

## INFORMATION ENTROPIES IN QUANTUM CHEMISTRY

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### ABSTRACT

The development of information theory and entropy has been traced from the time of Boltzmann to the present. Various forms of the information entropy functional have been scrutinized and the maximum entropy principle of Jaynes has been discussed. The problem of reconstructing probability distributions using moments of various orders has been examined in the light of the works of Dowson, Wragg and Einbu. A practical reconstruction of electron momentum densities by employing the first- and second moment constraints by Sears, Gadre and Koga has also been presented. Various aspects of information entropy encompassing kinetic energy functional, reaction dynamics, Loges, surprisal analysis have been discussed. The outstanding contribution of Bialynicki-Birula and Mycielski, giving the entropy sum in dual spaces the meaning of an uncertainty relation, has also been presented. The problem of characterizing the quality of atomic and molecular wavefunctions has been considered in the light of information entropies. A new entropy maximization principle for  $S_\rho + S_\gamma$  has been postulated and some of its applications in judging wavefunction quality and refinement of density distributions have also been presented in detail.

### HISTORICAL PREVIEW<sup>1</sup>

ACCORDING to the first and second laws of thermodynamics, entropy is a state function of a system. This function was used to identify a vanishing path integral in the theory of generalised Carnot cycles,

$$dq/T > 0 \quad (1)$$

where

$$dS = dq/T, \quad (2)$$

$S$  is the entropy;  $dq$  is a differential of heat; and  $T$ , the temperature. Equation (1) is also a statement of the second law of thermodynamics. The next major advance in the development in the concept of entropy was due to Boltzmann, through his famous measure of statistical entropy,

$$S = k \ln W, \quad (3)$$

where  $k$  is Boltzmann's constant. For the case where all the energy levels are nondegenerate,

$S = -k N \sum_i p_i \ln p_i$  where  $p_i = N_i/N$ , the frequency of finding a particle in the  $i$ th energy level. Later Gibbs introduced the idea of an

ensemble of systems, leading to an expression identical to that of Boltzmann,

$$S = - \sum_i p_i \ln p_i \quad (4)$$

however Boltzmann's  $p_i$ s are single particle probabilities. These statistical concepts of entropy were utilized by Shannon<sup>2</sup> in laying the foundation of information theory. Following Gibbs and preceding Shannon, several important advances in the development of the statistical entropy concept were made. Fischer<sup>3</sup> introduced a new measure of information in the context of statistical estimation theory. The pioneering work in information theory was carried out by Shannon, who in 1948, proved the basic theorems of this new field of statistical mathematics. Shannon's accomplishments lay in the revelation of the universality of the entropy functional (4),

$-\sum_i p_i \ln p_i$ , which may be said to represent the entropy of any probability distribution. It was this realization that prompted Jaynes<sup>4, 5</sup> to postulate his principle of entropy maximization.

### SHANNON'S INFORMATION ENTROPY FUNCTIONAL

Shannon's solution to the problem of obtaining a quantitative measure of uncertainty or entropy is axiomatic. For a statement of Shannon's axioms we will adopt the following notations and conditions:

(1)  $S(p)$  is the average uncertainty of the probability distribution,

$p = (p_1, p_2, \dots)$ , corresponding to the  $N$  element event space  $X = (x_1, x_2, \dots)$ .

$$(2) p_i \geq 0 \text{ for all } i \text{ and } \sum_i p_i = 1 \quad (5)$$

Shannon's entropy has been characterized by different axioms by various workers in the field. We state these axioms below:

(1) *Continuity*:  $S(p)$  is a continuous function of  $p$ .

(2) For a uniform probability distribution with  $N$  outcomes,  $S(p)$  is a monotonically increasing function of  $N$ , the number of outcomes *i.e.*

$$S(1/N \dots 1/N) > S(1/(N+1), \dots 1/(N+1)). \quad (6)$$

(3) *Recursivity*: If a choice can be broken down into two successive choices then the original entropy should be the weighted sum of the individual entropies

$$S(p_1 \dots p_{m-1}, p_m q_1 \dots p_m q_{n-m+1}) = S(p_1 \dots p_m) + p_m \cdot S(q_1 \dots q_{n-m+1}) \quad (7)$$

where

$$\sum_i^m p_i = 1 \text{ and } \sum_i^{n-m+1} q_i = 1. \quad (8)$$

(4) *Normalization*:  $S(0.5, 0.5) = 1$

(5)  $S(p) = \hat{A} S(p)$ , where  $\hat{A}$  is a permutation operator which arbitrarily scrambles the order of the probabilities. This symmetry axiom states that the uncertainty does not depend on the order in which the outcomes are presented.

The only functional form obeying the above axioms is

$$S = -k \sum_i p_i \ln p_i \quad (9)$$

The five properties above uniquely characterise the uncertainty measure in (10). Various other

characterisation measures lead to the same logarithmic measure in (9).

Generalization of the above discussion of discrete probability distributions to continuous ones has caused difficulty. The problem arose due to the deceptively simple assumption by Shannon<sup>2</sup>,

$$-\sum_i p_i \ln p_i \rightarrow -\int p(x) \ln p(x) dx, \quad (10)$$

for the transition from the discrete to continuous probabilities.

It was noticed that the form of continuous probability distribution is not invariant to a transformation of variable, *i.e.* the numerical value of entropy depends upon the co-ordinate system used. The lack of invariance is easily demonstrated:

If  $y = g(x)$ , where  $x$  is the variable, then the transformation of probability density is

$$q(y) = p(x) (dg/dx)^{-1} = p[g^{-1}(y)] J(x/y) \quad (11)$$

where  $g(y) = x$  is the unique inverse relation between  $x$  and  $y$  and  $J(x/y)$  is the Jacobian. Thus,

$$S[q(y)] = -\int p(x) \ln [p(x) J(x/y)] dx \quad (12)$$

$$= S[p(x)] - \int p(x) \ln [J(x/y)] dx \quad (13)$$

the last integral in (13) is generally non-zero, thus  $S[q(y)]$  differs from  $S[p(x)]$ . This invariance problem was addressed by Jaynes<sup>7</sup> who introduced a measure function,  $m(x)$  such that

$$S[p(x)] = -\int p(x) \ln [p(x)/m(x)] dx \quad (14)$$

and since  $p(x)$  and  $m(x)$  transform in the same way, the Jacobian term vanishes in (13). This is justified in being a necessary step in the proper description of continuous entropy;  $m(x)$  and  $x$  are related in the sense that if  $x$  is the natural variable then  $m(x)$  is simply a unit bearing constant.

### MAXIMUM ENTROPY PRINCIPLE

Jaynes' maximum entropy principle (MEP) may be paraphrased well in the words of Hobson<sup>6</sup>.

Given data  $D = (d_1, d_2, \dots)$  for a certain experiment, the probability distribution  $p$

$= (p_1, p_2, \dots)$ , which describes  $D$  must maximize the entropy expression  $S = -\sum p_i \ln p_i$ , with respect to all  $p$  satisfying  $D$ . If there are more than one probability distribution satisfying the constraints imposed by the data, then the single probability distribution having the greatest value of  $S$  will be the 'proper' one to select. Thus the mathematical description of information is inextricably connected with missing information, therefore uncertainty and entropy.

The MEP of Jaynes<sup>7</sup> has been used in literature for reconstruction of a probability distribution with the knowledge of some of its moments. Dowson and Wragg<sup>8</sup> investigated this MEP for approximating an absolutely continuous one-dimensional distribution with the knowledge of the first and second moments. Their investigation reveals the form for the density function of a distribution to be:

$$p(x) = \exp\left(-\sum_{r=0}^m \lambda_r x^r\right), \quad (15)$$

where  $\lambda_r, r = 0, 1, \dots, m$  are chosen to satisfy moment constraints of the form:

$$\mu_n = \int_a^b x^n \exp\left(-\sum_{r=0}^m \lambda_r x^r\right) dx; n = 0, 1, \dots, m, \quad (16)$$

with  $\mu_0 = 1$ . The validity of this result has been exhaustively dealt with and the existence of a solution to the above equation is considered for cases of  $p$ . Further they have proved that a unique solution to this equation exists for the case  $m = 2$  only the relation

$$\mu_2 \leq 2 \cdot \mu_1^2. \quad (17)$$

For a range  $[0, \infty)$  and no solution can exist for the case where

$$\mu_2 > 2 \cdot \mu_1^2. \quad (18)$$

Another interesting aspect studied is the limiting behaviour of maximum entropy distributions on  $[0, R]$  as  $R \rightarrow \infty$ , where they have shown that these distributions do not converge to a limiting distribution, which however is not a maximum

entropy distribution because convergence of the moments breaks down.

This work has been further extended by Einbu<sup>9</sup> to problems having more than two moment constraints. Also lower bounds for even order moments have been proven as a theorem:

If

$$\exp\left(-\sum_{j=1}^{N-1} x^j \lambda_j\right), \text{ with } N = 2i,$$

is the maximum-entropy distribution for the moments  $\mu_0, \dots, \mu_{N-1}$ , then maximum entropy-distributions exist for the moments  $\mu_0, \dots, \mu_N$  only if  $\mu_N = \mu_{2i} > \mu_{2i, \min}$ , where  $\mu_{2i, \min}$  is defined by

$$\mu_{2i, \min} = - \left| \begin{array}{c|c} 1 \ \mu_1 \ \dots \ \mu_i & 1 \ \mu_1 \ \dots \ \mu_{i-1} \\ \mu_1 \ \mu_2 \ \dots & \mu_1 \ \mu_2 \ \dots \\ \vdots & \vdots \\ \mu_i \ \dots \ 0 & \mu_{i-1} \ \dots \ \mu_{2(i-1)} \end{array} \right|^{-1} \quad (19)$$

The uniqueness of the solution of the moment problem has also been discussed in detail where they have proved that if a maximum entropy distribution exists for a given moment vector, then that distribution is unique.

An important aspect of the generalization of Shannon's entropy which, in the continuous case is invariant to co-ordinate transformation, is the discrimination information or Kullback-Liebler information<sup>10</sup>, defined as:

$$S[p_1/p_0] = -\sum p_{1i} \ln p_{1i}/p_0 \quad (20)$$

and in the continuous case as:

$$S[p_1/p_0] = -\int p_1(x) \ln [p_1(x)/p_0(x)] dx \quad (21)$$

where  $p_1(x)$  and  $p_0(x)$  are normalised probability density functions in the continuous case. Kullback has described  $S[p_1/p_0]$  as the mean information per observation for discrimination of  $p_1(x)$  over  $p_0(x)$  and is known as cross entropy. From an application point of view an important consideration is the minimum entropy deficiency, which states that given the expectation values of several operators  $F_i(x)$  and the

information:

$$\int p(x) F_i(x) dx = \langle F_i(x) \rangle \quad (i = 1, \dots, n) \quad (22)$$

and

$$\int p(x) dx = 1. \quad (23)$$

From an experiment, then the assimilation of this information in an unbiased manner is possible by Jaynes' principle of entropy maximization or the minimum entropy deficiency, subject to the given constraints:

$$\delta \left\{ \int p(x) \ln [p(x)/p_0(x)] + \sum_{i=1}^N \lambda_i \langle F_i(x) \rangle \right\} = 0, \quad (24)$$

where  $\lambda_i$  are the Lagrange multipliers. The solution is

$$p(x) = p_0(x) \exp \left[ -\lambda_0 - \sum_{i=1}^N \lambda_i F_i(x) \right] \quad (25)$$

thus

$$S[p/p_0] = -\lambda_0 - \sum_{i=1}^N \lambda_i \langle F_i(x) \rangle \quad (26)$$

and the 'surprisal' of the distribution is given by

$$I(p/p_0) = \sum_{i=1}^N \lambda_i F_i(x) \quad (27)$$

An important observation here is that the surprisal (27) immediately identifies the constraints used in minimum entropy deficiency procedure, the implication being that one can determine the operators important in reconstructing the distribution, by inspection of a surprisal plot. With this introduction to information theory entropy and its properties we shall now survey some of its applications to chemical physics.

#### APPLICATIONS OF INFORMATION ENTROPIES IN CHEMICAL PHYSICS

One of the applications has been to the problems of chemical kinetics. Levine and Bernstein<sup>11</sup> pioneered the application of information theory using surprisal analysis. Here information theory approach has been used to

describe non-equilibrium situations. As an example consider a diatomic reactive collision:



The products vibrational state distribution  $p(v, t)$  (where  $v$  is the vibrational quantum number and  $t$  the time), is of interest and is experimentally monitored. The tool for analysis here is the surprisal:

$$I(v, t) = -\ln [p(v, t)/p_0(v)], \quad (29)$$

the reference distribution is often taken to be the equilibrium distribution *i.e.*  $p(v, t = \infty)$ . Thus surprisal analysis offers a clear compact representation of non-equilibrium distributions. The time evolution of  $p(v, t)$  is also attractively depicted as a function of the number of constraints active during the relaxation process.

An interesting concept using information entropy ideas is that of 'loge'. Daudel and co-workers<sup>12</sup> introduced this concept to quantum chemistry. A loge is a region of space in an atomic or molecular system in which there is a high probability of finding a given number of electrons.

The probability of finding  $n$  and only  $n$  electrons in a region of space  $\Omega$ , is given by

$$p_n = \binom{N}{n} \int_{\Omega} dr_1 \dots \int_{\Omega} dr_n \int_{R^3-\Omega} | \psi(r_1 \dots r_N) |^2 dr_{n+1} \dots dr_N \quad (30)$$

'Events' are defined as assignments of a given number of electrons to the loges of a system. Originally the 'best' loges of a given system were identified by considering one of the events and allowing the other loges to relax until the probability of that particular partition is maximum. In systems where more than one event is equally probable the problem becomes severe. To overcome this Aslangul<sup>13</sup> suggested the use of Shannon's missing information measure

$$S(p) = - \sum_{i=1}^m p_i \ln p_i, \quad (31)$$

where  $m$  is the number of events as a means of accounting for all the events in a particular loge

partitioning. The best loge partitioning is defined as that division of physical space which gives the lowest value to the missing information functional.

In recent years, the increasing use of density matrices and density functional theories of electronic structure, has focussed attention on the electron density function and the one-matrix. Information theory provides particularly useful tools for the analysis of these functions. We present below some of these features.

The electron density is defined in the atomic or molecular case as:

$$\rho_{(1)} = N \int \psi^*(1, \dots, N) \psi(1, \dots, N) dr_2 \dots dr_N, \quad (32)$$

where  $\psi(1, \dots, N)$  is a many-particle wavefunction. The surprisal in this case is defined as

$$I[\rho/\rho_0] = -\ln[\rho/\rho_0], \quad (33)$$

where  $\rho_0$  is the arbitrary prior density. For the case where  $\rho_0 = 1$  for a reference density the surprisal becomes

$$I[\rho/1] = -\ln \rho. \quad (34)$$

Wang and Parr<sup>14</sup> also carried out computations on HF densities, plotting surprisal in  $r$  over the core and valence regions, suggesting a double exponential model for second row atoms and also revealing the constraints necessary for a surprisal synthesis construction of density. This also reveals that a great deal of electronic information is contained in the first moment of the distribution.

Gadre and Sears<sup>15</sup> and Sears and Gadre<sup>16</sup> employed the information theoretic technique of entropy maximization to Compton profile (CP) data, employing single and double distribution moments as constraints. The CP's reconstructed by employing  $\langle p \rangle$  as well as  $\langle p^2 \rangle$  constraints agree fairly well with their theoretical counterparts. Koga<sup>17</sup> extended this analysis to the case of molecular hydrogen at various internuclear distances. Sears *et al*<sup>18</sup> examined the connection between the kinetic energy functional and information measures like Shannon entropy, Fischer's

information and locality information matrix, and Kullback and Leibler's information measure.

#### UNCERTAINTY RELATIONS FOR INFORMATION ENTROPY

Bialynicki-Birula and Mycielski<sup>19</sup> presented new uncertainty relations in quantum mechanics using canonically conjugate variables in terms of corresponding information entropies. The new uncertainty relation has the form:

$$-\langle \ln |\psi(\mathbf{r})|^2 \rangle - \langle \ln |\phi(\mathbf{p})|^2 \rangle \geq n(1 + \ln \pi), \quad (36)$$

where  $|\psi(\mathbf{r})|^2$  and  $|\phi(\mathbf{p})|^2$  are probability densities in  $n$ -dimensional position and momentum space, noting that the wavefunctions generating these distribution are related by a Fourier transform relationship. The two terms appearing on the left side of the above inequality represent information entropies. Each entropy taken separately decreases without bound when the corresponding probability density becomes more concentrated, *i.e.* information increases. The boundedness from below of the sum of two entropies means that the total uncertainty in positions and momenta cannot be decreased beyond the value given in the inequality above. On further reduction, the above bound reduces to

$$S_\rho + S_\gamma \geq 3N(1 + \ln \pi) - 2N \ln N. \quad (37)$$

Gadre<sup>20</sup> has tested this interesting new uncertainty relation by Bialynicki-Birula and Mycielski<sup>19</sup> within the Thomas-Fermi framework and has obtained the following expressions for Shannon entropies:  $S_\rho = N(5.59 - 2 \ln N)$ ;  $S_\gamma = N(1.06 + \ln N)$  and  $S_\rho + S_\gamma = N(6.65 - \ln N)$ . He further conjectured that for atoms in their ground states, the entropies can be fairly well-represented by the form

$$S = aN + bN \ln N, \quad (38)$$

where  $a$  and  $b$  are more or less universal constants. The NHF entropies fitted to this form<sup>21</sup> are given by:  $S_\rho + S_\gamma = N(6.257 - 0.933 \ln N)$ ;  $S_\rho = N(4.171 - 1.715 \ln N)$  and  $S_\gamma = N(2.086 + 0.784 \ln N)$ .

## RECENT WORKS INVOLVING INFORMATION ENTROPIES IN DUAL SPACES

A detailed study of the application of the bound due to Bialynicki-Birula and Mycielski has been carried out by the authors several interesting results from which are presented below.

Some model systems such as the harmonic oscillator were examined<sup>21</sup>. The Shannon entropies and their sum for the harmonic oscillator increases with increasing quantum number  $n$ . For the hydrogen atom, the co-ordinate space information entropy  $S_\rho$  is a minimum for the ground state and increases monotonically with the excited state energies, whereas the momentum space entropy  $S_\gamma$  decreases monotonically. Investigations on  $S_\rho$  and  $S_\gamma$  for atoms helium through xenon in their ground states were also carried out and are presented pictorially in figure 1. The general trends show that  $S_\rho$  decreases and  $S_\gamma$  increases with increasing  $Z$ . Notable exceptions occur around fully-filled shells such as neon. A further application is the use of the entropy sum  $S_\rho + S_\gamma$  as a measure of

wavefunction quality. For this purpose wavefunctions of single-zeta (sz), double zeta (dz) and near Hartree-Fock (NHF) quality were employed. Atomic information entropies for some randomly selected atoms are presented in table 1. In particular  $S_\rho + S_\gamma$  increases with increasing quality wavefunction (ones that give better atomic properties). Another point in favour of the entropy sum  $S_\rho + S_\gamma$  is its scale invariance, which cannot be said about its components  $S_\rho$  and  $S_\gamma$  individually.

Maroulis *et al*<sup>22</sup> investigated the use of information theory for molecular properties and basis set quality. Here they have used information content with respect to various properties of a system. They have also formulated a procedure for construction of basis sets using information content. Simas *et al*<sup>23</sup> computed basis set quality for the helium atom using the procedure by Maroulis *et al*. This approach, however, demands the knowledge of exact expectation values, which are not easily obtainable for larger atoms.

Gadre and Bendale<sup>24</sup> have also studied the problem of wavefunction quality for the case of helium atom using Shannon information entropies  $S_\rho$ ,  $S_\gamma$  and their sum  $S_\rho + S_\gamma$ . The wavefunctions studied ranged from sz to NHF and ci quality, such as the ones by Taylor-Parr. The investigation revealed that the quantities  $S_\rho$  and  $S_\rho + S_\gamma$  increase monotonically with increasing kinetic energy. The quantity  $S_\gamma$  however steadily decreases. Gadre and Bendale<sup>25</sup> extended the MEP of Jaynes to the case involving constraints in complementary spaces. Conventionally, MEP is applied for the case of constructing the probability density in one space alone (subject to whatever is known). However, while applying the procedure to atomic systems, one should not ignore the deep-rooted physical reality, *viz* the Fourier transform (FT) relationship between the  $r$ - and  $p$ -spaces leading to complementary nature of the respective electron densities. Thus an enhancement in the information entropy in one space alone does not assure a gain in the combined information entropy,  $S_\rho + S_\gamma$ . Thus MEP has to be modified when combined sets of constraints,  $\{S_\rho\}$  and  $\{S_\gamma\}$  are available in  $r$ - and  $p$ -spaces respectively. The modified MEP (MMEP)

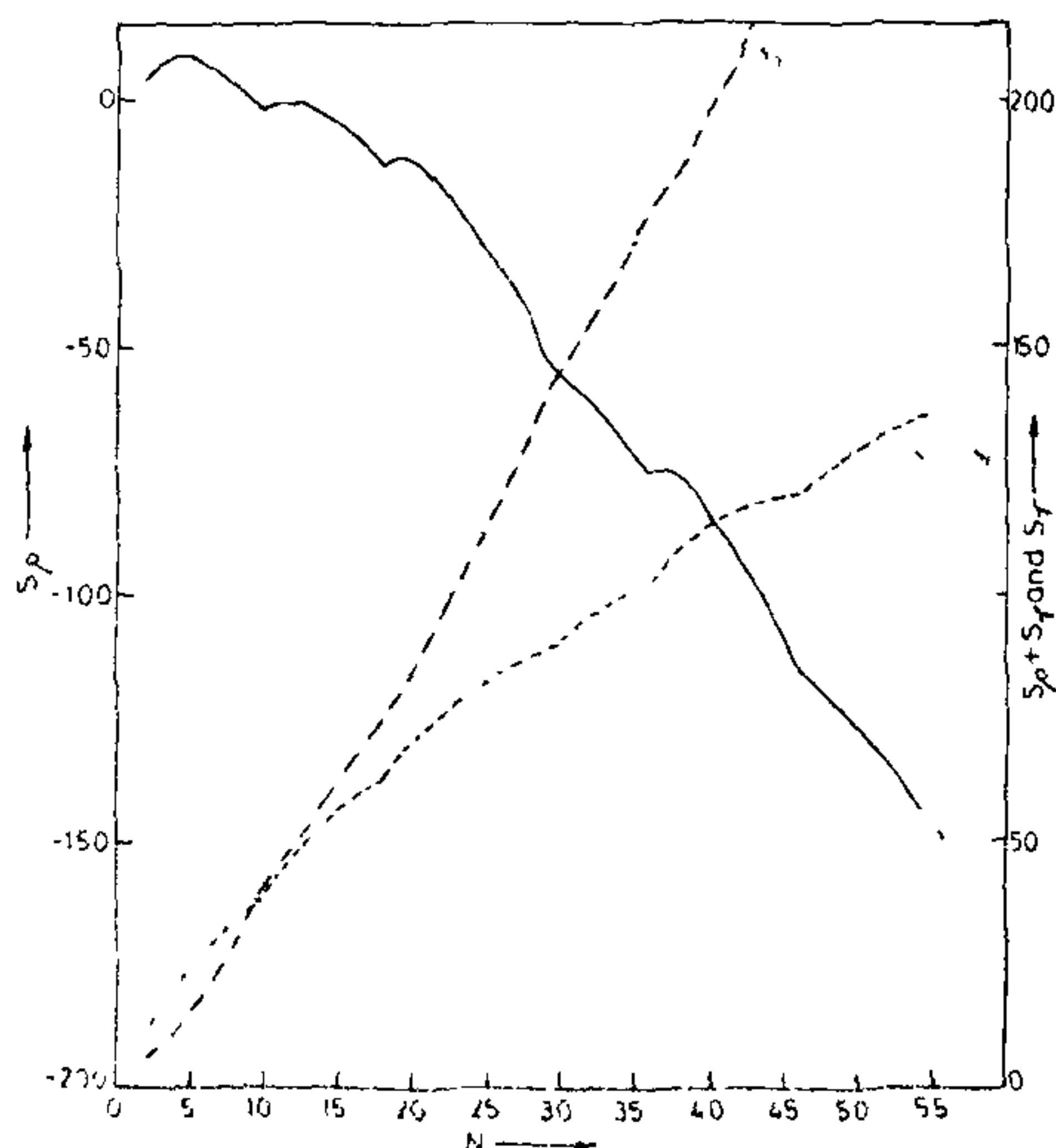


Figure 1. A plot of near-Hartree-Fock information entropies for neutral atoms with  $2 \leq N \leq 54$

**Table 1** Shannon entropies\*,  $S_\rho$ ,  $S_\gamma$  and their sum  $S_\rho + S_\gamma$  for some representative neutral atoms in their ground states computed from Near Hartree-Fock quality wavefunctions

Atom	NHF			DZ			SZ		
	$S_\rho$	$S_\gamma$	$S_\rho + S_\gamma$	$S_\rho$	$S_\gamma$	$S_\rho + S_\gamma$	$S_\rho$	$S_\gamma$	$S_\rho + S_\gamma$
Be	8.95	11.22	20.17	8.95	11.21	20.15	8.89	11.24	20.13
Ne	-2.47	41.35	38.87	-2.62	41.38	38.75	-4.67	42.43	37.76
P	-5.24	62.11	56.87	-5.59	62.11	56.86	-6.61	63.09	56.47
Zn	-55.35	146.3	90.98	-55.74	146.3	90.60	-60.15	148.4	88.26
Xe	-143.3	279.2	136.0	-143.3	279.2	135.9	-146.4	281.5	135.2

\* All values in a.u. Evaluated from near Hartree-Fock (NHF), double-zeta (DZ) and single-zeta (SZ) wavefunctions of E. Clementi and C. Roetti, *At. Data Nucl. Data Tables* 28 (1974) 477.

that emerges from these considerations may be stated as follows. The probability densities  $\rho(r)$  and  $\gamma(p)$  (which are connected through FT of the corresponding wavefunctions) and are subject to  $\{D_\rho\}$  and  $\{D_\gamma\}$  must maximize the sum  $S_\rho + S_\gamma$ . It is interesting to note<sup>25</sup> that the scaling of wavefunction in the  $r$ -space by a factor  $k$  leads to scaled entropies:  $S_{\rho_k} = S_\rho - 3N \ln k$  and  $S_{\gamma_k} = S_\gamma + 3N \ln k$ . Thus the sum of the entropies  $S_\rho + S_\gamma$  can be seen to be invariant to scaling.

The above considerations enable one to synthesize  $\rho(r)$  and  $\gamma(p)$  by considering the composite entropy maximization procedure. This synthesis may be effected by a suitable choice of variational forms for  $\psi(r_1 \dots r_N)$  incorporating various parameters and obtaining its FT,  $\phi(p_1 \dots p_N)$ , then computing and maximizing  $S_\rho + S_\gamma$ . The variational forms can be forced to show the proper asymptotic behaviour,<sup>26</sup> viz  $r^l \exp(-2\sqrt{2I}r)$  and  $p^{-8}$  where<sup>27</sup>  $I$  is the first ionization potential. A proper cusp can be forced by imposing Kato's theorem,

$$d\rho/dr|_{r=0} = -2Z\rho(0). \quad (39)$$

Another experimental constraint available in  $p$ -space is the  $\langle p^2 \rangle$  value. Thus it should be interesting to synthesize electron densities in coordinate and momentum spaces using the above mentioned constraints.

A further application by Gadre *et al*<sup>28</sup> is the refinement of a given momentum distribution using novel information theoretic techniques. In a practical implementation of this method, an approximate electron density is obtained from

knowledge of the momentum density only without any a-priori knowledge of the wavefunction itself. By constraining a refined density  $\gamma(p)$  to differ minimally from the original one  $\gamma_0(p)$  one obtains an expression for the momentum density as:

$$\gamma(p) = \gamma_0(p) + \gamma_0^k(p) (\lambda + \mu p^2), \quad (40)$$

where  $k$  is a parameter and  $\lambda$  and  $\mu$  are Lagrange multipliers. Various values of  $k$  were employed and the Shannon entropies evaluated for both coordinate and momentum densities; it turns out that for  $k = 1.25$  the entropy sum  $S_\rho + S_\gamma$  is a maximum. It should be noted that  $k$  cannot be less than 1.25 to ensure the  $p^{-8}$  asymptotic decay. The Compton profile generated with  $k = 1.25$  compares remarkably well with the experimental one. Thus it is clearly demonstrated that in MEP the key quantity for atomic and molecular systems is the net information content  $S_\rho + S_\gamma$  and not the individual entropies themselves.

Recently, significant advances have been made in the density-based approaches<sup>29</sup> to atoms and molecules. It may thus be hoped that the newer developments in information entropies would open many new avenues for synthesis and analysis of atomic and molecular electron densities.

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## ANNOUNCEMENT

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### AKHIL BHARTIYA JEEVRAKSHA VISHNOI SABHA, JODHPUR (India)

The Sabha is actively engaged in creating public awareness in environmental issues facing the country. The Sabha is planning to organise a national level competition in September 1986, wherein certificates and cash prizes will be awarded to those who have done commendable work in areas of wildlife protection, plantation, development of habitats and such

associated fields.

Nominations for the awards are invited before **15th November 1985**.

Further particulars may be had from Shri Purkha Ram Vishnoi, Secretary, Akhil Bhartiya Jeevraksha Vishnoi Sabha, 1 Cha 6, Madhuban Nagar, Basani Housing Board, Jodhpur 342 005.