

A quantum uncertainty relation based on Fisher's information

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Abstract

We explore quantum uncertainty relations involving the Fisher information functionals I_x and I_p evaluated, respectively, on a wavefunction $\Psi(\mathbf{x})$ defined on a D -dimensional configuration space and the concomitant wavefunction $\tilde{\Psi}(\mathbf{p})$ on the conjugate momentum space. We prove that the associated Fisher functionals obey the uncertainty relation $I_x I_p \geq 4D^2$ when either $\Psi(\mathbf{x})$ or $\tilde{\Psi}(\mathbf{p})$ is real. On the other hand, there is no lower bound to the above product for arbitrary complex wavefunctions. We give explicit examples of complex wavefunctions not obeying the above bound. In particular, we provide a parametrized wavefunction for which the product $I_x I_p$ can be made arbitrarily small.

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1. Introduction

The application of Fisher's information measure to the analysis of diverse physical systems and processes has been an active field of research in recent years [1–25]. Fisher's measure has been applied to the study of a variety of subjects, ranging from black hole physics [5] and the characterization of the arrow of time in irreversible processes [6, 7] to avoided crossing phenomena [23] and the information–theoretical aspects of chemical reactions [24]. Various recent developments indicate that Fisher's information plays a fundamental role in quantum mechanics and its applications [1–4, 10–25]. In particular, it allows for the formulation of new quantum uncertainty principles [17–21].

Uncertainty relations have played a distinguished role in the historical development of quantum mechanics and constitute a basic ingredient of its conceptual foundations [26–28]. In addition to the standard variance-based uncertainty relations, new uncertainty relations formulated in terms of Shannon's and other entropic measures (such as Rényi's and Tsallis')

have been proposed (see [29–31] and references therein). Uncertainty relations entirely based upon Fisher’s information have also been advanced, but most of them apply only to the eigenstates of particular systems [17–21]. The main motivation behind these undertakings is the following. The form of Fisher’s functional distinguishes it as a very special uncertainty measure. In contrast to ‘global’ ways of characterizing uncertainty (such as those provided by the variance, or by Shannon’s entropy), Fisher’s information depends not only on the relevant probability density ρ , but also on its gradient. Consequently, Fisher’s information is strongly sensitive to the local oscillatory character of ρ . It would be of considerable interest to obtain universal uncertainty relations based upon the Fisher informations $I_{\mathbf{x}}$ and $I_{\mathbf{p}}$, respectively, evaluated on the conjugate position and momentum spaces. A first step towards this end was recently done in [21], where it was proved that all real, even, one-dimensional wavefunctions $\Psi(x)$ comply with the uncertainty relation:

$$I_x I_p \geq 4. \tag{1}$$

The aim of this effort is to establish a substantial generalization of that result. We are going to prove that quantum states described by a wavefunction $\Psi(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^D$, satisfy the uncertainty relation:

$$I_x I_p \geq 4D^2, \tag{2}$$

when either $\Psi(\mathbf{x})$ or the corresponding momentum–space wavefunction $\tilde{\Psi}(\mathbf{p})$ is real. We shall also prove that this result cannot be extended to general (complex) wavefunctions.

This paper is organized as follows. In section 2, we briefly review the main expressions for the Fisher measures position and in momentum spaces. In section 3, we derive an uncertainty principle based on the above-mentioned Fisher functionals. This principle is valid for quantum states of a spinless particle in D dimensions and having a real position wavefunction or, alternatively, a real momentum wavefunction. In section 4, we provide examples of complex wavefunctions not complying with this Fisher uncertainty principle. Finally, some conclusions are drawn in section 5.

2. Fisher’s information in position and momentum spaces

The Fisher information I_θ corresponding to a family of probability densities $F(\mathbf{x}; \theta)$ defined on \mathbb{R}^D and depending on a parameter θ is given by [1, 2]

$$I_\theta = \int \frac{1}{F(\mathbf{x}; \theta)} \left(\frac{\partial F}{\partial \theta} \right)^2 \mathbf{d}\mathbf{x}, \tag{3}$$

where $\mathbf{d}\mathbf{x} = \prod_{k=1}^D dx_k$ is the volume element in \mathbb{R}^D . When dealing with a probability density $F(\mathbf{x}; \bar{\theta})$ depending on a set of parameters $\bar{\theta} = (\theta_1, \dots, \theta_m)$ one defines a Fisher matrix with matrix elements:

$$I_{jk} = \int \frac{1}{F(\mathbf{x}; \bar{\theta})} \left(\frac{\partial F}{\partial \theta_j} \right) \left(\frac{\partial F}{\partial \theta_k} \right) \mathbf{d}\mathbf{x}. \tag{4}$$

Of special importance are the translational families of probability densities having the form

$$F(\mathbf{x} - \bar{\theta}), \tag{5}$$

with $\bar{\theta} \in \mathbb{R}^D$. All the members of such a family of probability densities share the same shape and differ only on a shift given by the vector $\bar{\theta}$. In this case the elements of the Fisher matrix are $I_{jk} = \int \frac{1}{F} \left(\frac{\partial F}{\partial x_j} \right) \left(\frac{\partial F}{\partial x_k} \right) \mathbf{d}\mathbf{x}$. The trace of this Fisher matrix, given by

$$I = \int \frac{1}{F} \left[\sum_{k=1}^D \left(\frac{\partial F}{\partial x_k} \right)^2 \right] \mathbf{d}\mathbf{x} \tag{6}$$

is of particular relevance for the study of information theoretical aspects of wavefunctions in quantum mechanics. This information measure proved to be a very useful indicator of the uncertainty of the probability densities associated with quantum mechanical wavefunctions, because it takes into account local features of these densities [17–25]. The Fisher measure (6), and the analogous measure defined in momentum space, are the natural ones for the formulation of uncertainty relations for quantum systems with a D -dimensional configuration space, and are the ones that we are going to consider in this study.

Let us consider a normalized wavefunction $\Psi(\mathbf{x})$ defined on a D -dimensional configuration space characterized by the vector position $\mathbf{x} \in \mathbb{R}^D$. The corresponding momentum-space wavefunction is then given by

$$\tilde{\Psi}(\mathbf{p}) = \frac{1}{(2\pi)^{D/2}} \int \exp(-i\mathbf{x} \cdot \mathbf{p}) \Psi(\mathbf{x}) \, d\mathbf{x}, \quad (7)$$

where we have set $\hbar = 1$. The associated probability densities in both position and momentum spaces are, respectively,

$$\begin{aligned} \rho(\mathbf{x}) &= |\Psi(\mathbf{x})|^2, \\ \tilde{\rho}(\mathbf{p}) &= |\tilde{\Psi}(\mathbf{p})|^2, \end{aligned} \quad (8)$$

with the corresponding Fisher measures respectively given by

$$I_{\mathbf{x}} = \int \frac{1}{\rho} [\nabla_{\mathbf{x}} \rho]^2 \, d\mathbf{x} = 4 \int [\nabla_{\mathbf{x}} u]^2 \, d\mathbf{x} \quad (9)$$

and

$$I_{\mathbf{p}} = \int \frac{1}{\tilde{\rho}} [\nabla_{\mathbf{p}} \tilde{\rho}]^2 \, d\mathbf{p} = 4 \int [\nabla_{\mathbf{p}} \tilde{u}]^2 \, d\mathbf{p}, \quad (10)$$

where $\nabla_{\mathbf{x}} = (\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_D})$ and $\nabla_{\mathbf{p}} = (\frac{\partial}{\partial p_1}, \dots, \frac{\partial}{\partial p_D})$ are, respectively, the D -dimensional ∇ -operators in position and momentum space, $d\mathbf{p} = \prod_{k=1}^D dp_k$, $u(\mathbf{x}) = |\Psi(\mathbf{x})|$, and $\tilde{u}(\mathbf{p}) = |\tilde{\Psi}(\mathbf{p})|$. From here on we shall drop the subindex ‘ \mathbf{x} ’ from the ∇ -operator in position space.

3. An uncertainty relation based upon Fisher’s information

In this section we are going to derive an uncertainty principle based upon the Fisher measures $I_{\mathbf{x}}$ and $I_{\mathbf{p}}$. More specifically, we are going to show that the product $I_{\mathbf{x}} I_{\mathbf{p}}$ admits a non trivial (that is, non zero) lower bound when either $\Psi(\mathbf{x})$ or $\tilde{\Psi}(\mathbf{p})$ is real. We shall assume that all the integrals appearing in the derivations that follow converge. In particular, we shall assume that $I_{\mathbf{x}}$ and $I_{\mathbf{p}}$ adopt finite values.

Let us consider first the case of a real momentum wavefunction:

$$\tilde{\Psi}(\mathbf{p}) = \tilde{\Psi}^*(\mathbf{p}). \quad (11)$$

The momentum Fisher measure is then

$$I_{\mathbf{p}} = 4 \int [\nabla_{\mathbf{p}} \tilde{\Psi}]^2 \, d\mathbf{p} = -4 \int \tilde{\Psi} \nabla_{\mathbf{p}}^2 \tilde{\Psi} \, d\mathbf{p}, \quad (12)$$

where the last equality was obtained by integrating by parts (we assume that $\tilde{\Psi} \rightarrow 0$ fast enough when $|p| \rightarrow \infty$, so that the surface terms appearing when integrating by parts vanish). Now, in the momentum representation (7) the position observable x_k is represented by the operator

$$i \frac{\partial}{\partial p_k}. \quad (13)$$

Therefore, taking (11) into account, it is plain that the last expression for $I_{\mathbf{p}}$ appearing in equation (12) is proportional to the expectation value of the Hermitian operator corresponding (in the momentum representation) to the observable

$$\mathbf{x}^2 = \sum_{k=1}^D x_k^2. \quad (14)$$

That is,

$$I_{\mathbf{p}} = 4\langle \mathbf{x}^2 \rangle. \quad (15)$$

Consequently, the minimum value $G_{\min.}$ adopted by the functional

$$G = 4\langle \mathbf{x}^2 \rangle I_{\mathbf{x}} = 16 \left[\int u^2(\mathbf{x}) \mathbf{x}^2 d\mathbf{x} \right] \left\{ \int [\nabla u]^2 d\mathbf{x} \right\}, \quad (16)$$

when minimized over all functions $u(\mathbf{x})$ complying with the normalization condition

$$\int u^2(\mathbf{x}) d\mathbf{x} = 1, \quad (17)$$

provides a lower bound for the possible values adopted by the product $I_{\mathbf{x}} I_{\mathbf{p}}$ when $\tilde{\Psi}(\mathbf{p})$ is real.

Before considering the minimization of (16) under constraint (17) it is important to realize that the functional G is invariant under the re-scaling transformation:

$$u(\mathbf{x}) \longrightarrow u_{\lambda}(\mathbf{x}) = \lambda^{D/2} u(\lambda \mathbf{x}). \quad (18)$$

Indeed, under transformation (18) the quantities $\langle \mathbf{x}^2 \rangle$ and $I_{\mathbf{x}}$ scale as

$$\begin{aligned} \langle \mathbf{x}^2 \rangle [u_{\lambda}] &= \lambda^{-2} \langle \mathbf{x}^2 \rangle [u_{\lambda=1}] \\ I_{\mathbf{x}} [u_{\lambda}] &= \lambda^2 I_{\mathbf{x}} [u_{\lambda=1}], \end{aligned} \quad (19)$$

which leaves the product $\langle \mathbf{x}^2 \rangle I_{\mathbf{x}}$ invariant. Due to this invariance, the minimum value adopted by G does not change if, besides normalization, we incorporate a second constraint of the form

$$\int \mathbf{x}^2 u^2(\mathbf{x}) d\mathbf{x} = b, \quad (20)$$

where b is some constant. But now, the minimization of G under constraints (17) and (20) is tantamount to the minimization of $I_{\mathbf{x}}$ under these two constraints. This constrained variational problem can be tackled with the method of Lagrange multipliers, which leads to the variational equation:

$$\delta \left\{ 4 \int [\nabla u]^2 d\mathbf{x} + \alpha \left[\int u^2(\mathbf{x}) d\mathbf{x} - 1 \right] + \beta \left[\int \mathbf{x}^2 u^2(\mathbf{x}) d\mathbf{x} - b \right] \right\} = 0, \quad (21)$$

where α and β are the Lagrange multipliers corresponding to the normalization and $\langle \mathbf{x}^2 \rangle$ constraints, respectively. The Euler–Lagrange equations associated with the variational problem (21) are

$$\sum_{k=1}^D \frac{\partial}{\partial x_k} \left(\frac{\partial \mathcal{L}}{\partial w_k} \right) - \frac{\partial \mathcal{L}}{\partial u} = 0, \quad (22)$$

where $(w_k, k = 1, \dots, D)$ are the components of the vector $\mathbf{w} = \nabla u$ and the Lagrangian density \mathcal{L} is given by

$$\mathcal{L}(u, \mathbf{w}, \mathbf{x}) = 4\mathbf{w}^2 + \alpha u^2 + \beta \mathbf{x}^2 u^2. \quad (23)$$

The Euler–Lagrange equations (22) can be cast under the guise of a Schrödinger equation:

$$-\frac{1}{2} \nabla^2 u(\mathbf{x}) + V(\mathbf{x}) u(\mathbf{x}) = -\frac{1}{8} \alpha u(\mathbf{x}) \quad (24)$$

characterized by the potential function

$$V(\mathbf{x}) = \frac{1}{8}\beta\mathbf{x}^2. \quad (25)$$

The optimum function $u_m(\mathbf{x})$ (that is, the one minimizing the quantity G defined in equation (16) under the normalization constraint or, equivalently, the one minimizing I_x under the constraints given by normalization and $\langle \mathbf{x}^2 \rangle$) corresponds to the ground state of potential (25):

$$u_m(\mathbf{x}) = \frac{1}{(\pi^{1/2}a)^{D/2}} \exp[-\mathbf{x}^2/(2a^2)], \quad (26)$$

where

$$a = \left(\frac{4}{\beta}\right)^{1/4}. \quad (27)$$

Note that the Lagrange parameter β must be positive in order to obtain a function that complies with the normalization constraint. Finally, for the Gaussian wavefunction (26) we have

$$I_x[u_m]I_p[u_m] = 4D^2. \quad (28)$$

Consequently, if $\tilde{\Psi}(\mathbf{p})$ is real we have $I_x I_p \geq 4D^2$. It is clear that, due to the dual relationship between the x -representation and the p -representation, a similar argument holds in the case that the position-space wavefunction $\Psi(\mathbf{x})$ is real. Note that, in order to obtain the lower bound for $I_x I_p$, we only need to consider the ground state solution of the Schrödinger equation (24). Any solution corresponding to an excited state leads to a larger value of $I_x I_p$.

Summing up, we have proved that *if either the momentum-space wavefunction $\tilde{\Psi}(\mathbf{p})$ or the position-space wavefunction $\Psi(\mathbf{x})$ is real, then the associated Fisher measures satisfy the Fisher-based uncertainty relation:*

$$I_x I_p \geq 4D^2. \quad (29)$$

By recourse to the identity $I_x + I_p \geq 2\sqrt{I_x I_p}$ one can see that relation (29) also implies the uncertainty inequality

$$I_x + I_p \geq 4D. \quad (30)$$

Finally, let us say for the sake of completeness that the uncertainty relation (29) was previously found to hold for the particular case of eigenfunctions of central potentials [17–20].

4. General wavefunctions

The results reported in the previous section suggest the natural next step of considering the behaviour of the product $I_x I_p$ for general wavefunctions. As we will soon see, this product can be made arbitrarily small in the general case. We are now going to consider some particular examples where the aforementioned product does not comply with the uncertainty inequality (29).

4.1. Linear combinations of a finite number of Hermite wavefunctions

As a first example let us consider the bi-parametric family of wavefunctions:

$$\psi(x) = \frac{1}{\pi^{1/4}} e^{-\frac{x^2}{2}} \left(a_0 H_0(x) + a_1 \frac{1}{\sqrt{2}} H_1(x) \right), \quad (31)$$

where the $H_n(x)$ stand for the Hermite polynomials and

$$\begin{aligned} a_0 &= \epsilon_0 + i\sqrt{\frac{3}{4} - \epsilon_0^2}, \\ a_1 &= \epsilon_1 + i\sqrt{\frac{1}{4} - \epsilon_1^2}, \end{aligned} \quad (32)$$

with ϵ_0 and ϵ_1 real. Note that $|a_0|^2 + |a_1|^2 = 1$ (that is, wavefunction (31) is properly normalized) if $\epsilon_0 \leq \sqrt{\frac{3}{4}}$ and $\epsilon_1 \leq \frac{1}{2}$. It is possible to find values of ϵ_0 and ϵ_1 such that $I_x I_p < 4$. For instance, if $\epsilon_0 = 0.3$ and $\epsilon_1 = 0.4$, we obtain $I_x \simeq 2.22$, $I_p \simeq 1.68$, and

$$I_x I_p \simeq 3.73 < 4. \quad (33)$$

Let us consider now the linear space spanned by n one-dimensional Hermite wavefunctions. That is, we consider wavefunctions of the form

$$\psi_n(x) = \frac{1}{\pi^{\frac{1}{4}}} e^{-\frac{x^2}{2}} \sum_{k=0}^n a_k \frac{1}{\sqrt{2^k k!}} H_k(x), \quad (34)$$

where a_k are complex coefficients such that $\sum_{k=0}^n |a_k|^2 = 1$. Wavefunctions of the form (34) are not solutions of any specific, single Schrödinger equation. They constitute a linear subspace of the general space of normalized wavefunctions $\Psi(x)$ with $x \in \mathbb{R}$. Our purpose now is to determine the fraction F_n of states in this space that do not satisfy inequality (29) (with $D = 1$).

To evaluate the fraction F_n we use a numerical Monte Carlo approach. We generate random states in the above space, uniformly distributed according to the Haar measure (see [32, 33] and references therein) and compute, for different values of n , the fraction F_n of states satisfying $I_x I_p < 4$. In other words, we generate a large number A_n of n -tuples (a_1, \dots, a_n) (that is, a large number A_n of states of the form (34)) and determine how many of them do not comply with the inequality $I_x I_p \geq 4$. The numerical estimate of F_n is then given by $F_n \approx B_n/A_n$, where B_n is the number of generated states violating this inequality (one always has, of course, that $0 \leq B_n \leq A_n$). The details of the procedure for generating the aforementioned A_n sets of coefficients a_k are as follows. Let us first write the complex coefficients a_k as $a_k = r_k \exp(i\alpha_k)$, with r_k, α_k real, $r_k \geq 0$, and $\alpha_k \in [0, 2\pi)$. To generate each set of complex coefficients (a_1, \dots, a_n) we have to generate the n moduli (r_1, \dots, r_n) and the n phases $(\alpha_1, \dots, \alpha_n)$. The n numbers (r_1, \dots, r_n) can be regarded as the coordinates of a point on the positive hyperoctant of the hypersphere defined by the equation $r_1^2 + \dots + r_n^2 = 1$. To generate a set (r_1, \dots, r_n) is tantamount to generating a point on the above hyperoctant. On the basis of this geometric representation, the n -tuples (r_1, \dots, r_n) are generated randomly according to a uniform distribution on the surface of the above-mentioned hyperoctant. On the other hand, each of the phases α_k are randomly generated according to a uniform distribution on the interval $[0, \pi)$.

The values of F_n corresponding to different values of n are given in table 1. An interesting trend observed in this table is that F_n decreases quickly as n increases. Indeed, the results of our Monte Carlo study suggest that F_n decreases exponentially with n . This numerical evidence motivates us to make the conjecture that the fraction F_n of states violating the uncertainty relation (29) actually tends to zero when $n \rightarrow \infty$.

Table 1. Ratio F_n as a function of n .

n	F_n
2	0.33 ± 0.01
3	0.092 ± 0.009
4	0.030 ± 0.005
5	0.0093 ± 0.0009
6	0.0025 ± 0.0006

4.2. Time-dependent Gaussian wavepacket

Now we are going to discuss a particular example where the product $I_x I_p$ adopts arbitrarily small values. Let us consider a time-dependent, one-dimensional Gaussian wavepacket $\Psi(x, t)$ evolving according to the free-particle time-dependent Schrödinger equation:

$$i \frac{\partial \Psi}{\partial t} = -\frac{1}{2} \frac{\partial^2 \Psi}{\partial x^2}, \tag{35}$$

corresponding to a particle of unit mass (for a detailed discussion on time-dependent Gaussian wavepackets see [34]). We assume the following initial (that is, corresponding to $t = 0$) wavefunctions in position and momentum spaces:

$$\begin{aligned} \Psi(x, 0) &= \left(\frac{1}{\Delta \sqrt{\pi}} \right)^{1/2} \exp(-x^2/(2\Delta^2)) \\ \tilde{\Psi}(p, 0) &= \left(\frac{\Delta}{\sqrt{\pi}} \right)^{1/2} \exp(-\Delta^2 p^2/2), \end{aligned} \tag{36}$$

with $\Delta > 0$. The time-dependent solution $\Psi(x, t)$ to Schrödinger's equation (35) corresponding to the initial conditions (36) is then

$$\Psi(x, t) = \left(\frac{1}{\Delta \sqrt{\pi} (1 + it/\Delta^2)} \right)^{1/2} \exp\left(-\frac{x^2}{2\Delta^2 (1 + it/\Delta^2)} \right). \tag{37}$$

The time-dependent wavepacket (37) has group velocity equal to zero. The corresponding probability density in position space is

$$\rho(x, t) = \frac{1}{\Delta \sqrt{\pi} (1 + t^2/\Delta^4)} \exp\left(-\frac{x^2}{\Delta^2 (1 + t^2/\Delta^4)} \right). \tag{38}$$

On the other hand, due to the fact that momentum is conserved during free particle motion, the probability density in momentum space remains constant in time and is given by

$$\tilde{\rho}(p) = \frac{\Delta}{\sqrt{\pi}} \exp(-\Delta^2 p^2). \tag{39}$$

Evaluating now the product of the Fisher information associated with the probability densities (38) and (39) we obtain

$$I_x I_p = 4 \left(1 + \frac{t^2}{\Delta^4} \right)^{-1}. \tag{40}$$

We can see that $I_x I_p < 4$ when $t > 0$. In other words, wavefunction (37) does not satisfy the uncertainty relation $I_x I_p \geq 4D^2$ when $t > 0$. Moreover, $I_x I_p \rightarrow 0$ when $t \rightarrow \infty$.

5. Conclusions

We have investigated quantum uncertainty relations expressed in terms of the Fisher information measures I_x and I_p , respectively, evaluated on a wavefunction $\Psi(\mathbf{x})$ defined on a D -dimensional configuration space and on the associated wavefunction $\tilde{\Psi}(\mathbf{p})$ on the conjugate momentum space. Generalizing previous results recently presented in the literature, we proved that the above-mentioned Fisher functionals satisfy the uncertainty relation $I_x I_p \geq 4D^2$ when either $\Psi(\mathbf{x})$ or $\tilde{\Psi}(\mathbf{p})$ is real. On the other hand, we have shown that the product $I_x I_p$ does not admit a non-trivial lower bound in the case of arbitrary, complex wavefunctions. In point of fact, we provided an explicit example of a parameterized wavefunction for which the product $I_x I_p$ can be made arbitrarily small.

Our present findings unify and generalize previously reported results that apply only to the eigenfunctions of particular systems [17–21], or to real wavefunctions satisfying special requirements (such as, for instance, being even [21]). It is worth stressing, however, that in some special cases it is possible to obtain lower bounds to $I_x I_p$ that are stronger than the general ones derived here. Indeed, in the case of the eigenfunctions of spherically symmetric potentials there is a better (that is, higher than $4D^2$) bound to the product of the Fisher measures in position and momentum spaces [17–20].

As a final remark, it is worth mentioning that the real-valued character of either the wavefunction in position space or the one in momentum space that we assumed in order to derive the inequality $I_x I_p \geq 4D^2$ is, strictly speaking, only a sufficient condition to have this relation, but not a necessary one. In fact, the numerical study described in section 4.1 indicates that there are actually plenty of complex wavefunctions complying with the above inequality. Consequently, it may be the case that the validity of our present uncertainty relation may be extended to incorporate more general (complex) wavefunctions satisfying some appropriate (yet to be discovered) conditions. This means that our inequality $I_x I_p \geq 4D^2$, as referred to real $\Psi(\mathbf{x})$ or real $\tilde{\Psi}(\mathbf{p})$, may not be the most ‘universal’ uncertainty relation expressible as a lower bound to the product of the Fisher measures I_x and I_p . Any further research conducted along these lines will be welcomed.

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