International Journal of Theoretical Physics, Vol. 37, No. 6, 1998

Quantal Information Entropies for Atoms

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Received September 26, 1997

The polynomials occurring in the wave functions of hydrogenic excited states are found to present difficulties for a straightforward analytical approach to the study of associated information entropies. A method is suggested to deal with them. It is then applied to calculate the information entropy for the Jacobi polynomial. A model calculation is presented to examine the effect of screening on the entropy sum. It is seen that the sum does not depend on the choice of screening.

1. INTRODUCTION

A rigorous mathematical treatment of the theory of information (Shannon, 1949) first appeared with the birth of cybernetics, the science of control and automation of dynamical processes. Currently, information-theoretic approaches are widely used to study the properties of complex microscopic systems (Angulo *et al.*, 1993; Antolin *et al.*, 1994, 1997; Macia *et al.*, 1994; Nagy and Parr, 1996). Some studies on the foundation of quantum mechanics have been based on similar procedures (Kadomstev, 1994).

An information measure closely related to the concept of entropy in thermodynamics plays a role in atomic theories and is defined by (Shannon, 1994)

$$S_\omega = -\int \omega(\varepsilon) \ln \omega(\varepsilon)\, d\varepsilon \tag{1}$$

The quantal entropy S_ω measures the lack of information about the probability

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distribution $\omega(\varepsilon)$ in ε space. Problems in quantum mechanics are formulated either in the coordinate (r) space or in momentum (p) space, depending on which is more convenient for the problem under consideration. Thus from (1) we can write

$$S_\rho = -\int \rho(r) \ln \rho(r)\, dr \tag{2}$$

and

$$S_\gamma = -\int \gamma(p) \ln \gamma(p)\, dp \tag{3}$$

for the position and momentum space entropies with

$$\rho(r) = |\Psi(\bar{r})|^2 \qquad \text{and} \qquad \gamma(p) = |\overline{\Psi}(\bar{p})|^2 \tag{4}$$

Here $\overline{\Psi}(\bar{p})$ stands for the Fourier transform of $\Psi(\bar{r})$, the r-space eigenfunction of a central potential. The conjugate expressions in (2) and (3) allowed Bialynicki-Birula and Mycielski (1975) to derive a new and stronger version of the Heisenberg uncertainity relation:

$$S_\rho + S_\gamma \geq D(1 + \ln \pi) \tag{5}$$

where D corresponds to the dimensionality of the space for motion of the system. The information sum in (5) is often called the BBM inequality.

Yáñez *et al.* (1994) studied (2) and (3) for the D-dimensional hydrogen atom for arbitrary values of n and l, the principal and angular momentum quantum numbers, respectively. They found simple results for the ground states, $n = l + 1$, of a spectral series (constant l and varying n). But inordinate complications were encountered in treating the cases for excited states. The reason for this may be attributed to the fact that the ground-state hydrogenic wavefunctions consist of a single term, while the excited states involve polynomials. The logarithm of these polynomials presents difficulties in evaluating the entropy integral. One of our objectives in this work is to elucidate this point and derive a straightforward calculational procedure for S_ρ and S_γ for hydrogenic excited states. We shall work in three spatial dimensions. Our other aim is to examine the effect of screening on the entropy sum (5), the BBM inequality, and thus gain some physical insight about the internal structure of S_ω.

We devote Section 2 to evaluate the entropy integrals (2) and (3) for the 2s hydrogenic state. The calculational procedure will serve as a guide for dealing with other hydrogenic states characterized by associated Laguerre and Gegenbauer polynomials. It is important to note that evaluation of physical entropies ultimately reduces to calculation of the entropy integral E_n for classical orthogonal polynomials, and in this context evaluation of E_n for the Jacobi polynomial $P_n^{\alpha,\beta}(x)$ is an open problem (Yáñez *et al.*, 1994). In Section 3 we construct an exact analytical expression for E_n for the Jacobi polynomial and make some comments on the result. In Section 4 we investigate the effect of screening on S_ρ and S_γ by using the Hulthén potential (Hulthén, 1942) as a model for the screened Coulomb interaction.

2. INFORMATION ENTROPIES FOR HYDROGENIC EXCITED STATES

The wavefunction for the ground state of the *s* spectral series or hydrogenic state is given by

$$\Psi_{1s}(\bar{r}) = \frac{1}{\sqrt{\pi}} e^{-r} \tag{6}$$

We shall use Hartree atomic units throughout this work. The quantity S_ρ for this wavefunction (6) can be evaluated by using the standard integral

$$\int_0^\infty x^n e^{-ax}\, dx = \frac{\Gamma(n+1)}{a^{n+1}} \tag{7}$$

For similar calculations involving ground states of the *p, d, f, . . . ,* spectral series one can proceed by using different derivatives of the integral (Gradshteyn and Ryzhik, 1965)

$$\int_0^\infty e^{-\mu x} \ln x\, dx = \frac{1}{\mu}(C + \ln \mu) \tag{8}$$

with respect to μ and finally setting $\mu = 1$. The angular integrals for higher l values have been given by Yáñez*et al.* (1994). For ground states the calulation of S_γ is also equally straightforward. In the following we show that this is not true even for the hydrogenic 2*s* state.

The 2*s* wavefunction is given by

$$\Psi_{2s}(\bar{r}) = \frac{1}{4\sqrt{2\pi}}(2 - r)e^{-r/2} \tag{9}$$

and

$$\overline{\Psi}_{2s}(\bar{p}) = \frac{16}{\pi}\frac{1 - 4k^2}{(1 + 4k^2)^3} \tag{10}$$

For (9) the position-space entropy S_ρ can be written as

$$S_\rho = 5 \ln 2 + \ln \pi + 6 - \tfrac{1}{8} I_3 \tag{11}$$

involving a nontrivial integral

$$I_3 = \int_0^\infty r^2 (r - 2)^2 e^{-r} \ln(r - 2)^2 \, dr \tag{12}$$

To evaluate I_3 we introduce

$$\ln(r - 2)^2 = \lim_{\varepsilon \to 0} \frac{\partial}{\partial \varepsilon} (r - 2)^{2\varepsilon} \tag{13}$$

and make a change of variable by substituting

$$y = r - 2 \tag{14}$$

This gives

$$I_3 = \frac{1}{e^2} \lim_{\varepsilon \to 0} \frac{\partial}{\partial \varepsilon} [I_4(\varepsilon) + I_5(\varepsilon)] \tag{15}$$

where

$$I_4(\varepsilon) = \int_0^\infty e^{-y} y^{2+2\varepsilon} (y + 2)^2 \, dy \tag{16}$$

and

$$I_5(\varepsilon) = \int_{-2}^0 e^{-y} y^{2+2\varepsilon} (y + 2)^2 \, dy \tag{17}$$

The result for $I_4(\varepsilon)$ can be expressed in terms of the gamma function, while (17) needs separate consideration. For the latter we make a further change of variable,

$$y = 2x - 2 \tag{18}$$

and get

$$I_5(\varepsilon) = 2^{5+2\varepsilon} e^2 \int_0^1 e^{-2x} x^2 (1 - x)^{2+2\varepsilon} \, dx \tag{19}$$

The integral in (19) can be written in terms of confluent hypergeometric functions by using

$${}_1F_1[a, c; x] = \frac{\Gamma(c)}{\Gamma(a)\Gamma(c - a)} \int_0^1 e^{xt} t^{a-1} (1 - t)^{c-a-1} \, dt \tag{20}$$

From all these considerations we finally obtain

$$S_\rho = 5 \ln 2 + \ln \pi + 6 - \frac{1}{e^2}\left[-14\gamma + \frac{79}{3} + \left(\frac{4 \ln 2}{15} - \frac{47}{225}\right) {}_1F_1[3, 6; -2] \right] - \frac{16}{e^2} \sum_n \frac{\Gamma(3+n)}{\Gamma(6+n)} \frac{x^n}{n!} [\psi(6+n) - \psi(6)] \tag{21}$$

where $\psi(x)$ stands for the logarithmic derivative of the gamma function. In writing (21), we have also used

$$\frac{\partial}{\partial c}\, {}_1F_1[a, c; z] = -\sum_{j=1}^{\infty} \frac{(a)_j}{(c)_j} \frac{z^j}{j!} \sum_{n=1}^{j} \frac{1}{c + n - 1} \tag{22}$$

as given by Slater (1960) with $(a)_j$ the Pochchammer symbol.

The momentum-space entropy integral S_γ the present case (10) is given by

$$S_\gamma = -\frac{32^2}{\pi}\left[2\ln\frac{16}{\pi} \int_0^\infty \frac{(1-4k^2)^2}{(1+4k^2)^6} k^2\, dk + \int_0^\infty \frac{(1-4k^2)^2}{(1+4k^2)^6} \ln \frac{(1-4k^2)^2}{(1+4k^2)^6} k^2\, dk \right] \tag{23}$$

As in the treatment of S_ρ, the first integral in (23) is quite simple and can be evaluated analytically. Using (13), the second integral can be written in terms of the hypergeometric ${}_2F_1[\cdot]$ functions. The final expression for S_γ is found to be

$$S_\gamma = 4 \ln 2 + 2 \ln \pi - \frac{59}{10} - \frac{631 \times 32}{315\pi}\, {}_2F_1[6, 3; 11/2; 1/2] - \frac{1}{5\sqrt{2\pi}} \sum_n \frac{\Gamma(3/2+n)\Gamma(-3/2+n)}{\Gamma(-7/2+n)} \frac{x^n}{n!} [\psi(-3/2+n) - \psi(-3/2)] - \frac{3}{160\sqrt{\pi}} \sum_n \frac{\Gamma(6+n)\Gamma(3+n)}{\Gamma(11/2+n)} \frac{x^n}{n!} [\psi(3+n) - \psi(3)] \tag{24}$$

The associated Laguerre polynomials that enter into the hydrogenic wavefunctions can always be written in the form

$$(r-a)(r-b)(r-c)\ldots \tag{25}$$

where *a, b, c*, etc., are the roots of the polynomial. Using the representation

(25), one can follow our prescription for the 2s state to obtain S_ρ and S_γ for any excited state. The same approach can be followed to calculate the entropy for any orthogonal polynomial. In the next section we demonstrate this with reference to the Jacobi polynomial, which has a host of connections with other members of the family.

3. ENTROPY FOR JACOBI POLYNOMIAL

If $q_n(x)$ with $n = 0, 1, 2, \ldots$ are polynomials orthogonal with respect to the weight function $w(x)$ on the interval $[-1, +1]$, the corresponding information entropies are given by (Yáñez *et al.*, 1994)

$$E_n = -\int q_n^2(x) \ln q_n^2(x) w(x)\, dx \tag{26}$$

As already stated, the polynomial of interest is the generalized Jacobi polynomial $P_n^{\alpha,\beta}(x)$. The weight function for $P_n^{\alpha,\beta}(x)$ is

$$w(x) = (1 - x)^\alpha (1 + x)^\beta \tag{27}$$

The series and product representations for the Jacobi polynomial are given by (Abramowitz and Stegun, 1970)

$$P_n^{\alpha,\beta}(x) = 2^{-n} \sum_{m=0}^{n} (-1)^{n-m} C_m (1 - x)^{n-m} (1 + x)^m \tag{28}$$

and

$$P_n^{\alpha,\beta}(x) = k_n \prod_{i=0}^{n} (x - x_i) \tag{29}$$

where x_i stands for the ith root of $P_n^{\alpha,\beta}(x) = 0$. It should be noted that x_i is a real number lying between -1 and $+1$. The quantities C_n and k_n have the values

$$C_n = \binom{n + \alpha}{m} \binom{n + \beta}{n - m} \tag{30}$$

and

$$k_n = 2^{-n} \binom{2n + \alpha + \beta}{n} \tag{31}$$

with $\binom{p}{r}$ the binomial coefficients. The orthonormality relation for the Jacobi polynomial is expressed as

$$\int P_n^{\alpha,\beta}(x)\, P_{n'}^{\alpha,\beta}(x) w(x)\, dx = h_{n'}\delta_{nn'} \tag{32}$$

with

$$h_n = \frac{2^{\alpha+\beta+1}\,\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{n!\,(2n+\alpha+\beta+1)\Gamma(n+\alpha+\beta+1)}, \qquad \text{if} \quad \alpha > -1, \quad \beta > -1 \tag{33}$$

Combining the results (26) and (33), we have

$$E_n = -\left[2h_n \ln k_n + \sum_{i=1}^{n} J_i\right] \tag{34}$$

where

$$J_i = 2^{-2n} \sum_{m=0}^{n} \sum_{m'=0}^{n} (-1)^{m+m'} C_m C_{m'} \times \int_{-1}^{1} (1-x)^{2n+\alpha-m-m'}\,(1+x)^{m+m'+\beta} \ln(x-x_i)^2\, dx \tag{35}$$

To evaluate the integral in (35) analytically, we split it into two parts such that

$$J_i = 2^{1-2n} \sum_{m=0}^{n} \sum_{m'=0}^{n} (-1)^{m+m'}\, C_m\, C_{m'}\, [I_1 + I_2] \tag{36}$$

where

$$I_1 = \lim_{\varepsilon\to 0} \frac{\partial}{\partial\varepsilon} \int_{-1}^{x_i} (1-x)^p (1+x)^q (x_i - x)^\varepsilon\, dx \tag{37}$$

and

$$I_2 = \lim_{\varepsilon\to 0} \frac{\partial}{\partial\varepsilon} \int_{x_i}^{1} (1-x)^p (1+x)^q (x_i - x)^\varepsilon\, dx \tag{38}$$

with $p = 2n + \alpha - m - m'$ and $q = m + m' + \beta$.

Using the transformation $x_i - x = y$ in (37), we write

$$I_1 = \lim_{\varepsilon\to 0} \frac{\partial}{\partial\varepsilon} \int_{0}^{u} (y+v)^p (u-y)^q y^\varepsilon\, dx \tag{39}$$

with $u = 1 + x_i$ and $v = 1 - x_i$. Fortunately, the result of the integral in (39) is given (Gradshteyn and Ryzhik, 1965) in terms of a Gauss hypergeometric function and we have

$$I_1 = \lim_{\varepsilon \to 0} \frac{\partial}{\partial \varepsilon} (1 - x_i)^p (1 + x_i)^q B(q + 1, \varepsilon + 1)$$

$$_2F_1\left[-p, 1 + \varepsilon; 2 + q + \varepsilon; -\frac{1 + x_i}{1 - x_i} \right] \tag{40}$$

In order to make the $_2F_1[\cdot]$ function convergent everywhere, we use the transformation

$$_2F_1 [a, b; c; z] = (1 - z)^{-a} \, _2F_1 [a, c - b; c; z/ (z - 1)] \tag{41}$$

to obtain

$$I_1 = \lim_{\varepsilon \to 0} \frac{\partial}{\partial \varepsilon} [2^p (1 + x_i)^{q+1+\varepsilon} B(q + 1, \varepsilon + 1) \tag{42}$$

$$_2F_1[-p, 1 + q; 2 + q + \varepsilon; (1 + x_i)/2]]$$

in which the argument of the $_2F_1[\cdot]$ function $(1 + x_i)/2$ is always less than 1. The following argument will be useful to perform the derivative in (42):

$$\lim_{\varepsilon \to 0} \frac{\partial}{\partial \varepsilon} (1 + x_i)^{q+1+\varepsilon} = \ln(1 + x_i) \tag{43}$$

$$\lim_{\varepsilon \to 0} \frac{\partial}{\partial \varepsilon} B(q + 1, 1 + \varepsilon) = \frac{1}{q + 1} [\psi(1) - \psi(q + 1)] \tag{44}$$

and

$$\lim_{\varepsilon \to 0} \frac{\partial}{\partial \varepsilon} \, _2F_1 [-p, 1 + q; 2 + q + \varepsilon; (1 + x_i)/2] =$$

$$- \sum_{r=1}^{\infty} \frac{(-p)_r \, (q + 1)_r [(1 + x_i)/2]^r}{r! \, (q + 2)_r} \sum_{s=1}^{r} \frac{1}{q + s + 1} \tag{45}$$

The finite summation over s has resulted from the differentiation of the $_2F_1[\cdot]$ function (Slater, 1960) with respect to ε. The final result for I_1 is obtained in the form

$$I_1 = \frac{2^p (1 + x_i)^{q+1}}{q + 1} \Bigg((\ln(1 + x_i) + \psi(1) - \psi(q + 2))$$

$$\times \, _2F_1[-p, 1 + q; 2 + q + \varepsilon(1 + x_i)/2]$$

$$- \sum_{r=1}^{\infty} \frac{(-p)_r (q+1)_r [(1+x_i)/2]^r}{r!\ (q+2)_r} \sum_{s=1}^{r} \frac{1}{q+s+1} \Bigg) \tag{46}$$

A similar result for I_2 can be constructed which is the same as the expression (46) with p and q interchanged and x_i replaced by $-x_i$.

4. EFFECT OF CORRELATION ON THE INFORMATION ENTROPY

The Yukawa potential is often used as a model for screened and cutoff Coulomb interactions. But the eigenvalue for this interaction cannot be solved analytically. We have therefore chosen to work with the two-parameter (V_0, a) Hulthén potential given by (Hulthén, 1942)

$$V(r) = -V_0 \frac{e^{-r/a}}{1 - e^{-r/a}} \qquad \text{where} \quad V_0 a > 0 \tag{47}$$

This potential behaves like a Coulomb potential $V_c = -V_0 a/r$ at small values of r, whereas for large values of r it decreases exponentially so that its capacity for bound states is smaller than that of V_c. Alternatively, (47) will exhibit the same behavior as $a \rightarrow \infty$. If we work in atomic units, the correct Coulomb limit will be obtained as $a \rightarrow \infty$ and $V_0 a \rightarrow 1$. Regarding a as a screening parameter, the Hulthén potential has been widely used as a judicious model for the screened interaction. The Schrodinger equation for (47) is partially solvable in that it can be solved in terms of Gauss hypergeometric function for the s wave only (Flugge, 1974). Laha *et al.* (1988), studied the Hamiltonian hierarchy problem for the potential in (47) in the context of supersymmetric quantum mechanics (Witten, 1981) and found that the associated 'supersymmetric partners' belong to the Eckart class of potentials. Interestingly, the partner potentials could simulate the effect of the centrifugal barrier fairly accurately at least for a few lower partial waves. In the following we make use of wavefunctions given in Flugge (1974) and Laha *et al.* (1988) to study the effect of screening on the position and momentum information entropies.

The normalized ground-state (1s) coordinate-space wavefunction for the Hulthén potential can be written as

$$\Psi_{1s}(\bar{r}) = \frac{1}{\sqrt{\pi}} \left(\frac{\alpha_1}{a} \right)^{3/2} e^{-(\alpha_1/a)r} \tag{48}$$

with

$$\alpha_1 = V_0 a^2 - \tfrac{1}{2} \tag{49}$$

The momentum-space wavefunction corresponding to (48) is given by

$$\bar{\Psi}_{1s}(\bar{p}) = \frac{\alpha_1(2\alpha_1 a)^{3/2}}{\pi(\alpha_1^2 + a^2p^2)^2} \tag{50}$$

From (2), (3), (48), and (50) we get

$$S_\rho^H = 3 + \ln \pi - 3 \ln(\alpha_1/a) \tag{51}$$

and

$$S_\gamma^H = 2 \ln \pi + 5 \ln 2 + 3 \ln(\alpha_1/a) - 10/3 \tag{52}$$

Here we have used the superscript H to indicate that S_ρ and S_γ given in (51) and (52) refer to the Hulthén potential. The same convention will also be used for the Coulomb potential. The results for the Coulomb potential for (51) and (52) are given by

$$S_\rho^C = 3 + \ln \pi \tag{53}$$

and

$$S_\gamma^C = 2 \ln \pi + 5 \ln 2 - 10/3 \tag{54}$$

In the unscreening limit $\alpha_1/a \to 1$, one thus easily recovers the results in (53) and (54) from those in (51) and (52). Further, the equality of $S_\rho^H + S_\gamma^H$ with $S_\rho^C + S_\gamma^C$ implies that the entropy sum is independent of screening although it influences the values of S_ρ and S_γ.

Using the supersymmetry-inspired radial ladder operators, Laha *et al.* (1988) obtained the 2p radial wave function for the Hulthén potential from the exact 2s function given in Flugge (1974). The normalized 2p wavefunction is given by

$$\Psi_{2p}(\bar{r}) = \frac{1}{2^{1/2}}\left[\frac{f(V_0, a)}{a}\right]^{3/2} e^{-(\alpha_2/a)r}(1 - e^{-r/a})\, Y_{1m}(\Omega_r) \tag{55}$$

with

$$\alpha_2 = \frac{V_0 a^2}{2} - 1 \tag{56}$$

$$[f(V_0, a)]^{-3} = (V_0 a^2 - 2)^{-3} - 2\,(V_0 a^2 - 1)^{-3} + (V_0 a^2)^{-3} \tag{57}$$

and $Y_{1m}(\Omega_r)$ a scalar spherical harmonic. The corresponding momentum-space wavefunction is

$$\overline{\Psi}_{2p}(\bar{p}) = -\frac{2ip(2\alpha_2+1)a^4}{\sqrt{\pi}}\left(\frac{f(V_0,a))}{a}\right)^{3/2} \times \frac{(\alpha_2^2+a^2p^2)+[(\alpha_2+1)^2+a^2p^2]}{[(\alpha_2^2+a^2p^2)[(\alpha_2+1)^2+a^2p^2]]^2} Y_{1m}(\Omega_p) \tag{58}$$

From (57) we find

$$\lim_{a\to\infty}[f(V_0,a)]^{-3} = 12(V_0a^2)^{-5} \tag{59}$$

Interestingly, the results in (59) can be used to verify that (56) and (58) give the exact Coulomb functions in the unscreening limit. This serves as a check for the correctness of the results obtained within the framework of supersymmetric quantum mechanics.

From (2) and (56) we can write the $2p$ position-space information entropy as

$$\begin{aligned} S_\rho = &-\frac{1}{2}\left[\frac{f(V_0,a)}{a}\right]^3\left(\left[\ln\left(\frac{1}{2}\left[\frac{f(V_0,a)}{a}\right]^3\right)+I_3\right]\right. \\ &\times\int_0^\infty e^{-(\alpha_2/a)r}(1-e^{-r/a})r^2\,dr - \frac{2\alpha_2}{a} \\ &\times\int_0^\infty e^{-(2\alpha_2/a)r}(1-e^{-r/a})r^2\,dr \\ &\left.+2\int_0^\infty e^{-(\alpha_2/a)r}(1-e^{-r/a})^2\ln(1-e^{-r/a})r^2\,dr\right) \end{aligned} \tag{60}$$

where

$$I_3 = \int |Y_{1m}(\Omega)|^2 \ln|Y_{1m}(\Omega)|^2\,d\Omega \tag{61}$$

The result for I_3 has been given by Yáñez *et al.* (1994). The first and second integrals in (60) are standard and can be obtained as

$$2\left[\frac{a}{f(V_0,a)}\right]^3 \quad \text{and} \quad -\frac{a^3}{Y_0}\frac{\partial}{\partial a}\left[\frac{1}{f(V_0,a)}\right]^3$$

The evaluation of the third integral, however, requires a little care. Denoting it by I_2, we work this out as follows.

Introducing the change of variables $x = e^{-r/a}$, we rewrite I_2 as

$$I_2 = a^3 \lim_{\mu\to 0} \lim_{\varepsilon\to 0} \frac{\partial^2}{\partial\mu^2} \frac{\partial}{\partial\varepsilon} \int_0^1 x^{\delta-1} (1 - x)^{2+\varepsilon} \, dx \tag{62}$$

where $\delta = 2\alpha_2 + \mu$. The definite integral in (62) is the beta function $B(\delta, 3 + \varepsilon)$. Expressing $B(\delta, 3 + \varepsilon)$ in terms of gamma function, we carry out the derivatives and finally take the limits to get

$$\begin{aligned} I_2 = {} & \frac{a^3}{2\alpha_2(\alpha_2 + 1)(2\alpha_2 + 1)} \\ & \times (([\psi^1(2\alpha_2) - \psi^1(2\alpha_2 + 3)] + [\psi(2\alpha_2) - \psi(2\alpha_2 + 3)]^2) \\ & \times [\psi(3) - \psi(2\alpha_2 + 3)] - 2[\psi(2\alpha_2) \\ & - \psi(2\alpha_2 + 3)]\psi^1(2\alpha_2 + 3) - \psi^2(2\alpha_2 + 3)) \end{aligned} \tag{63}$$

where $\psi^n(x) = (d^n/dx^n)\,\psi(x)$. We can thus write

$$\begin{aligned} S_\rho^H = -\left[\frac{f(V_0, a)}{a}\right]^3 & \left(\left[\ln\left(\frac{1}{2}\left[\frac{f(V_0, a)}{a}\right]^3\right) + I_3\right]\left[\frac{a}{f(V_0, a)}\right]^3 \right. \\ & \left. + \frac{\alpha a^2}{V_0}\frac{\partial}{\partial a}\left[\frac{1}{f(V_0, a)}\right]^3 + I_2\right) \end{aligned} \tag{64}$$

We find

$$\lim_{a\to\infty} \lim_{V_0 a\to 1} S_\rho^H = 3\ln 2 + \ln 3 + 2\gamma + 5/6 - I_3 \tag{65}$$

which is indeed the correct expression for Coulomb $2p$ position-space information entropy.

From (3) and (58) the momentum-space entropy corresponding to (64) is obtained as

$$\begin{aligned} S_\gamma^H = -C & \left((\ln C + I_3) \int_0^\infty \frac{(g + 2a^2p^2)^2 p^4 \, dp}{(\alpha_2^2 + a^2p^2)^4\,[(\alpha_2 + 1)^2 + a^2p^2]^4} \right. \\ & + 2\int_0^\infty \frac{(g + 2a^2p^2)^2 p^4 \ln(g + 2a^2p^2)\, dp}{(\alpha_2^2 + a^2p^2)^4\,[(\alpha_2 + 1)^2 + a^2p^2]^4} \\ & - 4\int_0^\infty \frac{(g + 2a^2p^2)^2 p^4 \ln[(\alpha_2 + 1)^2 + a^2p^2]\, dp}{(\alpha_2^2 + a^2p^2)^4\,[(\alpha_2 + 1)^2 + a^2p^2]^4} \\ & \left. - 4\int_0^\infty \frac{(g + 2a^2p^2)^2 p^4 \ln(\alpha_2^2 + a^2p^2)\, dp}{(\alpha_2^2 + a^2p^2)^4\,[(\alpha_2 + 1)^2 + a^2p^2]^4} \right. \end{aligned} \tag{66}$$

$$+ 2\int_0^\infty \frac{(g + 2a^2p^2)^2p^4 \ln p dp}{(\alpha_2^2 + a^2p^2)^4 [(\alpha_2 + 1)^2 + a^2p^2]^4}\Bigg)$$

with

$$C = \frac{4a^8}{\pi}(2\alpha_2 + 1)^2 \left[\frac{f(V_0, a)}{a}\right]^3 \tag{67}$$

and $g = \alpha_2^2 + (\alpha_2 + 1)^2$. The integrals in (66) can be evaluated by the appropriate use of results given in Gradshteyn and Ryzhik (1965). Hence we can write

$$\lim_{a\to\infty} \lim_{V_0 a\to 1} S_\gamma^H = \ln \pi + \ln 3 - 43/10 - I_3 \tag{68}$$

Yáñez *et al.* (1994) analytically calculated the results for the position and momentum information entropies of the hydrogen atom in D spatial dimensions and used them to analyze the decrement or increment of S_ρ and S_γ as the information increases or decreases. Here we have dealt with a screened Coulomb potential and found that the information sum is independent of the screening parameter. On very general grounds one knows that in a screened hydrogenic system an electron experiences a more repulsive environment than in a pure Coulomb field. A screened Coulomb wavefunction is thus likely to be pushed apart leading to a relatively diffused probability density in position space. Consequently, S_ρ^H should be greater than S_ρ^C. Our result in (51) clearly indicates this since for all real situations $\alpha_1/a < 1$. Understandably, the opposite will happen for S_γ^H. After some algebraic simplification the same can be demonstrated for (64).

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