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BRIEF COMMUNICATION

Complex entropy and resultant information measures

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Abstract Classical and nonclassical contributions to Author's resultant Shannon- and Fisher-type measures of the information content in general electronic state $\varphi(\boldsymbol{r}) = R(\boldsymbol{r})\exp[\mathrm{i}\phi(\boldsymbol{r})]$, due to the state probability density $p(\boldsymbol{r}) = R(\boldsymbol{r})^2$ and its phase $\phi(\boldsymbol{r})$ or current $\boldsymbol{j}(\boldsymbol{r}) = (\hbar/m)p(\boldsymbol{r})\nabla\phi(\boldsymbol{r})$ distributions, respectively, are reexamined. The components of the overall entropy,

$$S[\varphi] \equiv -\int p(\boldsymbol{r})[\ln p(\boldsymbol{r}) + 2\phi(\boldsymbol{r})]\, d\boldsymbol{r} \equiv S[p] + S[\phi],$$

are shown to determine the real and imaginary parts of the state *complex* Shannon entropy,

$$H[\varphi] \equiv -2\,\langle\varphi|\ln\varphi|\varphi\rangle = S\,[p] + \mathrm{i}S[\phi],$$

a natural quantum-amplitude generalization of the classical Shannon entropy. Its contributions are related to the associated terms in the state resultant Fisher information,

$$I[\varphi] \equiv -4\langle\varphi|\nabla^2|\varphi\rangle \equiv \int p(\boldsymbol{r})\{[\nabla\ln p(\boldsymbol{r})]^2 + [2\nabla\phi\,(\boldsymbol{r})]^2\}\, d\boldsymbol{r} \equiv I[p] + I[\phi]$$
$$= I[p] + \int p(\boldsymbol{r})[(2m/\hbar)\boldsymbol{j}(\boldsymbol{r})/p(\boldsymbol{r})]^2\, d\boldsymbol{r} \equiv I[p] + I[\boldsymbol{j}],$$

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and the gradient entropy:

$$\tilde{I}[\varphi] \equiv \langle\varphi|[(\nabla \ln p)^2 + (\mathrm{i}2\nabla\phi)^2]|\varphi\rangle = I[p] - I[\phi] = \tilde{I}[p] + \tilde{I}[\phi].$$

Keywords Complex entropy · Fisher information · Information theory · Nonclassical information · Resultant information measures · Shannon entropy

1 Introduction

The crucial problem in entropic theories of molecular electronic structure is the quantum generalization of the classical entropy/information concepts of Fisher [1] and Shannon [2], appropriate for complex amplitudes (wavefunctions). Both the particle *probability* distribution and its *phase* or *current* densities ultimately contribute to the resultant information descriptors of molecular systems. Such *resultant* measures of the information content in electronic states, combining the classical contributions due to wavefunction modulus and their nonclassical supplements due to state phase, have been recently proposed, e.g., [3–8]. The electron density generates only the *classical* part of the overall information content, while the wavefunction phase or its gradient (probability-current) generate its *nonclassical* complement in the associated *resultant* measure. The quantum extension of the classical Fisher (gradient) information has been proposed using its association with the average kinetic energy of electrons and the corresponding resultant *global* entropy has been subsequently inferred using the relation between densities of the classical Fisher and Shannon measures [3–8]. Although, for simplicity, in what follows we assume the *one*-electron case the modulus (density) and phase (current) aspects of general electronic states can be separated using the Harriman [9], Zumbach and Maschke [10] construction of Slater determinants yielding the specified electron density [4,11].

In the present communication we relate the classical and nonclassical components of such generalized entropy/information descriptors of molecular states to the real and imaginary parts of the *complex entropy* concept, a natural extension of the classical Shannon entropy, provided by the functional of the system complex electronic wavefunction (quantum probability amplitude).

2 Information components

The average Fisher [1] measure of the gradient-information content in the probability density $p(\boldsymbol{r}) = |\varphi(\boldsymbol{r})|^2 = R(\boldsymbol{r})^2$ of the *single*-particle state $|\varphi\rangle$ described by the wavefunction $\varphi(\boldsymbol{r}) = \langle \boldsymbol{r}|\varphi\rangle = R(\boldsymbol{r}) \exp[\mathrm{i}\phi(\boldsymbol{r})]$ is reminiscent of von Weizsäcker's [12] inhomogeneity correction to the kinetic energy functional,

$$\begin{aligned} I[p] &= \int [\nabla p(\boldsymbol{r})]^2/p(\boldsymbol{r})\, d\boldsymbol{r} = \int p(\boldsymbol{r})[\nabla \ln p(\boldsymbol{r})]^2\, d\boldsymbol{r} \equiv \int p(\boldsymbol{r}) I_p(\boldsymbol{r})\, d\boldsymbol{r} \\ &= 4\int [\nabla R(\boldsymbol{r})]^2\, d\boldsymbol{r} \equiv I[R]. \end{aligned} \tag{1}$$

Its amplitude form $I[R]$ reveals that it measures the average length of the *modulus*-gradient. This classical descriptor characterizes an effective compactness ("narrowness") of the particle position distribution. The complementary descriptor of the classical Shannon [2] entropy,

$$S[p] = -\int p(\boldsymbol{r}) \ln p(\boldsymbol{r})\, d\boldsymbol{r} \equiv \int p(\boldsymbol{r}) S_p(\boldsymbol{r})\, d\boldsymbol{r} \equiv -2\int R^2(\boldsymbol{r}) \ln R(\boldsymbol{r})\, d\boldsymbol{r} \equiv S[R], \tag{2}$$

reflects the average indeterminacy ("spread") of this random variable. It provides the amount of information received, when this uncertainty is removed by an appropriate localization experiment: $I^{\mathrm{S}}[p] \equiv S[p]$. The densities-per-electron of these probability/modulus functionals are seen to satisfy the classical (nonlinear) relation

$$I_p(\boldsymbol{r}) = [\nabla S_p(\boldsymbol{r})]^2. \tag{3}$$

The resultant entropy/information descriptors of state $|\varphi\rangle$ combine these familiar classical contributions and the associated nonclassical supplements due to the state spatial phase or probability current [3–8]:

$$\begin{aligned} I[\varphi] &= -4\langle\varphi|\nabla^2|\varphi\rangle \equiv \langle\varphi|\hat{\mathrm{I}}|\varphi\rangle = 4\int |\nabla\varphi(\boldsymbol{r})|^2\, d\boldsymbol{r} \equiv \int p(\boldsymbol{r}) I(\boldsymbol{r})\, d\boldsymbol{r} \\ &= I[p] + 4\int p(\boldsymbol{r})[\nabla\phi(\boldsymbol{r})]^2\, d\boldsymbol{r} \equiv \int p(\boldsymbol{r})[I_p(\boldsymbol{r}) + I_\phi(\boldsymbol{r})]\, d\boldsymbol{r} \equiv I[p] + I[\phi] \\ &= I[p] + \left(\frac{2m}{\hbar}\right)^2 \int \boldsymbol{j}^2(\boldsymbol{r})/p(\boldsymbol{r})\, d\boldsymbol{r} \\ &= \int p(\boldsymbol{r})[I_p(\boldsymbol{r}) + I_j(\boldsymbol{r})]\, d\boldsymbol{r} \equiv I[p] + I[\boldsymbol{j}], \end{aligned} \tag{4}$$

$$\begin{aligned} S[\varphi] &= -\langle\varphi|\ln p + 2\phi|\varphi\rangle \equiv \langle\varphi|\hat{\mathrm{S}}|\varphi\rangle = \int \varphi(\boldsymbol{r})^* \hat{\mathrm{S}}(\boldsymbol{r})\varphi(\boldsymbol{r})\, d\boldsymbol{r} \\ &= \int p(\boldsymbol{r})[S_p(\boldsymbol{r}) - 2\phi(\boldsymbol{r})]\, d\boldsymbol{r} \equiv \int p(\boldsymbol{r})[S_p(\boldsymbol{r}) + S_\phi(\boldsymbol{r})]\, d\boldsymbol{r} \\ &= \int p(\boldsymbol{r}) S(\boldsymbol{r})\, d\boldsymbol{r} \equiv S[p] + S[\phi], \end{aligned} \tag{5}$$

$$\begin{aligned} \tilde{I}[\varphi] &= I[p] - I[\phi] \equiv \tilde{I}[p] + \tilde{I}[\phi] = \int p(\boldsymbol{r}) \left[\tilde{I}_p(\boldsymbol{r}) + \tilde{I}_\phi(\boldsymbol{r})\right] d\boldsymbol{r} \\ &\equiv \int p(\boldsymbol{r}) \tilde{I}(\boldsymbol{r})\, d\boldsymbol{r}. \end{aligned} \tag{6}$$

Above, these information components have been expressed as expectation values of the related real (multiplicative) "operators" in position representation, measuring the resultant densities-per-electron of the gradient information and entropy,

$$I(\boldsymbol{r}) = [\nabla \ln p(\boldsymbol{r})]^2 + 4[\nabla\phi(\boldsymbol{r})]^2 \quad \text{and} \quad \tilde{I}(\boldsymbol{r}) = [\nabla \ln p(\boldsymbol{r})]^2 - 4[\nabla\phi(\boldsymbol{r})]^2,$$

and of the overall entropy:

$$S(\boldsymbol{r}) = -[\ln p(\boldsymbol{r}) + 2\phi(\boldsymbol{r})].$$

The generalized gradient-*information* of Eq. (4), the expectation value of quantum-mechanical operator $\hat{\mathrm{I}} = -4\nabla^2 = (8m/\hbar^2)\hat{\mathrm{T}}$, is proportional to the average kinetic energy $T[\varphi] = \langle\varphi|\hat{\mathrm{T}}|\varphi\rangle$ corresponding to the Hermitian operator $\hat{\mathrm{T}}(\boldsymbol{r}) = -[\hbar^2/(2m)]\Delta$,

$$I[\varphi] = (8m/\hbar^2)T[\varphi], \tag{7}$$

and reflects the state gradient-*deterministic* aspect. The nonclassical densities of the resultant gradient information [Eq. (4)] and global entropy [Eq. (5)], respectively, obey the classical relation of Eq. (3):

$$I_\phi(\boldsymbol{r}) = [\nabla S_\phi(\boldsymbol{r})]^2. \tag{8}$$

One observes, however, that in the resultant gradient-*entropy* [Eq. (6)], which describes the state gradient-*indeterminicity* facet, the nonclassical contribution changes sign, $\tilde{I}[\phi] = -I[\phi]$, so that the nonclassical Shannon and Fisher entropy densities satisfy the modified relation:

$$\tilde{I}_\phi(\boldsymbol{r}) = -[\nabla S_\phi(\boldsymbol{r})]^2. \tag{9}$$

3 Complex entropy concept

Thus, the resultant entropy/information functionals combine the classical and nonclassical contributions, which separately obey the nonlinear relation of Eqs. (3) and (8). However, the nonlinear character of the mutual dependencies between these Shannon and Fisher components precludes this relation to be also satisfied by the resultant densities themselves, unless the two Shannon components are regarded as components of the *vector* entity $\vec{S}(\boldsymbol{r}) \equiv \boldsymbol{e}_p S_p(\boldsymbol{r}) + \boldsymbol{e}_\phi S_\phi(\boldsymbol{r})$, in the geometrical framework of the probability and phase *degrees-of-freedom* then determining the *independent* (orthogonal) directions represented by the *perpendicular* unit vectors $\boldsymbol{e}_p$ and $\boldsymbol{e}_\phi$, $\boldsymbol{e}_p \cdot \boldsymbol{e}_\phi = 0$ [3],

$$I(\boldsymbol{r}) = I_p(\boldsymbol{r}) + I_\phi(\boldsymbol{r}) = [\nabla \cdot \vec{S}(\boldsymbol{r})]^2 = [\nabla S_p(\boldsymbol{r})]^2 + [\nabla S_\phi(\boldsymbol{r})]^2. \tag{10}$$

However, this vector interpretation does not justify the change of sign in Eq. (9). The proper explanation calls for the density of the *complex entropy* concept, defined in an alternative vector framework of the *complex* plane,

$$H(\boldsymbol{r}) = S_p(\boldsymbol{r}) + \mathrm{i}S_\phi(\boldsymbol{r}) \equiv = -[\ln p(\boldsymbol{r}) + 2\mathrm{i}\phi(\boldsymbol{r})], \tag{11}$$

with the Shannon *phase*-entropy component S_ϕ $(\boldsymbol{r})$ being then attributed to the imaginary part. This generalized entropy indeed naturally follows from the classical entity, when one refers to the *multi*-valued logarithmic function of the complex argument $z = |z| \exp(\mathrm{i}\alpha)$,

$$\mathrm{Ln}z = \ln|z| + \mathrm{i}(\alpha + 2\pi k), \quad k = 0, \pm 1, \pm 2, \ldots, \tag{12}$$

or its *single*-valued branch $k = 0$:

$$\ln z = \ln|z| + \mathrm{i}\alpha. \tag{13}$$

Indeed, the resultant entropy of Eq. (5) then reflects the expectation value of the complex (multiplicative) logarithmic operator of Eq. (11) expressed in terms of the electronic state φ itself,

$$\hat{\mathrm{H}}(\boldsymbol{r}) = H(\boldsymbol{r}) = -2\ln\varphi(\boldsymbol{r}) = -[\ln p(\boldsymbol{r}) + 2\mathrm{i}\phi(\boldsymbol{r})] \equiv H_p(\boldsymbol{r}) + H_\phi(\boldsymbol{r}), \tag{14}$$

$$\begin{aligned} H[\varphi] &= \langle\varphi| - 2\ln\varphi|\varphi\rangle \equiv \langle\varphi|\hat{\mathrm{H}}|\varphi\rangle = S[p] + \mathrm{i}S[\phi] \\ &= S[R] + \mathrm{i}S[\phi] \equiv H[p] + H[\phi] \end{aligned} \tag{15}$$

The complex entropy thus provides a natural *complex*-amplitude generalization of the the familiar classical measure of the entropy content in probability distribution. The non-Hermitian entropy operator $\hat{\mathrm{H}} = -2\ln\varphi$ [Eq. (14)] then generates the probability and phase Shannon-type contributions as the real and imaginary parts of the resultant complex entropy.

Thus, the Hermitian operator $\hat{\mathrm{I}} = -4\nabla^2 = (8m/\hbar^2)\hat{\mathrm{T}}$ gives rise to the *real* expectation value of the state resultant *information* content $I[\varphi]$, while the *non*-Hermitian entropy operator $\hat{\mathrm{H}}(\boldsymbol{r}) = -2\ln\varphi(\boldsymbol{r})$ generates the state complex average quantity $H[\varphi]$. The gradient analogs in Eq. (6) then follow from the same type of a mutual relation [Eqs. (3) and (8)] between the information and entropy densities [compare Eq. (9)]:

$$\tilde{I}_p(\boldsymbol{r}) = [\nabla H_p(\boldsymbol{r})]^2 \quad \text{and} \quad \tilde{I}_\phi(\boldsymbol{r}) = [\nabla H_\phi(\boldsymbol{r})]^2 = [\mathrm{i}\nabla S_\phi(\boldsymbol{r})]^2 = -[\nabla S_\phi(\boldsymbol{r})]^2. \tag{16}$$

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