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ORIGINAL PAPER

On probability flow descriptors in position and momentum spaces

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Abstract The current density concepts of the position and momentum probability distributions are examined and the associated continuity equations are explored. The modified flow measure in the *momentum*-space is introduced in terms of which the non-classical (current-related) functionals of the entropy/information content in quantum states assume forms isomorphic with the corresponding *position*-space expressions, when expressed in terms of the state modulus (density) and phase (current) degrees-of-freedom. These concepts are illustrated for the stationary states as well as the plane waves and wave packets of the free particle.

Keywords Continuity equations · Current/phase information measures · Information theory · Momentum fluxes · Quantum entropy/information · Position/momentum representations

1 Introduction

The Information Theory (IT) of Fisher and Shannon [1–8] introduces *classical* measures of the information contained in the molecular quantum state, exploring only the probability distribution of the system electrons. They have proven their utility in extracting the chemical interpretation of the molecular electronic structure in

Throughout the article x denotes a scalar quantity, $\boldsymbol{x}$ stands for the *row*- or *column*-vector, and $\mathbf{x}$ represents a square or rectangular matrix. The natural logarithm $\log = \ln$ used in the Shannon entropy expresses the amount of information in *nats* (natural units): 1 nat = 1.44 bits.

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terms of bonded atoms and chemical bonds [9–17], providing an *entropic representation* of molecular states [18,19]. However, as recently argued elsewhere [20–23], the full (resultant) measure of the overall entropy/information content in the electronic state should include contributions from densities of both the particle probability, related to the wave-function modulus, and the state phase or its gradient determining the electronic current. The *nonclassical*, (phase, current)-related contributions in such generalized IT concepts complement the familiar *classical* measures, functionals of the particle probability distribution alone. The corresponding extension of the classical information-distance (entropy–deficiency) functionals has also been proposed and communication channels of the probability propagation in molecules have been supplemented by their nonclassical companions of the phase/current scattering [24].

This Quantum IT (QIT) description also generates a thermodynamic-like approach to *rates* of specific reorganizations in the system electronic structure [25,26]. It recognizes both the density and phase/current degrees-of-freedom of molecular states and its conceptual framework formally resembles that used in the ordinary irreversible thermodynamics [27]. The nonclassical entropy/information components have been shown to be essential for describing the system *phase*-equilibria [20–23] and extracting the resultant patterns of the chemical bond multiplicities [24–26] or reactivity behavior [28]. This *position* (r-space) QIT development has been recently supplemented by a similar *momentum* (p-space) description [29], following many earlier explorations of the momentum densities, e.g. [30–32].

The momentum representation generates a nonvanishing source term in the associated continuity equation for the electronic probability density [29], in contrast to the position representation where the probability source exactly vanishes. This net effect in the momentum distribution, a competition between the time rate of the density from the Schrödinger equation (SE) and the local inflow (the flux divergence), is current dependent, with different flux definitions only reshuffling the known local time rate between the inflow and source parts of the continuity equation for the momentum probability density.

In this analysis we reexamine the flow concept in the electronic momentum space, seeking the maximum symmetry between expressions in the r- and p-spaces, respectively, for the nonclassical functionals of the system entropy/information content in terms of the state moduli and phases in these two representations. To simplify theoretical considerations we limit ourselves to *one*-electron case. Its generalization to N-electron systems involves the wave functions in the Harriman representation [33], using the Harriman–Zumbach–Maschke (HZM) [33,34] construction of the modern Density Functional Theory (DFT) [35–37]. Such antisymmetric wave functions of N fermions, the Slater determinants of equidensity orbitals yielding the specified particle distribution, adopt the crucial insights due to Macke [38] and Gilbert [39]. The corresponding continuity equations will be used to determine probability sources associated with alternative definitions of the momentum flow measure. These momentum current concepts will be illustrated using stationary states and the free particle model (plane waves and wave packets).

2 Summary of alternative representations and dynamical pictures

In the context of Heisenberg's uncertainty principle one invokes two canonical (continuous) representations in the Hilbert space of molecular quantum states, corresponding to the sharply specified electron *positions* $\{\boldsymbol{r}_i\}$ or *momenta* $\{\boldsymbol{p}_i = \hbar\boldsymbol{k}_i\}$, respectively. For a single particle these bases combine the state vectors $\{|\boldsymbol{r}_1\rangle\}$ and $\{|\boldsymbol{p}_1\rangle \equiv \hbar^{-3/2}|\boldsymbol{k}_1\rangle\}$ corresponding to the sharply specified electron position $\boldsymbol{r}_1$ and momentum $\boldsymbol{p}_1 = \hbar\boldsymbol{k}_1$. These eigenvectors of the "geometric" quantum observables $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$, acting on state vectors in the molecular Hilbert space,

$$\hat{\mathbf{r}}|\boldsymbol{r}_1\rangle = \boldsymbol{r}_1|\boldsymbol{r}_1\rangle \quad \text{and} \quad \hat{\mathbf{p}}|\boldsymbol{p}_1\rangle = \boldsymbol{p}_1|\boldsymbol{p}_1\rangle, \tag{1}$$

form the complete sets,

$$\int d\boldsymbol{r}_1|\boldsymbol{r}_1\rangle\langle\boldsymbol{r}_1| = \int d\boldsymbol{p}_1|\boldsymbol{p}_1\rangle\langle\boldsymbol{p}_1| = \int d\boldsymbol{k}_1|\boldsymbol{k}_1\rangle\langle\boldsymbol{k}_1| = 1,$$

and define the associated wavefunctions (Dirac deltas), i.e., their (*diagonal*) representations in the r- and p-spaces, respectively,

$$\begin{aligned} &\langle\boldsymbol{r}|\boldsymbol{r}_1\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}_1) = u_{\boldsymbol{r}_1}(\boldsymbol{r}) \text{ and} \\ &\langle\boldsymbol{p}|\boldsymbol{p}_1\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}_1) = \bar{u}_{\boldsymbol{p}_1}(\boldsymbol{p}) \text{ or } \langle\boldsymbol{k}|\boldsymbol{k}_1\rangle = \delta(\boldsymbol{k}-\boldsymbol{k}_1) = \bar{u}_{\boldsymbol{k}_1}(\boldsymbol{k}). \end{aligned} \tag{2}$$

Here, $d\boldsymbol{r} \equiv d^3r$ and $d\boldsymbol{p} \equiv d^3p$ or $d\boldsymbol{k} \equiv d^3k = \hbar^{-3}d\boldsymbol{p}$ stand for the infinitesimal volume elements in the position and momentum/wave-number spaces, respectively, and integration is over the whole space involved.

Projections of the momentum eigenvectors onto position states similarly define the wave functions in the mixed (*off-diagonal*) representations (the amplitudes of plane waves),

$$\begin{aligned} u_{\boldsymbol{p}}(\boldsymbol{r}) &= \langle\boldsymbol{r}|\boldsymbol{p}\rangle = (2\,\pi\,\hbar)^{-3/2}\exp[\mathrm{i}(\boldsymbol{p}/\hbar)\cdot\boldsymbol{r}] = \bar{u}_{\boldsymbol{r}}(\boldsymbol{p})^* \quad \text{or} \\ u_{\boldsymbol{k}}(\boldsymbol{r}) &= \langle\boldsymbol{r}|\boldsymbol{k}\rangle \equiv (2\,\pi)^{-3/2}\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}) = \bar{u}_{\boldsymbol{r}}(\boldsymbol{k})^*, \end{aligned} \tag{3}$$

where $\bar{u}_{\boldsymbol{r}}(\boldsymbol{p}) = \langle\boldsymbol{p}|\boldsymbol{r}\rangle = u_{\boldsymbol{p}}(\boldsymbol{r})^*$ and $\bar{u}_{\boldsymbol{r}}(\boldsymbol{k}) = \langle\boldsymbol{k}|\boldsymbol{r}\rangle = u_{\boldsymbol{k}}(\boldsymbol{r})^*$. The position and momentum operators in these two bases are represented by diagonal operator kernels:

$$\begin{aligned} &\langle\boldsymbol{r}|\hat{\mathbf{r}}|\boldsymbol{r}'\rangle = \boldsymbol{r}'\delta(\boldsymbol{r}-\boldsymbol{r}'), \quad \langle\boldsymbol{p}|\hat{\mathbf{r}}|\boldsymbol{p}'\rangle = -\mathrm{i}\hbar\,\nabla_{\boldsymbol{p}}\,\delta(\boldsymbol{p}-\boldsymbol{p}') = \mathrm{i}\hbar\,\delta(\boldsymbol{p}-\boldsymbol{p}')\nabla_{\boldsymbol{p}}, \\ &\langle\boldsymbol{p}|\hat{\mathbf{p}}|\boldsymbol{p}'\rangle = \boldsymbol{p}'\delta(\boldsymbol{p}-\boldsymbol{p}'), \quad \langle\boldsymbol{r}|\hat{\mathbf{p}}|\boldsymbol{r}'\rangle = \mathrm{i}\hbar\,\nabla_{\boldsymbol{r}}\,\delta(\boldsymbol{r}-\boldsymbol{r}') = -\mathrm{i}\hbar\,\delta(\boldsymbol{r}-\boldsymbol{r}')\nabla_{\boldsymbol{r}}, \end{aligned} \tag{4}$$

where we have used identities from the integration by parts, and $\nabla_{\boldsymbol{r}}$, $\nabla_{\boldsymbol{p}}$ stand for the position and momentum gradients, respectively. These continuous "matrices" generate the effective operators acting on wavefunctions $\varphi(\boldsymbol{r}) = \langle\boldsymbol{r}|\varphi\rangle$ and $\bar{\varphi}(\boldsymbol{p}) = \langle\boldsymbol{p}|\varphi\rangle$ in the two canonical representations:

$$\langle \boldsymbol{r}|\hat{\mathbf{p}}|\varphi\rangle \equiv \hat{\mathbf{p}}(\boldsymbol{r})\varphi(\boldsymbol{r}), \quad \hat{\mathbf{p}}(\boldsymbol{r}) = -\mathrm{i}\hbar\nabla_{\boldsymbol{r}} \quad \text{and}$$
$$\langle \boldsymbol{p}|\hat{\mathbf{r}}|\varphi\rangle \equiv \hat{\mathbf{r}}(\boldsymbol{p})\bar{\varphi}(\boldsymbol{p}), \quad \hat{\mathbf{r}}(\boldsymbol{p}) = \mathrm{i}\hbar\nabla_{\boldsymbol{p}}. \tag{5}$$

One observes that the particle wave functions $\varphi(\boldsymbol{r})$ and $\bar{\varphi}(\boldsymbol{p})$ corresponding to the same state vector at time t_0, $|\varphi\rangle = |\varphi(t_0 \equiv 0)\rangle$, are the Fourier transforms of each other:

$$\begin{aligned}
\varphi(\boldsymbol{r}) = \int d\boldsymbol{p}\, \langle \boldsymbol{r}|\boldsymbol{p}\rangle\langle \boldsymbol{p}|\varphi\rangle &= \int d\boldsymbol{p}\, \bar{u}_{\boldsymbol{r}}(\boldsymbol{p})^*\bar{\varphi}(\boldsymbol{p}) \\
&= (2\,\pi\,\hbar)^{-3/2}\int d\boldsymbol{p}\ \exp[\mathrm{i}(\boldsymbol{p}/\hbar)\cdot\boldsymbol{r}]\bar{\varphi}(\boldsymbol{p}) \equiv \bar{\mathscr{F}}[\bar{\varphi}(\boldsymbol{p})], \\
\bar{\varphi}(\boldsymbol{p}) = \int d\boldsymbol{r}\langle \boldsymbol{p}|\boldsymbol{r}\rangle\langle \boldsymbol{r}|\varphi\rangle &= \int d\boldsymbol{r}\, u_{\boldsymbol{p}}(\boldsymbol{r})^*\varphi(\boldsymbol{r}) \\
&= (2\,\pi\,\hbar)^{-3/2}\int d\boldsymbol{r}\ \exp[-\mathrm{i}(\boldsymbol{p}/\hbar)\cdot\boldsymbol{r}]\varphi(\boldsymbol{r}) \equiv \mathscr{F}[\varphi(\boldsymbol{r})],
\end{aligned} \tag{6}$$

and hence

$$\bar{\mathscr{F}}\{\mathscr{F}[\varphi(\boldsymbol{r})]\} = \varphi(\boldsymbol{r}), \quad \mathscr{F}\{\bar{\mathscr{F}}[\bar{\varphi}(\boldsymbol{p})]\} = \bar{\varphi}(\boldsymbol{p}). \tag{7}$$

In particular, for $\bar{\varphi}(\boldsymbol{p}) = \bar{u}_{\boldsymbol{r}}(\boldsymbol{p})$ and $\varphi(\boldsymbol{r}) = u_{\boldsymbol{p}}(\boldsymbol{r})$, respectively, one finds the diagonal representations of Eq. (2): $u_{\boldsymbol{r}}(\boldsymbol{r}') = \delta(\boldsymbol{r}' - \boldsymbol{r})$ and $\bar{u}_{\boldsymbol{p}}(\boldsymbol{p}') = \delta(\boldsymbol{p}' - \boldsymbol{p})$.

In this short summary one also mentions the useful relations summarizing the mixed representations of functions $f(\hat{\mathbf{r}})$ and $g(\hat{\mathbf{p}})$ of the particle position and momentum operators, respectively [40],

$$\begin{aligned}
\langle \boldsymbol{p}|f(\hat{\mathbf{r}})|\boldsymbol{p}'\rangle &= \int d\boldsymbol{r}'\langle \boldsymbol{p}|f(\hat{\mathbf{r}})|\boldsymbol{r}'\rangle\langle \boldsymbol{r}'|\boldsymbol{p}'\rangle \\
&= \int d\boldsymbol{r}'\, f(\boldsymbol{r}')\,\langle \boldsymbol{p}|\boldsymbol{r}'\rangle\langle \boldsymbol{r}'|\boldsymbol{p}'\rangle = \int d\boldsymbol{r}'\ f(\boldsymbol{r}')\, u^*_{\boldsymbol{p}}(\boldsymbol{r}')u_{\boldsymbol{p}'}(\boldsymbol{r}') \\
&= (2\,\pi\,\hbar)^{-3}\int d\boldsymbol{r}'\ \exp[-\mathrm{i}\,(\boldsymbol{p}-\boldsymbol{p}')\cdot\boldsymbol{r}/\hbar)]\, f(\boldsymbol{r}') = (2\,\pi\,\hbar)^{-3/2}\bar{f}(\boldsymbol{p}-\boldsymbol{p}'),
\end{aligned} \tag{8}$$

$$\begin{aligned}
\langle \boldsymbol{r}|g(\hat{\mathbf{p}})|\boldsymbol{r}'\rangle &= \int d\boldsymbol{p}'\langle \boldsymbol{r}|g(\hat{\mathbf{p}})|\boldsymbol{p}'\rangle\langle \boldsymbol{p}'|\boldsymbol{r}'\rangle \\
&= \int d\boldsymbol{p}'\, g(\boldsymbol{p}')\,\langle \boldsymbol{r}|\boldsymbol{p}'\rangle\langle \boldsymbol{p}'|\boldsymbol{r}'\rangle = \int d\boldsymbol{p}'\, g(\boldsymbol{p}')\, u^*_{\boldsymbol{r}}(\boldsymbol{p}')\, u_{\boldsymbol{r}'}(\boldsymbol{p}') \\
&= (2\,\pi\,\hbar)^{-3}\int d\boldsymbol{p}'\, g(\boldsymbol{p}')\ \exp[\mathrm{i}\,(\boldsymbol{r}-\boldsymbol{r}')\cdot\boldsymbol{p}'/\hbar)] \\
&= (2\,\pi\,\hbar)^{-3/2}\bar{\mathscr{F}}[g(\boldsymbol{p}-\boldsymbol{p}')] \equiv (2\,\pi\,\hbar)^{-3/2}\tilde{g}(\boldsymbol{r}-\boldsymbol{r}'),
\end{aligned} \tag{9}$$

where $\tilde{g}(\boldsymbol{r}-\boldsymbol{r}') = \bar{\mathscr{F}}[g(\boldsymbol{p}-\boldsymbol{p}')]$ is the inverse Fourier transform of the momentum function $g(\boldsymbol{p}-\boldsymbol{p}')$.

We further recall that the quantum dynamics can be formulated in several alternative pictures, related by the time-dependent unitary operations. They all provide fully

equivalent physical theories. For example, the familiar Schrödinger (S) picture uses the time-independent operators $\{\hat{\mathrm{A}} \equiv \hat{\mathrm{A}}_S\}$ of physical quantities $\{A\}$, which do not depend on time explicitly, e.g., the operators of Eq. (1). Therefore, the evolution of quantum objects in time is then embodied in the time-dependent state vectors,

$$\left\{|\varphi_S(t)\rangle \equiv |\varphi(t)\rangle = \hat{\mathrm{U}}(t - t_0)|\varphi(t_0)\rangle \equiv \hat{\mathrm{U}}(\tau)|\varphi(t_0)\rangle\right\}, \tag{10}$$

determined by the unitary operator of time evolution,

$$\hat{\mathrm{U}}(\tau) = \exp[-(\mathrm{i}/\hbar)\tau\hat{\mathrm{H}}], \tag{11a}$$

where $\hat{\mathrm{H}}$ stands for the system Hamiltonian. The reverse propagation operator,

$$\hat{\mathrm{U}}(\tau)^{-1} = \hat{\mathrm{U}}(-\tau) = \hat{\mathrm{U}}(\tau)^{\dagger}, \tag{11b}$$

acting on $|\varphi(t)\rangle$ recovers the initial state vector at $t = t_0$:

$$|\varphi(t_0)\rangle = \hat{\mathrm{U}}(t_0 - t)|\varphi(t)\rangle \equiv \hat{\mathrm{U}}(\tau)^{-1}|\varphi(t)\rangle. \tag{12}$$

In the Heisenberg (H) picture the state vectors do not change in time $\{|\varphi_H\rangle \equiv |\varphi(t_0)\rangle \equiv |\varphi\rangle\}$, e.g., eigenvectors of Eq. (1), but the operators become time dependent:

$$\left\{\hat{\mathrm{A}}_H(\tau) \equiv \hat{\mathrm{U}}(\tau)^{-1}\hat{\mathrm{A}}_S\hat{\mathrm{U}}(\tau) \equiv \hat{\mathrm{A}}(\tau)\right\}. \tag{13}$$

The *state* dynamics is determined by the *Schrödinger equation* (SE),

$$\mathrm{i}\hbar[d|\varphi_S(t)\rangle/dt] = \hat{\mathrm{H}}|\varphi_S(t)\rangle, \tag{14}$$

which implies the associated derivative of expectation values $\langle A\rangle_\varphi = \langle\varphi_S(t)|\hat{\mathrm{A}}|\varphi_S(t)\rangle$:

$$d\langle A\rangle_\varphi/dt = (\mathrm{i}/\hbar)\langle[\hat{\mathrm{H}}, \hat{\mathrm{A}}]\rangle_\varphi. \tag{15}$$

The important consequence of the preceding relation is the *Ehrenfest principle*, that in quantum mechanics the expectation values of quantum observables obey the associated classical relations, e.g.,

$$d\langle \boldsymbol{r}\rangle_\varphi/dt = \langle \boldsymbol{p}\rangle_\varphi/m, \quad d\langle \boldsymbol{p}\rangle_\varphi/dt = -\langle\nabla v\rangle_\varphi = \langle \boldsymbol{F}\rangle_\varphi; \tag{16}$$

here $v(\boldsymbol{r})$ stands for the external potential due to the fixed nuclei and $\langle \boldsymbol{F}\rangle_\varphi$ is the average force acting on an electron in a molecule.

The corresponding *Heisenberg equation of motion* for the time-dependent quantum observable reads:

$$\mathrm{i}\hbar\frac{d\hat{\mathrm{A}}_H(\tau)}{dt} = [\hat{\mathrm{A}}_H(\tau), \hat{\mathrm{H}}_H(\tau)] = [\hat{\mathrm{A}}, \hat{\mathrm{H}}], \tag{17}$$

since the commutators are picture invariant. It implies the same time dependence of expectation values as in the Schrödinger picture [see Eq. (15)], since the expectation values and commutators are also invariants of the unitary transformation between the two pictures, e.g., $\langle A(t)\rangle_\varphi = \langle\varphi_S(t)|\hat{\mathrm{A}}|\varphi_S(t)\rangle = \langle\varphi|\hat{\mathrm{A}}_H(t)|\varphi\rangle$, and generates the classical relations between *operators*, instead their expectation values [compare Eq. (16)],

$$\frac{d\hat{\mathbf{r}}_H(\tau)}{dt} = \hat{\mathbf{p}}_H(\tau)/m, \quad \frac{d\hat{\mathbf{p}}_H(\tau)}{dt} = -\nabla_{\hat{\mathbf{r}}_H} v[\hat{\mathbf{r}}_H(\tau)] = \hat{\mathbf{F}}_H(\tau). \tag{18}$$

3 Densities and currents

To simplify the present considerations we limit ourselves to a single electron in a general state described by the complex wavefunction in the position representation at time $t_0 \equiv 0$,

$$\varphi(\boldsymbol{r}) = \langle\boldsymbol{r}|\varphi\rangle = R(\boldsymbol{r})\exp[\mathrm{i}\phi(\boldsymbol{r})], \tag{19}$$

moving in the molecular external potential $v(\boldsymbol{r})$ of the Born–Oppenheimer approximation which defines the electronic Hamiltonian $\langle\boldsymbol{r}|\hat{\mathrm{H}}|\boldsymbol{r}'\rangle = \hat{\mathrm{H}}(\boldsymbol{r})\delta(\boldsymbol{r}' - \boldsymbol{r})$,

$$\hat{\mathrm{H}}(\boldsymbol{r}) = (2m)^{-1}\hat{\mathbf{p}}(\boldsymbol{r})^2 + v(\boldsymbol{r}) = -(\hbar^2/2m)\nabla_{\boldsymbol{r}}^2 + v(\boldsymbol{r}) \equiv \hat{\mathrm{T}}(\boldsymbol{r}) + v(\boldsymbol{r}). \tag{20}$$

Here, $\hat{\mathrm{T}}(\boldsymbol{r})$ stands for the kinetic energy operator and $\nabla_{\boldsymbol{r}}^2 = \Delta_{\boldsymbol{r}}$ denotes the *position*-Laplacian. In this representation the SE (14) assumes a simple (diagonal) form:

$$\mathrm{i}\hbar[d\langle\boldsymbol{r}|\varphi(t)\rangle/dt] = \mathrm{i}\hbar[d\varphi(\boldsymbol{r},t)/dt] = \int d\boldsymbol{r}'\langle\boldsymbol{r}|\hat{\mathrm{H}}|\boldsymbol{r}'\rangle\langle\boldsymbol{r}'|\varphi(t)\rangle = \hat{\mathrm{H}}(\boldsymbol{r})\varphi(\boldsymbol{r},t), \tag{21}$$

while its momentum space variant reads [see Eq. (8)]:

$$\begin{aligned}\mathrm{i}\hbar[d\langle\boldsymbol{p}|\varphi(t)\rangle/dt] = \mathrm{i}\hbar[d\bar{\varphi}(\boldsymbol{p},t)/dt] &= \int d\boldsymbol{p}'\langle\boldsymbol{p}|\hat{\mathrm{H}}|\boldsymbol{p}'\rangle\langle\boldsymbol{p}'|\varphi(t)\rangle \\ &= [\boldsymbol{p}^2/(2m)]\bar{\varphi}(\boldsymbol{p},t) + (2\,\pi\,\hbar)^{-3/2}\int d\boldsymbol{p}'\bar{v}(\boldsymbol{p}-\boldsymbol{p}')\bar{\varphi}(\boldsymbol{p}',t).\end{aligned} \tag{22}$$

The wavefunction $\varphi(\boldsymbol{r})$ of Eq. (19) is defined by two (real) functions representing the state *modulus* $R(\boldsymbol{r})$, and (spatial) *phase* $\phi(\boldsymbol{r})$, respectively. These components generate the state two principal distributions, of the *position* probability, $\rho(\boldsymbol{r})$, and current, $\boldsymbol{j}(\boldsymbol{r})$, densities. The former represents the expectation value of the geometric (projection) operator $\hat{\rho}(\boldsymbol{r}) = |\boldsymbol{r}\rangle\langle\boldsymbol{r}|$, when it acts on the state *vectors* $\{|\varphi\rangle\}$ in the electronic Hilbert space, or its effective position representation $\hat{\rho}(\boldsymbol{r}_1;\boldsymbol{r})$,

$$\hat{\rho}(\boldsymbol{r}_1;\boldsymbol{r})\varphi(\boldsymbol{r}) \equiv \langle\boldsymbol{r}_1|\hat{\rho}(\boldsymbol{r})|\varphi\rangle = \langle\boldsymbol{r}_1|\boldsymbol{r}\rangle\langle\boldsymbol{r}|\varphi\rangle = \delta(\boldsymbol{r}_1 - \boldsymbol{r})\varphi(\boldsymbol{r}), \tag{23}$$

when it acts on *wavefunctions* $\{\varphi(\boldsymbol{r})\}$ in the adopted representation,

$$\rho(\boldsymbol{r}) = \langle\varphi|\hat{\rho}(\boldsymbol{r})|\varphi\rangle = |\varphi(\boldsymbol{r})|^2 = R(\boldsymbol{r})^2 = \int \varphi(\boldsymbol{r}_1)^*\hat{\rho}(\boldsymbol{r}_1;\boldsymbol{r})\varphi(\boldsymbol{r})d\boldsymbol{r}_1. \tag{24}$$

The local current density corresponds to the geometric (Hermitian) operator

$$\hat{\mathbf{j}}(\boldsymbol{r}) = \frac{1}{2m}\left[\hat{\rho}(\boldsymbol{r})\hat{\mathbf{p}} + \hat{\mathbf{p}}\hat{\rho}(\boldsymbol{r})\right] = \frac{1}{2}\left[\hat{\rho}(\boldsymbol{r})\hat{\mathbf{V}} + \hat{\mathbf{V}}\hat{\rho}(\boldsymbol{r})\right] \equiv \hat{\mathbf{j}}_S(\boldsymbol{r}) \tag{25}$$

or its effective position representation $\hat{\mathbf{j}}(\boldsymbol{r}_1;\boldsymbol{r})\varphi(\boldsymbol{r}_1) \equiv \langle\boldsymbol{r}_1|\hat{\mathbf{j}}(\boldsymbol{r})|\varphi\rangle$,

$$\begin{aligned}\hat{\mathbf{j}}(\boldsymbol{r}_1;\boldsymbol{r}) &= \frac{1}{2m}\left\{\hat{\rho}(\boldsymbol{r}_1;\boldsymbol{r})\hat{\mathbf{p}}(\boldsymbol{r}) + [\hat{\rho}(\boldsymbol{r}_1;\boldsymbol{r})\hat{\mathbf{p}}(\boldsymbol{r})]^\dagger\right\} \\ &\equiv \frac{1}{2}\left\{\hat{\rho}(\boldsymbol{r}_1;\boldsymbol{r})\hat{\mathbf{V}}(\boldsymbol{r}_1) + \hat{\mathbf{V}}(\boldsymbol{r}_1)\hat{\rho}(\boldsymbol{r}_1;\boldsymbol{r})\right\}.\end{aligned} \tag{26}$$

The average quantum current of the position probability at $\boldsymbol{r}$ thus reads:

$$\begin{aligned}\boldsymbol{j}(\boldsymbol{r}) = \langle\varphi|\hat{\mathbf{j}}(\boldsymbol{r})|\varphi\rangle &= \int \varphi(\boldsymbol{r}_1)^*\hat{\mathbf{j}}(\boldsymbol{r}_1;\boldsymbol{r})\varphi(\boldsymbol{r}_1)d\boldsymbol{r}_1 \equiv \rho(\boldsymbol{r})\boldsymbol{V}(\boldsymbol{r}) \\ &= (1/2)\left\{\langle\varphi|\boldsymbol{r}\rangle\langle\boldsymbol{r}|\frac{\hat{\mathbf{p}}}{m}|\varphi\rangle + [\langle\boldsymbol{r}|\frac{\hat{\mathbf{p}}}{m}|\varphi\rangle]^\dagger\langle\boldsymbol{r}|\varphi\rangle\right\} \\ &= \frac{1}{2}\left\{\varphi^*(\boldsymbol{r})\hat{\mathbf{V}}(\boldsymbol{r})\varphi(\boldsymbol{r}) + [\hat{\mathbf{V}}(\boldsymbol{r})\varphi(\boldsymbol{r})]^*\varphi(\boldsymbol{r})\right\} \\ &= \frac{\hbar}{2m\mathrm{i}}\left[\varphi^*(\boldsymbol{r})\nabla_{\boldsymbol{r}}\varphi(\boldsymbol{r}) - \varphi(\boldsymbol{r})\nabla_{\boldsymbol{r}}\varphi^*(\boldsymbol{r})\right] = \frac{\hbar}{m}\rho(\boldsymbol{r})\nabla_{\boldsymbol{r}}\phi(\boldsymbol{r}).\end{aligned} \tag{27}$$

The magnitude of this flux density represents the position probability transported through unit area in unit time.

In the preceding equation the *effective* local velocity density $\boldsymbol{V}(\boldsymbol{r})$ of the probability "fluid" is determined by the corresponding current-per-particle,

$$\boldsymbol{V}(\boldsymbol{r}) = \boldsymbol{j}(\boldsymbol{r})/\rho(\boldsymbol{r}) = \frac{\hbar}{m}\nabla_{\boldsymbol{r}}\phi(\boldsymbol{r}), \tag{28}$$

shaped by the gradient of the spatial phase alone, while the operator $\hat{\mathbf{V}}$ in Eqs. (25) and (27),

$$\hat{\mathbf{V}} = \hat{\mathbf{p}}/m \quad \text{or} \quad \hat{\mathbf{V}}(\boldsymbol{r}_1)\varphi(\boldsymbol{r}_1) \equiv \langle\boldsymbol{r}_1|\hat{\mathbf{V}}|\varphi\rangle = -\mathrm{i}(\hbar/m)\nabla_{\boldsymbol{r}_1}\varphi(\boldsymbol{r}_1). \tag{29a}$$

corresponds to the classical velocity $\boldsymbol{V}$ (momentum per unit mass) of the probability "fluid".

It also follows from Eq. (4) that

$$\hat{\mathbf{V}}(\boldsymbol{p}_1)\bar{\varphi}(\boldsymbol{p}_1) \equiv \langle\boldsymbol{p}_1|\hat{\mathbf{V}}|\varphi\rangle = \frac{d\hat{\mathbf{r}}(\boldsymbol{p}_1)}{dt} = \mathrm{i}\hbar\frac{d}{dt}[\nabla_{\boldsymbol{p}_1}\bar{\varphi}(\boldsymbol{p}_1)] = \mathrm{i}\hbar\nabla_{\boldsymbol{p}_1}\frac{d\bar{\varphi}(\boldsymbol{p}_1)}{dt}, \tag{29b}$$

where we have recognized that two differential operators with respect to different variables, d/dt and $\nabla_{\boldsymbol{p}} \equiv \partial/\partial \boldsymbol{p}$, commute with one another. The average position velocity in state $|\varphi\rangle$,

$$\begin{aligned}\langle \boldsymbol{V}\rangle_\varphi = \langle\varphi|\hat{\mathbf{V}}|\varphi\rangle &= \int \varphi^*(\boldsymbol{r}_1)[\hat{\mathbf{V}}(\boldsymbol{r}_1)\varphi(\boldsymbol{r}_1)]d\boldsymbol{r}_1 = \int [\hat{\mathbf{V}}(\boldsymbol{r}_1)\varphi(\boldsymbol{r}_1)]^*\varphi(\boldsymbol{r}_1)d\boldsymbol{r}_1 \\ &= \int \boldsymbol{j}(\boldsymbol{r})d\boldsymbol{r} = \langle \boldsymbol{j}\rangle_\varphi = \int \rho(\boldsymbol{r})\boldsymbol{V}(\boldsymbol{r})d\boldsymbol{r} \\ &= (\hbar/m)\int \rho(\boldsymbol{r})\nabla_{\boldsymbol{r}}\phi(\boldsymbol{r})d\boldsymbol{r} = (\hbar/m)\langle\nabla_{\boldsymbol{r}}\phi\rangle_\varphi, \end{aligned} \tag{30}$$

then reflects the state average current, $\langle \boldsymbol{j}\rangle_\varphi$, related to the average gradient of the spatial phase, $\langle\nabla_{\boldsymbol{r}}\phi\rangle_\varphi$.

The time-dependent distributions, equal in both dynamical pictures as expectation values,

$$\begin{aligned}\rho(\boldsymbol{r},t) &= \langle\varphi(t)|\hat{\rho}(\boldsymbol{r})|\varphi(t)\rangle = \langle\varphi|\hat{\rho}_H(\boldsymbol{r},t)|\varphi\rangle \quad \text{and} \\ \boldsymbol{j}(\boldsymbol{r},t) &= \langle\varphi(t)|\hat{\mathbf{j}}(\boldsymbol{r})|\varphi(t)\rangle = \langle\varphi|\hat{\mathbf{j}}_H(\boldsymbol{r},t)|\varphi\rangle, \end{aligned} \tag{31}$$

satisfy the "hydrodynamical" equations [41] [see Eqs. (15) and (17)]:

$$\partial\rho(\boldsymbol{r},t)/\partial t = -\nabla_{\boldsymbol{r}}\cdot\boldsymbol{j}(\boldsymbol{r},t) \quad \text{or} \tag{32}$$

$$\sigma_\rho(\boldsymbol{r},t) \equiv d\rho(\boldsymbol{r},t)/dt = \partial\rho(\boldsymbol{r},t)/\partial t + \nabla_{\boldsymbol{r}}\cdot\boldsymbol{j}(\boldsymbol{r},t) = 0, \tag{33}$$

and

$$\partial\boldsymbol{j}(\boldsymbol{r},t)/\partial t = (\mathrm{i}\hbar)^{-1}\left\langle[\hat{\mathbf{j}}_H(t),\hat{\mathrm{H}}_H(t)]\right\rangle_\varphi = (\mathrm{i}\hbar)^{-1}\left\langle[\hat{\mathbf{j}},\hat{\mathrm{H}}]\right\rangle_{\varphi(t)}. \tag{34}$$

The first of them represents the *continuity equation* for the particle spatial probability distribution. It signifies the sourceless ($\sigma_p = 0$) evolution in time of the system electron density, with the local change in the particle distribution [l.h.s. of Eq. (32)], being effected by the probability outflow alone [r.h.s. of Eq. (32)].

The current density of Eqs. (27) and (31) represents a "flow" aspect of the particle probability distribution in the physical, r-space. It combines the *non-commuting* aspects of the particle position and momentum (velocity). Therefore, in accordance with the Heisenberg's uncertainty principle, it unites the concepts related to the simultaneous measurements of the two incompatible particle properties.

One similarly introduces the probability density and flow concepts in the p-space [29]. The momentum density represents the expectation value of the geometric (projection) operator $\hat{\pi}(\boldsymbol{p}) = |\boldsymbol{p}\rangle\langle\boldsymbol{p}|$, when it acts on state *vectors* $\{|\varphi\rangle\}$ in the electronic Hilbert space, or its effective position representation $\hat{\pi}(\boldsymbol{p}_1;\boldsymbol{p})$,

$$\hat{\pi}(\boldsymbol{p}_1;\boldsymbol{p})\bar{\varphi}(\boldsymbol{p}) \equiv \langle\boldsymbol{p}_1|\hat{\pi}(\boldsymbol{p})|\varphi\rangle = \langle\boldsymbol{p}_1|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\varphi\rangle = \delta(\boldsymbol{p}_1-\boldsymbol{p})\bar{\varphi}(\boldsymbol{p}_1), \tag{35}$$

when it acts on wavefunctions,

$$\bar{\varphi}(\boldsymbol{p}) = M(\boldsymbol{p}) \exp[\mathrm{i}\chi(\boldsymbol{p})], \tag{36}$$

in this representation:

$$\pi(\boldsymbol{p}) = \langle\varphi|\hat{\pi}(\boldsymbol{p})|\varphi\rangle = |\bar{\varphi}(\boldsymbol{p})|^2 = M(\boldsymbol{p})^2 = \int \bar{\varphi}(\boldsymbol{p}_1)^* \hat{\pi}(\boldsymbol{p}_1;\boldsymbol{p})\bar{\varphi}(\boldsymbol{p}_1)d\boldsymbol{p}_1. \tag{37}$$

The density of momentum current now corresponds to the geometric operator

$$\hat{\mathbf{J}}(\boldsymbol{p}) = \frac{1}{m}\hat{\pi}(\boldsymbol{p})\hat{\mathbf{p}} = \hat{\pi}(\boldsymbol{p})\hat{\mathbf{V}} \equiv \hat{\mathbf{J}}_S(\boldsymbol{p}) \tag{38}$$

or its effective momentum representation $\hat{\mathbf{J}}(\boldsymbol{p}_1;\boldsymbol{p})\bar{\varphi}(\boldsymbol{p}_1) \equiv \langle \boldsymbol{p}_1|\hat{\mathbf{J}}(\boldsymbol{p})|\varphi\rangle$,

$$\hat{\mathbf{J}}(\boldsymbol{p}_1;\boldsymbol{p}) = \frac{1}{m}\hat{\pi}(\boldsymbol{p}_1;\boldsymbol{p})\hat{\mathbf{p}}(\boldsymbol{p}_1). \tag{39}$$

For the average current of the momentum probability at $\boldsymbol{p}$ one then finds the following classical flux expression:

$$\begin{aligned}\boldsymbol{J}(\boldsymbol{p}) &= \langle\varphi|\hat{\mathbf{J}}(\boldsymbol{p})|\varphi\rangle = \int \bar{\varphi}(\boldsymbol{p}_1)^*\hat{\mathbf{J}}(\boldsymbol{p}_1;\boldsymbol{p})\bar{\varphi}(\boldsymbol{p}_1)d\boldsymbol{p}_1 \\ &= \langle\varphi|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\frac{\hat{\mathbf{p}}}{m}|\varphi\rangle = \langle\varphi|\boldsymbol{p}\rangle(\boldsymbol{p}/m)\langle\boldsymbol{p}|\varphi\rangle = P(\boldsymbol{p}|\varphi)\boldsymbol{V}(\boldsymbol{p}),\end{aligned} \tag{40}$$

where $P(\boldsymbol{p}|\varphi) = |\langle\boldsymbol{p}|\varphi\rangle|^2 = \pi(\boldsymbol{p})$ stands for the *conditional* probability of observing $|\boldsymbol{p}\rangle$ in $|\varphi\rangle$, $\int P(\boldsymbol{p}|\varphi)d\boldsymbol{p} = 1$, which determines the momentum probability density itself.

This classical momentum current combines the momentum-density $\pi(\boldsymbol{p})$ and the classical particle velocity for the specified momentum $\boldsymbol{p}$, $\boldsymbol{V}(\boldsymbol{p}) = \boldsymbol{p}/m$, i.e., the two *commuting* observables in the p-space, with the momentum density reflecting the momentum-localization aspect of the electronic state $|\varphi\rangle$. Its momentum divergence,

$$\nabla_p \cdot \boldsymbol{J}(\boldsymbol{p},t) = \boldsymbol{V}(\boldsymbol{p}) \cdot \nabla_p\, \pi(\boldsymbol{p},t) + 3\pi(\boldsymbol{p},t)/m, \tag{41}$$

determines the outflow part of the associated continuity equation for momentum probability density [29]:

$$\partial\pi(\boldsymbol{p},t)/\partial t = -\nabla_p \cdot \boldsymbol{J}(\boldsymbol{p},t) + \sigma_\pi(\boldsymbol{p},t). \tag{42}$$

Its nonvanishing source,

$$\sigma_\pi(\boldsymbol{p},t) \equiv d\pi(\boldsymbol{p},t)/dt = \partial\pi(\boldsymbol{p},t)/\partial t + \nabla_p \cdot \boldsymbol{J}(\boldsymbol{p},t) \neq 0, \tag{43}$$

corresponds to the known probability rate $\partial\pi(\boldsymbol{p},t)/\partial t$ resulting from the SE in momentum representation [Eq. (22)] and its Hermitian conjugate:

$$\partial\pi(\boldsymbol{p},t)/\partial t = (2/\hbar)(2\,\pi\,\hbar)^{-3/2}\int d\boldsymbol{p}'\mathrm{Im}\left[\bar{v}(\boldsymbol{p}-\boldsymbol{p}')\gamma(\boldsymbol{p}',\boldsymbol{p};t)\right], \tag{44}$$

where the momentum density matrix [42,43]

$$\gamma(\boldsymbol{p},\boldsymbol{p}';t) = \bar{\varphi}(\boldsymbol{p},t)\bar{\varphi}^*(\boldsymbol{p}',t), \quad \pi(\boldsymbol{p},t) = \gamma(\boldsymbol{p},\boldsymbol{p};t). \tag{45}$$

To summarize, the classical momentum flux gives rise to a generally finite momentum source [29], contrary to the vanishing source term in the position-space.

Interpreting the velocity operator as time-derivative of the position operator [Eq. (29b)],

$$\hat{\mathbf{V}}(\boldsymbol{p};t) = \frac{d}{dt}\hat{\mathbf{r}}(\boldsymbol{p}) = \mathrm{i}\hbar\nabla_p\frac{d}{dt}, \tag{46}$$

generates the alternative expression for the momentum-current operator,

$$\hat{\mathbf{J}}(\boldsymbol{p},t) = \frac{1}{2}\left\{\hat{\pi}(\boldsymbol{p})\frac{d\hat{\mathbf{r}}}{dt} + \frac{d\hat{\mathbf{r}}}{dt}\hat{\pi}(\boldsymbol{p})\right\} \equiv \frac{1}{2}[\hat{\pi}(\boldsymbol{p})\hat{\mathbf{V}}(t) + \hat{\mathbf{V}}(t)\hat{\pi}(\boldsymbol{p})], \tag{47}$$

or its effective form in the momentum representation:

$$\begin{aligned}\hat{\mathbf{J}}(\boldsymbol{p}_1;\boldsymbol{p},t) &= \frac{1}{2}\left\{\hat{\pi}(\boldsymbol{p}_1;\boldsymbol{p},t)\frac{d\hat{\mathbf{r}}(\boldsymbol{p}_1)}{dt} + \frac{d\hat{\mathbf{r}}(\boldsymbol{p}_1)}{dt}\hat{\pi}(\boldsymbol{p}_1;\boldsymbol{p},t)\right\}\\ &= \frac{i\hbar}{2}\left\{\delta(\boldsymbol{p}_1-\boldsymbol{p})\left[\frac{d}{dt}\nabla_{p_1}\right] + \left[\frac{d}{dt}\nabla_{p_1}\right]\delta(\boldsymbol{p}_1-\boldsymbol{p})\right\}.\end{aligned} \tag{48}$$

The expectation value of this flow operator thus combines the momentum density, corresponding to operator $\hat{\pi}(\boldsymbol{p})$, and the momentum-gradient of the time derivative of the wave function $\bar{\varphi}(\boldsymbol{p},t) = \langle\boldsymbol{p}|\varphi(t)\rangle$ [compare Eq. (27)]:

$$\begin{aligned}\boldsymbol{J}(\boldsymbol{p},t) &= \langle\varphi(t)|\hat{\mathbf{J}}(\boldsymbol{p},t)|\varphi(t)\rangle = \int\bar{\varphi}(\boldsymbol{p}_1,t)^*\hat{\mathbf{J}}(\boldsymbol{p}_1;\boldsymbol{p},t)\bar{\varphi}(\boldsymbol{p}_1,t)d\boldsymbol{p}_1\\ &= \frac{i\hbar}{2}\left\{\bar{\varphi}^*(\boldsymbol{p},t)\nabla_p\left[\frac{\partial\bar{\varphi}(\boldsymbol{p},t)}{\partial t}\right] - \bar{\varphi}(\boldsymbol{p},t)\nabla_p\left[\frac{\partial\bar{\varphi}^*(\boldsymbol{p},t)}{\partial t}\right]\right\}\\ &= -\hbar\,\mathrm{Im}\left[\bar{\varphi}^*\nabla_p(\partial\bar{\varphi}/\partial t)\right] \equiv \pi(\boldsymbol{p},t)\boldsymbol{V}(\boldsymbol{p},t).\end{aligned} \tag{49}$$

For a general quantum state of Eq. (36), defined by the (real) modulus (M) and phase (χ) components in the momentum representation,

$$\bar{\varphi}(\boldsymbol{p},t) = M(\boldsymbol{p},t)\exp[\mathrm{i}\chi(\boldsymbol{p},t)], \tag{50}$$

when $\pi(\boldsymbol{p},t) = M(\boldsymbol{p},t)^2$, Eq. (49) gives:

$$\boldsymbol{J}(\boldsymbol{p},t) = -\hbar\, M(\boldsymbol{p},t)\left\{M(\boldsymbol{p},t)\left[\nabla_p\left(\frac{\partial\chi(\boldsymbol{p},t)}{\partial t}\right)\right] + [\nabla_p M(\boldsymbol{p},t)]\left(\frac{\partial\chi(\boldsymbol{p},t)}{\partial t}\right) + \left(\frac{\partial M(\boldsymbol{p},t)}{\partial t}\right)[\nabla_p\chi(\boldsymbol{p},t)]\right\}. \tag{51}$$

This expression also identifies the effective quantum velocity of the momentum fluid [see Eqs. (40) and (49)] defined by the associated current per particle: $\boldsymbol{V}(\boldsymbol{p},t) = \overline{\boldsymbol{J}}(\boldsymbol{p},t)/\pi(\boldsymbol{p},t)$.

4 Alternative "flux" in momentum space and its entropy/information descriptors

One observes that the above classical momentum current is independent of the phase $\chi(\boldsymbol{p})$ in Eq. (36), in terms of which the proposed nonclassical information functionals in p-space have been formulated [29]. Therefore, the two components of $\bar{\varphi}(\boldsymbol{p})$ play distinctly different roles in shaping the nonclassical gradient information contribution in the momentum space, compared to the associated expression in the position space. Moreover, this classical flow concept of the *momentum* probability [Eqs. (25) and (38)] is lacking the conjugate *spatial* input. We recall, that such a mixture of the simultaneous momentum and position descriptors was present in the probability current $\boldsymbol{j}(\boldsymbol{r})$, combining the r-space distributions of both the particle position probability and its momentum (velocity).

In what follows we shall attempt to design an alternative, *phase*-dependent "flux" quantity in p-space, which unites these two incompatible aspects of the particle quantum state and makes expressions for the nonclassical gradient information term isomorphic in two representations [29]. This feature gives an interpretative advantage of using our present, r-space understanding of the roles the modulus (density) and phase (current) degrees-of-freedom of molecular electronic states play in shaping the resultant entropy/information content also in the complementary p-space.

It follows from Eq. (25) that the spatial current operator represents the symmetrized product of the *position*-density and *momentum* operators, thus representing density of the first *momentum*-moment (per unit mass) of spatial probability distribution:

$$\left[position\text{-probability density}\right] \times [momentum]\,/\,[mass]\,.$$

The "symmetrical" concept in the momentum space, though no longer representing the physical flux of the momentum probability distribution, should involve an analogous product of the (noncommuting) *momentum*-density and *position* operators:

$$\hat{\tilde{\mathbf{J}}}(\boldsymbol{p}) = \frac{1}{2m}\left[\hat{\pi}(\boldsymbol{p})\hat{\mathbf{r}} + \hat{\mathbf{r}}\hat{\pi}(\boldsymbol{p})\right] \quad \text{or}$$
$$\hat{\tilde{\mathbf{J}}}(\boldsymbol{p}_1;\boldsymbol{p}) = \frac{1}{2m}\left[\hat{\pi}(\boldsymbol{p}_1;\boldsymbol{p})\hat{\mathbf{r}}(\boldsymbol{p}_1) + \hat{\mathbf{r}}(\boldsymbol{p}_1)\hat{\pi}(\boldsymbol{p}_1;\boldsymbol{p})\right]. \tag{52}$$

This new concept now represents a density of the first *position*-moment (per unit mass) of the momentum probability distribution:

$$\left[momentum\text{-probability density}\right] \times \left[position\right]/\text{mass}.$$

Its expectation value again becomes related to the probability-weighted gradient of the momentum phase function of Eq. (36) [compare Eq. (27)]:

$$\begin{aligned}\overline{\boldsymbol{J}}(\boldsymbol{p}) &= \langle\varphi|\hat{\tilde{\mathbf{J}}}(\boldsymbol{p})|\varphi\rangle = \int \bar{\varphi}^*(\boldsymbol{p}_1)\hat{\tilde{\mathbf{J}}}(\boldsymbol{p}_1;\boldsymbol{p})\bar{\varphi}(\boldsymbol{p}_1)d\boldsymbol{p}_1 \\ &= \left\{\langle\varphi|\boldsymbol{p}\rangle\langle\boldsymbol{p}|\hat{\mathbf{r}}(\boldsymbol{p}_1)|\varphi\rangle + [\langle\boldsymbol{p}|\hat{\mathbf{r}}(\boldsymbol{p}_1)|\varphi\rangle]^\dagger\langle\boldsymbol{p}|\varphi\rangle\right\}/(2m) \\ &= -\frac{\hbar}{2m\mathrm{i}}\left[\bar{\varphi}^*(\boldsymbol{p})\nabla_{\boldsymbol{p}}\bar{\varphi}(\boldsymbol{p}) - \bar{\varphi}(\boldsymbol{p})\nabla_{\boldsymbol{p}}\bar{\varphi}^*(\boldsymbol{p})\right] \\ &= -\frac{\hbar}{m}\pi(\boldsymbol{p})\nabla_{\boldsymbol{p}}\chi(\boldsymbol{p}). \end{aligned} \tag{53}$$

Therefore, this *symmetrical* "flux" concept reflects the negative gradient of the momentum-phase, $-\nabla_{\boldsymbol{p}}\chi(\boldsymbol{p})$. This parallels the role of the position-probability current, which measures the gradient of the spatial phase, $\nabla_{\boldsymbol{r}}\phi(\boldsymbol{r})$.

It is of interest to examine the nonclassical (current related) supplements to the classical (probability based) average entropy/information measures in the two representations. The r-space functionals of such current supplements to the classical Shannon entropy,

$$S^{class.}[\varphi] = S[\rho] = -\int \rho(\boldsymbol{r})\,\log\rho(\boldsymbol{r})d\boldsymbol{r}, \tag{54}$$

and Fisher information,

$$I^{class.}[\varphi] = I[\rho] = \int [\nabla_{\boldsymbol{r}}\rho(\boldsymbol{r})]^2/\rho(\boldsymbol{r})d\boldsymbol{r} = 4\int [\nabla_{\boldsymbol{r}}R(\boldsymbol{r})]^2 d\boldsymbol{r}, \tag{55}$$

respectively, read [20–23]:

$$S^{nclass.}[\varphi] = -2\int \rho(\boldsymbol{r})\phi(\boldsymbol{r})d\boldsymbol{r} \equiv S[\rho,\phi], \tag{56}$$

$$\begin{aligned} I^{nclass.}[\varphi] &= 4\int \rho(\boldsymbol{r})[\nabla_{\boldsymbol{r}}\phi(\boldsymbol{r})]^2 d\boldsymbol{r} \equiv I[\rho,\phi] \\ &= (2m/\hbar)^2\int \rho(\boldsymbol{r})[\boldsymbol{j}(\boldsymbol{r})/\rho(\boldsymbol{r})]^2 d\boldsymbol{r} \equiv I[\rho,\boldsymbol{j}]. \end{aligned} \tag{57}$$

With the selection of the modified "flux" of Eq. (53) the resulting general forms of these functionals remain preserved in the p-space:

$$\begin{aligned} S^{class.}[\bar{\varphi}] &= S[\pi] = -\int \pi(\boldsymbol{p})\, \log\pi(\boldsymbol{p}) d\boldsymbol{p}, \\ S^{nclass.}[\bar{\varphi}] &= -2\int \pi(\boldsymbol{p})\chi(\boldsymbol{p}) d\boldsymbol{p} \equiv S[\pi, \chi], \\ I^{class.}[\bar{\varphi}] &= I[\pi] = \int [\nabla_p \pi(\boldsymbol{p})]^2/\pi(\boldsymbol{p}) d\boldsymbol{p} = 4\int [\nabla_p M(\boldsymbol{p})]^2 d\boldsymbol{p}, \\ I^{nclass.}[\bar{\varphi}] &= 4\int \pi(\boldsymbol{p})[\nabla_p \chi(\boldsymbol{p})]^2 d\boldsymbol{p} \equiv I[\pi, \chi] \\ &= (2m/\hbar)^2 \int \pi(\boldsymbol{p})[\overline{\boldsymbol{J}}(\boldsymbol{p})/\pi(\boldsymbol{p})]^2 d\boldsymbol{p} \equiv I[\pi, \overline{\boldsymbol{J}}]. \end{aligned} \tag{58}$$

(59)

This modified momentum "current" thus makes the associated nonclassical information terms in p-space isomorphic with their corresponding expressions in r-space. The modulus and phase components now play analogous roles in shaping the classical and nonclassical information components of quantum states in both representations: the nonclassical supplements of the Shannon entropy reflect the state average phases, while the nonclassical Fisher terms measure the average magnitudes of the phase gradients, i.e., of the corresponding currents per particle.

The new p-flux measure determines the associated momentum divergence [compare Eq. (41)]:

$$\nabla_p \cdot \overline{\boldsymbol{J}}(\boldsymbol{p}, t) = -\frac{\hbar}{m}\left[\nabla_p \pi(\boldsymbol{p}) \cdot \nabla_p \chi(\boldsymbol{p}) + \pi(\boldsymbol{p})\Delta_p \chi(\boldsymbol{p})\right]. \tag{60}$$

It defines the corresponding outflow part of the momentum probability density in the associated p-space continuity relation [see Eqs. (42)–(44)]:

$$\partial\pi(\boldsymbol{p}, t)/\partial t = -\nabla_p \cdot \overline{\boldsymbol{J}}(\boldsymbol{p}, t) + \bar{\sigma}_\pi(\boldsymbol{p}, t). \tag{61}$$

The latter introduces the modified momentum-probability source,

$$\bar{\sigma}_\pi(\boldsymbol{p}, t) \equiv d\pi(\boldsymbol{p}, t)/dt = \partial\pi(\boldsymbol{p}, t)/\partial t + \nabla_p \cdot \overline{\boldsymbol{J}}(\boldsymbol{p}, t), \tag{62}$$

where the local rate of change in the momentum density, $\partial\pi(\boldsymbol{p}, t)/\partial t$, is defined by Eq. (44).

To conclude this section, we emphasize that the quantum estimate of the particle velocity, the time derivative of the position operator, remains invariant of the adopted dynamical picture [see Eqs. (16) and (18)],

$$\boldsymbol{V}_S(\boldsymbol{r}, t) \equiv \langle\varphi(t)|\hat{\mathbf{p}}/m|\varphi(t)\rangle = \langle\varphi|\hat{\mathbf{p}}_H(t)/m|\varphi\rangle \equiv \boldsymbol{V}_H(\boldsymbol{r}, t). \tag{63}$$

and so is the classical momentum current [compare Eq. (31)]:

$$\boldsymbol{J}_S(\boldsymbol{p},t) \equiv \langle\varphi(t)|\hat{\mathbf{J}}(\boldsymbol{p})|\varphi(t)\rangle = \langle\varphi|\hat{\mathbf{J}}_H(\boldsymbol{p},t)|\varphi\rangle \equiv \boldsymbol{J}_H(\boldsymbol{p},t)$$
$$= \langle\varphi(t)|\boldsymbol{p}\rangle(\boldsymbol{p}/m)\langle\boldsymbol{p}|\varphi(t)\rangle = P[(\boldsymbol{p}|\varphi);t]\boldsymbol{V}(\boldsymbol{p}). \quad (64)$$

5 Illustrative examples

As an illustration of these flow concepts let us first consider the simplest case of a free motion along x-axis with momentum $p_x \equiv p = k\hbar \equiv Vm$. When the position is sharply specified at $x = x'$, for the vanishing position dispersion, the particle exhibits the infinitely sharp probability distribution $\rho(x) = \delta(x - x')$ in state $u_{x'}(x) = \langle x|x'\rangle = \delta(x - x') \equiv \varphi(x)$, which can be expressed in terms of eigenstates $u_k(x') = \langle x'|k\rangle = (2\,\pi)^{-1/2}\exp(\mathrm{i}kx')$ of the momentum operator,

$$\varphi(x) = \langle x|x'\rangle = \int \langle x|k\rangle\langle k|x'\rangle dk = \int u_k(x)u_k(x')^* dk = \delta(x - x'), \quad (65)$$

In accordance with the superposition principle of quantum mechanics the modulus square of the expansion coefficient,

$$u_k(x')^* = \langle k|x'\rangle = u_{x'}(k) = (2\,\pi)^{-1/2}\int \exp(-\mathrm{i}kx)u_{x'}(x)dx$$
$$= (2\,\pi)^{-1/2}\exp(-\mathrm{i}kx') = \bar{\varphi}(k), \quad (66)$$

dertermines the state uniform momentum probability, giving rise to its infinite dispersion,

$$\pi(k) = \langle x'|k\rangle\langle k|x'\rangle = u_{x'}(k)^* u_{x'}(k) = (2\,\pi)^{-1} = const. \quad (67)$$

The associated time-dependent (stationary) wavefunctions then read:

$$\varphi(x,t) = \varphi(x)\exp(-\mathrm{i}\omega t) \quad \text{and} \quad \bar{\varphi}(k,t) = \bar{\varphi}(k)\exp(-\mathrm{i}\omega t),$$
$$\omega = p^2/(2m\hbar) = k^2\hbar/(2m). \quad (68)$$

The resultant momentum phase of $\bar{\varphi}(k,t)$ thus reads:

$$\chi(k,t) = -kx' - [\hbar k^2/(2m)]t. \quad (69)$$

For this *position*-localized model state one predicts the following probability fluxes:

$$j(x,t) = \frac{\hbar}{m}\rho(x,t)\frac{\partial\phi(x,t)}{\partial x} = 0,$$
$$J(p,t) = (2\,\pi)^{-1}V = [\pi(k)/m]\,\hbar k \equiv \hbar J(k) \quad \text{and}$$
$$\overline{J}(p,t) = -\frac{\hbar}{m}\pi(p,t)\frac{\partial\chi(p,t)}{\partial p} = (2\,\pi\,m)^{-1}(x' + Vt). \quad (70)$$

The vanishing position current $j(x,t)$ is due to the vanishing spatial phase $\phi(x)=0$. In the classical momentum current $J(p,t)=J(p)$ the uniform distribution $\pi(p,t)=\pi(p)$ of the momentum probability density is flowing with constant classical velocity $V=p/m$, while the modified concept $\overline{J}(p)$ combines the constant momentum distribution with the particle time-dependent position $x(t)=x'+Vt$.

Consider next the localized case in p-space, for the vanishing momentum dispersion, when the particle momentum is sharply specified at $p=p'=\hbar k'=mV'$ for $\pi(p)=\delta(p-p')$. The particle is then in the state $u_{k'}(k)=\langle k|k'\rangle=\delta(k-k')\equiv\bar{\varphi}(k)$ or in its time-dependent, stationary form for the kinetic energy $E'=\hbar\omega'=(p')^2/(2m)$:

$$\begin{aligned}\bar{\varphi}(k,t)&=\bar{\varphi}(k)\exp(-\mathrm{i}\omega' t)\equiv\delta(k-k')\exp[\mathrm{i}\chi(k',t)],\\ \omega'&=(p')^2/(2m\hbar)=k'^2\hbar/(2m).\end{aligned}\tag{71}$$

Its expansion in terms of eigenstates of the position operator,

$$u_x(k)=\langle k|x\rangle=u_k(x)^*=(2\,\pi)^{-1/2}\exp(-\mathrm{i}kx),\tag{72}$$

$$\bar{\varphi}(k)=\langle k|k'\rangle=\int\langle k|x\rangle\langle x|k'\rangle dx=\int u_x(k)u_x(k')^*dx=\delta(k-k'),\tag{73}$$

now gives the uniform distribution of the position probability, i.e., the infinite dispersion of the particle spatial location. It is determined by the modulus square of the expansion coefficient, the inverse Fourier transform of $\bar{\varphi}(k)$,

$$\begin{aligned}&u_x(k')^*=u_{k'}(x)=(2\,\pi)^{-1/2}\exp(\mathrm{i}k'x)=\varphi(x)=(2\,\pi)^{-1/2}\exp[\mathrm{i}\phi(x)],\\ &\text{or }\varphi(x,t)=\varphi(x)\exp[\mathrm{i}\omega' t],\end{aligned}\tag{74}$$

$$\rho(x)=\langle k'|x\rangle\langle x|k'\rangle=u_{k'}(x)^*\,u_{k'}(x)=(2\,\pi)^{-1}=const.\tag{75}$$

The *momentum*-localized state of Eq. (71) corresponds to the resultant momentum phase $\chi(k,t)=-\omega' t$ and gives the following current predictions [see Eq. (70)]:

$$\begin{aligned}j(x,t)&=\frac{\hbar}{m}\rho(x)\frac{d\phi(x)}{dx}=(2\,\pi\,m)^{-1}\hbar k'=\rho(x)V',\\ J(p,t)&=\delta(p-p')(p/m)=\pi(p)V(p),\\ \overline{J}(p,t)&=-\frac{\hbar}{m}\pi(p,t)\frac{\partial\chi(p,t)}{\partial p}=\delta(p-p')V't/m.\end{aligned}\tag{76}$$

Next, let us examine the *stationary* electronic states $\{|\psi(t;E)\rangle\}$ corresponding to the sharply specified energy $E=const.$, one of the Hamiltonian eigenvalues and generating the time-independent probability distribution. They have been previously classified [20–23] as being either the *strong*- or *weak*-stationary in character, when they give rise to zero or finite current of the position probability, respectively. The former correspond to the vanishing spatial phase $\phi(\boldsymbol{r})$, e.g., in the standing-wave state of the free particle or nondegenerate molecular state, while the latter exhibit a finite

spatial phase, e.g., in the *plane*-wave state of the free motion or in degenerate states of molecules.

In the position representation the wave-function of a stationary electronic state reads

$$\psi(\boldsymbol{r}, t; E) = \varphi(\boldsymbol{r}; E) \exp[-\mathrm{i}\omega(E)t], \quad \omega(E) = E/\hbar. \tag{77}$$

It marks the time-independent probability distribution in the physical space:

$$\rho(\boldsymbol{r}, t; E) = |\psi(\boldsymbol{r}, t; E)|^2 = |\varphi(\boldsymbol{r}; E)|^2 = \rho(\boldsymbol{r}; E). \tag{78}$$

In such states the associated current density is also stationary:

$$\boldsymbol{j}(\boldsymbol{r}, t; E) = \langle \psi(t; E)|\hat{\mathbf{j}}(\boldsymbol{r})|\psi(t; E)\rangle = \int \varphi(\boldsymbol{r}_1; E)^* \hat{\mathbf{j}}(\boldsymbol{r}_1; \boldsymbol{r})\varphi(\boldsymbol{r}_1; E) d\boldsymbol{r}_1 = \boldsymbol{j}(\boldsymbol{r}; E). \tag{79}$$

In fact, this is true for the expectation value of any observable, which does not depend on time explicitly, e.g., $\hat{\mathrm{F}} = \{\hat{\rho}(\boldsymbol{r}) \quad \text{or} \quad \hat{\mathbf{j}}(\boldsymbol{r})\}$,

$$\langle F \rangle = \langle \psi(t; E)|\hat{\mathrm{F}}|\psi(t; E)\rangle = \int \varphi(\boldsymbol{r}; E)^* \, \hat{\mathrm{F}}(\boldsymbol{r})\varphi(\boldsymbol{r}; E) d\boldsymbol{r}. \tag{80}$$

It should be recalled, however, that the physical quantity F is sharply specified, as one of the $\hat{\mathrm{F}}$ eigenvalues $\{F_i\}, \hat{\mathrm{F}}|\zeta_i\rangle = F_i|\zeta_i\rangle$, only when $[\hat{\mathrm{F}}, \hat{\mathrm{H}}] = 0$. For example, for the free motion of a particle, when $v(\boldsymbol{r}) = 0, \hat{\mathrm{H}} = \hat{\mathrm{T}} = \hat{\mathbf{p}}^2/(2m)$, and $E(\boldsymbol{p}) = \boldsymbol{p}^2/(2m) \equiv \hbar\omega(\boldsymbol{p})]$, the system stationary state of plane-wave,

$$\psi(\boldsymbol{r}, t; \boldsymbol{p}) = \langle \boldsymbol{r}|\psi[t; E(\boldsymbol{p})]\rangle = A \exp\{\mathrm{i}[\boldsymbol{k} \cdot \boldsymbol{r} - \omega(\boldsymbol{p})t]\}, \tag{81}$$

constitutes the common eigenstate of the Hamiltonian, momentum and current operators, since then $[\hat{\mathbf{j}}(\boldsymbol{r}), \hat{\mathrm{H}}] = [\hat{\mathbf{j}}(\boldsymbol{r}), \hat{\mathrm{T}}] = 0$. Such (*weak*) stationary state generate a finite classical current of the position probability in the direction of the system specified momentum $\boldsymbol{p} = \hbar\boldsymbol{k}$:

$$\boldsymbol{j}(\boldsymbol{r}, t; \boldsymbol{p}) = \frac{\hbar}{m}|A|^2\boldsymbol{k}, \tag{82}$$

while the classical momentum current of Eq. (40) reads: $\boldsymbol{J}(\boldsymbol{p}', t; \boldsymbol{p}) = (\boldsymbol{p}/m)\delta(\boldsymbol{p}' - \boldsymbol{p})$.

The Fourier transform of the stationary state also involves the time-independent modulus component $M(\boldsymbol{p}; E)$ of the classical amplitude $\bar{\varphi}(\boldsymbol{p}; E)$ of the momentum density:

$$\begin{aligned} &\pi(\boldsymbol{p}, t; E) = |\bar{\psi}(\boldsymbol{p}, t; E)|^2 = |\bar{\varphi}(\boldsymbol{p}; E)|^2 = \pi(\boldsymbol{p}; E) = M(\boldsymbol{p}; E)^2, \\ &\bar{\psi}(\boldsymbol{p}, t; E) = \bar{\varphi}(\boldsymbol{p}; E) \exp[-\mathrm{i}\omega(E)t], \quad \bar{\varphi}(\boldsymbol{p}; E) \equiv M(\boldsymbol{p}; E) \exp[\mathrm{i}\chi(\boldsymbol{p}; E)]. \end{aligned} \tag{83}$$

It exhibits the resultant p-space phase, combining the momentum and time contributions,

$$\chi(\boldsymbol{p}, t; E) = \chi(\boldsymbol{p}; E) - \omega(E)t. \tag{84}$$

Therefore, for the stationary state $\partial M/\partial t = 0, \partial\chi/\partial t = -\omega(E) = const.$, and hence $\nabla_{\boldsymbol{p}}(\partial\chi/\partial t) = \boldsymbol{0}$. Thus, only the second term in Eq. (51) contributes to the quantum current in p-space. One then predicts a finite density of the quantum current of momentum probability shaped by the gradient of momentum density alone:

$$\overline{\boldsymbol{J}}(\boldsymbol{p}, t; E) = EM(\boldsymbol{p}; E)\nabla_{\boldsymbol{p}} M(\boldsymbol{p}; E) = (E/2)\nabla_{\boldsymbol{p}}\pi(\boldsymbol{p}; E). \tag{85}$$

Thus, the *strong*-stationary (*zero*-current) state in the r-space generally implies the *weak*-stationary (*finite*-current) state in the p-space. This reemphasizes a need for the nonclassical (current-related) information measures of the QIT description in the momentum-space [29].

For the free motion in 3 dimensions, $v(\boldsymbol{r}) = 0$, at constant energy $E(\boldsymbol{p}) = \boldsymbol{p}^2/(2m) = \hbar\omega(\boldsymbol{p})$ determined by the fixed particle momentum $\boldsymbol{p} = \hbar\boldsymbol{k} = m\boldsymbol{V}$, i.e., $\pi[\boldsymbol{p}', t; E(\boldsymbol{p})] = \delta(\boldsymbol{p}' - \boldsymbol{p})$, the stationary state of a particle is described by the *plane*-wave of Eq. (81), which predicts a constant density of the space probability distribution, $\rho(\boldsymbol{r}, t; E) = |A|^2$. i.e., the infinite position dispersion, and the spatial current in the $\boldsymbol{p}$ direction [Eq. (82)]. This is in accord with the state momentum representation

$$\bar{\psi}(\boldsymbol{p}', t; \boldsymbol{p}) = \langle \boldsymbol{p}'|\boldsymbol{p}\rangle \exp[-\mathrm{i}\omega(\boldsymbol{p})t] = \delta(\boldsymbol{p}' - \boldsymbol{p}) \exp[-\mathrm{i}\omega(\boldsymbol{p})t], \tag{86}$$

which implies the vanishing momentum dispersion. Its infinitely sharp amplitude gives rise to the classical momentum current $\boldsymbol{J}(\boldsymbol{p}, t) = \delta(\boldsymbol{p}' - \boldsymbol{p})(\boldsymbol{p}/m) = (\hbar/m)\delta(\boldsymbol{k}' - \boldsymbol{k})\boldsymbol{k}$, while the modified momentum current of Eq. (53) reads:

$$\overline{\boldsymbol{J}}(\boldsymbol{p}, t; E) = \pi(\boldsymbol{p}, t; E)\boldsymbol{V}t/m. \tag{87}$$

Finally, let us briefly examine the wave-packets, again limiting ourselves, for reasons of simplicity, to the one-dimensional case. The initial Gaussian "signal" in r-space,

$$\psi(x, t = 0) = a^{-1/2}(2\,\pi)^{-1/4} \exp\{-[x/(2a)]^2\} \exp(\mathrm{i}k_0 x), \tag{88}$$

which generates the normalized *position*-probability distribution

$$\rho(x, t = 0) = a^{-1}(2\,\pi)^{-1/2} \exp[-x^2/(2a^2)], \quad \int \rho(x, t = 0)dx = 1, \tag{89}$$

of height $h_x(t = 0) = a^{-1}(2\,\pi)^{-1/2}$, represents a particle localized around $x = 0$ in the range $\Delta x = a \equiv w_x(t = 0)$, as measured by the width of $\rho(x, t = 0)$, moving with the average momentum $\langle p\rangle = \hbar k_0$.

In the p-space this state also generates the Gaussian wave-function

$$\bar{\psi}(k, t=0) = a^{-1/2}(2\pi)^{-3/4} \int \exp\left\{-[x'/(2a)]^2\right\} \exp[\mathrm{i}x'(k_0 - k)]dx' = [2a/(2\pi)^{1/2}]^{1/2} \exp[-a^2(k_0 - k)^2] = M(k, t), \quad (90)$$

and the associated momentum distribution

$$\pi(k, t=0) = [2a/(2\pi)^{1/2}] \exp[-2a^2(k_0 - k)^2]. \quad (91)$$

The latter corresponds to the wave-number distribution of height $h_k(t=0) = [2a/(2\pi)^{1/2}]$ in the range $\Delta k = (2a)^{-1} \equiv w_k(t=0)$ around k_0, or the momentum width $\Delta p = (2a)^{-1}\hbar \equiv w_p(t=0)$ around $p_0 = \hbar k_0$, thus generating the Heisenberg product of simultaneous "uncertainties" of the particle position and momentum:

$$\Delta x\, \Delta p = \Delta x\, \hbar\, \Delta k = \hbar/2. \quad (92)$$

The r-space current in this state reads:

$$j(x, t=0) = (\hbar/m)\rho(x, t=0)k_0 = \rho(x, t=0)[\langle p\rangle/m] = \rho(x, t=0)\langle V\rangle, \quad (93)$$

where the classical *group* velocity $\langle V\rangle = \langle p\rangle/m = \hbar(k_0/m) \equiv V_0$. The associated current in p-space gives

$$J(p, t=0) = \pi(k, t=0)V_0. \quad (94)$$

Since in the wavefunction of Eq. (90) the momentum phase $\chi(k, t)$ identically vanishes, one finds from Eq. (53) the vanishing modified flow descriptor of the particle momentum probability:

$$\overline{J}(p, t=0) = 0. \quad (95)$$

These predictions remain valid in any finite time $t > 0$, when one replaces the initial width (w) and hight (h) descriptors with their desolved analogs after time t:

$$w_x(t=0) \to w_x(t) = w_x(t=0)[1 + (t/\tau_0)^2]^{1/2} \equiv w_x(t=0)f(t), \quad \text{around } x_0(\mathrm{t}) = V_0 t, \quad \tau_0 = k_0^2 a^2/\omega_0, \quad \omega_0 = \hbar k_0^2/(2m); \quad (96)$$

$$w_k(t=0) \to w_k(t) = w_k(t=0)/f(t), \quad \text{around } k_0, \quad (97)$$

$$h_x(t=0) \to h_x(t) = h_x(t=0)/f(t). \quad (98)$$

6 Conclusion

To accommodate the complex wavefunctions of molecular electronic states the non-classical (phase/current)-related supplements of the classical (probability) descriptors

of the entropy/ information content are required in the resultant QIT approach. In the position representation the quantum-generalized gradient measure of the Fisher (*determinicity*) information involves a contribution due to the probability current (phase gradient), which gives rise to a *non*-vanishing information source. It is related to the dimentionless ("reduced") expectation value of the system electronic kinetic energy. The resultant entropy of the Shannon (*indeterminicity*) information descriptor similarly involves the negative average phase contribution, which complements the familiar Shannon functional of the electron probability distribution. This extension satisfies the requirement that the relation between the classical Shannon and Fisher information densities extends into the nonclassical (quantum) domain, between the entropy/information densities due to the state phase/current. Similar generalized descriptors of both the resultant information content and entropy-deficiency (information-distance [5,6]) have been introduced in p-space [29]. The continuity equation for the momentum density has been shown to exhibit a nonvanishing probability source. The Fourier transforms of the *strong*-stationary (*zero*-current) states in the position representation, were shown to give rise to the *weak*-stationary (*finite*-current) states in the momentum space. This observation strengthens the need for the nonclassical information supplements in the molecular quantum mechanics.

A composition of the probability and current distributions in the position and momentum spaces is quite different. The chemically most important *external* (large r) valence region of the electron density corresponds to the *internal* (low p) region of the momentum density. The former gives rise to a sourceles continuity relation, while the latter exhibits a finite source term conditional on the adopted flux definition. The states exhibiting vanishing flow term in r-space generally exhibit a finite current in p-space, so that the importance of nonclassical information terms increases in the momentum representation of quantum mechanics. Their transparent interpretation in terms of the moduli and phases of the complex wavefunctions in position space facilitates a discussion of the information origins of the chemical bond, promotion of bonded atoms, etc. [23,25,26]. Since different current definitions only redistribute the time-rate of change in the momentum density (determined by SE) between the outflow (divergence) and source contributions in the momentum-continuity equation [26], for interpretative purposes it is desirable to define the momentum flux concept in such a way, that the resulting expressions for the nonclassical information supplements remain isomorphic in the two spaces. In this work we have succeded in defining such a very momentum-probability "flow" concept, a quantity "symmetrical" with respect to the known position-probability current.

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