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Entropic descriptors of quantum communications in molecules

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Abstract The *classical* Information Theory (IT) deals with entropic descriptors of the probability distributions and probability-propagation (communication) systems, e.g., the electronic channels in molecules reflecting the information scattering via the system chemical bonds. The *quantum* IT additionally accounts for the *non-classical* (current/phase)-related contributions in the resultant information content of electronic states. The classical and non-classical terms in the quantum Shannon entropy and Fisher information are reexamined. The associated *probability*-propagation and *current*-scattering networks are introduced and their Fisher- and Shannon-type descriptors are identified. The *non-additive* and *additive* information descriptors of the probability channels in both the *Atomic Orbital* and *local* resolution levels are related to the network *conditional-entropy* and *mutual-information*, which represent the IT *covalency* and *ionicity* components in the classical communication theory of the chemical bond. A similar partition identifies the associated bond indices in the molecular current/phase channels. The resultant bond descriptors combining the classical and non-classical terms, due to the probability and current distributions, respectively, are proposed as generalized *communication-noise* (covalency) and *information-flow* (iconicity) concepts in the quantum IT.

Keywords Bond multiplicity descriptors · Communication systems · Local communications · Orbital communications · Probability/current distributions · Quantum information measures

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1 Introduction

Concepts and techniques of *Information Theory* (IT) [1–8] have been widely and successfully applied to explore the molecular electron probabilities and the associated patterns of chemical bonds, e.g., [9–18]. In Schrödinger's quantum mechanics the electronic state is determined by the system wave function, the (complex) amplitude of the particle *probability*-distribution, which ultimately carries the *resultant* information content. Both the electron density or its shape factor, the *probability* distribution determined by the wave-function *modulus*, and the system *current*-distribution, related to the gradient of the wave-function *phase*, ultimately contribute to the quantum information descriptors of molecular states. The former reveals the *classical* information component, while the latter determines its *non-classical* complement in the resultant information measure [9,10,16,17,19]. As shown elsewhere [19–25], these two contributions are vital for determining the so called *vertical* (density-constrained) and *horizontal* (density-unconstrained) equilibria in molecular systems and their constituent fragments.

The *classical* communication systems [3,4,7] reveal the *probability* scattering in information networks, reflected by the conditional probabilities of the "output" events, given the "input" events appropriate for the resolution in question. These molecular channels constitute the basis of the *Communication Theory of the Chemical Bond* (CTCB) [11] and its newest version—the *Orbital Communication Theory* (OCT) [12,13], in which the input probability "signal" is propagated via the system chemical bonds. This approach has established the overall entropic descriptors of the system bond multiplicities ("orders") and their "covalent" (communication-noise) and "ionic" (information-flow) components. It has also identified the novel, intermediate ("bridge") mechanism of the chemical bond formation in molecules [13,26].

In the present analysis we address the natural question about the *non-classical* complements of such *classical* molecular channels, which additionally reflect the *current/phase*-scattering in electronic states. We shall also inquire about the associated bond-multiplicity descriptors, which supplement the corresponding classical IT bond-order measures. They will be expressed in terms of the *additive* and *non-additive* components of the total information contained in the 1-electron density matrix or its orbitally resolved analog—the Charge-and-Bond-Order (CBO) matrix. We begin this analysis with a brief summary of the (phase/current)-related complements of the classical Fisher [1] and Shannon [3] information measures in the resultant quantum measure of the information content in the given electronic state. This outline also presents the relevant *non*-classical supplements of the classical *cross* (relative) *entropy* (information distance) descriptors within both the Fisher and Shannon measures of the information content.

Throughout the article the following tensor notation is used: A denotes a scalar quantity, $\boldsymbol{A}$ stands for the *row* or *column* vector, and $\mathbf{A}$ represents a square or rectangular matrix. The logarithm of the Shannon-type information measure is taken to an arbitrary but fixed base. In keeping with the custom in works on IT the logarithm taken to base 2 corresponds to the information measured in *bits* (binary digits), while selecting $\log = \ln$ expresses the amount of information in *nats* (natural units): 1 nat = 1.44 bits.

2 Entropy/information contributions due to probabilities and currents

Consider the electron density $\rho(\boldsymbol{r}) = Np(\boldsymbol{r})$, or its shape (probability) factor $p(\boldsymbol{r})$, and the current density $\boldsymbol{j}(\boldsymbol{r})$ in the quantum state $\Psi(N)$ of N electrons, defined by the corresponding quantum-mechanical expectation values,

$$\rho(\boldsymbol{r}) = \langle\Psi|\hat{\rho}(\boldsymbol{r})|\,\Psi\rangle \quad \text{and} \quad \boldsymbol{j}(\boldsymbol{r}) = \langle\Psi|\hat{\mathbf{j}}(\boldsymbol{r})|\,\Psi\rangle, \tag{1}$$

of the corresponding observables in the position representation,

$$\begin{aligned}\hat{\rho}(\boldsymbol{r}) &= \sum_{k=1}^{N}\delta(\boldsymbol{r}_k - \boldsymbol{r}) \equiv \sum_{k=1}^{N}\hat{\rho}_k(\boldsymbol{r}) \quad \text{and}\\ \hat{\mathbf{j}}(\boldsymbol{r}) &= \frac{1}{2m}\sum_{k=1}^{N}\left[\delta(\boldsymbol{r}_k - \boldsymbol{r})\hat{\mathbf{p}}_k + \hat{\mathbf{p}}_k\delta(\boldsymbol{r}_k - \boldsymbol{r})\right]\\ &= \frac{\hbar}{2m\mathrm{i}}\sum_{k=1}^{N}[\delta(\boldsymbol{r}_k - \boldsymbol{r})\nabla_k + \nabla_k\delta(\boldsymbol{r}_k - \boldsymbol{r})] \equiv \sum_{k=1}^{N}\hat{\mathbf{j}}_k(\boldsymbol{r}),\end{aligned} \tag{2}$$

where m denotes the electronic mass and the momentum operator $\hat{\mathbf{p}}_k = -\mathrm{i}\hbar\nabla_k$. These average values assume simple forms in the *Molecular Orbital* (MO) approximation,

$$\Psi(N) = (1/\sqrt{N!})\det(\varphi_1, \varphi_2, \ldots, \varphi_N) \equiv |\varphi_1, \varphi_2, \ldots, \varphi_N|, \tag{3}$$

e.g., in the familiar Hartree–Fock (HF) or Kohn–Sham (KS) *Self-Consistent-Field* (SCF) theories, in which $\Psi(N)$ is given by the *anti*-symmetrized product (Slater determinant) of N orthonormal *one*-particle functions, the system *Molecular Orbitals* (MO)

$$\{\varphi_k(\boldsymbol{r}) \equiv R_k(\boldsymbol{r})\exp[\mathrm{i}\phi_k(\boldsymbol{r})]\,, \quad k = 1, 2, \ldots, N\}. \tag{4}$$

Since the observables of Eq. (2) combine *one*-electron operators their expectation values are given by the sum of the corresponding orbital expectation values:

$$\rho(\boldsymbol{r}) = \sum_{k=1}^{N}\langle\varphi_k|\,\hat{\rho}_k(\boldsymbol{r})\,|\varphi_k\rangle = \sum_k R_k^2(\boldsymbol{r}) = \sum_k \rho_k(\boldsymbol{r}), \tag{5}$$

$$\boldsymbol{j}(\boldsymbol{r}) = \sum_{k=1}^{N}\langle\varphi_k|\,\hat{\mathbf{j}}_k(\boldsymbol{r})\,|\varphi_k\rangle = \frac{\hbar}{m}\sum_k \rho_k(\boldsymbol{r})\nabla\phi_k(\boldsymbol{r}) = \sum_k \boldsymbol{j}_k(\boldsymbol{r}), \tag{6}$$

where $\{\rho_k(\boldsymbol{r})\}$ and $\{\boldsymbol{j}_k(\boldsymbol{r})\}$ denote contributions due to an electron occupying φ_k.

In the simplest case of a *single* ($N = 1$) electron occupying the complex MO,

$$\varphi(\boldsymbol{r}) = R(\boldsymbol{r})\,\exp[\mathrm{i}\phi(\boldsymbol{r})], \tag{7}$$

the modulus factor $R(\boldsymbol{r})$ thus determines the particle spatial distribution,

$$\rho(\boldsymbol{r}) = \langle\varphi|\hat{\rho}(\boldsymbol{r})|\varphi\rangle = \varphi^*(\boldsymbol{r})\varphi(\boldsymbol{r}) = R(\boldsymbol{r})^2 = p(\boldsymbol{r}), \quad \int p(\boldsymbol{r})d\boldsymbol{r} = 1, \tag{8}$$

while the gradient of its phase generates the associated current density:

$$\boldsymbol{j}(\boldsymbol{r}) = \langle\varphi|\hat{\mathbf{j}}(\boldsymbol{r})|\varphi\rangle = \frac{\hbar}{2m\mathrm{i}}\left[\varphi^*(\boldsymbol{r})\nabla\varphi(\boldsymbol{r}) - \varphi(\boldsymbol{r})\nabla\varphi^*(\boldsymbol{r})\right] = \frac{\hbar p(\boldsymbol{r})}{m}\nabla\phi(\boldsymbol{r}). \tag{9}$$

The *phase*-gradient is proportional to the current-per-particle, "velocity" field $\boldsymbol{V}(\boldsymbol{r}) = \boldsymbol{j}(\boldsymbol{r})/p(\boldsymbol{r})$,

$$\boldsymbol{V}(\boldsymbol{r}) = (\hbar/m)\,\nabla\phi(\boldsymbol{r}). \tag{10}$$

The probability and current densities manifest the complementary facets of electron distributions in molecules. They respectively generate the classical and *non*-classical contributions to the generalized measures of the resultant information content in the quantum electronic state [9,10,16,17,24,25], which we shall now briefly summarize. As already remarked above, these phase/current complements have to be used in diagnosing the full (resultant) information content of electronic states, exploring the quantum molecular equilibria, probing the chemical bond multiplicities due to the orbital bridges, and in treating the associated multiple (cascade) communications in molecular information channels.

The key element in this quantum IT approach to molecular electronic structure is an adequate definition of a generalized measure of the information content in the given (generally complex) quantum state of electrons in molecules. The system electron distribution, related to the wave-function *modulus*, reveals only the classical, *probability* aspect of the molecular information content, while the *phase/current* component gives rise to the associated *non*-classical entropy/information terms [9,10,16,17,24,25] in the corresponding overall quantum measure. The *resultant* quantities monitor the full information content in the *non*-equilibrium or variational states, thus providing the *complete* quantum information description of their evolution towards the final equilibrium.

In *Density Functional Theory* (DFT) [27,28] one often refers to the density-constrained principles [9,10,29] and states [29–33], which correspond to the fixed electronic probability distribution. Thermodynamic-like information searches over such constrained wave-function ultimately give rise to the "vertical" equilibria in molecules. They are determined solely by the *non*-classical (phase/current-related) entropy/information functionals [16,17,23–25]. The density-unrestricted extrema of the resultant information measure similarly determine the *horizontal* (probability-unconstrained) equilibria in molecules [9–11,23–25].

Of interest in the electronic structure theory also are the *cross* (or relative) *entropy* quantities, which measure the *information distance* between two probability distributions and reflect the information *similarity* between different states or molecules. Communication approaches to bond multiplicities use entropic descriptors of the information propagation, via system chemical bonds, between bonded atoms, orbitals or local volume elements. For example, in OCT molecular systems are regarded as the Atomic Orbital (AO)-resolved information channels. The spread of information in such classical communication networks is described by the average *conditional-entropy* (communication "noise") and *mutual-information* (information-flow) descriptors [3,4,7,11–13]. They provide a resolution of the overall IT bond multiplicities into the associated ("chemical") *covalent* and *ionic* bond components, respectively [11–13,18].

Consider the classical Shannon (S) entropy [3] in the normalized probability vector $\boldsymbol{p} = \{p_i\}$ or density distribution $p(\boldsymbol{r})$,

$$\sum_i p_i = \int p(\boldsymbol{r})\, d\boldsymbol{r} = 1. \tag{11}$$

For the discrete elementary events the entropy function becomes

$$S(\boldsymbol{p}) = -\sum_i p_i \log p_i, \tag{12}$$

while for the *continuous* labels of the electron locality events $\{\boldsymbol{r}\}$ the entropy functional of the spatial probability distribution $p(\boldsymbol{r}) = R^2(\boldsymbol{r})$, determined by its classical amplitude $R(\boldsymbol{r})$, reads:

$$S[p] = S^{class.}[\varphi] = -\int p(\boldsymbol{r}) \log p(\boldsymbol{r})\, d\boldsymbol{r} \equiv \int p(\boldsymbol{r}) S^{class.}(\boldsymbol{r})\, d\boldsymbol{r} \equiv \int s^{class.}(\boldsymbol{r})\, d\boldsymbol{r}. \tag{13}$$

These Shannon quantities provide a measure of the average indeterminacy (spread, width, "disorder", "uncertainty") in the argument probability distribution. They also measure the corresponding amount of information $I^{\mathrm{S}}(\boldsymbol{p}) = S(\boldsymbol{p})$ or $I^{\mathrm{S}}[p] = S[p]$ obtained when the distribution indeterminacy is removed by an appropriate measurement (experiment).

This global information measure is *classical* in character, being determined by the probabilities alone. This property distinguishes it from the corresponding quantum concept of the *non*-classical entropy contribution due to the phase of the complex electronic state. As argued elsewhere [16,17,25], for a single electron in the complex MO state of Eq. (7) the classical information in the state probability distribution $p(\boldsymbol{r})$, $S[p] = S^{class.}[\varphi]$, while the density $s^{nclass.}(\boldsymbol{r})$ of the *non*-classical entropy complement to the classical Shannon entropy of Eq. (13) is proportional to the *negative* magnitude of the spatial phase function, $|\phi(\boldsymbol{r})| = [\phi^2(\boldsymbol{r})]^{1/2}$, the square root of the *phase*-density $\pi(\boldsymbol{r}) = \phi^2(\boldsymbol{r})$, with the local particle probability density providing the relevant weighting factor:

$$\begin{aligned} S^{nclass.}[\varphi] &= -2\int p(\boldsymbol{r})|\phi(\boldsymbol{r})|\, d\boldsymbol{r} \equiv S[p,\phi] \equiv -2\langle|\phi|\rangle \equiv \int p(\boldsymbol{r}) S^{nclass.}(\boldsymbol{r})\, d\boldsymbol{r} \\ &\equiv \int s^{nclass.}(\boldsymbol{r})\, d\boldsymbol{r}. \end{aligned} \tag{14}$$

The two components $S[p] = S^{class.}[\varphi]$ and $S[p,\phi] = S^{nclass.}[\varphi]$ determine the *resultant* entropy descriptor of the complex MO state:

$$S[\varphi] = S^{class.}[\varphi] + S^{nclass.}[\varphi] = S[p] + S[p, \phi]. \quad (15)$$

The classical gradient (Fisher) measure of the information content for locality events [1,2], called the *intrinsic accuracy* in the probability density $p(\boldsymbol{r})$, reads:

$$I[p] = \int p(\boldsymbol{r}) \left[\nabla \ln p(\boldsymbol{r})\right]^2 d\boldsymbol{r} = \int \left[\nabla p(\boldsymbol{r})\right]^2 / p(\boldsymbol{r})\, d\boldsymbol{r} = 4 \int \left[\nabla R(\boldsymbol{r})\right]^2 d\boldsymbol{r} \equiv I[R], \quad (16)$$

where $R(\boldsymbol{r}) = \sqrt{p(\boldsymbol{r})}$ again denotes the *classical* amplitude of this continuous probability distribution. It is reminiscent of von Weizsäcker's [34] inhomogeneity correction to the electronic kinetic energy in the Thomas–Fermi theory and characterizes the average determinacy (compactness, narrowness, "order") of the probability density $p(\boldsymbol{r})$. The classical Shannon entropy and Fisher information thus describe the complementary facets of the system probability density: the former reflects a degree of distribution's *delocalization*, while the latter characterizes its *localization* aspect.

The classical amplitude form of Eq. (16) is naturally generalized into the domain of the *quantum* (complex) probability amplitudes, the wave functions of Schrödinger's quantum mechanics. For the *one*-electron state of Eq. (7), when $p(\boldsymbol{r}) = \varphi^*(\boldsymbol{r})\, \varphi(\boldsymbol{r}) = |\varphi(\boldsymbol{r})|^2 = R^2(\boldsymbol{r}) = \rho(\boldsymbol{r})$, the resultant Fisher measure,

$$\begin{aligned} I[\varphi] &= 4 \int |\nabla \varphi(\boldsymbol{r})|^2\, d\boldsymbol{r} \equiv \int p(\boldsymbol{r}) \left[I^{class.}(\boldsymbol{r}) + I^{nclass.}(\boldsymbol{r}) \right] d\boldsymbol{r} \\ &\equiv \int \left[f^{class.}(\boldsymbol{r}) + f^{nclass.}(\boldsymbol{r}) \right] d\boldsymbol{r}, \end{aligned} \quad (17)$$

is related to the average kinetic energy $T[\varphi]$:

$$T[\varphi] \equiv \langle \varphi | \hat{\mathrm{T}} | \varphi \rangle = -\frac{\hbar^2}{2m} \int \varphi^*(\boldsymbol{r}) \Delta \varphi(\boldsymbol{r})\, d\boldsymbol{r} = \frac{\hbar^2}{2m} \int |\nabla \varphi(\boldsymbol{r})|^2\, d\boldsymbol{r} = \frac{\hbar^2}{8m} I[\varphi]. \quad (18)$$

The latter separates into the classical, Fisher contribution, depending solely upon the electron probability distribution $p(\boldsymbol{r})$,

$$T^{class.}[\varphi] = T[p] = \frac{\hbar^2}{8m} \int \frac{|\nabla p(\boldsymbol{r})|^2}{p(\boldsymbol{r})}\, d\boldsymbol{r} = \frac{\hbar^2}{2m} \int \left[\nabla R(\boldsymbol{r})\right]^2 d\boldsymbol{r}, \quad (19)$$

and the *non*-classical, (phase/current)-related term,

$$T^{nclass.}[\varphi] = T[p, \boldsymbol{j}] = \frac{m}{2} \int \left[\boldsymbol{j}(\boldsymbol{r}) / R(\boldsymbol{r})\right]^2 d\boldsymbol{r} = \frac{\hbar^2}{2m} \int R^2(\boldsymbol{r}) \left[\nabla \phi(\boldsymbol{r})\right]^2 d\boldsymbol{r}, \quad (20)$$

$$T[\varphi] = T^{class.}[\varphi] + T^{nclass.}[\varphi] = T[p] + T[p, \boldsymbol{j}]. \quad (21)$$

A similar partitioning of the generalized information functional of Eq. (17) gives:

$$I[\varphi] \equiv I^{class.}[\varphi] + I^{nclass.}[\varphi] = I[p] + 4\int p(\boldsymbol{r})[\nabla\phi(\boldsymbol{r})]^2\, d\boldsymbol{r}$$
$$= I[p] + \left(\frac{2m}{\hbar}\right)^2 \int \boldsymbol{j}^2(\boldsymbol{r})/p(\boldsymbol{r})\, d\boldsymbol{r}$$
$$\equiv I[p] + I[p,\phi] \equiv I[p] + I[p,\boldsymbol{j}]. \quad (22)$$

It should be observed that while the non-classical Shannon term of Eq. (14) is negative, thus decreasing the structural uncertainty/information, the complementary Fisher term of the preceding equation, related to electronic kinetic energy, is positive—increasing the information content of MO state.

The vanishing spatial phase in the ground (stationary) state signifies the complete absence of the current aspect in the molecular electronic structure. Any displacement from this extreme situation is manifested in the non-classical entropy/information quantities either by the average magnitude of phase (in Shannon's measure) or its gradient (in Fisher's descriptor). Increased average presence of currents implies more overall "structure" (order) in the system, thus less global electronic "uncertainty" (disorder). This intuition rationalizes the negative sign of the *global* descriptor of $S^{nclass.}[\varphi]$.

The intuitively correct sign of the related Fisher-type measure $I^{nclass.}[\varphi]$ is less certain [35]. On one hand, the "order" ("localization", probability-narrowness) descriptor $I^{class.}[\varphi]$ increases when its complementary measure, the *global* "disorder" ("delocalization", probability-speed) measure $S^{class.}[\varphi]$ decreases. Can this intuition be used to guess the influence of electronic currents on information content? Such an information increasing behavior would conform to the *positive* sign of the non-classical gradient determinicity-*information* $I^{nclass.}[\varphi]$. This choice of sign links this non-classical information contribution to the dimensionless kinetic energy. However, the negative sign of $S^{nclass.}[\varphi]$ implies the negative information received, when reaching the stationary state of the same probability distribution, and this would also suggest the *negative* sign of the current supplement in the resultant gradient *entropy* (indeterminicity information).

To justify the negative sign of the current-related entropy term let us compare the (*one*-dimensional) stationary distribution of the "standing" wave, resulting from the equal, 50% probabilities of the "left" and "right" "traveling" waves of the same amplitude, i.e., of the total ignorance of a direction of the wave vector and the vanishing values of the average current and the nonclassical entropy-information supplements $S[p,\phi] = I[p,\phi] = 0$, with the 100 % "right" traveling-wave representing a finite current in this direction and hence nonvanishing $S[p,\phi]$ and $I[p,\phi]$. Clearly, the pure traveling-wave situation represents a lower degree of the electronic "uncertainty",i.e., entropy(indeterminicity information), $S[p,\phi] < 0$, or $S[\varphi] < S[p]$, and thus a higher degree of the electronic determinicity information $I[p,\phi] > 0$, or $I[\varphi] > I[p]$. As argued elsewhere [35], the negative of the non-classical information term, $-I[p,\phi] \leq 0$, then represents an appropriate phase/current contribution to the gradient measure of the system resultant entropy (indeterminicity information).

The relevant information densities-per-electron [Eq. (17)] thus read:

$$I^{class.}(\boldsymbol{r}) = [\nabla p(\boldsymbol{r})/p(\boldsymbol{r})]^2 = [2\nabla R(\boldsymbol{r})]^2,$$
$$I^{nclass.}(\boldsymbol{r}) = [2\nabla\phi(\boldsymbol{r})]^2 = (2m/\hbar)^2 \left[\boldsymbol{j}(\boldsymbol{r})/p(\boldsymbol{r})\right]^2. \tag{23}$$

The classical and *non*-classical densities-per-electron of the complementary Shannon and Fisher measures of the information content are thus mutually related via the common-type dependence [9,10,16,17]:

$$I^{class.}(\boldsymbol{r}) = [\nabla \ln p(\boldsymbol{r})]^2 = [\nabla S^{class.}(\boldsymbol{r})]^2 \quad \text{and}$$
$$I^{nclass.}(\boldsymbol{r}) = \left(\frac{2m\boldsymbol{j}(\boldsymbol{r})}{\hbar p(\boldsymbol{r})}\right)^2 \equiv [\nabla S^{nclass.}(\boldsymbol{r})]^2. \tag{24}$$

Thus, the square of the gradient of the local Shannon probe of the state quantum "indeterminicity" (disorder) generates (up to the sign) the density of the corresponding Fisher measure of the state quantum "determinicity" (order).

An important generalization of Shannon's entropy concept, called the *relative* (cross) *entropy*, also known as the *entropy deficiency*, *missing information* or *directed divergence*, has been proposed by Kullback and Leibler [5] and Kullback [6]. It measures the information "distance" between the two (normalized) probability distributions for the same set of events. For example, in the discrete probability scheme identified by events $\boldsymbol{a} = \{a_i\}$ and their probabilities $\boldsymbol{P}(\boldsymbol{a}) = \{P(a_i) = p_i\} \equiv \boldsymbol{p}$, this discrimination information in $\boldsymbol{p}$ with respect to the reference distribution $\boldsymbol{P}(\boldsymbol{a}^0) = \{P(a_i^0) = p_i^0\} \equiv \boldsymbol{p}^0$ is defined as follows:

$$\Delta S(\boldsymbol{p}|\boldsymbol{p}^0) = \sum_i p_i \log(p_i/p_i^0) \geq 0. \tag{25}$$

This quantity provides a measure of the information resemblance between the two compared probability distributions. The more the two vectors differ from one another, the larger the information distance. For individual events the logarithm of probability ratio $I_i = \log(p_i/p_i^0)$, called the (probability) *surprisal*, provides a measure of the event information in $\boldsymbol{p}$ relative to that in the reference distribution $\boldsymbol{p}^0$. Notice that the equality in preceding equation takes place only for the vanishing surprisal for all events, i.e., when the two probability distributions are identical. The directed-divergence between the continuous probability density $p(\boldsymbol{r}) = |\varphi(\boldsymbol{r})|^2$ and the reference distribution $p^0(\boldsymbol{r}) = |\varphi^0(\boldsymbol{r})|^2$, measuring the average *probability*-surprisal $I_p(\boldsymbol{r})$, similarly reads:

$$\Delta S[p|p^0] = \int p(\boldsymbol{r}) \log[p(\boldsymbol{r})/p^0(\boldsymbol{r})]d\boldsymbol{r} \equiv \int p(\boldsymbol{r}) I_p(\boldsymbol{r}) d\boldsymbol{r}$$
$$\equiv \int p(\boldsymbol{r}) \Delta S^{class.}(\boldsymbol{r}) d\boldsymbol{r} \equiv \Delta S^{class.}[\varphi|\varphi^0]. \tag{26}$$

Similar classical concepts of the information distance can be advanced within the Fisher measure [11,24,25]:

$$\Delta I[p|p^0] = \int p(\boldsymbol{r})[\nabla I_p(\boldsymbol{r})]^2\, d\boldsymbol{r} \equiv \int p(\boldsymbol{r})\Delta I^{class.}(\boldsymbol{r})\, d\boldsymbol{r} \equiv \Delta I^{class.}[\varphi|\varphi^0] \geq 0. \tag{27}$$

One can also design appropriate measures of the *non*-classical information distance, related to the phase/current degrees-of-freedom of the compared quantum states φ and φ^0, which generate the associated (probability, phase, current) components $(p, \phi, \boldsymbol{j})$ and $(p^0, \phi^0, \boldsymbol{j}^0)$, respectively. In the positive phase convention, $|\phi| = \phi \geq 0$, the *non*-classical Shannon measure $S[p, \phi]$ generates the following information distance measuring the average *phase*-surprisal $I_\phi(\boldsymbol{r})$:

$$\begin{aligned}\Delta S[\phi|\phi^0] \equiv \Delta S^{nclass.}[\varphi|\varphi^0] &= \int p(\boldsymbol{r})|\log[\phi(\boldsymbol{r})/\phi^0(\boldsymbol{r})]|\; d\boldsymbol{r} \\ &\equiv \int p(\boldsymbol{r})I_\phi(\boldsymbol{r})\; d\boldsymbol{r} \equiv \int p(\boldsymbol{r})\Delta I^{nclass.}(\boldsymbol{r})\; d\boldsymbol{r}.\end{aligned} \tag{28}$$

Two components of Eqs. (26) and (28) then determine the following resultant entropy-deficiency between the two complex MO wave functions:

$$\begin{aligned}\Delta S[\varphi|\varphi^0] &= \Delta S^{class.}[\varphi|\varphi^0] + \Delta S^{nclass.}[\varphi|\varphi^0] = \Delta S[p|p^0] + \Delta S[\phi|\phi^0] \\ &= \int p(\boldsymbol{r})[I_p(\boldsymbol{r}) + I_\phi(\boldsymbol{r})]d\boldsymbol{r}.\end{aligned} \tag{29}$$

In establishing the *non*-classical Fisher-information distance,

$$\Delta I^{nclass.}[\varphi|\varphi^0] \equiv \int p(\boldsymbol{r})\Delta I^{nclass.}(\boldsymbol{r})d\boldsymbol{r}, \tag{30}$$

one again uses the relation between the complementary Shannon and Fisher information densities-per-electron [Eq. (24)]. For comparing the two complex MO states one finds [24,25]:

$$\Delta I^{nclass.}(\boldsymbol{r}) = \left\{\nabla[\Delta S^{nclass.}(\boldsymbol{r})]\right\}^2 = [\nabla I_\phi(\boldsymbol{r})]^2 = \left\{\nabla|\ln[\phi(\boldsymbol{r})/\phi^0(\boldsymbol{r})]|\right\}^2, \tag{31}$$

$$\begin{aligned}\Delta I^{nclass.}[\varphi|\varphi^0] &= \int p(\boldsymbol{r})\left\{\nabla \ln[\phi(\boldsymbol{r})/\phi^0(\boldsymbol{r})]\right\}^2 d\boldsymbol{r} \\ &= \int p(\boldsymbol{r})[\nabla I_\phi(\boldsymbol{r})]^2\, d\boldsymbol{r} \equiv \Delta I[\phi|\phi^0].\end{aligned} \tag{32}$$

The two components of Eqs. (27) and (32) determine the resultant Fisher-information distance between two complex MO:

$$\begin{aligned}\Delta I[\varphi|\varphi^0] &= \Delta I^{class.}[\varphi|\varphi^0] + \Delta I^{nclass.}[\varphi|\varphi^0] = \Delta I[p|p^0] + \Delta I[\phi|\phi^0] \\ &= \int p(\boldsymbol{r})\left\{[\nabla I_p(\boldsymbol{r})]^2 + [\nabla I_\phi(\boldsymbol{r})]^2\right\} d\boldsymbol{r}.\end{aligned} \tag{33}$$

3 Classical molecular channels and their bond descriptors

We continue this short overview with the entropy/information descriptors of a transmission of the electron-assignment "signals" in molecular *communication systems* [11–13]. The *classical* orbital networks [3,4,7,11–13,18] propagate probabilities of electron assignments to basis functions of SCF MO calculations, while the *quantum* channels [20,24] scatter wave functions, the complex probability amplitudes, between such elementary states. The former loose memory of the phase aspect of this information propagation, which becomes crucial in the *multi*-stage (cascade, bridge) propagations [26]. In determining the underlying conditional probabilities of the *output*-orbital events given the *input*-orbital events, or the scattering amplitudes of the *emitting* (input) states among the *monitoring/receiving* (output) states [11–13,25], one uses [36–38] the bond-projected *Superposition Principle* (SP) of quantum mechanics [39].

In a classical communication device the signal emitted from n "inputs" $\boldsymbol{a} = (a_1, a_2, \ldots, a_n)$ of the channel *source* **A** is characterized by the probability distribution $\boldsymbol{P}(\boldsymbol{a}) = \boldsymbol{p} = (p_1, p_2, \ldots, p_n)$, which describes the way the channel is exploited/probed. It can be received at m "outputs" $\boldsymbol{b} = (b_1, b_2, \ldots, b_m)$ of the system *receiver* **B**. The transmission of signals in such communication network is randomly disturbed thus exhibiting a typical communication *noise*. This feature of communication systems is described by the conditional probabilities of the *outputs-given-inputs*, $\mathbf{P}(\mathbf{B}|\mathbf{A}) \equiv \mathbf{P}(\boldsymbol{b}|\boldsymbol{a}) = \{P(b_j|a_i) = P(a_i \wedge b_j)/P(a_i) \equiv P(j|i)\}$, where the probability matrix for simultaneous events $\mathbf{P}(\boldsymbol{a} \wedge \boldsymbol{b}) \equiv \mathbf{P}(\boldsymbol{a}, \boldsymbol{b}) = \{P(a_i \wedge b_j) \equiv P(i, j)\}$ groups probabilities of the joint occurrence of the specified pair of the input–output events. The output signal distribution among the detection events $\boldsymbol{b}$ is thus given by the (output) probability distribution

$$\boldsymbol{P}(\boldsymbol{b}) = \boldsymbol{q} = (q_1, q_2, \ldots, q_m) = \boldsymbol{p}\,\mathbf{P}(\boldsymbol{b}|\boldsymbol{a}). \tag{34}$$

The input and output probabilities are mutually dependent. One decomposes the joint probabilities of the simultaneous events $\boldsymbol{a} \wedge \boldsymbol{b} = \{a_i \wedge b_j = (i, j)\}$ in these two distributions, $\mathbf{P}(\boldsymbol{a}, \boldsymbol{b}) = \{P(i, j) = \pi_{i,j}\} \equiv \boldsymbol{\pi}$, as products of the "marginal" probabilities of events in one set, say $\boldsymbol{P}(\boldsymbol{a})$, and the corresponding conditional probabilities $\mathbf{P}(\boldsymbol{b}|\boldsymbol{a}) = \{P(j|i)\}$ of outcomes in the other set $\boldsymbol{b}$, given that events $\boldsymbol{a}$ have already occurred:

$$\mathbf{P}(\boldsymbol{a}, \boldsymbol{b}) = \{P(i, j) = p_i P(j|i)\}. \tag{35}$$

The relevant normalization conditions for such joint and conditional probabilities read:

$$\sum_j P(i, j) = p_i, \quad \sum_i P(i, j) = q_j, \quad \sum_i \sum_j P(i, j) = 1,$$
$$\text{and} \quad \sum_j P(j|i) = 1, \quad i = 1, 2, \ldots \tag{36}$$

The Shannon entropy of the joint distribution $\mathbf{P}(\boldsymbol{a}, \boldsymbol{b})$ can be then expressed as the sum of the average entropy $S(\boldsymbol{p})$ in the marginal probability distribution and the average *conditional entropy* in $\boldsymbol{q}$ given $\boldsymbol{p}$,

$$S(\boldsymbol{q}|\boldsymbol{p}) = -\sum_i \sum_j P(i,j)\ \log P(j|i)] = -\sum_i p_i \left[\sum_j P(j|i)\ \log P(j|i) \right], \tag{37}$$

$$\begin{aligned} S(\mathbf{P}(\boldsymbol{a},\boldsymbol{b})) &= -\sum_i \sum_j P(i,j) \log P(i,j) = -\sum_i \sum_j p_i P(j|i)[\log p_i + \log P(j|i)], \\ &= -\sum_i p_i \log p_i - \sum_i \sum_j P(i,j)\ \log P(j|i)] \equiv S(\boldsymbol{p}) + S(\boldsymbol{q}|\boldsymbol{p}). \end{aligned} \tag{38}$$

The conditional entropy represents the extra amount of the uncertainty/information about the occurrence of events $\boldsymbol{b}$, given that the events $\boldsymbol{a}$ are known to have occurred. The information obtained as a result of simultaneously observing events $\boldsymbol{a}$ and $\boldsymbol{b}$ thus equals to the amount of information in set $\boldsymbol{a}$, supplemented by the extra information provided by the occurrence of events in the other set $\boldsymbol{b}$, when $\boldsymbol{a}$ are known to have occurred already.

One also introduces the channel complementary descriptor, called the *mutual information* in the two probability distributions,

$$\begin{aligned} I(\boldsymbol{p}:\boldsymbol{q}) &= \sum_i \sum_j P(i,j) \log \left[P(i,j) / \left(p_i p_j \right) \right] \\ &\equiv \sum_i \sum_j P(i,j) \log \left[P(i,j) / P^{ind.}(i,j) \right] \\ &\equiv \Delta S[\mathbf{P}(\boldsymbol{a},\boldsymbol{b})\,|\mathbf{P}^{ind.}(\boldsymbol{a},\boldsymbol{b})] = S(\boldsymbol{p}) + S(\boldsymbol{q}) - S(\boldsymbol{\pi}) \\ &= S(\boldsymbol{p}) - S(\boldsymbol{p}|\boldsymbol{q}) = S(\boldsymbol{q}) - S(\boldsymbol{q}|\boldsymbol{p}) \geq 0. \end{aligned} \tag{39}$$

The equality holds only for the independent distributions, when $P(i,j) = P^{ind.}(i,j) = p_i q_j$. The amount of uncertainty in $\boldsymbol{q}$ can only decrease, when $\boldsymbol{p}$ has been known beforehand, $S(\boldsymbol{q}) \geq S(\boldsymbol{q}|\boldsymbol{p}) = S(\boldsymbol{q}) - I(\boldsymbol{p}:\boldsymbol{q})$. As also indicated above, the average mutual information is an example of the entropy deficiency, measuring the missing information between the joint probabilities $\mathbf{P}(\boldsymbol{a},\boldsymbol{b}) = \boldsymbol{\pi}$ of the *dependent* events $\boldsymbol{a}$ and $\boldsymbol{b}$, and the joint probabilities $\mathbf{P}^{ind.}(\boldsymbol{a},\boldsymbol{b}) = \boldsymbol{p}^{\mathrm{T}}\boldsymbol{q}$ for the *independent* events. The average mutual information thus reflects a degree of a dependence between the input and output events. A similar information-distance interpretation can be attributed to the average conditional entropy: $S(\boldsymbol{p}|\boldsymbol{q}) = S(\boldsymbol{p}) - \Delta S[\mathbf{P}(\boldsymbol{a},\boldsymbol{b})|\mathbf{P}^{ind.}(\boldsymbol{a},\boldsymbol{b})]$.

The input probabilities $\boldsymbol{p}$ reflect the way the channel is used (probed). The Shannon entropy $S(\boldsymbol{p})$ of these *source* probabilities determines the channel a priori entropy. The average *conditional entropy* of the outputs-given-inputs, $S(\boldsymbol{q}|\boldsymbol{p}) \equiv H(\mathbf{B}|\mathbf{A})$, is then determined by the input signal $\boldsymbol{p}$ and the scattering probabilities $\mathbf{P}(\boldsymbol{b}|\boldsymbol{a})$. It measures the average noise in the $\mathbf{A} \rightarrow \mathbf{B}$ transmission. The so called a posteriori entropy, of the input given output, $S(\boldsymbol{p}|\boldsymbol{q}) \equiv H(\mathbf{A}|\mathbf{B})$, is similarly defined by the conditional probabilities of the $\mathbf{B} \rightarrow \mathbf{A}$ propagation: $\mathbf{P}(\mathbf{A}|\mathbf{B}) = \mathbf{P}(\boldsymbol{a}|\boldsymbol{b}) = \{P(a_i|b_j) = P(a_i \wedge b_j)/P(b_j) = P(i|j)\}$. It reflects the residual indeterminacy about the input signal, when the output signal has already been received. An observation of the output signal thus provides on average the amount of information given by the difference between the a priori and a posteriori uncertainties, $S(\boldsymbol{p}) - S(\boldsymbol{p}|\boldsymbol{q}) = I(\boldsymbol{p}:\boldsymbol{q})$, which defines the *mutual information* in the source and receiver. In other words, the mutual information measures the net amount of information transmitted through this classical communication channel, while the conditional entropy $S(\boldsymbol{p}|\boldsymbol{q})$ reflects a fraction of $S(\boldsymbol{p})$ transformed into "noise" as a result of the input signal being scattered in the information channel. Accordingly, $S(\boldsymbol{q}|\boldsymbol{p})$ reflects the noise part of $S(\boldsymbol{q}) = S(\boldsymbol{q}|\boldsymbol{p}) + I(\boldsymbol{p}:\boldsymbol{q})$.

For example, in OCT the orbital molecular channels [11–13] propagate probabilities of electron assignments to basis functions of typical SCF MO calculations, e.g., AOs $\boldsymbol{\chi} = (\chi_1, \chi_2, \ldots, \chi_m)$. The underlying conditional probabilities of the *output* AO events, given the input AO events, $\mathbf{P}(\boldsymbol{\chi}'|\boldsymbol{\chi}) = \{P(\chi_j|\chi_i) \equiv P(j|i) \equiv P_{i\to j} \equiv A(j|i)^2 \equiv (A_{i\to j})^2\}$, or the associated scattering amplitudes $\mathbf{A}(\boldsymbol{\chi}'|\boldsymbol{\chi}) = \{A(j|i) = A_{i\to j}\}$ of the *emitting* (input) states $\boldsymbol{a} = |\boldsymbol{\chi}\rangle = \{|\chi_i\rangle\}$ among the *monitoring/receiving* (output) states $\boldsymbol{b} = |\boldsymbol{\chi}'\rangle = \{|\chi_j\rangle\}$, results from the bond-projected SP. The local description (LCT) similarly invokes the basis functions $\{|\boldsymbol{r}\rangle\}$ of the position representation, identified by the continuous labels of the spatial coordinates determining the location $\boldsymbol{r}$ of an electron. This complete basis set then determines both the input $\boldsymbol{a} = \{|\boldsymbol{r}\rangle\}$ and output $\boldsymbol{b} = \{|\boldsymbol{r}'\rangle\}$ events of the *local* molecular channel determined by the relevant kernel of conditional-probabilities: $P(\boldsymbol{r}'|\boldsymbol{r}) = P_{\boldsymbol{r}\to\boldsymbol{r}'} = (A_{\boldsymbol{r}\to\boldsymbol{r}'})^2$ [22]. The corresponding products of the elementary (*direct*) probabilities $\mathbf{P}(\boldsymbol{\chi}'|\boldsymbol{\chi})$ or $P(\boldsymbol{r}'|\boldsymbol{r})$ then determine the corresponding *multi*-stage (cascade/bridge) communications [13,22,26].

In OCT the entropy/information indices of the covalent/ionic components of the system chemical bonds represent the complementary descriptors of the average communication *noise* and amount of information *flow*, respectively, in the AO-resolved molecular channel. One observes that the *molecular* input $\boldsymbol{P}(\boldsymbol{a}) \equiv \boldsymbol{p}$ generates the same distribution in the output of this network, $\boldsymbol{q} = \boldsymbol{p}\mathbf{P}(\boldsymbol{b}|\boldsymbol{a}) = \{\sum_i p_i P(j|i) \equiv \sum_i P(i\wedge j) = p_j\} = \boldsymbol{p}$, thus identifying $\boldsymbol{p}$ as the *stationary* vector of AO-probabilities in the molecular ground state. This purely molecular channel is devoid of any reference (history) of the chemical bond formation and generates the average noise index of the IT bond-*covalency* measured by the average conditional-entropy of the system outputs-given-inputs: $S(\boldsymbol{P}(\boldsymbol{b})|\boldsymbol{P}(\boldsymbol{a})) = S(\boldsymbol{q}|\boldsymbol{p}) \equiv S$.

The AO channel with the *promolecular* input signal, $\boldsymbol{P}(\boldsymbol{a}^0) = \boldsymbol{p}^0 = \{p_i^0\}$, of AO in the system *free* constituent atoms, refers to the initial stage in the bond-formation process. It corresponds to the ground-state occupations of the AO contributed by the system constituent atoms to the system chemical bonds, before their mixing into MO. These reference input probabilities give rise to the average information *flow* index of the system IT bond-*ionicity*, given by the *mutual-information* in the channel *promolecular* inputs and *molecular* outputs:

$$\begin{aligned} I(\boldsymbol{P}(\boldsymbol{a}^0):\boldsymbol{P}(\boldsymbol{b})) = I(\boldsymbol{p}^0:\boldsymbol{q}) &= \sum_i\sum_j P(i,j)\log\left[p_i P(i,j)/(p_i q_j p_i^0)\right] \\ &= \sum_i\sum_j P(i,j)[-\log q_j + \log(p_i/p_i^0) \\ &\quad + \log P(j|i)] \\ &= S(\boldsymbol{q}) + \Delta S(\boldsymbol{p}|\boldsymbol{p}^0) - S \equiv I^0. \end{aligned} \tag{40}$$

This amount of information reflects the fraction of the initial (promolecular) information content $S(\boldsymbol{p}^0)$ which has not been dissipated as noise in the molecular communication system. In particular, for the molecular input, $\boldsymbol{p}^0 = \boldsymbol{p}$ and hence $\Delta S(\boldsymbol{p}|\boldsymbol{p}^0) = 0$,

$$I(\boldsymbol{p}{:}\boldsymbol{q}) = S(\boldsymbol{q}) - S \equiv I. \tag{41}$$

The sum of these two bond components, e.g.,

$$M(\boldsymbol{P}(\boldsymbol{a}^0); \boldsymbol{P}(\boldsymbol{b})) = \boldsymbol{M}(\boldsymbol{p}^0; \boldsymbol{q}) = S + I^0 = S(\boldsymbol{q}) + \Delta S(\boldsymbol{p}|\boldsymbol{p}^0) \equiv M^0, \tag{42}$$

measures the *absolute* overall IT bond-multiplicity index relative to the *promolecular* reference, of all bonds in the molecular system under consideration. For the *molecular* input this quantity preserves the Shannon entropy of the molecular input probabilities:

$$M(\boldsymbol{p}; \boldsymbol{q}) = S(\boldsymbol{q}|\boldsymbol{p}) + I(\boldsymbol{p}{:}\boldsymbol{q}) = S(\boldsymbol{q}) \equiv M. \tag{43}$$

The *relative* index [22],

$$\Delta M = M - M^0 = \Delta S(\boldsymbol{p}|\boldsymbol{p}^0), \tag{44}$$

reflecting the IT-multiplicity changes due to the chemical bonds alone, is then interaction dependent. It correctly vanishes in the atomic dissociation limit of *separated atoms*, when $\boldsymbol{p}^0$ and $\boldsymbol{p}$ become identical. The entropy deficiency index $\Delta S(\boldsymbol{p}|\boldsymbol{p}^0)$, reflecting the information distance between the *molecular* electron distribution, generated by the constituent bonded atoms, and the *promolecular* density, due to the molecularly placed non-bonded (free) atoms, thus represents the overall IT difference-index of the system chemical bonds.

4 Additive and non-additive information terms in molecular communications

In the simplest *single*-configuration approximation of typical (HF or KS) SCF MO calculations the occupied MO $\boldsymbol{\varphi} = (\varphi_1, \varphi_2, \ldots, \varphi_N)$ are expanded in the (orthogonalized) AO basis functions $\boldsymbol{\chi} = (\chi_1, \chi_2, \ldots, \chi_m)$: $\boldsymbol{\varphi} = \boldsymbol{\chi}\mathbf{C}$; here the columns $\{\boldsymbol{C}_s\}$ of the unitary matrix $\mathbf{C}$, $\mathbf{C}^\dagger\mathbf{C} = \mathbf{I}$, group the expansion coefficients of $\{\varphi_s = \boldsymbol{\chi}\boldsymbol{C}_s\}$. The *bond subspace* $\boldsymbol{\varphi}$ is defined by the associated MO projector $\hat{\mathrm{P}}_\varphi \equiv |\boldsymbol{\varphi}\rangle\langle\boldsymbol{\varphi}|$, which gives rise to the (idempotent) *Charge and Bond-Order* (CBO) matrix in the AO representation:

$$\begin{aligned} \boldsymbol{\gamma} &= \{\gamma_{i,j}\} = \langle\boldsymbol{\chi}|\boldsymbol{\varphi}\rangle\,\langle\boldsymbol{\varphi}|\boldsymbol{\chi}\rangle \equiv \langle\boldsymbol{\chi}|\,\hat{\mathrm{P}}_{\boldsymbol{\varphi}}\,|\boldsymbol{\chi}\rangle = \mathbf{C}\mathbf{C}^\dagger, \\ \boldsymbol{\gamma}^2 &= \mathbf{C}\left(\mathbf{C}^\dagger\mathbf{C}\right)\mathbf{C}^\dagger = \mathbf{C}\mathbf{C}^\dagger = \boldsymbol{\gamma}. \end{aligned} \tag{45}$$

The molecular joint probabilities of the given pair of the *input–output* AO in the bond system are then proportional to the square of the corresponding CBO matrix element [12,13]:

$$P(\chi_i \wedge \chi_j) \equiv P(i, j) = \gamma_{i,j}\gamma_{j,i}/N = (\gamma_{i,j})^2/N,$$
$$\sum_j P(i, j) = N^{-1}\sum_j \gamma_{i,j}\gamma_{j,i} = \gamma_{i,i}/N = p_i. \tag{46}$$

The conditional probabilities between AO [13,36–38], $\mathbf{P}(\boldsymbol{\chi}'|\boldsymbol{\chi}) = \{P(j|i) = P(i, j)/p_i\}$,

$$P(j|i) \equiv P_{i\to j} = (A_{i\to j})^2 = (\gamma_{i,j})^2/\gamma_{i,i}\}, \quad \sum_j P(j|i) = 1, \tag{47}$$

then reflect the electron delocalization in the occupied MO system and identify the associated classical scattering amplitudes $\mathbf{A}(\boldsymbol{\chi}'|\boldsymbol{\chi}) = \{A(j|i) = A_{i\to j}\}$:

$$A_{i\to j} = \gamma_{i,j}/[\gamma_{i,i}]^{1/2}. \tag{48}$$

These amplitudes are seen to represent the *input*-renormalized elements of the CBO matrix $\boldsymbol{\gamma}$, which connect the specified input (i) and output (j) AO states.

The noise descriptor of Eq. (37) can be then decomposed into the following difference between *total* and *additive* communication contributions,

$$\begin{aligned} S(\boldsymbol{q}|\boldsymbol{p}) &= -\sum_i\sum_j P(i, j)\ \log\left[P(i, j)/p_i\right] = S[\mathbf{P}(\boldsymbol{a}, \boldsymbol{b})] - S(\boldsymbol{p}) \\ &= N^{-1}\left[-\sum_i\sum_j \gamma_{i,j}\gamma_{j,i}\log(\gamma_{i,j}\gamma_{j,i}) + \sum_i \gamma_{i,i}\log\gamma_{i,i}\right] \\ &\equiv N^{-1}\{S^{total}(\boldsymbol{\gamma}) - S^{add.}(\boldsymbol{\gamma})\} \equiv N^{-1}S^{nadd.}(\boldsymbol{\gamma}). \end{aligned} \tag{49}$$

The preceding equation also defines the associated *non-additive* component of the Shannon entropy contained in the CBO matrix $\boldsymbol{\gamma}$. A similar partitioning of the information-flow quantity of Eq. (39) identifies it as the difference between these two components of $S^{total}(\boldsymbol{\gamma})$:

$$\begin{aligned} I(\boldsymbol{p}:\boldsymbol{q}) &= \sum_i\sum_j P(i, j)\log\left[P(i, j)/\left(p_i q_j\right)\right] = S(\boldsymbol{p}) + S(\boldsymbol{q}) - S[\mathbf{P}(\boldsymbol{a}, \boldsymbol{b})] \\ &= N^{-1}[2S^{add.}(\boldsymbol{\gamma}) - S^{total}(\boldsymbol{\gamma})] + \log N \\ &= N^{-1}[S^{add.}(\boldsymbol{\gamma}) - S^{nadd.}(\boldsymbol{\gamma})] + \log N. \end{aligned} \tag{50}$$

These two bond-multiplicity components generate the following molecular bond-order index:

$$M(\boldsymbol{p}; \boldsymbol{q}) = S(\boldsymbol{q}|\boldsymbol{p}) + I(\boldsymbol{p}:\boldsymbol{q}) = S(\boldsymbol{q}) = N^{-1}S^{add.}(\boldsymbol{\gamma}) + \log N. \tag{51}$$

This resultant bond-multiplicity index in AO resolution reflects the *additive* component of

$$S^{total}(\boldsymbol{\gamma}) = N\{S[\mathbf{P}(\boldsymbol{a}, \boldsymbol{b})] - \log N\} \tag{52}$$

$$S^{add.}(\boldsymbol{\gamma}) = N[M(\boldsymbol{p}; \boldsymbol{q}) - \log N] = N[S(\boldsymbol{p}) - \log N], \tag{53}$$

while the *non*-additive part reads:

$$S^{nadd.}(\boldsymbol{\gamma}) = S^{total}(\boldsymbol{\gamma}) - S^{add.}(\boldsymbol{\gamma}) = N\,\{S\,[\mathbf{P}(\boldsymbol{a}, \boldsymbol{b})] - M(\boldsymbol{p}; \boldsymbol{q})\}. \tag{54}$$

To summarize, in this single-determinant approximation of molecular states the *additive* part of the Shannon entropy due to the molecular AO communications represents the overall bond-multiplicity index, the *non-additive* part reflects the channel covalent (noise) descriptor, while their difference measures the complementary ionic (deterministic) descriptor.

This demonstration can be straightforwardly generalized into the ultimate, *local* resolution, in which the simultaneous $P(\boldsymbol{r}, \boldsymbol{r}')$ and conditional $P(\boldsymbol{r}'|\boldsymbol{r})$ probabilities of observing the input $\{\boldsymbol{r}\}$ and output $\{\boldsymbol{r}'\}$ locations of an electron in the molecular bond system are determined by the corresponding elements of the (idempotent) 1-electron density matrix

$$\gamma(\boldsymbol{r}, \boldsymbol{r}') = \langle \boldsymbol{r}|\boldsymbol{\varphi}\rangle\langle\boldsymbol{\varphi}|\boldsymbol{r}'\rangle = \boldsymbol{\varphi}(\boldsymbol{r})\boldsymbol{\varphi}^{\dagger}(\boldsymbol{r}'), \quad \int \gamma(\boldsymbol{r}, \boldsymbol{r}')\,\gamma(\boldsymbol{r}', \boldsymbol{r})\,d\boldsymbol{r}' = \gamma(\boldsymbol{r}, \boldsymbol{r}). \tag{55}$$

The relevant probability kernels and their normalizations now read:

$$P(\boldsymbol{r}, \boldsymbol{r}') = N^{-1}\gamma(\boldsymbol{r}, \boldsymbol{r}')\,\gamma(\boldsymbol{r}', \boldsymbol{r}), \qquad \int P(\boldsymbol{r}, \boldsymbol{r}')\,d\boldsymbol{r}' = N^{-1}\gamma(\boldsymbol{r}, \boldsymbol{r}) = p(\boldsymbol{r}); \tag{56}$$

$$P(\boldsymbol{r}'|\boldsymbol{r}) = \gamma(\boldsymbol{r}, \boldsymbol{r}')\,\gamma(\boldsymbol{r}', \boldsymbol{r})\,/\gamma(\boldsymbol{r}, \boldsymbol{r}), \qquad \int P(\boldsymbol{r}'|\boldsymbol{r})d\boldsymbol{r}' = 1. \tag{57}$$

The conditional entropy (noise) descriptor of this local molecular channel also reflects the non-additive component,

$$\begin{aligned} S[p'|p] &= -\int\!\!\int P(\boldsymbol{r}, \boldsymbol{r}')\log\big[P(\boldsymbol{r}', \boldsymbol{r})\,/\,p(\boldsymbol{r})\big]\,d\boldsymbol{r}'d\boldsymbol{r} \equiv S[P] - S[p] \\ &= N^{-1}\Big\{-\int\!\!\int \gamma(\boldsymbol{r}, \boldsymbol{r}')\,\gamma(\boldsymbol{r}', \boldsymbol{r})\;\log[\gamma(\boldsymbol{r}, \boldsymbol{r}')\,\gamma(\boldsymbol{r}', \boldsymbol{r})]d\boldsymbol{r}'d\boldsymbol{r} \\ &\quad + \int \gamma(\boldsymbol{r}, \boldsymbol{r})\log\gamma(\boldsymbol{r}, \boldsymbol{r})\,d\boldsymbol{r}\Big\} \\ &\equiv N^{-1}\{S^{total}[\gamma] - S^{add.}[\gamma]\} \equiv N^{-1}S^{nadd.}[\gamma]. \end{aligned} \tag{58}$$

The corresponding partitioning of the mutual-information (flow) descriptor of this local channel similarly gives

$$\begin{aligned} I[p{:}p'] &= \int\int P\left(\boldsymbol{r},\boldsymbol{r}'\right)\log\left\{P\left(\boldsymbol{r}',\boldsymbol{r}\right)/\left[p(\boldsymbol{r})p\left(\boldsymbol{r}'\right)\right]\right\}d\boldsymbol{r}'d\boldsymbol{r} \equiv S[p]+S\left[p'\right]-S[P] \\ &= N^{-1}\left\{2S^{add.}[\gamma]-S^{total}\left[\gamma\right]\right\}+\log N \\ &= N^{-1}\left\{S^{add.}[\gamma]-S^{nadd.}\left[\gamma\right]\right\}+\log N, \end{aligned} \tag{59}$$

thus giving rise to the overall bond-multiplicity descriptor at this resolution level:

$$M[p;\, p'] = S[p'|p] + I[p{:}p'] = N^{-1}S^{add.}[\gamma] + \log N. \tag{60}$$

5 Non-classical channels

A presence of the non-classical, (phase/current)-related supplements of the classical measures of the information content in quantum molecular states impresses the need for supplementing the classical communication system, i.e., the *probability channel*, with an appropriate non-classical companion, of the current or phase propagation in the molecular bond system. We call such quantum communication systems for generating the non-classical Fisher- and Shannon-type descriptors the *current* and *phase* channels, respectively.

In designing the information indices of these new IT constructs we request that their *total* entropic descriptors reproduce the corresponding non-classical Fisher or Shannon information contributions. Following the classical development of the preceding section, we further require that their *noise* (IT "covalency") parts are related to the corresponding *non-additive* parts of the relevant non-classical entropy/information measures in the resolution under consideration. Accordingly, the overall bond-multilicities should reflect the corresponding *additive* information terms, while the associated *determinicity* (IT "iconicity") bond orders should measure the difference between the additive and non-additive components.

Since the electronic current concept combines both the probability and phase factors, we retain in this non-classical construct the same input signal as in the classical channel, shaped by the molecular probability distribution $\boldsymbol{p} = \{p_i\}$ or $\{p(\boldsymbol{r})\}$. Indeed, these probability distributions characterize the molecular identity, i.e., the molecular ground-state, the same in both the classical and non-classical channels. The overall information in the molecular electronic state is thus parallelly propagated via both the probability and current/phase networks for the same, *molecular* input signal.

Another hint comes from examining the molecular *phase*-equilibria: all constituent structural units of the composite system, which determine the elementary "events" of the adopted resolution of the molecular electron distribution, in the system equilibrium state exhibit equalized thermodynamic phases, identical with the phase of the whole molecule. In other words, the state phase or its gradient constitute the bona fide molecular "intensity", equal to all subsystems. Therefore, the basis functions $\boldsymbol{\chi} = \{\chi_i\}$ of the

AO-resolution or the localized-electron states $\{|\boldsymbol{r}\rangle\}$ in the local-resolution, are all characterized by the same, spatial (thermodynamic) phase $\phi(\boldsymbol{r})$ of the whole molecular system under consideration. This important observation also implies that any *two*-orbital or *two*-point partitioning of the electronic currents (or phase distribution) must originate from the exhaustive division of the relevant molecular "extensive" parameter, e.g., the electron occupations $\{N_i\}$ of the basis functions in the AO resolution,

$$\left\{N_i = \gamma_{i,i} = Np_i = \sum_j \gamma_{i,j}\gamma_{j,i} = N\sum_j P(i,j)\right\}, \tag{61}$$

or of their local (density) analogs:

$$\left\{\rho(\boldsymbol{r})=\gamma(\boldsymbol{r},\boldsymbol{r}) = Np(\boldsymbol{r}) = \int \gamma\left(\boldsymbol{r},\boldsymbol{r}'\right)\gamma\left(\boldsymbol{r}',\boldsymbol{r}\right)d\boldsymbol{r}'=N\int P\left(\boldsymbol{r},\boldsymbol{r}'\right)d\boldsymbol{r}'\right\}. \tag{62}$$

Alternatively, the associated partitioning of the corresponding probabilities can be used. The joint probabilities

$$\{P(i,j) = p_i P(j|i)\} \text{ and } \left\{P\left(\boldsymbol{r},\boldsymbol{r}'\right) = p(\boldsymbol{r})\ P(\boldsymbol{r}'|\boldsymbol{r})\right\} \tag{63}$$

provide a convenient tool for performing such a division. Therefore, for the adopted molecular inputs $\boldsymbol{p}$ or $\{p(\boldsymbol{r})\}$ the network of the associated conditional probabilities $\{P(j|i)\}$ or $\{P(\boldsymbol{r}'|\boldsymbol{r})\}$ fully determines the associated branches of the *two*-orbital or *two*-point (current/phase)-"communications" in a molecule.

For example, this way of partitioning the probability factor $p(\boldsymbol{r})$ in $\boldsymbol{j}(\boldsymbol{r})$ into AO-resolved probability links between the specified input and output AO events,

$$\left\{P_{i,j}(\boldsymbol{r}) \equiv\ P(i,j)p(\boldsymbol{r}) = p_i P(j|i)p(\boldsymbol{r})\right\}, \tag{64}$$

where p_i stands for the input signal at χ_i, subsequently defines the partial currents between inputs $\{\chi_i\}$ and outputs $\{\chi_j\}$ in AO resolution:

$$\left\{\boldsymbol{j}_{i,j}(\boldsymbol{r}) \equiv P(i,j)\boldsymbol{j}(\boldsymbol{r}) = p_i\left[(\hbar/m)\ P(j|i)p(\boldsymbol{r})\nabla\phi(\boldsymbol{r})\right] \equiv p_i\boldsymbol{j}_{(j|i)}(\boldsymbol{r})\right\}. \tag{65}$$

They also identify the elementary *conditional currents* $\{\boldsymbol{j}_{i,j}(\boldsymbol{r})/p_i \equiv \boldsymbol{j}_{(j|i)}(\boldsymbol{r})\}$ in this AO *current*-channel. These *two*-orbital probabilities also define the partial and conditional phases of the associated AO *phase*-channel:

$$\left\{\phi_{i,j}(\boldsymbol{r}) = P_{i,j}(\boldsymbol{r})\phi(\boldsymbol{r}) = p_i P(j|i)p(\boldsymbol{r})\phi(\boldsymbol{r}) \equiv p_i\phi_{(j|i)}(\boldsymbol{r})\right\}. \tag{66}$$

The local current channel involves two (input $\boldsymbol{r}$ and output $\boldsymbol{r}'$) locations of an electron in the molecule. The probability factor $p(\boldsymbol{r}') = \int P(\boldsymbol{r},\boldsymbol{r}')d\boldsymbol{r}$ of the molecular current $\boldsymbol{j}(\boldsymbol{r}')$ in the specified output location is now partitioned into the corresponding *two*-point contributions $\{P(\boldsymbol{r},\boldsymbol{r}')\}$ due to the specified input locations $\{\boldsymbol{r}\}$, thus defining the associated partial $\boldsymbol{j}(\boldsymbol{r},\boldsymbol{r}')$ and conditional $\boldsymbol{j}(\boldsymbol{r}'|\boldsymbol{r}) = \boldsymbol{j}(\boldsymbol{r},\boldsymbol{r}')/p(\boldsymbol{r})$ currents in this fine-grained resolution of the *current*-channel generating the non-classical Fisher-type information descriptors:

$$\{j(r,r') = P(r,r')j(r') = p(r)\left[(\hbar/m)\,P(r'|r)\nabla\phi(r)\right] \equiv p(r)\,j(r'|r)\}. \quad (67)$$

One similarly designs the non-classical partial and conditional links in the local *phase*-channel,

$$\{\phi(r,r') \equiv P(r,r')\,\phi(r') = p(r)[P(r'|r)\phi(r')] \equiv p(r)\,\phi(r'|r)\}, \quad (68)$$

which generates the non-classical complement of the classical Shannon entropy.

6 Information bond descriptors of local *current*-channel

Consider first the local *current*-channel shown in Fig. 1. For simplicity we again assume the $N = 1$ case. One recalls that in the Harriman–Zumbach–Maschke (HZM) construction [16,17,32,33] of the Slater determinants corresponding to the fixed electron density the equilibrium phases of the *plane-wave*-like orbitals include contributions of the optimum "orthogonality" phase and of the "thermodynamic" contribution common to all MO. The former ultimately do not contribute to the *resultant current* of the whole molecule [24,25]. The overall current due to all occupied MO is thus fully determined by the molecular probability density $p(r)$ and the gradient of the (equalized) equilibrium *thermodynamic phase*:

$$\phi(r) = \phi_{eq.}(r) = -\,(1/2)\,\ln p(r). \quad (69)$$

For the local volume elements in equilibrium their thermodynamic phases are determined by the molecular density alone. The local current network of Fig. 1, resulting from the *two*-point partitioning of the probability distribution, in fact partitions the molecular *output*-velocity field, $V(r') = j(r')/p(r') = (\hbar/m)\nabla\phi(r')$, defining the kernel of *conditional* currents,

$$j(\mathbf{B}|\mathbf{A}) = \{j(r'|r) = (\hbar/m)\,P(r'|r)\nabla\phi\,(r') \equiv j(r,r')\,/p(r)\}, \quad (70)$$

which establish the "communication" connections of this non-classical channel, and the elementary *partial flows* connecting the specified input (r) and output (r') locations:

$$\begin{aligned} j(\mathbf{A},\mathbf{B}) = \{j(r,r') &= p(r)j(r'|r) = (\hbar/m)\,p(r)P(r'|r)\nabla\phi(r') \\ &= (\hbar/m)\,P(r,r')\,\nabla\phi(r')\}. \end{aligned} \quad (71)$$

Let us examine the sum rules of this current system. As expected, the resultant effect of the current propagations originating from all *input* locations $\{r\}$ produces the molecular current at the given *output* location r':

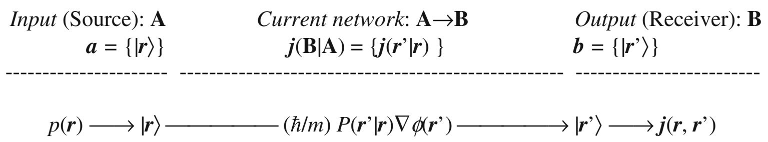

Fig. 1 Schematic diagram of the *local* current system $\mathbf{A} \rightarrow \mathbf{B}$. It is characterized by the molecular input signal $p(\boldsymbol{r})$, the network of *conditional* currents of outputs $\{|\boldsymbol{r}'\rangle\}$ given inputs $\{|\boldsymbol{r}\rangle\}$, $\boldsymbol{j}(\mathbf{B}|\mathbf{A}) = \{\boldsymbol{j}(\boldsymbol{r}'|\boldsymbol{r}) = (\hbar/m)P(\boldsymbol{r}'|\boldsymbol{r})\nabla\phi(\boldsymbol{r}')\}$, and *partial* output currents $\{\boldsymbol{j}(\boldsymbol{r},\boldsymbol{r}') = p(\boldsymbol{r})\boldsymbol{j}(\boldsymbol{r}'|\boldsymbol{r}) = (\hbar/m)P(\boldsymbol{r},\boldsymbol{r}')\nabla\phi(\boldsymbol{r}')\}$

$$\int p(\boldsymbol{r})\,\boldsymbol{j}(\boldsymbol{r}'|\boldsymbol{r})\,d\boldsymbol{r} = \int \boldsymbol{j}\left(\boldsymbol{r},\boldsymbol{r}'\right)d\boldsymbol{r} = (\hbar/m)\left[\int P\left(\boldsymbol{r},\boldsymbol{r}'\right)d\boldsymbol{r}\right]\nabla\phi\left(\boldsymbol{r}'\right)$$
$$= (\hbar/m)\;p\left(\boldsymbol{r}'\right)\nabla\phi\left(\boldsymbol{r}'\right) = \boldsymbol{j}\left(\boldsymbol{r}'\right). \tag{72}$$

The corresponding sum over the output locations $\{\boldsymbol{r}'\}$ of the partial currents $\{\boldsymbol{j}(\boldsymbol{r},\boldsymbol{r}')\}$ originating from the specified input location $\boldsymbol{r}$ defines the effective input current at this position, for the adopted molecular input signal $p(\boldsymbol{r})$,

$$\int p(\boldsymbol{r})\,\boldsymbol{j}(\boldsymbol{r}'|\boldsymbol{r})\,d\boldsymbol{r}' = \int \boldsymbol{j}\left(\boldsymbol{r},\boldsymbol{r}'\right)d\boldsymbol{r}' = (\hbar/m)\int P\left(\boldsymbol{r},\boldsymbol{r}'\right)\nabla\phi\left(\boldsymbol{r}'\right)d\boldsymbol{r}' = \boldsymbol{j}[p;\boldsymbol{r}]\,. \tag{73}$$

Notice, that when the input signal probes only a single infinitesimal volume element around $\boldsymbol{r}$, $p(\boldsymbol{r}) = \delta(\boldsymbol{r}' - \boldsymbol{r})$, this quantity reproduces the overall molecular current at this input location:

$$\boldsymbol{j}[\delta(\boldsymbol{r}' - \boldsymbol{r});\boldsymbol{r}] = (\hbar/m)\int \delta(\boldsymbol{r}' - \boldsymbol{r})P(\boldsymbol{r}'|\boldsymbol{r})\nabla\phi\left(\boldsymbol{r}'\right)\,d\boldsymbol{r}'$$
$$= (\hbar/m)\;P(\boldsymbol{r}|\boldsymbol{r})\nabla\phi(\boldsymbol{r}) = N\boldsymbol{j}(\boldsymbol{r}) = \boldsymbol{j}(\boldsymbol{r}), \tag{74}$$

since $P(\boldsymbol{r}|\boldsymbol{r}) = \gamma(\boldsymbol{r},\boldsymbol{r}) = Np(\boldsymbol{r}) = p(\boldsymbol{r})$ [Eq. (62)]. Finally, integrating the partial flows in the non-classical channel of Fig. 1 over all local inputs and outputs generates the average *current* quantity of the system as a whole:

$$\boldsymbol{J} = \int\int \boldsymbol{j}\left(\boldsymbol{r},\boldsymbol{r}'\right)d\boldsymbol{r}\,d\boldsymbol{r}' = \int \boldsymbol{j}\left(\boldsymbol{r}'\right)d\boldsymbol{r}' = \int \boldsymbol{j}[p;\boldsymbol{r}]\,d\boldsymbol{r}. \tag{75}$$

Let us now examine the entropy/information bond descriptors of this local *current*-channel. Its overall *Fisher* information descriptor $I^{nclass.}_{total}[p;\boldsymbol{j}]$, defining the associated *total* functional $I^{nclass.}_{total}[\gamma]$ of the system density matrix, now reads:

$$I^{nclass.}_{total}[p;\boldsymbol{j}] = 4\int p\left(\boldsymbol{r}'\right)[\nabla\phi\left(\boldsymbol{r}'\right)]^2 d\boldsymbol{r}' = 4\int\int p(\boldsymbol{r})P(\boldsymbol{r}'|\boldsymbol{r})[\nabla\phi\left(\boldsymbol{r}'\right)]^2 d\boldsymbol{r}'d\boldsymbol{r}$$
$$= 4\int\int P\left(\boldsymbol{r},\boldsymbol{r}'\right)[\nabla\phi\left(\boldsymbol{r}'\right)]^2 d\boldsymbol{r}'d\boldsymbol{r}$$
$$= (4/N)\int\int \gamma\left(\boldsymbol{r},\boldsymbol{r}'\right)\gamma\left(\boldsymbol{r}',\boldsymbol{r}\right)[\nabla\phi\left(\boldsymbol{r}'\right)]^2 d\boldsymbol{r}'d\boldsymbol{r}$$
$$\equiv (4/N)\;I^{nclass.}_{total}[\gamma]. \tag{76}$$

Together with its additive contribution of the overall non-classical bond multiplicity,

$$\begin{aligned} I_{add.}^{nclass.}[p;\boldsymbol{j}] &= 4\int\int p(\boldsymbol{r})\delta(\boldsymbol{r}'-\boldsymbol{r})P(\boldsymbol{r}'|\boldsymbol{r})[\nabla\phi(\boldsymbol{r}')]^2 d\boldsymbol{r}'d\boldsymbol{r} \\ &= 4\int P(\boldsymbol{r}',\boldsymbol{r}')\left[\nabla\phi(\boldsymbol{r}')\right]^2 d\boldsymbol{r}' \\ &= (4/N)\int[\gamma(\boldsymbol{r}',\boldsymbol{r}')\,\nabla\phi(\boldsymbol{r}')]^2 d\boldsymbol{r}' = (4/N)\,I_{add.}^{nclass.}[\gamma], \end{aligned} \tag{77}$$

where

$$P(\boldsymbol{r}'|\boldsymbol{r}') = \left[\gamma(\boldsymbol{r}',\boldsymbol{r}')^2/N\right]/[\gamma(\boldsymbol{r}',\boldsymbol{r}')/N] = \gamma(\boldsymbol{r}',\boldsymbol{r}') = Np(\boldsymbol{r}'), \tag{78}$$

it subsequently defines the associated non-additive (indeterminicity, "noise") descriptor

$$\begin{aligned} I_{nadd.}^{nclass.}[p;\boldsymbol{j}] &= (4/N)\,(I_{total}^{nclass.}[\gamma] - I_{add.}^{nclass.}[\gamma]) \\ &= 4\int\int[1-\delta(\boldsymbol{r}'-\boldsymbol{r})]P(\boldsymbol{r},\boldsymbol{r}')[\nabla\phi(\boldsymbol{r}')]^2 d\boldsymbol{r}'d\boldsymbol{r} \\ &= (4/N)\int\int\gamma(\boldsymbol{r},\boldsymbol{r}')\,[1-\delta(\boldsymbol{r}'-\boldsymbol{r})]\gamma(\boldsymbol{r}',\boldsymbol{r})\,[\nabla\phi(\boldsymbol{r}')]^2 d\boldsymbol{r}'d\boldsymbol{r} \\ &= 4\int[p(\boldsymbol{r}') - P(\boldsymbol{r}',\boldsymbol{r}')][\nabla\phi(\boldsymbol{r}')]^2 d\boldsymbol{r}' \\ &= 4\int p(\boldsymbol{r}')[1-Np(\boldsymbol{r}')][\nabla\phi(\boldsymbol{r}')]^2 d\boldsymbol{r}' \\ &= (4/N)\int\gamma(\boldsymbol{r}',\boldsymbol{r}')\,[1-\gamma(\boldsymbol{r}',\boldsymbol{r}')][\nabla\phi(\boldsymbol{r}')]^2 d\boldsymbol{r}' \\ &\equiv (4/N)\,I_{nadd.}^{nclass.}[\gamma] \equiv I^{nclass.}[\boldsymbol{j}|p], \end{aligned} \tag{79}$$

which constitutes the non-classical "covalency" index of the local *current*-channel.

Following the development of the preceding section, we thus introduce the following bond "ionicity" (determinicity) descriptor for this current system:

$$\begin{aligned} I^{nclass.}[p:\boldsymbol{j}] &= (4/N)\,(I_{add.}^{nclass.}[\gamma] - I_{nadd.}^{nclass.}[\gamma]) = (4/N)\,(2I_{add.}^{nclass.}[\gamma] - I_{total}^{nclass.}[\gamma]) \\ &= (4/N)\int\int\gamma(\boldsymbol{r},\boldsymbol{r}')\,[2\delta(\boldsymbol{r}'-\boldsymbol{r})-1]\gamma(\boldsymbol{r}',\boldsymbol{r})\,[\nabla\phi(\boldsymbol{r}')]^2 d\boldsymbol{r}\,d\boldsymbol{r}' \\ &= 4\int p(\boldsymbol{r}')\,[2Np(\boldsymbol{r}')-1][\nabla\phi(\boldsymbol{r}')]^2 d\boldsymbol{r}'. \end{aligned} \tag{80}$$

Hence, the sum of the non-classical indices of the bond covalency and iconicity amount to the additive descriptor of the current network:

$$I^{nclass.}[p;\boldsymbol{j}] = I^{nclass.}[\boldsymbol{j}\,|p] + I^{nclass.}[p:\boldsymbol{j}] = I_{add.}^{nclass.}[p;\boldsymbol{j}]. \tag{81}$$

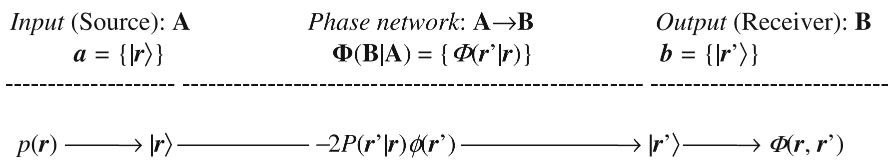

Fig. 2 Schematic diagram of the local phase system $\mathbf{A} \to \mathbf{B}$. It is characterized by the molecular input signal $p(\boldsymbol{r})$, the network of *conditional* phases of outputs $\{|\boldsymbol{r}'\rangle\}$ given inputs $\{|\boldsymbol{r}\rangle\}$, $\boldsymbol{\Phi}(\mathbf{B}|\mathbf{A}) = \{\Phi(\boldsymbol{r}'|\boldsymbol{r}) = -2P(\boldsymbol{r}'|\boldsymbol{r})\phi(\boldsymbol{r}')\}$, and *partial* output phases $\{\Phi(\boldsymbol{r}, \boldsymbol{r}')\}$

For the equilibrium molecular phase it gives for $N = 1$:

$$I^{nclass.}[p; \boldsymbol{j}_{eq.}] = \int \left[\int P\left(\boldsymbol{r}', \boldsymbol{r}'\right) \, d\boldsymbol{r} \right] [\nabla p\left(\boldsymbol{r}'\right) / p\left(\boldsymbol{r}'\right)]^2 d\boldsymbol{r}' = \int [\nabla p\left(\boldsymbol{r}'\right)]^2 / p\left(\boldsymbol{r}'\right) d\boldsymbol{r}'$$
$$= I^{class.}[\varphi] = I[p]. \quad (82)$$

Therefore, the overall bond index of the local *current*-channel for the system equilibrium phase measures the classical Fisher information in electronic distribution.

7 Bond indices of local *phase*-channel

The *phase*-gradient (current) network of the preceding section, generating the non-classical supplement of the classical *Fisher information*, can be also interpreted as the associated communication system involving directly the state-phase itself. Such a local *phase*-channel, shown in Fig. 2, is now related to the non-classical complement of the *Shannon entropy*.

One constructs the local *phase*-channel generating the non-classical entropy of the molecular state by reinterpreting the *current*-system of Fig. 1, for the same classical input signal of the molecular probability distribution $p(\boldsymbol{r})$. As an illustration we again examine the simplest $N = 1$ case, adopting the positive phase convention: $|\phi(\boldsymbol{r})| = \phi(\boldsymbol{r}) \geq 0$. The local phase network now results from the *two*-point partitioning of the molecular *output*-phase field $\phi(\boldsymbol{r}')$. It is effected by the corresponding division of the input probability distribution $p(\boldsymbol{r})$. Following the above current development one introduces the kernel of *conditional* phases defining "communications" in this non-classical local channel,

$$\boldsymbol{\Phi}(\mathbf{B}|\mathbf{A}) = \left\{\Phi(\boldsymbol{r}'|\boldsymbol{r}) \equiv \Phi\left(\boldsymbol{r}, \boldsymbol{r}'\right)/p(\boldsymbol{r}) = -2P(\boldsymbol{r}'|\boldsymbol{r})\, \phi\left(\boldsymbol{r}'\right)\right\}, \quad (83)$$

and the associated *partial* phases for the specified input ($\boldsymbol{r}$) and output ($\boldsymbol{r}$') locations (local "events"):

$$\boldsymbol{\Phi}(\mathbf{A}, \mathbf{B}) = \left\{\Phi\left(\boldsymbol{r}, \boldsymbol{r}'\right) = p(\boldsymbol{r})\, \Phi(\boldsymbol{r}'|\boldsymbol{r}) = -2P\left(\boldsymbol{r}, \boldsymbol{r}'\right) \phi\left(\boldsymbol{r}'\right)\right\}. \quad (84)$$

The resultant effect of the phase propagations originating from all *input* locations $\{\boldsymbol{r}\}$ now produces the non-classical entropy density at the specified *output* location $\boldsymbol{r}'$:

$$\int p(\boldsymbol{r})\ \Phi(\boldsymbol{r}'|\boldsymbol{r})\, d\boldsymbol{r} = \int \Phi\left(\boldsymbol{r},\boldsymbol{r}'\right) d\boldsymbol{r} = -2\left[\int P\left(\boldsymbol{r},\boldsymbol{r}'\right) d\boldsymbol{r}\right]\phi\left(\boldsymbol{r}'\right) = -2p\left(\boldsymbol{r}'\right)\phi\left(\boldsymbol{r}'\right) = s^{nclass.}\left(\boldsymbol{r}'\right). \tag{85}$$

The integration over the output locations $\{\boldsymbol{r}'\}$ of the partial phase $\{\Phi(\boldsymbol{r},\boldsymbol{r}')\}$ originating from the specified input location $\boldsymbol{r}$ similarly defines the input entropy density for the given molecular input signal $p(\boldsymbol{r})$,

$$\int p(\boldsymbol{r})\ \Phi(\boldsymbol{r}'|\boldsymbol{r})\, d\boldsymbol{r}' = \int \Phi\left(\boldsymbol{r},\boldsymbol{r}'\right) d\boldsymbol{r}' = -2\int P\left(\boldsymbol{r},\boldsymbol{r}'\right)\phi\left(\boldsymbol{r}'\right) d\boldsymbol{r}' = s^{nclass.}[p;\boldsymbol{r}], \tag{86}$$

which again reproduces the full entropy density ($N = 1$) for the localized, Dirac-delta input signal $p(\boldsymbol{r}) = \delta(\boldsymbol{r}' - \boldsymbol{r})$:

$$s^{nclass.}[\delta(\boldsymbol{r}'-\boldsymbol{r});\boldsymbol{r}] = -2\int \delta(\boldsymbol{r}'-\boldsymbol{r})P(\boldsymbol{r}'|\boldsymbol{r})\ \phi\left(\boldsymbol{r}'\right) d\boldsymbol{r}' = -2p(\boldsymbol{r})\ \phi(\boldsymbol{r}) = s^{nclass.}(\boldsymbol{r}). \tag{87}$$

Hence, the integrations of the partial phases in the non-classical channel of Fig. 2 over all input and output locations generates the overall non-classical entropy of the whole molecular system:

$$\int\int \Phi\left(\boldsymbol{r},\boldsymbol{r}'\right) d\boldsymbol{r}\, d\boldsymbol{r}' = \int s^{nclass.}\left(\boldsymbol{r}'\right) d\boldsymbol{r}' = \int s^{nclass.}(\boldsymbol{r};\, p)\, d\boldsymbol{r} = -2\int p(\boldsymbol{r})\,\phi(\boldsymbol{r})\, d\boldsymbol{r} = S^{nclass.}[\varphi]. \tag{88}$$

Let us now turn to the bond descriptors of this local channel. Consider first the non-classical complement $S[p,\phi] \equiv S^{nclass.}_{total}[p;\phi]$ of the Shannon entropy describing the overall degree of "uncertainty" in this phase-scattering network. It defines the associated total functional $S^{nclass.}_{total}[\gamma]$ of the state density matrix:

$$S^{nclass.}_{total}[p;\phi] = -2\int\int p(\boldsymbol{r})P(\boldsymbol{r}'|\boldsymbol{r})\ \phi\left(\boldsymbol{r}'\right) d\boldsymbol{r}'d\boldsymbol{r} = -2\int\int P\left(\boldsymbol{r},\boldsymbol{r}'\right)\phi\left(\boldsymbol{r}'\right) d\boldsymbol{r}'d\boldsymbol{r} = -\,(2/N)\int\int \gamma\left(\boldsymbol{r},\boldsymbol{r}'\right)\gamma\left(\boldsymbol{r}',\boldsymbol{r}\right)\phi\left(\boldsymbol{r}'\right) d\boldsymbol{r}'d\boldsymbol{r} \equiv (2/N)\, S^{nclass.}_{total}[\gamma]. \tag{89}$$

Its additive contribution,

$$S^{nclass.}_{add.}[p;\phi] = -2\int\int p(\boldsymbol{r})\delta(\boldsymbol{r}'-\boldsymbol{r})P(\boldsymbol{r}'|\boldsymbol{r})\,\phi\left(\boldsymbol{r}'\right)d\boldsymbol{r}'d\boldsymbol{r} = -2\int P\left(\boldsymbol{r}',\boldsymbol{r}'\right)\phi\left(\boldsymbol{r}'\right)d\boldsymbol{r}'$$
$$= -(2/N)\int\int \gamma\left(\boldsymbol{r}',\boldsymbol{r}'\right)^2\phi\left(\boldsymbol{r}'\right)d\boldsymbol{r}' = (2/N)\,S^{nclass}_{add.}[\gamma], \qquad (90)$$

generates the following non-additive (“noise”) descriptor of this *phase*-channel:

$$S^{nclass.}_{nadd.}[p;\phi] = (2/N)\left(S^{nclass.}_{total}[\gamma] - S^{nclass.}_{add.}[\gamma]\right)$$
$$= -2\int\int[1-\delta(\boldsymbol{r}'-\boldsymbol{r})]P(\boldsymbol{r},\boldsymbol{r}')\,\phi\left(\boldsymbol{r}'\right)d\boldsymbol{r}'d\boldsymbol{r}$$
$$= -2\int\left[p\left(\boldsymbol{r}'\right) - P\left(\boldsymbol{r}',\boldsymbol{r}'\right)\right]\phi\left(\boldsymbol{r}'\right)^2 d\boldsymbol{r}'$$
$$= -2\int p\left(\boldsymbol{r}'\right)\left[1-Np\left(\boldsymbol{r}'\right)\right]\phi\left(\boldsymbol{r}'\right)d\boldsymbol{r}'$$
$$= -(2/N)\int\gamma\left(\boldsymbol{r}',\boldsymbol{r}'\right)\left[1-\gamma\left(\boldsymbol{r}',\boldsymbol{r}'\right)\right]\phi\left(\boldsymbol{r}'\right)d\boldsymbol{r}'$$
$$\equiv (2/N)\,S^{nclass.}_{nadd.}[\gamma] \equiv S^{nclass.}[\phi\,|p]. \qquad (91)$$

It represents the non-classical bond-covalency index of the local phase-channel.

Following the development of the preceding section we again introduce the associated bond “ionicity” (determinicity) descriptor of this non-classical local channel:

$$S^{nclass.}[p{:}\phi] = (2/N)\left(S^{nclass.}_{add.}[\gamma] - S^{nclass.}_{nadd.}[\gamma]\right) = (2/N)\left(2S^{nclass.}_{add.}[\gamma] - S^{nclass.}_{total}[\gamma]\right)$$
$$= -(2/N)\int\int\left[2\gamma\left(\boldsymbol{r}',\boldsymbol{r}'\right)^2 - \gamma\left(\boldsymbol{r},\boldsymbol{r}'\right)\gamma\left(\boldsymbol{r}',\boldsymbol{r}\right)\right]\phi\left(\boldsymbol{r}'\right)\,d\boldsymbol{r}\,d\boldsymbol{r}'. \qquad (92)$$

Therefore, the sum of the non-classical bond indices of the bond covalency and iconicity again amount to the additive descriptor of the phase network,

$$S^{nclass.}[p;\phi] = S^{nclass.}[\phi\,|p] + S^{nclass.}[p{:}\phi] = S^{nclass.}_{add.}[p;\phi]. \qquad (93)$$

For the equilibrium molecular phase it gives ($N = 1$):

$$S^{nclass.}[p;\phi_{eq.}] = -2\int\left[\int P\left(\boldsymbol{r},\boldsymbol{r}'\right)\,d\boldsymbol{r}\right]\phi_{eq.}\left(\boldsymbol{r}'\right)d\boldsymbol{r}' = \left[\int p\left(\boldsymbol{r}'\right)\,\ln p\left(\boldsymbol{r}'\right)d\boldsymbol{r}'\right]$$
$$= -\int s^{class.}\left(\boldsymbol{r}'\right)d\boldsymbol{r}' \equiv -S^{class.}[\varphi] = -S\,[p]. \qquad (94)$$

Therefore, in such an equilibrium distribution of electrons the overall bond index of the *phase*-channel amounts to the negative classical Shannon entropy, thus giving rise to the vanishing resultant entropy in φ.

8 Non-classical AO channels

A natural resolution level for discussing the mechanisms of the chemical bond formation is provided by the (orthogonal) AO framework, in which the CBO matrix replaces the density matrix of the local perspective. The corresponding partition of the molecular AO probabilities is summarized in Eq. (64). It gives rise to the associated current [Eq. (65)] and phase [Eq. (66)] links between the input and output AO of the associated non-classical channels of Figs. 3 and 4. The corresponding molecular probabilities of the orbital events $\{\chi_i(\boldsymbol{r}) = \langle \boldsymbol{r}|i\rangle\}$ in this resolution are defined in Eqs. (46) and (47).

It can be straightforwardly verified that the relevant partial and total sum rules of these AO channels read:

$$\sum_k \boldsymbol{j}_{k,l}(\boldsymbol{r}) = p_l\,\boldsymbol{j}(\boldsymbol{r}),\ \ \sum_l \boldsymbol{j}_{k,l}(\boldsymbol{r}) = p_k\,\boldsymbol{j}(\boldsymbol{r}),$$
$$\sum_k \sum_l \boldsymbol{j}_{k,l}(\boldsymbol{r}) = \boldsymbol{j}(\boldsymbol{r}),\quad \sum_k \sum_l \int \boldsymbol{j}_{k,l}(\boldsymbol{r})d\boldsymbol{r} = \boldsymbol{J}; \tag{95}$$

$$\sum_k \Phi_{k,l}(\boldsymbol{r}) = p_l s^{nclass.}(\boldsymbol{r}),\ \sum_l \Phi_{k,l}(\boldsymbol{r}) = p_k s^{nclass.}(\boldsymbol{r}),\ \sum_k \sum_l \Phi_{k,l}(\boldsymbol{r}) = s^{nclass.}(\boldsymbol{r}),$$
$$\sum_k \sum_l \int \Phi_{k,l}(\boldsymbol{r})d\boldsymbol{r} = S^{nclass.}[\varphi] = S[p,\phi]. \tag{96}$$

Let us summarize the bond descriptors of such non-classical AO channels. As before, we have to identify the additive (IT-multiplicity) and non-additive (IT-covalency) measures of the information/entropy in the current/phase AO distributions, the differences of which ultimately establish the associated IT-ionicity components. In the AO current-channel of Fig. 3 the (total) non-classical gradient information can be decomposed into the associated AO-resolved pieces determined by the *two*-orbital probabilities $\{P(k,l)\}$, functions of the corresponding elements of the CBO matrix $\boldsymbol{\gamma}$:

Input (Source): **A**	*Current network*: **A→B**	*Output* (Receiver): **B**
$\boldsymbol{a} = \{\chi_k(\boldsymbol{r}) = \langle \boldsymbol{r}\|k\rangle\}$	$\boldsymbol{j}(\mathbf{B}\|\mathbf{A}) = \{\boldsymbol{j}_{(l\|k)}(\boldsymbol{r})\}$	$\boldsymbol{b} = \{\chi_l(\boldsymbol{r}) = \langle \boldsymbol{r}\|l\rangle\}$

$$p_k \longrightarrow \langle \boldsymbol{r}|k\rangle \text{———} (\hbar/m)P(l|k)p(\boldsymbol{r})\nabla\phi(\boldsymbol{r}) \longrightarrow \langle \boldsymbol{r}|l\rangle \longrightarrow \boldsymbol{j}_{k,l}(\boldsymbol{r})$$

Fig. 3 Representative current propagation in the AO current system **A** → **B**. It is characterized by the AO input probability signal $\boldsymbol{p} = \{p_k\}$, the network of *conditional* AO currents, $\boldsymbol{j}(\mathbf{B}|\mathbf{A}) = \{\boldsymbol{j}_{(l|k)}(\boldsymbol{r}) = (\hbar/m)P(l|k)p(\boldsymbol{r})\nabla\phi(\boldsymbol{r})\}$, and *partial* AO currents $\{\boldsymbol{j}_{k,l}(\boldsymbol{r})\}$

Input (Source): **A**	*Phase network*: **A→B**	*Output* (Receiver): **B**
$\boldsymbol{a} = \{\chi_k(\boldsymbol{r}) = \langle \boldsymbol{r}\|k\rangle\}$	$\mathbf{\Phi}(\mathbf{B}\|\mathbf{A}) = \{\Phi_{(l\|k)}(\boldsymbol{r})\}$	$\boldsymbol{b} = \{\chi_l(\boldsymbol{r}) = \langle \boldsymbol{r}\|l\rangle\}$

$$p_k \longrightarrow \langle \boldsymbol{r}|k\rangle \text{———} -2P(l|k)p(\boldsymbol{r})\phi(\boldsymbol{r}) \longrightarrow \langle \boldsymbol{r}|l\rangle \longrightarrow \Phi_{k,l}(\boldsymbol{r})$$

Fig. 4 Schematic diagram of the AO phase network **A** → **B**. It is characterized by the molecular input AO-probability signal $\boldsymbol{p} = \{p_k\}$, the network of *conditional* AO phases $\mathbf{\Phi}(\mathbf{B}|\mathbf{A}) = \{\Phi_{(l|k)}(\boldsymbol{r}) = -2P(l|k)\,p(\boldsymbol{r})\phi(\boldsymbol{r})\}$, and *partial* AO phases $\{\Phi_{k,l}(\boldsymbol{r}) = -2P(k,l)\,p(\boldsymbol{r})\phi(\boldsymbol{r})\}$

$$I_{total}^{nclass.}[\boldsymbol{p};\boldsymbol{j}] = I[p,\phi] = 4\int p(\boldsymbol{r})[\nabla\phi(\boldsymbol{r})]^2 d\boldsymbol{r} = \sum_k\sum_l P(k,l)\, I[p,\phi]$$
$$= (4/N)\left(\sum_k\sum_l \gamma_{k,l}\gamma_{l,k}\right)\int p(\boldsymbol{r})[\nabla\phi(\boldsymbol{r})]^2 d\boldsymbol{r} \equiv (4/N)\, I_{total}^{nclass.}(\boldsymbol{\gamma}). \tag{97}$$

Their AO-diagonal contributions define the associated additive information component, the overall non-classical bond-descriptor of the AO *current*-channel

$$I_{add.}^{nclass.}[\boldsymbol{p};\boldsymbol{j}] = I^{nclass.}\left[\boldsymbol{p};\boldsymbol{j}\right] = \left[\sum_k P(k,k)\, I[p,\phi]\right]$$
$$= (4/N)\left[\sum_k (\gamma_{k,k})^2\right]\int p(\boldsymbol{r})[\nabla\phi(\boldsymbol{r})]^2 d\boldsymbol{r} \equiv (4/N)\, I_{add.}^{nclass.}(\boldsymbol{\gamma}), \tag{98}$$

while the *off*-diagonal terms generate the non-additive part, the channel non-classical covalency (indeterminacy) descriptor

$$I_{nadd.}^{nclass.}[\boldsymbol{p};\boldsymbol{j}] = I^{nclass.}[\boldsymbol{j}|\boldsymbol{p}] = \sum_k\sum_l (1-\delta_{k,l}) P(k,l)\, I[p,\phi]$$
$$= (4/N)\left[\sum_k\sum_l (1-\delta_{k,l})\gamma_{k,l}\gamma_{l,k}\right]\int p(\boldsymbol{r})[\nabla\phi(\boldsymbol{r})]^2 d\boldsymbol{r} \equiv (4/N)\, I_{nadd.}^{nclass.}(\boldsymbol{\gamma}). \tag{99}$$

The associated IT iconicity index is then given by the difference of these two components,

$$I^{nclass.}[\boldsymbol{p}:\boldsymbol{j}] = I_{add.}^{nclass.}[\boldsymbol{p};\boldsymbol{j}] - I_{nadd.}^{nclass.}[\boldsymbol{p};\boldsymbol{j}] = (4/N)\,[2I_{add.}^{nclass.}(\boldsymbol{\gamma}) - I_{total}^{nclass.}(\boldsymbol{\gamma})]. \tag{100}$$

This AO-determinacy information descriptor thus measures the dominance of the AO diagonal current-scattering over the non-diagonal propagations.

One similarly decomposes the overall non-classical descriptor of the AO *phase*-channel (Fig. 4). The total descriptor is now given by the non-classical entropy $S[p,\phi]$,

$$S_{total}^{nclass.}[\boldsymbol{p};\phi] = S[p,\phi] = -2\int p(\boldsymbol{r})\,\phi(\boldsymbol{r})\,d\boldsymbol{r} = \sum_k\sum_l P(k,l)\, S[p,\phi]$$
$$= -(2/N)\left(\sum_k\sum_l \gamma_{k,l}\gamma_{l,k}\right)\int p(\boldsymbol{r})\,\phi(\boldsymbol{r})\,d\boldsymbol{r} \equiv (2/N)\, S_{total}^{nclass.}(\boldsymbol{\gamma}), \tag{101}$$

and it decomposes into the AO-additive part describing the channel overall non-classical IT bond-multiplicity,

$$S^{nclass.}_{add.}[\boldsymbol{p};\phi] = S^{nclass.}[\boldsymbol{p};\phi] = \sum_k P(k,k)]S[p,\phi]$$
$$= -(2/N)\left[\sum_k (\gamma_{k,k})^2\right]\int p(\boldsymbol{r})\,\phi(\boldsymbol{r})\,d\boldsymbol{r} \equiv (2/N)\,S^{nclass.}_{add.}(\boldsymbol{\gamma}), \tag{102}$$

and its non-additive complement, the bond-covalency (indeterminicity) descriptor

$$S^{nclass.}_{nadd.}[\boldsymbol{p};\phi] = S^{nclass.}[\phi|\boldsymbol{p}] = \sum_k\sum_l (1-\delta_{k,l})P(k,l)\,S[p,\phi]$$
$$= -(2/N)\left[\sum_k\sum_l (1-\delta_{k,l})\gamma_{k,l}\gamma_{l,k}\right]\int p(\boldsymbol{r})\,\phi(\boldsymbol{r})\,d\boldsymbol{r} \equiv (2/N)S^{nclass.}_{nadd.}(\boldsymbol{\gamma}). \tag{103}$$

Their difference again establishes the associated bond-ionicity (determinicity) index:

$$S^{nclass.}[\boldsymbol{p}:\phi] = S^{nclass.}_{add.}[\boldsymbol{p};\phi] - S^{nclass.}_{nadd.}[\boldsymbol{p};\phi] = (2/N)\left[2S^{nclass.}_{add.}(\boldsymbol{\gamma}) - S^{nclass.}_{nadd.}(\boldsymbol{\gamma})\right]. \tag{104}$$

Since $P(k,k) = p_k\gamma_{k,k} \equiv p_k N_k$, where $N_k = \gamma_{k,k}$ stands for the average electron occupation of χ_k in the molecular bond system, the sum in Eqs. (98) and (102) in fact stands for the average AO occupation in the molecule,

$$\sum_k P(k,k) = \sum_k p_k N_k = \langle N\rangle, \tag{105}$$

and hence the overall non-classical bond indices of AO channels read:

$$I^{nclass.}\left[\boldsymbol{p};\boldsymbol{j}\right] = \langle N\rangle I[p,\phi] \quad \text{and} \quad S^{nclass.}[\boldsymbol{p};\phi] = \langle N\rangle S[p,\phi]. \tag{106}$$

9 Conclusion

The quantum-generalized information measures have been summarized and the associated information-scattering networks have been introduced. This analysis has stressed the need for using the *resultant* information measures, which take into account both the *classical* and *non-classical* contributions due to the electronic probability and current (phase) distributions, respectively. The *non*-classical generalization of the gradient (Fisher) information introduces the information contribution due to the probability current, while the *quantum*-generalized Shannon entropy includes the additive contribution due to the average magnitude of the state phase. These quantum-information terms complement the corresponding classical Fisher and Shannon measures, functionals of the particle probability distribution alone. The resultant quantum measures are capable to extract the *full* information content of the complex probability amplitudes (wave functions), due to both the probability and current distributions. The relation between the classical Shannon and Fisher information densities-per-electron has been extended into their *non*-classical analogs. A similar generalization of the classical information-distance (entropy-deficiency) concept, for comparing probability distributions, has also been proposed in both the Shannon cross-entropy and Fisher missing-information representations.

The superposition principle of quantum mechanics applied to the bond system of the configuration occupied MO determines the conditional probabilities between the elementary quantum states, which generate the classical network of the molecular (probability) communications. In SCF MO theory their amplitudes in the AO and local resolutions are related to the corresponding elements of the CBO and the 1-electron density matrices, respectively. The standard conditional-entropy and mutual-information descriptors of these classical networks provide useful indices of the classical overall IT bond multiplicity and its covalency/iconicity components. These IT bond indices have been related to the additive and non-additive contributions of the adopted entropy/information measures. We have also introduced the non-classical companions of the classical probability-scattering (communication) systems, at both the local and AO resolution levels. These *current*- and *phase*-scattering *channels* generate the respective non-classical Fisher and Shannon information/entropy descriptors of the molecular electronic state in question and their associated bond descriptors.

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