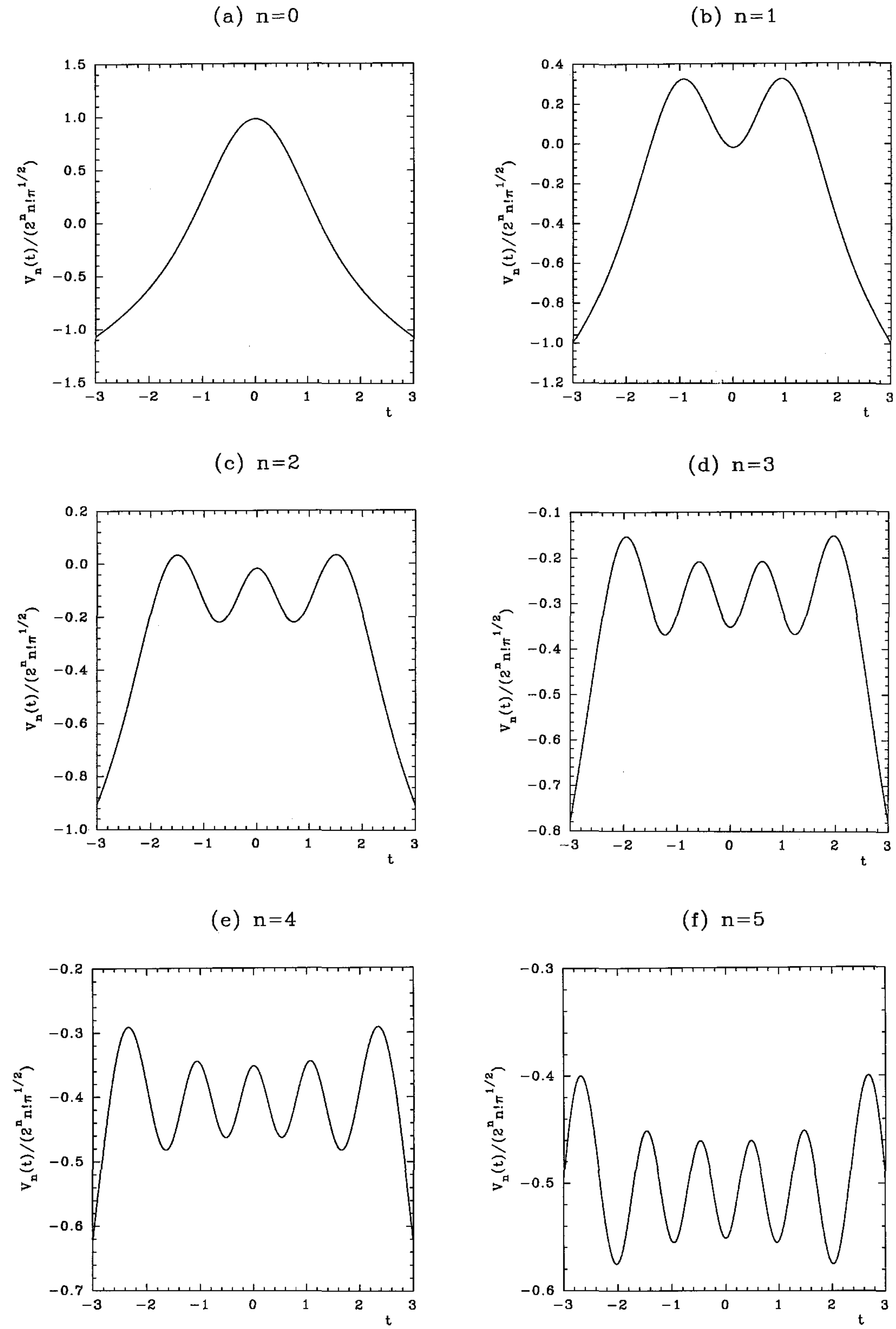

FIG. 1. Logarithmic potential $V_n(t)$ for $0 \leqslant n \leqslant 5$, as given by Eq. (27).

$$E_n(H)=2^n n!\sqrt{\pi}\left(n\gamma-2\sum_{i=1}^{n} x_{n,i}^2\ {}_2F_2\left(1,1;\frac{3}{2},2;-x_{n,i}^2\right)+\sum_{k=1}^{n}\binom{n}{k}\frac{(-1)^k 2^k}{k}\sum_{i=1}^{n} M\left(k,\frac{1}{2},-x_{n,i}^2\right)\right). \tag{32}$$

Alternatively, using Eq. (12) instead of (10), and taking into account Eqs. (29) and (31), we obtain

$$E_n(H)=2^n n!\sqrt{\pi}\left(n\gamma-2\epsilon\sum_{k=1}^{m+\epsilon}\frac{1}{2k-1}-4\sum_{i=1}^{m} x_{n,i}^2\ {}_2F_2\left(1,1;\ \frac{3}{2},2;-x_{n,i}^2\right)\right.$$
$$\left.+2\sum_{k=1}^{n}\binom{n}{k}\frac{(-1)^k 2^k}{k}\sum_{i=1}^{m} M\left(k,\ \frac{1}{2},-x_{n,i}^2\right)\right). \tag{33}$$

In turn, from these results, using Eq. (4), we obtain for S_n the expressions

$$S_n=\ln(2^n n!\sqrt{\pi})+n+\frac{1}{2}+n\gamma-2\sum_{i=1}^{n} x_{n,i}^2\ {}_2F_2\left(1,1;\ \frac{3}{2},2;-x_{n,i}^2\right)$$
$$+\sum_{k=1}^{n}\binom{n}{k}\frac{(-1)^k 2^k}{k}\sum_{i=1}^{n} M\left(k,\ \frac{1}{2},-x_{n,i}^2\right), \tag{34}$$

and

$$S_n=\ln(2^n n!\sqrt{\pi})+n+\frac{1}{2}+n\gamma-2\epsilon\sum_{k=1}^{m+\epsilon}\frac{1}{2k-1}-4\sum_{i=1}^{m} x_{n,i}^2\ {}_2F_2\left(1,1;\ \frac{3}{2},2;-x_{n,i}^2\right)$$
$$+2\sum_{k=1}^{n}\binom{n}{k}\frac{(-1)^k 2^k}{k}\sum_{i=1}^{m} M\left(k,\ \frac{1}{2},-x_{n,i}^2\right), \tag{35}$$

respectively, which are the generalizations of Eqs. (8) and (9) to arbitrary values of n. For example, in the $n=2$ case, the zeros of the polynomial $H_2(x)=4x^2-2$ are $\pm 1/\sqrt{2}$, so that we have

$$S_2=\ln(8\sqrt{\pi})+\frac{5}{2}+2\gamma-2\,{}_2F_2\left(1,1;\ \frac{3}{2},2;-\frac{1}{2}\right)-8M\left(1,\frac{1}{2},-\frac{1}{2}\right)+4M\left(2,\frac{1}{2},-\frac{1}{2}\right),$$

while in the $n=3$ case the zeros of $H_3(x)=8x^3-12x$ are 0 and $\pm\sqrt{3/2}$, and we have

$$S_3=\ln(48\sqrt{\pi})+\frac{5}{6}+3\gamma-6\,{}_2F_2\left(1,1;\ \frac{3}{2},2;-\frac{3}{2}\right)-12M\left(1,\frac{1}{2},-\frac{3}{2}\right)+12M\left(2,\frac{1}{2},-\frac{3}{2}\right)$$
$$-\frac{16}{3}M\left(3,\frac{1}{2},-\frac{3}{2}\right).$$

Fully analytic, though increasingly cumbersome, expressions of this kind may be written for every $n\leqslant 9$, since then $H_n(x)=x^{\epsilon}\widetilde{H}_m(x^2)$, where $\widetilde{H}_m(x)$ is a polynomial of degree $m\leqslant 4$.

Using Eqs. (10) and (29), the conjectured inequality (30) yields an upper bound for $E_n(H)$,

$$E_n(H)\leqslant -2^n n!\sqrt{\pi}\left(\ln(2^{2n})+n\psi\left(\frac{n+\epsilon+1}{2}\right)\right)=2^n n!\,n\sqrt{\pi}\left(\gamma-2\sum_{k=1}^{m+\epsilon}\frac{1}{2k-1}\right), \tag{36}$$

where, recalling Eq. (13), we have written $m+\epsilon$ in the equivalent form $(n+\epsilon)/2$, and the second expression is obtained from the first one by using (31). Introducing the previous equation into (4), we get

$$S_n \leqslant \ln\left(\frac{n!\sqrt{\pi}}{2^n}\right)+n+\frac{1}{2}-n\psi\left(\frac{n+\epsilon+1}{2}\right)=\ln(2^n n!\sqrt{\pi})+\frac{1}{2}+n\left(1+\gamma-2\sum_{k=1}^{m+\epsilon}\frac{1}{2k-1}\right). \tag{37}$$

This conjectured upper bound for S_n turns out to be stronger than that given by Eq. (7) when n is odd, and coincides with the exact value not only for $n=0$, but also for $n=1$ [see Eqs. (8) and (9)].

III. ALTERNATIVE EXPRESSIONS

Using Eq. (23) for $W_0(t)$, and Eq. (25) for $W_{2k}(t)$, $k>0$, Eq. (27) can be written as

$$V_n(t)=2^n n!\sqrt{\pi}\left(\frac{\gamma}{2}+\ln 2+\frac{1}{2}\sum_{r=1}^{\infty}\frac{(-1)^r(r-1)!}{(2r)!}(2t)^{2r}+\frac{1}{2}\sum_{k=1}^{n}\binom{n}{k}\frac{(-1)^k 2^k}{k!}\sum_{r=0}^{\infty}\frac{(-1)^r\Gamma(k+r)}{(2r)!}(2t)^{2r}\right),$$

which, taking advantage of Eq. (28), and writing again $(n+\epsilon)/2$ instead of $m+\epsilon$, simplifies to

$$V_n(t)=2^{n-1}n!\sqrt{\pi}\left(-\psi\left(\frac{n+\epsilon+1}{2}\right)+\sum_{r=1}^{\infty}\frac{(-1)^r(r-1)!}{(2r)!}(2t)^{2r}+\sum_{k=1}^{n}\binom{n}{k}\frac{(-1)^k 2^k}{k!}\sum_{r=1}^{\infty}\frac{(-1)^r\Gamma(k+r)}{(2r)!}(2t)^{2r}\right). \tag{38}$$

Taking into account Eq. (19), together with the identity[29]

$$\binom{n}{k}=\frac{(-1)^k(-n)_k}{k!},$$

the summation over k in the double series of Eq. (38) can be performed in terms of the Gauss hypergeometric function,

$$\sum_{k=1}^{n}\binom{n}{k}\frac{(-1)^k 2^k\Gamma(r+k)}{k!}=(r-1)!(F(-n,r;1;2)-1).$$

Substituting this equation into (38), we obtain

$$V_n(t)=2^{n-1}n!\sqrt{\pi}\left(-\psi\left(\frac{n+\epsilon+1}{2}\right)+\sum_{r=1}^{\infty}\frac{(-1)^r 2^{2r}(r-1)!}{(2r)!}F(-n,r;1;2)t^{2r}\right), \tag{39}$$

which is an alternative expression for the logarithmic potential $V_n(t)$.

The entropy of the Hermite polynomials defined by Eq. (10) can thus be written in the form

$$E_n(H)=2^n n!\sqrt{\pi}\left(-\ln(2^{2n})-n\psi\left(\frac{n+\epsilon+1}{2}\right)+n\sum_{r=1}^{\infty}\frac{(-1)^r 2^{2r}(r-1)!}{(2r)!}F(-n,r;1;2)\mu_{2r}(n)\right), \tag{40}$$

where $\mu_r(n)$ $(r=0,1,2,\dots)$ are the spectral moments around the origin of the Hermite polynomial $H_n(x)$, i.e., the quantities

$$\mu_r(n)=\frac{1}{n}\sum_{i=1}^{n}(x_{n,i})^r, \tag{41}$$

and Eq. (4) then yields

$$S_n=\ln\left(\frac{n!\sqrt{\pi}}{2^n}\right)+n+\frac{1}{2}-n\psi\left(\frac{n+\epsilon+1}{2}\right)+n\sum_{r=1}^{\infty}\frac{(-1)^r 2^{2r}(r-1)!}{(2r)!}F(-n,r;1;2)\mu_{2r}(n). \tag{42}$$

This new expression for S_n is less useful than Eqs. (34) and (35) for practical calculations, since, unfortunately, there are no global and compact expressions for the moments $\mu_{2r}(n)$, but they have to be recurrently generated. For Hermite polynomials, $\mu_r(n)$ vanishes when r is an odd integer, while it can be shown[30] that

$$\mu_0(n)=1,\quad \mu_2(n)=\frac{n-1}{2},$$

and for $r\geqslant 2$ the even spectral moments $\mu_{2r}(n)$ are determined by means of the nonlinear recurrent formula

$$(2n+2-s)\mu_{s-3}(n)-2\mu_{s-1}(n)+n\left(\sum_{t=1}^{s-4}\mu_{s-3-t}(n)\mu_t(n)\right)=0,\quad s\geqslant 5.$$

However, Eq. (42) turns out to be more appropriate than Eqs. (34) and (35) to display the relation between our exact results and the asymptotic approximation (6). Use of the well-known asymptotic expansions for the gamma and psi functions[29] gives

$$\ln(n!)\sim\left(n+\frac{1}{2}\right)\ln n-n+\frac{1}{2}\ln(2\pi)+O(n^{-1}),$$

$$\psi\left(\frac{n+\epsilon+1}{2}\right)\sim\ln\left(\frac{n+\epsilon}{2}\right)+O(n^{-2})\sim\ln n-\ln 2+\frac{\epsilon}{n}+O(n^{-2}),$$

where the remaining terms of these expansions can be explicitly written in terms of Bernoulli numbers. Substituting these results into Eq. (42), we obtain

$$S_n\sim\ln(\pi\sqrt{2n})+\frac{1}{2}-\epsilon+n\sum_{r=1}^{\infty}\frac{(-1)^r 2^{2r}(r-1)!}{(2r)!}F(-n,r;1;2)\mu_{2r}(n)+O(n^{-1}). \tag{43}$$

Comparison of this equation with (6) leads to the asymptotic formula

$$n\sum_{r=1}^{\infty}\frac{(-1)^r 2^{2r}(r-1)!}{(2r)!}F(-n,r;1;2)\mu_{2r}(n)\sim\epsilon-\frac{3}{2}+o(1). \tag{44}$$

Finally, we note that, comparing the exact formula for S_n, Eq. (42), with the conjectured upper bound (37), the latter turns out to be equivalent to the inequality

$$\sum_{r=1}^{\infty} \frac{(-1)^r 2^{2r}(r-1)!}{(2r)!} F(-n,r;1;2)\mu_{2r}(n) \leqslant 0, \tag{45}$$

which Eq. (44) implies to be, at least, asymptotically valid. When n is even, the validity of Eqs. (37) and (45) follows from that of Eq. (7), which then places a stronger upper bound on S_n than (37). For n odd, however, Eq. (37) is stronger than (7), so that the problem of finding a proof of its general validity remains open.

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APPENDIX: PROOF OF EQ. (28)

Equation (28) follows from the identity

$$\sum_{k=1}^{n} \binom{n}{k} \frac{(-1)^k 2^k}{k} = -\sum_{k=1}^{n} \frac{1-(-1)^k}{k}, \tag{A1}$$

which is the particular case $x=2$ of the more general formula

$$f(x) \equiv \sum_{k=1}^{n} \binom{n}{k} \frac{(-1)^k x^k}{k} = -\sum_{k=1}^{n} \frac{1-(1-x)^k}{k}. \tag{A2}$$

The validity of Eq. (A2) can be proved by induction over n, and also by considering the Newton binomial expansion of $f'(x)$,

$$f'(x) = \frac{1}{x} \sum_{k=1}^{n} \binom{n}{k} (-x)^k = \frac{(1-x)^n - 1}{x}.$$

Making the change of variables $1-x=t$, and taking into account that

$$\frac{t^n-1}{t-1} = \sum_{k=0}^{n-1} t^k,$$

we readily obtain

$$f(x) = \int \frac{(1-x)^n-1}{x}\, dx = \sum_{k=1}^{n} \frac{(1-x)^k}{k} + C.$$

Finally, the value of the integration constant C is determined from the condition $f(0)=0$, which leads to Eq. (A2).

The expression $1-(-1)^k$ vanishes if k is even, while it is equal to 2 if k is odd, so that only the odd values of k give a nonvanishing contribution to the right-hand side of (A1). If $n=2m+\epsilon$, with $m=[n/2]$ and $\epsilon=0,1$ for n even and odd, respectively, the last nonzero term in the summation is that corresponding to $k=2m+2\epsilon-1$ ($2m-1=n-1$ for n even and $2m+1=n$ for n odd). Writing $k=2l-1$, we have

$$\sum_{k=1}^{n} \frac{1-(-1)^k}{k} = \sum_{k=1}^{2m+2\epsilon-1} \frac{1-(-1)^k}{k} = 2\sum_{l=1}^{m+\epsilon} \frac{1}{2l-1},$$

and taking into account Eq. (31) we complete our proof of (28).

[1] P. Hohenberg and W. Kohn, ''Inhomogeneous electron gas,'' Phys. Rev. B **136**, 864–870 (1964).
[2] R. G. Parr and W. Yang, *Density Functional Theory of Atoms and Molecules* (Oxford U.P., New York, 1989).
[3] E. S. Kryachko and E. V. Ludeña, *Density Functional Theory of Many-Electron Systems* (Kluwer, Dordrecht, 1989).
[4] R. M. Dreizler and E. K. U. Gross, *Density Functional Theory An Approach to the Quantum Mechanics* (Springer-Verlag, Heidelberg, 1990).
[5] N. H. March, *Electron Density Theory of Atoms and Molecules* (Academic, New York, 1992).
[6] S. R. Gadre and R. D. Bendale, ''Rigorous relationships among quantum-mechanical kinetic energy and atomic information entropies: upper and lower bounds,'' Phys. Rev. A **36**, 1932–1935 (1987).
[7] J. C. Angulo and J. S. Dehesa, ''Tight rigorous bounds to atomic information entropies,'' J. Chem. Phys. **97**, 6485–6495 (1992).
[8] J. C. Angulo, ''Uncertainty relationships in many-body systems,'' J. Phys. A **26**, 6493–6497 (1993).
[9] J. C. Angulo, ''Information entropy and uncertainty in D-dimensional many-body systems,'' Phys. Rev. A **50**, 311–313 (1994).
[10] R. J. Yáñez, J. C. Angulo, and J. S. Dehesa, ''Information entropies of many-electron systems,'' Int. J. Quantum Chem. **56**, 489–498 (1995).
[11] W. Beckner, ''Inequalities in Fourier analysis,'' Ann. Math. **102**, 159–182 (1975).
[12] I. Bialynicki-Birula and J. Mycielski, ''Uncertainty relations for information entropy in wave mechanics,'' Commun. Math. Phys. **44**, 129–132 (1975).
[13] I. Bialynicki-Birula, ''Entropic uncertainty relations,'' Phys. Lett. A **103**, 253–254 (1984).
[14] M. Grabowski, ''The spreading of free wave packets and the entropy of position,'' J. Math. Phys. **22**, 303–305 (1981).
[15] M. Grabowski, ''The entropy of position and the spreading of wave packets,'' Rep. Math. Phys. **24**, 327–331 (1986).
[16] N. Canosa, A. Plastino, and R. Rossignoli, ''Ground-state wave functions and maximum entropy,'' Phys. Rev. A **40**, 519–525 (1989).
[17] N. Canosa, R. Rossignoli, and A. Plastino, ''Information theory and energy spectra,'' Phys. Rev. A **43**, 1145–1152 (1991).
[18] N. Balakrishnan and N. Sathyamurthy, ''Maximization of entropy during a chemical reaction,'' Chem. Phys. Lett. **164**, 267–269 (1989).
[19] R. J. Yáñez, W. Van Assche, and J. S. Dehesa, ''Position and momentum information entropies of the D-dimensional harmonic oscillator and hydrogen atom,'' Phys. Rev. A **50**, 3065–3079 (1994).
[20] J. S. Dehesa, W. Van Assche, and R. J. Yáñez, ''Logarithmic potential of Hermite polynomials and information entropies of the harmonic oscillator eigenstates,'' Meth. Appl. Anal. **4**, 91–110 (1997).
[21] A. I. Aptekarev, V. S. Buyarov, and J. S. Dehesa, ''Asymptotic behavior of L^p-norms and entropy for general orthogonal polynomials,'' Russ. Acad. Sci. Sb. Math. **82**, 373–395 (1995).
[22] A. I. Aptekarev, J. S. Dehesa, and R. J. Yáñez, ''Spatial entropy of central potentials and strong asymptotics of orthogonal polynomials,'' J. Math. Phys. **35**, 4423–4428 (1994).
[23] W. Van Assche, R. J. Yáñez, and J. S. Dehesa, ''Entropy of orthogonal polynomials with Freud weights and information entropies of the harmonic oscillator potential,'' J. Math. Phys. **36**, 4106–4118 (1995).
[24] A. I. Aptekarev, V. S. Buyarov, W. Van Assche, and J. S. Dehesa, ''Asymptotics of entropy integrals for orthogonal polynomials,'' Dokl. Math. **53**, 47–49 (1996).
[25] J. Sánchez-Ruiz, ''Asymptotic formula for the quantum entropy of position in energy eigenstates,'' Phys. Lett. A **226**, 7–13 (1997).
[26] V. Majerník and T. Opatrný, ''Entropic uncertainty relations for a quantum oscillator,'' J. Phys. A **29**, 2187–2197 (1996).
[27] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products*, 5th ed. (Academic, San Diego, 1994).
[28] H. Kleindienst and A. Lüchow, ''Multiplication theorems for orthogonal polynomials,'' Int. J. Quantum Chem. **48**, 239–247 (1993).
[29] Y. L. Luke, *The Special Functions and their Approximations* (Academic, New York, 1969), Vol. I.
[30] K. M. Case, ''Sum rules for zeros of polynomials. I,'' J. Math. Phys. **21**, 702–714 (1980).