International Journal of Theoretical Physics, Vol. 41, No. 9, September 2002 (© 2002)

Statistics of Local Value in Quantum Mechanics

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Received February 23, 2002

Given a quantum mechanical observable and a state, one can construct a *classical* observable, that is, a real function on the configuration space, such that it is the optimal estimate of the quantum observable, in the sense of minimum variance. This optimal estimate turns out to be the quantum mechanical local value, which arises from several contexts such as de Broglie–Bohm's casual approach to quantum mechanics, instantaneous frequency in time–frequency analysis, Nelson's quantum fluctuations formalism, and phase-space approach to quantum mechanics. Accordingly, any observable can be decomposed into a local value part and a quantum fluctuation part, which are independent, both geometrically and statistically. Furthermore, the current density in quantum mechanics, the osmotic velocity in stochastic mechanics, and the Fisher information in classical statistical inference, arise naturally in connection with local value. In particular, Heisenberg uncertainty principle can be quantified more precisely by virtue of local value.

KEY WORDS: local value; classical observable; Fisher information; conditional expectation; Heisenberg uncertainty principle.

1. INTRODUCTION

Classical mechanics is a deterministic theory, and there is no room for fluctuations in principle, except when we are content to make some approximations (e.g. in statistical mechanics). In quantum mechanics, things change radically, since quantum mechanics is inherently probabilistic, and the Heisenberg uncertainty principle places the irreducible fluctuations in a principle place. However, de Broglie and Bohm have demonstrated that deterministic particle trajectories is compatible with quantum mechanics (Bohm, 1952; Bohm and Hiley, 1995; Holland, 1993; the idea dates back to de Broglie in 1927). Their quantum potential theory points to the possibility and usefulness of assigning values of quantum observables at each point of the configuration space. This is in contrast to the orthodox quantum theory, which lays undue emphasis on global quantities (global

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averages). The notion of quantum mechanical local value manipulates a balance between a quantum observable itself (which cannot be exactly measured in a representation diagonalizing its conjugate observable) and its simple global average. As emphasized by Bell (1987), Bohmian mechanics is essentially equivalent to the standard quantum mechanics, but the pictures and viewpoints are somewhat different. The fact that it is not as widely accepted as Feynman's imaginary time path integral approach may be purely due to historical accidents. While Heisenberg uncertainty principle prohibits the possibility of simultaneously assigning exact values to conjugate observables, it is possible to reconcile the complementarity by assigning *exact* value to one observable (served as a reference observable, representation observable) and an optimum *statistical average* to the conjugated one at each value of the reference observable. The notion of local value implements such a idea (Cohen, 1996; Holland, 1993; Wan and Sumner, 1988). A local value of an observable in a state (wave function) is the representing operator acting on the wave function, divided by the wave function, and taking the real part. Prominent examples are quantum mechanical current density, Bohm's quantum potential, and instantaneous frequency. See the remarkable monographs of Holland (1993) and of Bohm and Hiley (1995) for extensive accounts.

The main point of local value is to exploit the complex structure inherent in the mathematical formalism of quantum mechanics, and may be briefly summarized as follows. First fix a reference observable (e.g. the position), and let the quantum system Hilbert space be $\mathcal{H}$ and a wave function $\psi \in \mathcal{H}$ be realized as a function in the representation diagonalizing the fixed reference observable. Let another observable A be represented as a self-adjoint operator on $\mathcal{H}$; we may take $\mathcal{H} = L^2(\mathbb{R})$. Consider the average

$$\langle A\rangle_\psi = \int \psi^* A\psi \, dq = \int \mathrm{Re}\left(\frac{\psi^* A\psi}{\psi^*\psi}\right) |\psi|^2 \, dq + i \int \mathrm{Im}\left(\frac{\psi^* A\psi}{\psi^*\psi}\right) |\psi|^2 \, dq.$$

Since $\langle A\rangle_\psi$ is a real number, the contribution of the average is only from the first term, $\mathrm{Re}(\frac{\psi^* A\psi}{\psi^*\psi})$. This motivates to split $\frac{\psi^* A\psi}{\psi^*\psi} = \frac{A\psi}{\psi}$ into its real and imaginary parts as

$$\frac{A\psi}{\psi} = \mathrm{Re}\left(\frac{A\psi}{\psi}\right) + i\,\mathrm{Im}\left(\frac{A\psi}{\psi}\right).$$

This seemingly simple and naive decomposition has intuitive physical significance and interesting mathematical consequences. Phrased roughly, the real part (local value) corresponds to a classical approximation of A. The imaginary part (the local spread) is of purely fluctuation character, and is connected with Nelson's quantum fluctuations in his stochastic mechanics formalism (Nelson, 1966, 1985). In this formalism, Nelson derived the Schrödinger equation from Newtonian mechanics plus stochastic perturbation (fluctuation), an assumed Markov diffusion process induced by various fluctuations of a background field. The mysteries and counterintuitive effects of quantum phenomena have their origin in the imaginary part (quantum fluctuations). The key issue related to local value is this: for any physical observable, it is possible to decompose it as a systematic part (local value) relative to a reference observable, and an irreducible fluctuation part (local spread) arising from the incompatible nature of the observable with the reference one. The notion of local value is introduced in several contexts and has been studied by a lot of authors (Bohm, 1952; Cohen, 1996; Holland, 1993; Wan and Summer, 1988).

If ψ is an eigenvector of A with eigenvalue a, that is, $A\psi = a\psi$, then

$$\mathrm{Re}\left(\frac{A\psi}{\psi}\right) = a, \qquad \mathrm{Im}\left(\frac{A\psi}{\psi}\right) = 0$$

as desired. Thus in an eigenvector of A, the local value of A is exactly its eigenvalue, and the local spread is zero. Otherwise, the local spread is not zero in general, which represents a fluctuation arising from the imaginary part. Moreover, we have $\langle A\rangle_\psi = \langle \mathrm{Re}(\frac{A\psi}{\psi})\rangle_\psi$ and

$$\begin{aligned}\mathrm{Var}_\psi(A) = &\int \left(\mathrm{Re}\left(\frac{A\psi}{\psi}\right) - \langle A\rangle_\psi\right)^2 |\psi(q)|^2\, dq \\ &+ \int \left(\mathrm{Im}\left(\frac{A\psi}{\psi}\right)\right)^2 |\psi(q)|^2\, dq.\end{aligned} \tag{1}$$

From Eq. (1), Cohen (1996) interprets $\mathrm{Re}(\frac{A\psi}{\psi})$ as the local value of the observable A (it is "local" in virtue of being a function in configuration space of the reference observable), and $\mathrm{Im}(\frac{A\psi}{\psi})$ as its local spread. Thus the variance of an observable consists of as two terms: one of local value and one of local spread.

The purpose of this paper is to present some statistical interpretations of the notion of local value and to investigate its fundamental properties. We focus on its mathematical and physical aspects, ignoring completely its philosophy in relation to Bohmian mechanics. In the course, we see how the quantum mechanical current density, the Heisenberg uncertainty relations, and the Fisher information arise naturally. We will relate local value to conditional expectation and the properties of phase-space quasi-probabilities. The paper is organized as follows: In Section 2, we address a statistical inference problem motivated by simultaneous measurement of two conjugate quantum observables, and demonstrate how local value manifests itself as the optimum solution. Local value interpolates between the quantum observable and its global average. Some fundamental properties of local value are uncovered, and several examples are illustrated. In Section 3, we study the relationships between local value and Fisher information, and examine the origin of the uncertainty in the Heisenberg uncertainty principles. In Section 4, we relate local value with conditional expectation and phase-space distributions, and show that local value is consistent with conditional expectation if we employ phase-space formulation of quantum mechanics. Section 5 is devoted to the extension of local value to non-self-adjoint operators, which may find applications in quantum detection and estimation theory. Finally, Section 6 concludes with some discussions.

2. QUANTUM OBSERVABLE, LOCAL VALUE, AND STATISTICAL ESTIMATION

Consider a quantum system, whose pure state space is the complex Hilbert space $L^2(\mathbb{R})$ (we will only work in position representation). Let $\psi \in L^2(\mathbb{R})$ be a normalized wave function, and A be a quantum mechanical observable, which is a self-adjoint operator on $L^2(\mathbb{R})$. The probability space $(\mathbb{R}, |\psi(q)|^2\, dq)$ may be considered as a classical world in which the position observable and all observables commuting with it can be assigned exact values. The following statistical estimation problem arise naturally: What is the best classical estimate of A, when the quantum system is in the state ψ? More precisely, we want to find a classical observable, that is, a *real function* $\overline{A} = \overline{A}(q)$ on $\mathbb{R}$ (rather than an operator on $L^2(\mathbb{R})$), such that the variance

$$\mathrm{Var}_\psi(A - \overline{A})$$

is minimized subject to the condition $\langle \overline{A} \rangle_\psi = \langle A \rangle_\psi$. Here we have interpreted $\overline{A}$ as a multiplication operator on $L^2(\mathbb{R})$. Alternatively, we may also interpreted $\overline{A} = \overline{A}(q)$ as a classical random variable on the probability space $(\mathbb{R}, |\psi(q)|^2\, dq)$. By the spectral theorem of self-adjoint operators in Hilbert spaces, $\overline{A}$ is essentially a real function of the position observable Q, and thus commutes with Q.

Theorem 1. *The unique solution of the optimization problem*

$$\min_{\overline{A}} \ \mathrm{Var}_\psi(A - \overline{A}), \qquad \textit{subject to} \quad \langle \overline{A} \rangle_\psi = \langle A \rangle_\psi$$

is

$$\overline{A}(q) = \mathrm{Re}\left(\frac{A\psi}{\psi}\right)(q). \tag{2}$$

Moreover, we have

$$\mathrm{Var}_\psi(A - \overline{A}) = \int \left(\mathrm{Im}\left(\frac{A\psi}{\psi}\right)\right)^2 |\psi|^2\, dq.$$

Proof: The result follows from a simple application of the Lagrangian multiplier method and calculus of variations. Consider the Lagrangian

$$L(\overline{A}) := \mathrm{Var}_\psi(A - \overline{A}) - \lambda(\langle \overline{A} \rangle_\psi - \langle A \rangle_\psi).$$

In order to minimize $L(\bar{A})$, taking variation with respect to $\bar{A}$ (perturbing $\bar{A}$ by a small quantity $t\delta\bar{A}$, $\delta\bar{A}$ is a real function on $\mathbb{R}$), we have

$$\frac{\partial}{\partial t}L(\bar{A}+t\delta\bar{A}) = -\psi|A\delta\bar{A}|\psi\rangle - \langle\psi|\delta\bar{A}A|\psi\rangle + 2\langle\psi|\bar{A}\delta\bar{A}|\psi\rangle_{\psi} + 2t\langle\psi|(\delta\bar{A})^2|\psi\rangle - \lambda\langle\psi|\delta\bar{A}|\psi\rangle,$$

$$\frac{\partial^2}{\partial t^2}L(\bar{A}+t\delta\bar{A}) = 2\langle\psi|(\delta\bar{A})^2|\psi\rangle > 0.$$

The first-order condition

$$\frac{\partial}{\partial t}L(\bar{A}+t\delta\bar{A})\ |_{t=0}\ = 0$$

leads to

$$\int(-(A\psi)^*(q)\psi(q) - \psi^*(q)(A\psi)(q) + 2\bar{A}(q)\psi^*(q)\psi(q) - \lambda\psi^*(q)\psi(q))\delta\bar{A}(q)\,dq = 0.$$

Since $\delta\bar{A}$ is an arbitrary perturbation, we have

$$\bar{A}(q) = \frac{1}{2\psi^*(q)\psi(q)}((A\psi)^*(q)\psi(q) + \psi^*(q)(A\psi)(q)) + \lambda = \mathrm{Re}\left(\frac{A\psi}{\psi}\right)(q) + \lambda.$$

The multiplier λ is determined as $\lambda = 0$ by the condition $\langle\bar{A}\rangle_{\psi} = \langle A\rangle_{\psi}$.

Now since $\bar{A} = \mathrm{Re}(\frac{A\psi}{\psi})$, we have

$$(A-\bar{A})\psi = \left(\frac{A\psi}{\psi} - \mathrm{Re}\left(\frac{A\psi}{\psi}\right)\right)\psi = i\ \mathrm{Im}\left(\frac{A\psi}{\psi}\right)\psi, \qquad \langle\psi|(A-\bar{A})|\psi\rangle = 0.$$

Consequently,

$$\mathrm{Var}_{\psi}(A-\bar{A}) = \langle\psi|(A-\bar{A})^2)|\psi\rangle - \langle\psi|(A-\bar{A})|\psi\rangle^2 = \int\left(i\ \mathrm{Im}\left(\frac{A\psi}{\psi}\right)\psi\right)^*\left(i\ \mathrm{Im}\left(\frac{A\psi}{\psi}\right)\psi\right)dq = \int\left(\mathrm{Im}\left(\frac{A\psi}{\psi}\right)\right)^2|\psi|^2\,dq. \qquad \square$$

Remark. We see that $\bar{A}$ is precisely the quantum mechanical local value arising from several other contexts (Cohen, 1996; Holland, 1993; Wan and Summer, 1988). We should emphasize that $\bar{A}$ is dependent on the relevant state ψ, but for notational simplicity, we have suppressed this dependence since it is always clear from the context which state is involved.

Put $\tilde{A} = A - \overline{A}$ (the tilde indicates fluctuations); then we have the decomposition

$$A = \overline{A} + \tilde{A}. \tag{3}$$

Clearly, both $\overline{A}$ and $\tilde{A}$ are Hermitian operators on $L^2(\mathbb{R})$. In the decomposition equality (3), $\overline{A}$ is a classical estimate of A, some object intermediate between the precise knowledge of A and the global average $\langle A \rangle_\psi$. In other words, $\overline{A}$ "tracks" the observable A (optimally in the sense of Theorem 1), which is in a quantum world, from the classical world. The residual part $\tilde{A}$ represents inherent quantum fluctuations of A in the state ψ. Since $\langle \overline{A} \rangle_\psi = \langle A \rangle_\psi$, we have $\langle \tilde{A} \rangle_\psi = 0$. Moreover, if A_1 and A_2 are two quantum observables, then we have

$$\overline{A_1 + A_2} = \overline{A}_1 + \overline{A}_2, \quad \widetilde{A_1 + A_2} = \tilde{A}_1 + \tilde{A}_2.$$

But in general, it is *not* true that $\overline{A_1 A_2} = \overline{A}_1 \overline{A}_2$, $\widetilde{A_1 A_2} = \tilde{A}_1 \tilde{A}_2$.

Theorem 2. *It holds that* $\langle \overline{A} \rangle_\psi = \langle A \rangle_\psi$, $\langle \tilde{A} \rangle_\psi = 0$, *and*

$$\overline{\overline{A}} = \overline{A}, \quad \tilde{\tilde{A}} = \tilde{A}; \qquad \overline{\tilde{A}} = 0, \quad \tilde{\overline{A}} = 0.$$

Proof: The first two equalities are clear.

Since $\overline{A} = \mathrm{Re}(\frac{A\psi}{\psi})$ is a real-valued function, and can be considered as a multiplication operator on $L^2(\mathbb{R})$, we have

$$\overline{\overline{A}} = \mathrm{Re}\left(\frac{\overline{A}\psi}{\psi}\right) = \overline{A}\,\mathrm{Re}\left(\frac{\psi}{\psi}\right) = \overline{A}.$$

Now by linearity,

$$\overline{\tilde{A}} = \overline{A - \overline{A}} = \overline{A} - \overline{\overline{A}} = 0.$$

$$\tilde{\overline{A}} = \overline{A} - \overline{\overline{A}} = 0.$$

$$\tilde{\tilde{A}} = A \widetilde{-} \overline{A} = \tilde{A} - \tilde{\overline{A}} = \tilde{A}. \qquad \square$$

Remark. The above result demonstrates that in certain sense, $\overline{A}$ and $\tilde{A}$ are geometrically independent (orthogonal). It is reminiscent of the orthogonal decomposition of a Hilbert space vector via orthogonal projection. The operation of taking local value mimics the orthogonal projection.

If we indicate the dependence of the local value $\overline{A}$ in two different wave functions as $\overline{A}_1$, $\overline{A}_2$, and denote the corresponding quantum fluctuation parts as

$\tilde{A}_1$, $\tilde{A}_2$, then we have the following generalization of Theorem 2:

$$\overline{(\overline{A}_1)_2} = \overline{A}_1, \quad (\widetilde{\tilde{A}_1})_2 = \tilde{A}_2; \qquad \overline{(\tilde{A}_1)_2} = \overline{A}_2 - \overline{A}_1, \quad (\widetilde{\overline{A}_1})_2 = 0.$$

These identities demonstrate the nice interactions among local values and quantum fluctuations.

Let $\overline{A} \circ \tilde{A} := \frac{1}{2}(\overline{A}\tilde{A} + \tilde{A}\overline{A})$ be the Jordan product of $\overline{A}$ and $\tilde{A}$, and following Bohm (1951), let

$$\mathrm{Cov}_\psi(\overline{A}, \tilde{A}) := \langle \psi | \overline{A} \circ \tilde{A} | \psi \rangle - \langle \overline{A} \rangle_\psi \langle \tilde{A} \rangle_\psi$$

be the covariance between $\overline{A}$ and $\tilde{A}$ in the state ψ. The following result shows that the decomposition $A = \overline{A} + \tilde{A}$ as a local value part and quantum fluctuation part is statistically independent, complementing the geometrical independence as stated in Theorem 2.

Theorem 3. *We have* $\mathrm{Cov}_\psi(\overline{A}, \tilde{A}) = 0$ *and*

$$\mathrm{Var}_\psi(A) = \mathrm{Var}_\psi(\overline{A}) + \mathrm{Var}_\psi(\tilde{A}).$$

Proof: To prove the first assertion, note that

$$\begin{aligned}\langle \psi | \overline{A}\tilde{A} | \psi \rangle &= \int (\overline{A}\psi)^* \tilde{A}\psi \, dq \\ &= \int \left(\mathrm{Re}\left(\frac{A\psi}{\psi} \right) \psi \right)^* i \, \mathrm{Im}\left(\frac{A\psi}{\psi} \right) \psi \, dq. \\ &= i \int \mathrm{Re}\left(\frac{A\psi}{\psi} \right) \mathrm{Im}\left(\frac{A\psi}{\psi} \right) |\psi|^2 \, dq.\end{aligned}$$

Similarly,

$$\langle \psi | \tilde{A}\overline{A} | \psi \rangle = -i \int \mathrm{Re}\left(\frac{A\psi}{\psi} \right) \mathrm{Im}\left(\frac{A\psi}{\psi} \right) |\psi|^2 \, dq.$$

Thus noting $\langle \tilde{A} \rangle_\psi = 0$, we come to

$$\mathrm{Cov}_\psi(\overline{A}, \tilde{A}) = \frac{1}{2}(\langle \psi | \overline{A}\tilde{A} | \psi \rangle + \langle \psi | \tilde{A}\overline{A} | \psi \rangle) = 0.$$

The second assertion is due to Cohen (1996). The simple derivation is as follows:

$$\begin{aligned}&\mathrm{Var}_\psi(A) \\ &= \langle (A - \langle A \rangle_\psi)\psi | (A - \langle A \rangle_\psi)\psi_\theta \rangle\end{aligned}$$

$$= \int |(A - \langle A\rangle_\psi)\psi(q)|^2\, dq$$
$$= \int \left| \left(\frac{A\psi(q)}{\psi(q)} - \langle A\rangle_\psi \right) \psi(q) \right|^2\, dq$$
$$= \int \left| \mathrm{Re}\left(\frac{A\psi(q)}{\psi(q)} \right) - \langle A\rangle_\psi + i\,\mathrm{Im}\left(\frac{A\psi(q)}{\psi(q)} \right) \right|^2 |\psi(q)|^2\, dq$$
$$= \int \left(\mathrm{Re}\left(\frac{A\psi(q)}{\psi(q)} \right) - \langle A\rangle_\psi \right)^2 |\psi(q)|^2\, dq + \int \left(\mathrm{Im}\left(\frac{A\psi(q)}{\psi(q)} \right) \right)^2 |\psi(q)|^2\, dq$$
$$= \mathrm{Var}_\psi(\bar{A}) + \mathrm{Var}_\psi(\tilde{A}). \quad \text{(by Theorem 1)} \qquad \square$$

We consider some particular cases. Let the wave function ψ be written in the polar form: $\psi(q) = r(q)\, e^{i\phi(q)}$.

Example 1. If $A = Q$ (the position observable), the $Q\psi(q) = q\psi(q)$ and thus $\bar{Q} = Q$, $\tilde{Q} = 0$, in conformity with intuition. If $A = P = -i\frac{\partial}{\partial q}$ is the momentum operator (we put $\hbar = 1$), then

$$\bar{P} = \frac{1}{2i|\psi|^2} \left(\frac{\partial \psi}{\partial q} \psi^* - \frac{\partial \psi^*}{\partial q} \psi \right) = \frac{\partial \phi}{\partial q}$$

is the quantum mechanical current density (current velocity in Nelson's terminology; Nelson, 1985). The imaginary part

$$\mathrm{Im}\left(\frac{P\psi}{\psi} \right) = \frac{\partial \log |\psi|}{\partial q}$$

is the osmotic velocity of Nelson.

Example 2. If $A = \frac{1}{2}(PQ + QP)$ is the dilation operator, then $\bar{A}(q) = q\frac{\partial \phi(q)}{\partial q}$. Moreover,

$$\mathrm{Var}_\psi(A) = \int (\bar{A} - \langle A\rangle_\psi)^2 |\psi(q)|^2\, dq + \frac{1}{4} \int \left(1 + q \frac{\partial \ln |\psi(q)|^2}{\partial q} \right)^2 |\psi(q)|^2\, dq.$$

The last integral is connected with the scaling Fisher information of $|\psi|^2$ (see Section 3). On the other hand, if $A = PQ^{-1} + Q^{-1}P$ (which is related to the time-of-arrival operator of Aharonov and Bohm, 1961, in momentum representation), then

$$\bar{A} = \frac{2}{q} \frac{\partial \phi(q)}{\partial q} \quad \text{and} \quad \mathrm{Im}\left(\frac{A\psi}{\psi} \right) = -\frac{2}{q} \frac{\partial \ln r(q)}{\partial q} + \frac{1}{q^2}.$$

Example 3. If $A = P\beta(Q)P$, here β is a real-valued function on $\mathbb{R}$, then

$$\overline{A} = \beta \left(\frac{\partial \phi}{\partial q}\right)^2 - \frac{1}{r}\frac{\partial}{\partial q}\left(\beta \frac{\partial r}{\partial q}\right)$$

and

$$\mathrm{Im}\left(\frac{A\psi}{\psi}\right) = -\frac{\partial}{\partial q}\left(\beta \frac{\partial \phi}{\partial q}\right) - \frac{2\beta}{r}\frac{\partial r}{\partial q}\frac{\partial \phi}{\partial q}.$$

Theorem 4. *Let $P = -i\frac{\partial}{\partial q}$ be the momentum observable and $\tilde{P} = P - \overline{P}$ be the quantum fluctuation. Let $\psi(q) = r(q)\, e^{i\phi(q)}$ be the polar form of ψ, then*

$$\overline{(\tilde{P})^2} = -\frac{1}{r(q)}\frac{\partial^2 r(q)}{\partial q^2}.$$

Consequently, the local value of the squared quantum fluctuation is precisely Bohm's quantum potential.

Proof: From $\tilde{P} = P - \overline{P}$, and by the definition of local value, Eq. (2), we have

$$\overline{(\tilde{P})^2} = \mathrm{Re}\left(\frac{(\tilde{P})^2\psi}{\psi}\right) = \mathrm{Re}\left(\frac{(P^2 - P\overline{P} - \overline{P}P + \overline{P}^2)\psi}{\psi}\right).$$

Substituting $P = -i\frac{\partial}{\partial q}$ and $\psi(q) = r(q)\, e^{i\phi(q)}$ into the above expression, we obtain the desired result. □

3. FISHER INFORMATION, LOCAL VALUE, AND UNCERTAINTY PRINCIPLE

Let $\{f_\theta \colon \theta \in \mathbb{R}\}$ be a parametric family of probability densities on $\mathbb{R}$. From the theory of statistical inference (Cramér, 1946), the Fisher information of f_θ is defined as

$$I(f_\theta) = \int \left(\frac{\partial \ln f_\theta(q)}{\partial \theta}\right)^2 f_\theta(q)\, dq \tag{4}$$

$$= 4\int \left(\frac{\partial \sqrt{f_\theta(q)}}{\partial \theta}\right)^2 dq. \tag{5}$$

The definition (4) emphasizes the role of the statistical score function $\frac{\partial \ln f_\theta}{\partial \theta}$, and the definition (5) employs the gradient of probability amplitude $\sqrt{f_\theta}$. It is precisely the coincidence of these two definitions that renders statistics useful in treating quantum mechanical kinetic energy. The concept of Fisher information, originated in early days of the theory of statistical inference (Fisher, 1925), has found many interesting and inspiring applications in physics (Frieden, 1998). It is connected with the celebrated Cramér–Rao inequality and the theory of maximum likelihood estimation (Cramér, 1946). The significance and potential usefulness of the concept of Fisher information are well worth of further investigations. By virtue of Fisher information, we can even formulate the Heisenberg uncertainty principle concerning the position–momentum pair as an exact equality rather than an inequality concerning variances (Luo, 2001). This formulation quantifies Heisenberg's original idea (Heisenberg, 1928) more precisely. After all, Heisenberg's original formulation of uncertainty principle is expressed as an approximate equality.

When $f_\theta(q) = f(q-\theta)$, that is, the parameter θ is a location parameter, by the translation invariance of Lebesgue integral, we have

$$I(f_\theta) = 4\int\left(\frac{\partial\sqrt{f(q)}}{\partial q}\right)^2 dq,$$

which is indepedent of θ, and we may denote it as $I(f)$. This fact is in accordance with Mach's principle, since $I(f_\theta)$ describes in certain sense the shape of f_θ, and since all $f_\theta(q) = f(q-\theta)$ are of the same shape (or convey the same information, there is no absolute origin.)

Similarly, when $f_\theta(q) = \theta f(\theta q)$, that is, the parameter θ is a scale parameter, after some simple manipulation of changing variables, we obtain

$$I(f_\theta) = \frac{1}{\theta^2}\int\left(1 + q\frac{\partial \ln f(q)}{\partial q}\right)^2 f(q)\,dq.$$

Let $\psi_\theta \in L^2(\mathbb{R})$ satisfies the Schrödinger equation

$$i\frac{\partial\psi_\theta}{\partial\theta} = A\psi_\theta. \tag{6}$$

Here θ is interpreted as a parameter which may represent a temporal shift or a spatial displacement. According to the postulate of quantum mechanics, $f_\theta := |\psi_\theta|^2$ describes the probability density of the position observable, and its Fisher information is

$$I(|\psi_\theta|^2) = \int\left(\frac{\partial \ln|\psi_\theta(q)|^2}{\partial\theta}\right)^2 |\psi_\theta(q)|^2\,dq = 4\int\left(\frac{\partial|\psi_\theta(q)|}{\partial\theta}\right)^2 dq.$$

If $\hat{\theta}$ is an estimator (measurement) for θ, then the celebrated Cramér–Rao inequality states that (Cramér, 1946; Helstrom, 1976)

$$I(|\psi_\theta|^2) \geq \frac{\left(\frac{\partial}{\partial\theta}\langle\hat{\theta}\rangle_{\psi_\theta}\right)^2}{\mathrm{Var}_{\psi_\theta}(\hat{\theta})}.$$

In particular, if $\langle\hat{\theta}\rangle_{\psi_\theta} = \theta +$ constant, then

$$I(|\psi_\theta|^2) \geq \frac{1}{\mathrm{Var}_{\psi_\theta}(\hat{\theta})}. \tag{7}$$

This inequality places an upper bound of the estimation precision (reciprocal of variance) in terms of Fisher information.

Theorem 5. *Let ψ_θ satisfy the Schrödinger equation (6) and has polar form $\psi_\theta = r_\theta\, e^{i\phi\theta}$. Let $\bar{A} = \mathrm{Re}(\frac{A\psi_\theta}{\psi_\theta})$ be the local value of the observable A. Then*

$$\bar{A} = \frac{i}{2|\psi_\theta|^2}\left(\psi_\theta^* \frac{\partial\psi_\theta}{\partial\theta} - \frac{\partial\psi_\theta^*}{\partial\theta}\psi_\theta\right) = -\frac{\partial}{\partial\theta}\phi_\theta.$$

Moreover,

$$Var_{\psi_\theta}(A) = Var_{\psi_\theta}(\bar{A}) + \frac{1}{4}I(|\psi_\theta|^2), \tag{8}$$

or equivalently,

$$Var_{\psi_\theta}(\tilde{A}) = \frac{1}{4}I(|\psi_\theta|^2). \tag{9}$$

Thus the variance of the quantum fluctuation is essentially the Fisher information.

Proof: Noting that $A\psi_\theta = i\frac{\partial\psi_\theta}{\partial\theta}$, we readily get the first equality. Now

$$\begin{aligned}
\mathrm{Var}_{\psi_\theta}(A) &= \int |(A - \langle A\rangle_{\psi_\theta})\psi_\theta(q)|^2\, dq \\
&= \int \left|\left(\frac{A\psi_\theta(q)}{\psi_\theta(q)} - \langle A\rangle_{\psi_\theta}\right)\psi_\theta(q)\right|^2 dq \\
&= \int \left|\mathrm{Re}\left(\frac{A\psi_\theta(q)}{\psi_\theta(q)}\right) - \langle A\rangle_{\psi_\theta} + i\,\mathrm{Im}\left(\frac{A\psi_\theta(q)}{\psi_\theta(q)}\right)\right|^2 |\psi_\theta(q)|^2\, dq \\
&= \int \left(\mathrm{Re}\left(\frac{A\psi_\theta(q)}{\psi_\theta(q)}\right) - \langle A\rangle_{\psi_\theta}\right)^2 |\psi_\theta(q)|^2\, dq \\
&\quad + \int \left(\mathrm{Im}\left(\frac{A\psi_\theta(q)}{\psi_\theta(q)}\right)\right)^2 |\psi_\theta(q)|^2\, dq \\
&= \int (\bar{A}(q) - \langle A\rangle_{\psi_\theta})^2 |\psi_\theta(q)|^2\, dq + \int \left(\frac{\partial\, \ln r_\theta(q)}{\partial\theta}\right)^2 |\psi_\theta(q)|^2\, dq
\end{aligned}$$

$$= \mathrm{Var}_{\psi_\theta}(\overline{A}) + \frac{1}{4}\int \left(\frac{\partial \ln|\psi_\theta(q)|^2}{\partial\theta}\right)^2 |\psi_\theta(q)|^2\, dq$$

$$= \mathrm{Var}_{\psi_\theta}(\overline{A}) + \frac{1}{4} I(|\psi_\theta|^2).$$

By Theorem 3, the last assertion follows. □

Remark: When ψ_θ satisfies Eq. (6), the local value $\overline{A} = \frac{i}{2|\psi_\theta|^2}(\psi_\theta^* \frac{\partial\psi_\theta}{\partial\theta} - \frac{\partial\psi_\theta^*}{\partial\theta}\psi_\theta) = -\frac{\partial}{\partial\theta}\phi_\theta$ is a generalization of the quantum mechanical current per unit mass per unit density (when A is the momentum operator, we have $\psi_\theta(q) = \psi(q-\theta)$ and $\overline{A}$ reduces to the conventional current density).

In contrast to inequality (7), which places a lower bound of the Fisher information in terms of variance of an estimator of the parameter, Theorem 5 establishes a simple identity relating the Fisher information and the variance of the squared quantum fluctuation. In particular, Eq. (8) implies an upper bound for the Fisher information in terms of the variance of the generator A of the motion:

$$4\,\mathrm{Var}_{\psi_\theta}(A) \ge I(|\psi_\theta|^2). \tag{10}$$

Combining inequalities (7) and (10), we have the following inequality chain:

Corollary 6. *If ψ_θ satisfies Eq. (6), then*

$$4\,\mathrm{Var}_{\psi_\theta}(A) \ge I(|\psi_\theta|^2) \ge \frac{1}{\mathrm{Var}_{\psi_\theta}(\hat{\theta})}. \tag{11}$$

In particular, $\mathrm{Var}_{\psi_\theta}(\hat{\theta})\mathrm{Var}_{\psi_\theta}(A) \ge \frac{1}{4}$.

From the above result, we see that the Fisher information $I(|\psi_\theta|^2)$ already encodes more information about the uncertainty principle than the usual variance formulation. The inequality chain (11) also unifies and refines the conventional Heisenberg uncertainty relations concerning the conjugate pair of position and momentum, as well as the conjugate pair of time (interpreted as a parameter in the Schrödinger equation) and energy. This is explained as follows:

(1) Let $\hat{\theta} = Q$ be the position observable (measurement) defined as $Q\psi_\theta(q) = q\psi_\theta(q)$, and $A = P = -i\frac{\partial}{\partial q}$ be the momentum observable. Let $\psi = \psi_0 \in L^2(\mathbb{R})$ be any Schrödinger wave function; then $\psi_\theta(q) = e^{-i\theta P}\psi(q) = \psi(q-\theta)$. In this circumstance,

$$I(|\psi_\theta|^2) = I(|\psi|^2) = \int \left(\frac{\partial \ln|\psi(q)|^2}{\partial q}\right)^2 |\psi(q)|^2\, dq$$

is independent of the parameter θ, and we have

$$\langle Q\rangle_{\psi_\theta} = \theta + \langle Q\rangle_\psi, \quad \mathrm{Var}_{\psi_\theta}(P) = \mathrm{Var}_\psi(P), \quad \mathrm{Var}_{\psi_\theta}(Q) = \mathrm{Var}_\psi(Q),$$
$$I(|\psi_\theta|^2) = I(|\psi|^2).$$

Thus the inequality chain (11) reduces to

$$4\,\mathrm{Var}_\psi(P) \geq I(|\psi|^2) \geq \frac{1}{\mathrm{Var}_\psi(Q)},$$

which clearly implies the familiar Heisenberg uncertainty relation for the canonical pair of position and momentum. From Theorem 5, we also see that the uncertainty comes from two parts: the first is the intrinsic irreducible randomness of the state (wave function) and the second is from the incompatibility (complementarity, noncommutativity) of P with Q.

(2) The time–energy uncertainty relation is a more subtle, and even controversial, issue in the Hilbert space formalism of quantum mechanics. The reason is the lack of a time observable (in the sense of a self-adjoint operator). See Gislason *et al.* (1985) for a concise review. However, if we interpret time only as a parameter, we obtain the same form of uncertainty relation as the position–momentum pair by means of *classical* statistical inference. This is already incorporated in the inequality chain (11) if we regard A as an energy operator and θ as time t.

4. CONDITIONAL EXPECTATION, LOCAL VALUE, AND PHASE-SPACE DISTRIBUTIONS

In classical probability, if (X, Y) is a random vector on some probability space $(\Omega, \mathcal{F}, P)$ with joint probability density $p(x, y)$, then we have the conditional probability $p(y \mid x) = \frac{p(x,y)}{p(x)}$. We also have the conditional expectation $\mathrm{E}(X \mid Y)$ and the conditional variance $\mathrm{Var}(X \mid Y)$, both of which are essentially functions of the random variable Y, and thus are also random variables themselves. If $X \in L^2(\Omega, \mathcal{F}, P)$, then the conditional expectation $\mathrm{E}(X \mid Y)$ is the projection of X from $L^2(\Omega, \mathcal{F}, P)$ to the subspace $L^2(\Omega, \sigma(Y), P)$. Here $\sigma(Y)$ denotes the σ-algebra generated by the random variable Y. We have

$$\mathrm{E}(X) = \int \left(\int xp(x \mid y)\,dx\right) p(y)\,dy = \int\int xp(x, y)\,dx\,dy$$
$$\mathrm{Var}(X) = \int (x - \mathrm{E}(X))^2 p(x, y)\,dx\,dy$$
$$\mathrm{E}(X \mid Y) = \int xp(x \mid Y)\,dx$$
$$\mathrm{Var}(X \mid Y) = \int (x - \mathrm{E}(X))^2 p(x \mid Y)\,dx.$$

Moreover,

$$\mathrm{Var}(X) = \mathrm{Var}(\mathrm{E}(X \mid Y)) + \mathrm{E}(\mathrm{Var}(X \mid Y)).$$

This last identity is analogous to Eq. (1). Thus local value $\mathrm{Re}(\frac{A\psi}{\psi})$ is formally like the conditional expectation $\mathrm{E}(X \mid Y)$, and the local spread $\mathrm{Im}(\frac{A\psi}{\psi})$ is formally like the conditional variance $\mathrm{Var}(X \mid Y)$, with A corresponding to X, the reference observable to Y, and the state ψ to the probability P.

In quantum mechanics, various distribution functions have been introduced (Cohen, 1966; Hillery *et al.*, 1984; Lee, 1995). They are pseudo-probability densities in the sense that they may take negative values. The motivation is to express quantum expectation values as the average of a classical observable under a probability distribution on phase space (or configuration space). Cohen (1966) introduced a very general class of quantum mechanical phase-space (or time–frequency) distributions which incorporates all existing ones:

$$\Phi(q, p) = \frac{1}{4\pi^2} \int e^{-i\xi q - i\eta p + i\xi x} \psi^* \left(x - \frac{\eta}{2}\right) \psi \left(x + \frac{\eta}{2}\right) k(\xi, \eta)\, d\xi\, d\eta\, dx. \tag{12}$$

Here $k(\xi, \eta)$ is a kernel function. Alternatively, we may write

$$\Phi(q, p) = \frac{1}{4\pi^2} \int e^{-i\xi q - i\eta p} M(\xi, \eta)\, d\xi\, d\eta$$

with $M(\xi, \eta) = k(\xi, \eta) A(\xi, \eta)$, where

$$A(\xi, \eta) = \int e^{i\xi x} \psi^* \left(x - \frac{\eta}{2}\right) \psi \left(x + \frac{\eta}{2}\right) dx$$

is usually referred to as ambiguity function. In order to satisfy the desired marginal properties

$$\int \Phi(q, p)\, dp = |\psi(q)|^2, \qquad \int \Phi(q, p)\, dq = |\hat{\psi}(p)|^2,$$

we must impose the condition $k(\xi, 0) = k(0, \eta) = 1$. Here $\hat{\psi}(p) = \frac{1}{\sqrt{2\pi}} \int \psi(q) e^{-iqp}\, dq$ is the Fourier transform of ψ. The distribution (12) contains many previously introduced distributions as special cases. For example, when $k(\xi, \eta) = 1$, it is the prominent Wigner distribution.

Now $\Phi(q, p)$ is a general quantum mechanical phase-space distribution (although it may take negative values), and we may consider various quantities derived from it by following formally the classical probability procedures. One may wonder what is its behavior under conditional expectations. For example, we may define $\Phi(p \mid q) = \frac{\Phi(q,p)}{|\psi(q)|^2}$ as the conditional probability of P when $Q = q$

(although it may take negative values), and we can also define the conditional expectation

$$\mathrm{E}(P \mid q) = \int p\Phi(p \mid q)\, dp.$$

Theorem 7. *Let $P = -i\frac{\partial}{\partial q}$ be the momentum observable. If $\frac{\partial}{\partial \eta}k(\xi, \eta)\mid_{\eta=0} = 0$, then*

$$\bar{P}(q) = \mathrm{E}(P \mid q).$$

That is, the local value $\bar{P}$ is precisely the conditional expectation of P, given the position $Q = q$, under the phase-space distribution Φ.

Proof: Write ψ in polar form as $\psi(q) = r(q)\,e^{i\phi(q)}$, let $\delta(\eta)$ be the Dirac delta function, and note $\int e^{-i\eta p}\, dp = 2\pi\delta(\eta)$; therefore we have

$$\begin{aligned}
\mathrm{E}(P \mid q) &= \int p\Phi(p \mid q)\, dp \\
&= \frac{1}{|\psi(q)|^2}\int p\Phi(q,p)\, dp \\
&= \frac{1}{4\pi^2\psi(q)|^2}\int\int\int\int p\, e^{-i\xi q - i\eta p + i\xi x}\psi^*\left(x - \frac{\eta}{2}\right)\psi \\
&\quad \times \left(x + \frac{\eta}{2}\right)k(\xi, \eta)\, d\xi\, d\eta\, dx\, dp \\
&= \frac{1}{4\pi^2|\psi(q)|^2}\int\int\int 2\pi i\frac{\partial}{\partial\eta}\delta(\eta)\, e^{-i\xi q + i\xi x}\psi^*\left(x - \frac{\eta}{2}\right)\psi \\
&\quad \times \left(x + \frac{\eta}{2}\right)k(\xi, \eta)\, d\xi\, d\eta\, dx \\
&= \frac{1}{2\pi|\psi(q)|^2}\int\int |\psi(x)|^2\left(k(\xi, 0)\frac{\partial\phi(x)}{\partial x} - i\frac{\partial k(\xi, \eta)}{\partial\eta}\mid_{\eta=0}\right) \\
&\quad \times e^{i\xi(x-q)}\, d\xi\, dx \\
&= \frac{1}{2\pi|\psi(q)|^2}\int 2\pi|\psi(x)|^2\frac{\partial\phi(x)}{\partial x}\delta(q - x)\, dx \\
&= \frac{\partial\phi(q)}{\partial q} = \bar{P}(q).
\end{aligned}$$

□

Remark: There are infinitely many $k(\xi, \eta)$ satisfying the condition $\frac{\partial}{\partial \eta} k(\xi, \eta)|_{\eta=0} = 0$. Some physically motivated simple examples are

$$k(\xi, \eta) = 1,\ \cos(\xi\eta/2),\ \frac{\sin(\xi\eta/2)}{\xi\eta/2},\ e^{-\xi^2\eta^2/2}.$$

5. LOCAL VALUE OF NON-SELF-ADJOINT OPERATORS

In the theory of quantum detection and quantum estimation, the measurement of non-self-adjoint observables may turn out to be more useful than the measurement of self-adjoint observables in some circumstances (Helstrom, 1976; Yuen *et al.*, 1975; Yuen and Lax, 1973). Just like any complex number can be written as the combination of two real numbers, for a general operator A, we can also write

$$A = A_{\mathrm{R}} + iA_{\mathrm{I}}, \quad \text{with} \quad A_{\mathrm{R}} = \frac{A + A^*}{2},\ A_{\mathrm{I}} = \frac{A - A^*}{2i}.$$

Here both A_{R} and A_{I} are self-adjoint operators. Consequently we may define their local value $\bar{A}_{\mathrm{R}}$ and $\bar{A}_{\mathrm{I}}$ as in Section 2. From this we define the local value of A as

$$\bar{A} = \bar{A}_{\mathrm{R}} + i\bar{A}_{\mathrm{I}}.$$

Similarly, we have the quantum fluctuations $\widetilde{A_{\mathrm{R}}}$ and $\tilde{A}_{\mathrm{I}}$, and we may define

$$\tilde{A} = \widetilde{A_{\mathrm{R}}} + i\tilde{A}_{\mathrm{I}}.$$

By the linearity, we have the decomposition formally identical to Eq. (3).

$$A = \bar{A} + \tilde{A}.$$

To consider an example, let us determine the local value of a general operator in the ground state of the harmonic oscillator with one degree of freedom. Let an operator (not necessarily self-adjoint) A on $L^2(\mathbb{R})$ be represented in a series expansion of the canonical position–momentum pair (Q, P) as

$$A = \sum_{m,n=0}^{\infty} a_{m,n} Q^m P^n. \tag{13}$$

Here $a_{m,n}$'s are complex numbers. We want to find its local value in the ground state of the harmonic oscillator. For this purpose, it will be suffice to introduce the creation operator a^+ and the annihilation operator a^- (they are mutually adjoint)

$$a^+ = \frac{Q - ip}{\sqrt{2}}, \qquad a^- = \frac{Q + iP}{\sqrt{2}}.$$

Clearly, $[a^-, a^+] = 1$ and the Hamiltonian of the harmonic oscillator is $H = a^+a^- + \frac{1}{2}$. The orthonormal eigenfunctions $\{\psi_n(q)\}$ of H is given by the

Hermite functions

$$\psi_n(q) = (2^n n! \pi^{1/2})^{-1/2} h_n(q)\, e^{-q^2/2}, \quad n = 0, 1, 2, \ldots$$

and $h_n(q)$ is the Hermite polynomial given by

$$h_n(q) = (-1)^n\, e^{q^2}\, \frac{\partial^n}{\partial q^n}\, e^{-q^2}.$$

The ground state of H is

$$\psi(q) \equiv \psi_0(q) = \pi^{-1/4}\, e^{-q^2/2}.$$

Now by virtue of the commutation relation $[a^-, a^+] = 1$, we can arrange the series representation (13) in the Wick order (normal order) form in terms of a^+ and a^- (that is, the creation operator always occurs to the left of the annihilation operator):

$$A = \sum_{m,n=0}^{\infty} c_{m,n} a^{+m} a^{-n}.$$

Then

$$A^* = \sum_{m,n=0}^{\infty} c^*_{m,n} a^{+n} a^{-m} = \sum_{m,n=0}^{\infty} c^*_{n,m} a^{+m} a^{-n},$$

and thus

$$A_{\mathrm{R}} = \sum_{m,n=0}^{\infty} \frac{c_{m,n} + c^*_{n,m}}{2} a^{+m} a^{-n}, \qquad A_{\mathrm{I}} = \sum_{m,n=0}^{\infty} \frac{c_{m,n} - c^*_{n,m}}{2i} a^{+m} a^{-n}.$$

Consequently, note that $a^-\psi = 0$ and $a^{+m}\psi = (m!)^{1/2}\psi_m$, we have

$$\begin{aligned}\bar{A}_{\mathrm{R}} &= \sum_{m=0}^{\infty} \mathrm{Re}\left(\frac{c_{m,0} + c^*_{0,m}}{2}\right) \frac{(m!)^{1/2}\psi_m(q)}{\psi(q)} \\ &= \sum_{m=0}^{\infty} \mathrm{Re}\left(\frac{c_{m,0} + c^*_{0,m}}{2}\right) 2^{-m/2} h_m(q).\end{aligned}$$

Similarly,

$$\begin{aligned}\bar{A}_{\mathrm{I}} &= \sum_{m=0}^{\infty} \mathrm{Re}\left(\frac{c_{m,0} - c^*_{0,m}}{2i}\right) 2^{-m/2} h_m(q) \\ &= \sum_{m=0}^{\infty} \mathrm{Im}\left(\frac{c_{m,0} - c^*_{0,m}}{2}\right) 2^{-m/2} h_m(q).\end{aligned}$$

Finally, we obtain

$$\overline{A} = \overline{A}_{\mathrm{R}} + i\,\overline{A}_{\mathrm{I}} = \sum_{m=0}^{\infty} \frac{c_{m,0} + c_{0,m}}{2} 2^{-m/2} h_m(q).$$

By the above method, we can also calculate the local value of A in any state ψ_m by noting that $a^-\psi = 0$, $a^-\psi_n = n^{1/2}\psi_{n-1}$, $a^+\psi_n = (n+1)^{1/2}\psi_{n+1}$.

6. CONCLUSIONS

We have presented various statistical interpretations of the concept of quantum mechanical local value, which arises naturally in several contexts of quantum mechanics and time–frequency analysis. Local value provides a classical estimation and visualization of incompatible quantum observables. The basic idea is to fix one reference observable, and approximate the other one in the fixed representation, that is, assign a best statistical average value to the observable at each value of the reference observable. This method leading to local value is in complete parallel with projection technique, with the least square, and with conditional expectation in spirit. By decomposing a quantum observable into a local value part (classical) and a local spread part (quantum fluctuation), we see clearly how the uncertainty of the quantum observable comes from two statistically and geometrically independent parts. Moreover, the statistical notion of Fisher information enters naturally into this scenario, and the Heisenberg uncertainty relations can be analyzed more deeply, from both physical and mathematical aspects. The notion of local value may find more applications in the de Broglie–Bohm's casual and pilot wave interpretation of quantum mechanics. In particular, it may serve as an intuitive guidance in treating some quantum phenomena which seem so peculiar and mysterious in the standard formalism.

Finally, we point out that although we have worked only in the framework of position representation and pure state (wave function), the extensions to other representation and mixed state (density operator) are straightforward, and some new phenomena connected with the information contents of mixed state should be expected.

ACKNOWLEDGMENT

The work is supported by the Liu Bie Ju Center for Mathematical Sciences (Project No. 9360020), City University of Hong Kong, and by the Knowledge Innovation Program of the Chinese Academy of Sciences.

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