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# Fisher information, kinetic energy and uncertainty relation inequalities

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**Abstract**
By interpolating between Fisher information and mechanical kinetic energy, we introduce a general notion of kinetic energy *with respect to a parameter* of Schrödinger wavefunctions from a statistical inference perspective. Kinetic energy is the sum of Fisher information and an integral of a parametrized analogue of quantum mechanical current density related to phase. A family of integral inequalities concerning kinetic energy and moments are established, among which the Cramér–Rao inequality and the Weyl–Heisenberg inequality, are special cases. In particular, the integral inequalities involving the negative order moments are relevant to the study of electron systems. Moreover, by specifying the parameter to a scale, we obtain a family of inequalities of uncertainty relation type which incorporate the position and momentum observables symmetrically in a single quantity.

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## 1. Introduction

The notion of Fisher information arose from statistical inference [4, 6] and is now playing an increasingly popular role in the interactions among statistics, information theory, differential geometry and physics [1, 2, 9, 12]. Its main virtue comes from its formal resemblance to mechanical kinetic energy [8, 9], from the celebrated Cramér–Rao inequality and the asymptotical normality of maximum likelihood estimations [4]. Its various extensions to the non-commutative case play an important role in quantum estimation and quantum detection [12, 17]. Its usefulness in deriving the Heisenberg uncertainty relations was first noted by Stam [16]. Moreover, by virtue of Fisher information, the Heisenberg uncertainty relation concerning the canonical pair of position and momentum observables can even be formulated as an exact information conservation law [13], rather than as an inequality concerning variances [11, 14].

On the other hand, the mechanical kinetic energy is a basic notion in kinematical and dynamical theory of motions, and plays a crucial role in the Lagrangian approach to mechanics. The formal resemblance between the mathematical expressions of Fisher information and mechanical kinetic energy (both involve a square gradient integration) suggests that there may be some intimate and intrinsic connections between the statistical notion of Fisher information and the mechanical notion of kinetic energy, and thus renders the powerful and intuitive statistical inference method applicable in an informational approach to mechanics. In fact, Frieden proposed a principle of extreme physical information, in particular, the principle of minimum Fisher information, as a unified theme to derive physical motion equations [7–9]. His programme is fruitful and promising. In this paper, working in the spirit of Frieden in emphasizing the informational interpretation of mechanical kinetic energy, we first introduce a notion of kinetic energy *with respect to a parameter* as an informational concept, which incorporates both the notions of Fisher information and the conventional mechanical kinetic energy. Then we establish a family of integral inequalities involving the kinetic energy, which are of the type of uncertainty relations and include the Cramér–Rao inequality [4] and the Weyl–Heisenberg inequality [11, 14] as particular cases. We will only work in one spatial dimension for simplicity since our focus is to introduce a new notion and to clarify its relationship with mechanical kinetic energy and Fisher information. In the three spatial dimensional case, the inequalities involving negative order moments are useful in the study of the hydrogen atom. For example, Faris used an uncertainty relation inequality involving the radial expectation of the first negative order to establish an estimation of the ground state energy [5]. The other order moments are also of analytical relevance and have physical meaning in quantum chemistry [15], and the general uncertainty relation inequalities involving them are useful in establishing various moment bounds for the Weizsäcker energy of many electron systems.

## 2. Fisher information and kinetic energy

First, we recall the mathematical definition of Fisher information. Let $\{p_\theta : \theta \in \mathbb{R}\}$ be a family of probability densities (or more generally, likelihood functions) parametrized by a parameter $\theta$. The Fisher information of $p_\theta$ (with respect to the parameter $\theta$) is defined as (see [4])

$$I(p_\theta) := \int_{\mathbb{R}} \left(\frac{\partial \ln p_\theta(x)}{\partial \theta}\right)^2 p_\theta(x)\,\mathrm{d}x = 4\int_{\mathbb{R}} \left(\frac{\partial \sqrt{p_\theta(x)}}{\partial \theta}\right)^2 \mathrm{d}x$$

provided the integral is finite. Otherwise it is defined as infinite. Fisher information characterizes the information contents of probability densities and is also intimately related to the Shannon entropy via the elegant de Bruijin identity [3, 16]. More precisely, let $p_\theta$ be the convolution probability density of any probability density $p$ with the normal (Gaussian) density with zero mean and variance $\theta > 0$ and let $S(p_\theta) := -\int_{\mathbb{R}} p_\theta(x) \ln p_\theta(x)\,\mathrm{d}x$ be the Shannon entropy of $p_\theta$. Then

$$\frac{\partial}{\partial \theta} S(p_\theta) = \frac{1}{2} I(p_\theta).$$

However, in quantum mechanics, probability amplitudes, not probability densities, are fundamental quantities. Inspired by the above notion and for comparison with the notion of kinetic energy *with respect to a parameter* to be introduced shortly, we start from probability amplitudes (wavefunctions) and define their Fisher information as follows.

Let $\{\psi_\theta : \theta \in \mathbb{R}\} \subset L^2(\mathbb{R}, \mathrm{d}x)$ be a family of Schrödinger wavefunctions sufficiently well behaved with respect to the parameter $\theta$. The parameter $\theta$ may be interpreted as temporal or spatial shift, or other physical parameter. According to the statistical interpretation of wavefunctions proposed by Born, $p_\theta := |\psi_\theta|^2$ describes the distribution probability density of the particle if $\psi_\theta$ is normalized. In general, when $\psi_\theta$ is not necessarily normalized, $p_\theta := |\psi_\theta|^2$ may be interpreted as a likelihood function. The wavefunction $\psi_\theta$ is a probability amplitude corresponding to $p_\theta$ (for any real $\phi$, $\mathrm{e}^{\mathrm{i}\phi}\psi_\theta$ is also a probability amplitude corresponding to $p_\theta$). The Fisher information of $\{\psi_\theta : \theta \in \mathbb{R}\}$ *with respect to the parameter* $\theta$ is defined as

$$I(\psi_\theta) := \int_{\mathbb{R}} \left( \frac{\partial \ln |\psi_\theta(x)|^2}{\partial \theta} \right)^2 |\psi_\theta(x)|^2 \, \mathrm{d}x = 4 \int_{\mathbb{R}} \left( \frac{\partial |\psi_\theta(x)|}{\partial \theta} \right)^2 \mathrm{d}x$$

provided the integral is finite. Otherwise it is defined as infinite. This is essentially the Fisher information of the family of likelihood functions $p_\theta = |\psi_\theta|^2$. In particular, if $\psi_\theta(x) := \psi(x+\theta)$ for some $\psi \in L^2(\mathbb{R}, \mathrm{d}x)$, then

$$I(\psi_\theta) = 4 \int_{\mathbb{R}} \left( \frac{\partial |\psi(x+\theta)|}{\partial \theta} \right)^2 \mathrm{d}x = 4 \int_{\mathbb{R}} \left( \frac{\partial |\psi(x)|}{\partial x} \right)^2 \mathrm{d}x$$

is independent of the parameter $\theta$. We denote $I(\psi_\theta)$ simply by $I(\psi)$ in this particular case.

The notion of Fisher information of a wavefunction has one defect since the phase of $\psi_\theta$ does not play any role in this definition and the important phase information which is so fundamental in the quantum mechanical superposition principle is missing. To remedy this weak point and to take the phase into account, we define the kinetic energy of the wavefunction $\psi_\theta$ *with respect to the parameter* $\theta$ as

$$K(\psi_\theta) := \int_{\mathbb{R}} \left| \frac{\partial \psi_\theta(x)}{\partial \theta} \right|^2 \mathrm{d}x.$$

This definition should be useful in treating quantum mechanical quantities from the statistical inference point of view. In particular, if $\psi_\theta$ satisfies a Schrödinger type equation with respect to the parameter $\theta$: $\mathrm{i}\frac{\partial}{\partial\theta}\psi_\theta = H\psi_\theta$, then $K(\psi_\theta) = \langle H^2 \rangle_{\psi_\theta}$ coincides with the expectation value of the square of the Hamiltonian $H$ at the state $\psi_\theta$.

To see how the above definition generalizes the notion of conventional mechanical kinetic energy, consider $\psi_\theta(x) := \psi(x+\theta)$ for some $\psi \in L^2(\mathbb{R}, \mathrm{d}x)$, that is, $\theta$ is a location parameter. Due to the translation invariance of the Lebesgue integral, we have

$$K(\psi_\theta) = \int_{\mathbb{R}} \left| \frac{\partial \psi(x+\theta)}{\partial \theta} \right|^2 \mathrm{d}x = \int_{\mathbb{R}} \left| \frac{\partial \psi(x)}{\partial x} \right|^2 \mathrm{d}x.$$

Thus in this particular case, $K(\psi_\theta)$ is independent of the parameter $\theta$ and is just the conventional mechanical kinetic energy of $\psi$. In other words, the conventional mechanical kinetic energy may be viewed as our kinetic energy with respect to the *location parameter*. In this circumstance, we denote $K(\psi_\theta)$ simply by $K(\psi)$.

In general, $\psi_\theta$ is a complex wavefunction, but in the particular case when $\psi_\theta$ is a real positive wavefunction, it is clear from the definitions that $I(\psi_\theta) = 4K(\psi_\theta)$. In this case, Fisher information and kinetic energy are essentially the same quantity. In general, Fisher information and kinetic energy are related by the following identity taking into account the contribution of the phase part.

**Theorem 1.** *For any $\psi_\theta \in L^2(\mathbb{R},\ \mathrm{d}x)$, it holds that*

$$K(\psi_\theta) = \frac{1}{4}I(\psi_\theta) + \int_{\mathbb{R}} J^2_{\psi_\theta}(x)|\psi_\theta(x)|^2\,\mathrm{d}x.$$

*Here*

$$J_{\psi_\theta} = \frac{1}{2\mathrm{i}|\psi_\theta|^2}\left(\frac{\partial\psi_\theta}{\partial\theta}\psi^*_\theta - \psi_\theta\frac{\partial\psi^*_\theta}{\partial\theta}\right)$$

*is an analogue of the normalized quantum mechanical current density (with respect to the parameter $\theta$).*

**Proof.** Let $\psi_\theta(x) = r_\theta(x)\mathrm{e}^{\mathrm{i}\phi_\theta(x)}$ be the polar decomposition of the wavefunction $\psi_\theta$. Then both $r_\theta(x)$ (the amplitude) and $\phi_\theta(x)$ (the phase) are real-valued functions, and

$$|\psi_\theta(x)|^2 = r^2_\theta(x) \qquad \frac{\partial\psi_\theta}{\partial\theta} = \frac{\partial r_\theta}{\partial\theta}\,\mathrm{e}^{\mathrm{i}\phi_\theta} + \mathrm{i}r_\theta\,\mathrm{e}^{\mathrm{i}\phi_\theta}\frac{\partial\phi_\theta}{\partial\theta}.$$

Consequently,

$$\begin{aligned}
K(\psi_\theta) &= \int_{\mathbb{R}}\left|\frac{\partial r_\theta(x)}{\partial\theta}\,\mathrm{e}^{\mathrm{i}\phi_\theta(x)} + \mathrm{i}r_\theta(x)\,\mathrm{e}^{\mathrm{i}\phi_\theta(x)}\frac{\partial\phi_\theta}{\partial\theta}\right|^2\,\mathrm{d}x \\
&= \int_{\mathbb{R}}\left(\frac{\partial r_\theta(x)}{\partial\theta}\right)^2\,\mathrm{d}x + \int_{\mathbb{R}}\left(r_\theta(x)\frac{\partial\phi_\theta(x)}{\partial\theta}\right)^2\,\mathrm{d}x \\
&= \frac{1}{4}I(\psi_\theta) + \int_{\mathbb{R}} J^2_{\psi_\theta}(x)|\psi_\theta(x)|^2\,\mathrm{d}x.
\end{aligned}$$

□

## 3. Uncertainty relation inequalities

It was first noted by Stam that the conventional Heisenberg uncertainty relation is a consequence of the Cramér–Rao inequality [16]. We will establish a family of integral inequalities relating kinetic energy and moments (with both positive and negative order) which are of the characteristic of uncertainty relations.

For $k = 0,\ \pm 1, \pm 2, \ldots,$ we define the $k$th moment of $\psi_\theta$ centred at zero as

$$M_k(\psi_\theta) := \int_{\mathbb{R}} x^k|\psi_\theta(x)|^2\,\mathrm{d}x$$

provided the integral exists.

Let

$$Q_k\psi_\theta(x) = x^k\psi_\theta \qquad P\psi_\theta(x) = \frac{\partial}{\partial\theta}\psi_\theta(x).$$

Then

$$\langle Q_k\psi_\theta, P\psi_\theta\rangle = \int_{\mathbb{R}} x^k\psi_\theta(x)\frac{\partial}{\partial\theta}\psi^*_\theta(x)\,\mathrm{d}x.$$

Consequently, let Re denote the real part of a complex number, we have

$$\begin{aligned}
\mathrm{Re}\langle Q_k\psi_\theta, P\psi_\theta\rangle &= \frac{1}{2}\int_{\mathbb{R}} x^k\left(\psi_\theta(x)\frac{\partial\psi^*_\theta(x)}{\partial\theta} + \psi^*_\theta(x)\frac{\partial\psi_\theta(x)}{\partial\theta}\right)\mathrm{d}x \\
&= \frac{1}{2}\int_{\mathbb{R}} x^k\frac{\partial}{\partial\theta}|\psi_\theta(x)|^2\,\mathrm{d}x \\
&= \frac{1}{2}\frac{\partial}{\partial\theta}\int_{\mathbb{R}} x^k|\psi_\theta(x)|^2\,\mathrm{d}x \\
&= \frac{1}{2}\frac{\partial}{\partial\theta}M_k(\psi_\theta).
\end{aligned}$$

By Schwarz inequality,

$$|\mathrm{Re}\langle Q_k\psi_\theta, P\psi_\theta\rangle|^2 \leqslant \langle Q_k\psi_\theta, Q_k\psi_\theta\rangle \cdot \langle P\psi_\theta, P\psi_\theta\rangle.$$

Thus

$$\left(\frac{1}{2}\frac{\partial}{\partial\theta}M_k(\psi_\theta)\right)^2 \leqslant \int_{\mathbb{R}} |Q_k\psi_\theta(x)|^2\,\mathrm{d}x \cdot \int_{\mathbb{R}} |P\psi_\theta(x)|^2\,\mathrm{d}x = M_{2k}(\psi_\theta)\cdot K(\psi_\theta).$$

In summary, we have established the following result.

**Theorem 2.** *For* $k = 0, \pm1, \pm2, \ldots,\ \psi_\theta \in L^2(\mathbb{R},\ \mathrm{d}x)$*, it holds that*

$$K(\psi_\theta)\cdot M_{2k}(\psi_\theta) \geqslant \left(\frac{1}{2}\frac{\partial}{\partial\theta}M_k(\psi_\theta)\right)^2.$$

If $\psi_\theta$ is a positive wavefunction, that is, $\psi_\theta = \sqrt{|\psi_\theta|^2}$, then $I(\psi_\theta) = 4K(\psi_\theta)$ and we come to the following conclusion.

**Corollary 3.** *For* $k = 0, \pm1, \pm2, \ldots,\ \psi_\theta \in L^2(\mathbb{R},\ \mathrm{d}x), \psi_\theta \geqslant 0$*, it holds that*

$$I(\psi_\theta)\cdot M_{2k}(\psi_\theta) \geqslant \left(\frac{\partial}{\partial\theta}M_k(\psi_\theta)\right)^2.$$

In particular, when $k = 1$, we come to the celebrated Cramér–Rao inequality widely used in statistical inference [4].

For any $k = 0,\ \pm1,\ \pm2, \ldots,\ \psi \in L^2(\mathbb{R},\ \mathrm{d}x)$, and any $\theta \in \mathbb{R}$, we define the $k$th moment of $\psi$ centred at $\theta$ as

$$M_k(\psi, \theta) := \int_{\mathbb{R}} (x-\theta)^k |\psi(x)|^2\,\mathrm{d}x.$$

**Corollary 4.** *For* $k = 0,\ \pm1,\ \pm2, \ldots,\ \psi \in L^2(\mathbb{R},\ \mathrm{d}x), \theta \in \mathbb{R}$*, we have*

$$K(\psi)\cdot M_{2k}(\psi,\theta) \geqslant \left(\frac{k}{2}M_{k-1}(\psi,\theta)\right)^2.$$

**Proof.** Put $\psi_\theta(x) = \psi(x+\theta)$, and apply theorem 2. In this case, $K(\psi_\theta) = K(\psi)$ is independent of $\theta$, and

$$\begin{aligned}
M_k(\psi_\theta) &= \int_{\mathbb{R}} x^k |\psi(x+\theta)|^2\,\mathrm{d}x \\
&= \int_{\mathbb{R}} (x-\theta)^k |\psi(x)|^2\,\mathrm{d}x \\
&= M_k(\psi,\theta) \\
\frac{\partial}{\partial\theta}M_k(\psi_\theta) &= -k\int_{\mathbb{R}} (x-\theta)^{k-1}|\psi(x)|^2\,\mathrm{d}x \\
&= -kM_{k-1}(\psi,\theta).
\end{aligned}$$

The conclusion follows.

Two cases are of particular interest and simplicity. We assume that $\psi_\theta$ is normalized, that is, $\int_{\mathbb{R}} |\psi_\theta(x)|^2\,\mathrm{d}x = 1$.

(1) If $k = 1$, then we obtain the conventional Weyl–Heisenberg inequality [11, 14]

$$K(\psi)\cdot M_2(\psi) \geqslant \frac{1}{4}.$$

(2) If $k = -1$, we have a peculiar inequality

$$K(\psi) \cdot \frac{1}{M_{-2}(\psi)} \geqslant \frac{1}{4}$$

which may also be interpreted as a kind of uncertainty relation. □

Frieden introduced a notion of $F$-information for the purpose to establish a unitless analogue of Fisher information [10]. Generalizing this notion from probability densities to wavefunctions, we define for any $\psi \in L^2(\mathbb{R}, \mathrm{d}x)$, the $F$-information of $\psi$ as

$$F(\psi) := 4 \int_{\mathbb{R}} x^2 \left| \frac{\partial \psi(x)}{\partial x} \right|^2 \mathrm{d}x.$$

This notion of $F$-information is essentially connected with the Fisher information of $\psi_\theta(x) := \psi(\theta x)$, that is, Fisher information with respect to a *scale* parameter, and thus is also intimately connected with the kinetic energy with respect to a scale parameter. In theorem 2, specifying the parameter to a scale parameter, we have

**Corollary 5.** *For $k = 0, \pm 1, \pm 2, \ldots, \psi \in L^2(\mathbb{R}, \mathrm{d}x), \theta \in \mathbb{R}$, we have*

$$F(\psi) \geqslant \frac{(k+1)^2 M_k^2(\psi)}{M_{2k}(\psi)}.$$

*In particular, when $\psi$ is a normalized wavefunction and $k = 0$, we have*

$$F(\psi) \geqslant 1.$$

**Proof.** In theorem 2, let $\psi_\theta(x) := \psi(\theta x)$, then by definitions

$$K(\psi_\theta) = \int_{\mathbb{R}} \left| \frac{\partial \psi(\theta x)}{\partial \theta} \right|^2 \mathrm{d}x = \frac{1}{\theta^3} \int_{\mathbb{R}} x^2 \left| \frac{\partial \psi(x)}{\partial x} \right|^2 \mathrm{d}x = \frac{1}{4\theta^3} F(\psi)$$

$$M_k(\psi_\theta) = \int_{\mathbb{R}} x^k |\psi(\theta x)|^2 \,\mathrm{d}x = \frac{1}{\theta^{k+1}} M_k(\psi)$$

$$M_{2k}(\psi_\theta) = \frac{1}{\theta^{2k+1}} M_{2k}(\psi).$$

□

The desired result follows.

## 4. Discussions

By generalizing both the notion of Fisher information and the notion of conventional mechanical kinetic energy, we have introduced a general notion of kinetic energy with respect to a parameter. Since this notion interpolates between a fundamental statistical notion—the Fisher information, and a fundamental mechanical notion—the kinetic energy, it provides a bridge to connect the statistical information theory and the theory of mechanical motions. As applications, we have established a whole family of integral inequalities of the characteristic of uncertainty relations, which includes some familiar fundamental inequalities as special cases. We hope the notion of kinetic energy introduced here may serve as an intuitive tool in the informational approach to physics by connecting the notion of Fisher information and the classical Lagrangian approach to mechanics.

It should be emphasized that we have only worked on the one-dimensional case (in both parameter and the space). Although the extension to the multi-parameter case and higher dimensional spaces seems straightforward, we do not pursue it here. However, we remark that this extension is more relevant in applications to physical systems. Many new phenomena should be expected concerning the interaction of multi-parameter and higher dimensional spaces. In this respect, see [5, 15, 17] for some motivating physical examples.

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