Structure of the density matrix providing the minimum of generalized uncertainty relation for mixed states

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Abstract. For configurational space of arbitrary dimension a strict form of the uncertainty principle has been obtained, which takes into account the dependence of inequality limit on the effective number of pure states present in given statistical mixture. It is shown that in a state with minimal uncertainty the density operators eigenfunctions coincide with the stationary wavefunctions of a multidimensional harmonic oscillator. The mixed state obtained has a permutational symmetry which is typical for a system of identical bosons.

PACS numbers: 03.65.Bz

Submitted to: J. Phys. A: Math. Gen.

1. Introduction

As shown in the papers [1-3], the generalization of conventional uncertainty relation of the position-momentum type (see, e. g. Ref. 4) to the case of mixed states, determined by a density matrix $\rho(x, x')$, leads to a radically new result. It sounds as follows — the smallest allowable room $\Delta v_p$, occupied by system in the phase space, grows proportionally to the effective number $N_{\text{eff}}$ of pure states by whose statistical mixture the given density matrix is representable, that is

$$\min(\Delta v_p) \propto N_{\text{eff}}.$$ (1)

One of the possible variants of relation (1), which can be used in a real or configurational space $X = (x_1, \ldots, x_s)$ with an arbitrary number of dimensions $s$, has been obtained in [5] and is of the form

$$\frac{(\Delta x \Delta q)^s}{N_{\text{eff}}} \geq C(s) \left(\frac{1}{2}\right)^s.$$ (2)
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The next definitions are introduced here: $\Delta x$, $\Delta q$ the root mean square widths (additionally averaged over all $s$ degrees of freedom) correspondingly of coordinate and wave-vector distributions in the state $\rho(x, x')$

\[
(\Delta x)^2 = \frac{1}{s} \int d^sX X^2 \rho(X, X),
\]

\[
(\Delta q)^2 = -\frac{1}{s} \int d^sX \int d^sX' \delta(X - X') \nabla^2_X \rho(X, X'), \quad \left[ \nabla^2_X = \sum_{i=1}^s \frac{\partial^2}{\partial x_i^2} \right],
\]

\[
N_{eff} = \left( \int d^sX \int d^sX' |\rho(X, X')|^2 \right)^{-1}.
\]

Besides, it is assumed that the normalisation condition

\[
\int d^sX \rho(X, X) = 1,
\]

is met and the mean values of position and momentum are equal to zero (without loss of generality the latter can be done by choosing an appropriate reference frame). For convenience the right-hand side of inequality (2) is represented as two factors. One of which, $(1/2)^s$, is the minimum of usual uncertainty relation for pure states and, as known, is attained for Gaussian wave-packets [4]. The second factor, $C(s)$, can be named the “packing coefficient” and expresses the specificity of $N_{eff}$ definition and, properly, the influence of space multidimensionality [5]

\[
C(s) = \frac{2^{s+1}(s+1)!}{(s+2)^{s+1}}.
\]

The particular interest for the relation (2) is caused by its analogy with one of the basic statements of statistical mechanics [6, 7] concerning the partitioning of the phase space into cells with each of them corresponds to one quantum state. Indeed, the quantity $\Delta v_p = (\Delta x, \Delta q)^s$ is a peculiar kind of measure of a system phase volume, whereas $N_{eff}$ is a characteristic number of its possible states. It is therefore obvious that, despite the considerable differences in the formulations used, in either case one can speak about two possible ways of exhibiting one and the same fundamental property of quantum-mechanical objects.

On the other hand, inequality (2) holds not only for density matrix, but as well for correlation functions of wavefields of various nature and it can be seminally applied, after appropriate terminology corrections, in other fields of physics. In fact, the basic works [1-3], where one-dimensional case of relation (2) was obtained, deal with partially coherent light beams.

Given in [5] variant of the proof was based on the Carlson type integral inequalities for the Wigner function, that implies some disadvantages, in particular, because such approach does not determine the explicit form of the density matrix minimizing (2). This question is of interest in itself and, at the same time, is important for applications
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(for example, at the coherence theory [8]). Hence in the present paper we shall consider an alternative way to derive the relation (2). The aim is not only to solve the problem stated, but also reinforces the inequality by taking into account the dependence of packing coefficient on the effective number of states $C(s) \Rightarrow C(s, N_{\text{eff}})$.

2. Formulation of the problem and rigorous solution

The method to be applied constitutes a modification of approach, which was developed in Ref. 9 to analyze an analogous one-dimensional problem. It is based on the use of standard Lagrange procedure of search for the minimum of the system uncertainty volume (i.e. the value $\Delta x \Delta q$) under a constraint of given $N_{\text{eff}}$ (5). As common for such treatments [1-3, 5, 9], one should seek the extremum of auxiliary functional $F$

$$F[\rho(X, X')] = k^2(\Delta x)^2 + \frac{1}{k^2}(\Delta q)^2,$$

which has the property that its minimum for $k$ ($k$ is a variate scale factor) is attained simultaneously with the minimum of uncertainty volume

$$\min_k F = 2\Delta x \Delta q.$$

The substitution of definitions (3), (4) into (8) shows that the value of $F$ coincides in form with the mean value of energy of $s$-dimensional symmetrical harmonic oscillator with a Hamiltonian

$$\frac{1}{s} \left(-\frac{1}{k^2} \nabla_X^2 + k^2X^2\right),$$

which is in the mixed state $\rho(X, X')$. It is therefore natural for further treatment to represent $\rho(X, X')$ as a series expansion in the basis of this Hamiltonian eigenfunctions

$$\rho(X, X') = \sum_{n,n'} a_{n,n'}\Psi_n(X)\Psi_{n'}(X'),$$

where $n = (n_1, \ldots, n_s)$ is the “vector” index whose components range over nonnegative integer numbers,

$$\Psi_n(X) = \prod_{i=1}^s \psi_{n_i}(x_i),$$

$$\psi_n(x) = \sqrt{\frac{k}{2\pi n!}} e^{-k^2 x^2 / 2} H_n(kx),$$

$H_n(x) = \frac{1}{\sqrt{\pi}} e^{x^2} \frac{d^n}{dx^n} e^{-x^2} \text{ — Hermite polynomials, the functions } \Psi_n(X) \text{ are real and orthonormal. In view of the foregoing, the substitution of (9) into (8) gives}$

$$F = \sum_n a_{n,n} \left(\frac{2}{s} \|n\| + 1\right), \quad \|n\| = \sum_{i=1}^s n_i.$$
Now the additional condition, under which the effective number of states (5) is constant, can be written in the form

\[ \mu = \frac{1}{N_{eff}} = \sum_{n,n'} |a_{n,n'}|^2 = \text{const} \]  

(11)

(in statistical optics the parameter \( \mu \) is frequently referred to as global degree of coherence). One more constraint on expansion coefficients \( a_{n,n'} \) follows from the requirement for the density matrix (6) normalization

\[ \sum_n a_{n,n} = 1. \]  

(12)

Without going into details of elementary, although cumbersome intermediate calculations, we now turn to the analysis of the solution obtained. The first and most important consequence of minimization of \( \mathcal{F} \) (10) in coefficients \( a_{n,n} \) is that in the state of least uncertainty \( \rho_{\text{min}}(X,X') \) all off-diagonal elements of the matrix \([a_{n,n}]\) are equal to zero

\[ a_{n,n'} = a_{n,n} \delta_{n,n'}. \]

It means, that in this case the density operator’s eigenfunctions [6] (in optics — the decomposition modes) coincide in form with the eigenfunctions of energy operator of multidimensional harmonic oscillator. Accordingly, the diagonal elements of matrix \([a_{n,n'}]\) are the eigenvalues of density operator

\[ a_{n,n} \Psi_n(X) = \int d^sX' \rho_{\text{min}}(X,X') \Psi_n(X'). \]

They define the probabilities to find the system in the pure state \( \Psi_n(X) \) and satisfy the conditions \( \text{Im} a_{n,n} = 0 \) (as a consequence of \([a_{n,n'}]\) is Hermitian) and \( 0 \leq a_{n,n} \leq 1. \)

It should be noted here that the use of characteristic \( N_{eff} \) as a measure of number of possible pure states of the system is directly related to the operation of transition to the basis of density operator’s eigenfunctions in the representation (9). In the theory of stochastic processes [10] this procedure is referred to as Karhunen-Loève expansion of “correlation function” \( \rho(X,X') \) and gives, as known, the most compact and the most rapidly converging form of this series. Therefore, in this paper (as well as in [5]) under the term “state” is meant, as a rule, the eigenstate of density operator.

The second conclusion, directly following from the form of (10) – (12), is that the weights of states \( a_{n,n} \) can only depend on the vector index norm \( ||n|| \), and this dependence is linear and decreasing when \( ||n|| \) increases. Then it is obvious that at any finite value of \( N_{eff} \) the number of pure states \( \mathcal{N} \) present in the expansion \( \rho_{\text{min}} \) with a probability other then zero is also finite. And in the index domain, the coefficients \( a_{n,n} \neq 0 \) fill, layer by layer, the interior of \( s\)-dimensional equilateral pyramid with the total number of layers equal to \( \mathcal{L} \) (\( 0 \leq ||n|| < \mathcal{L} \)). The most probable pure state (\( n = 0 \)) corresponds to the pyramids vertex. The terms of expansion (9) pertaining to some particular layer are absolutely equivalent and make an equal contribution to
functional $\mathcal{F}$. Hence the spectrum of the eigenvalues in this mixed state is degenerate, and degeneration multiplicity in each layer is determined by value of $\|n\|$ and space dimensionality $s$

$$g_s(\|n\|) = \frac{(\|n\| + s - 1)!}{(\|n\|)! (s - 1)!}.$$ 

The total number of significant terms in $(9)$ is given by relation

$$N(\mathcal{L}) = \sum_{\|n\|=0}^{\mathcal{L}-1} g_s(\|n\|) = \frac{(\mathcal{L} + s - 1)!}{(\mathcal{L} - 1)! s!} = \frac{\mathcal{L}}{s} g_s(\mathcal{L}).$$

Finally, the sought state $\rho_{\min}$, which realizes the minimum of the generalized uncertainty relation, is described by series $(9)$ with coefficients

$$a_{n,n} = \begin{cases} \frac{1}{N(\mathcal{L})} \left[ 1 + ((\mathcal{L} - 1)s - \|n\|(s + 1)) \sqrt{\frac{(N(\mathcal{L}) - N_{\text{eff}})(s + 2)}{N_{\text{eff}} s(\mathcal{L} + s)(\mathcal{L} - 1)}} \right], & 0 \leq \|n\| < \mathcal{L}, \\ 0, & \|n\| \geq \mathcal{L} \end{cases}$$

and the inequality analogous to (2) takes the form

$$\Delta x \Delta q \geq \frac{(2\mathcal{L} + s - 1)!}{2(s + 1)} - \frac{\sqrt{(N(\mathcal{L}) - N_{\text{eff}})(\mathcal{L} + s)(\mathcal{L} - 1)}}{(s + 1) \sqrt{N_{\text{eff}} s(s + 2)}} = B(N_{\text{eff}}, \mathcal{L}(N_{\text{eff}})).$$

And it should be kept in mind that quantity $\mathcal{L}$, a certain positive integer, still remains a free parameter of the task and should be chosen proceeding from the condition of minimality of the right-hand side of inequality (14). By this means $\mathcal{L}$ will be a certain function of $N_{\text{eff}}$. The above requirements for the expansion coefficients $a_{n,n}$ (13) to be real and positive impose restrictions on allowable values of this parameter, namely, the quantity $\mathcal{L}$ should satisfy the following inequalities

$$N_{\text{eff}} \leq \frac{(\mathcal{L} + s - 1)!}{(\mathcal{L} - 1)! s!},$$

$$N_{\text{eff}} > \frac{(\mathcal{L} + s - 1)!}{(\mathcal{L} - 2)! (s + 1)!} \frac{s + 2}{s + 2(\mathcal{L} - 1)}.$$  

There exist certain ranges of values of $N_{\text{eff}}$ and $s$ (in particular, $s \gg 1$), in which inequalities (15), (16) determine $\mathcal{L}$ uniquely. But where it is not fulfilled and several integers fall within the interval given by formulas (15) and (16), the sought value of $\mathcal{L}$ turns to be largest of them (i.e. integer proximate to the upper boundary of (16)).

Inequality (14) is more hard than the previous inequality (2). On the plane of parameters with coordinates $\Delta x \Delta q$ and $N_{\text{eff}}$ it rigorously defines the region of physically realizable states. It is therefore apparent and can easily be proved that one should arrive at the same distributions of expansion coefficients (13) and the same region (14) by solving the inverse problem of seeking a mixed state with a largest possible value of $N_{\text{eff}}$ at a given measure $\Delta v_p$ of phase volume occupied by this state.
3. Approximate form of uncertainty relation

By virtue of the fact that with increasing \( N_{\text{eff}} \) the quantity \( L \) goes through a set of discrete values, the boundary of physical region \( B(N_{\text{eff}}) \) in (14) is not a perfectly smooth curve and is not described by analytical expression. Even though the numerical calculation of the right-hand side of inequality (14) presents no problem, it would be desirable to have its approximate analytical form in order to analyse the obtained relation and compare it with (2).

To this end we have investigated the behaviour of the function \( B(N_{\text{eff}}, \tilde{L}) \) at a given value of \( N_{\text{eff}} \), formally regarding \( \tilde{L} \) as an independent continuous variable. Analytical and numerical calculations show that in the vicinity of the true value of \( L \) the dependence of \( B \) on \( \tilde{L} \) is extremely weak. As well, in this region slightly different neighbouring local minimum and maximum for \( B(\tilde{L}) \) occur. This gives grounds to use the continuous parameter \( \tilde{L} \) instead of discrete number \( L \) when approximately describing the boundary of inequality (14). There are several ways of choosing the specific condition determining the value of \( \tilde{L} \).

The following one seems to be fairly simple and logically substantiated. In the expression for expansion coefficients (13), one can formally require “continuous” transition of its first part to the second one\footnote{Naturally, in this case, the variable \( ||n|| \) in (13) should also be regarded as continuous.}, which, after a little algebraic manipulations, yields a transcendental equation for determining \( \tilde{L} \) in the form

\[
a_{\tilde{L}, \tilde{L}} = 0 \Rightarrow N_{\text{eff}} = \frac{(s + 2) \Gamma(\tilde{L} + s + 1)}{(s + 2 \tilde{L})(s + 1)! \Gamma(\tilde{L})}; \tag{17}
\]

(because of \( \tilde{L} \) being continuous the factorials entering into the formula for \( N(\tilde{L}) \) have been replaced here by Euler gamma-functions). Accordingly, with such a way of defining \( L \), the approximate expression for inequality (14) can be written in the parametric form

\[
\Delta x \Delta q \geq \frac{s + 2 \tilde{L}(N_{\text{eff}})}{2(s + 2)}. \tag{18}
\]

It should be noted that the approximate boundary of physical domain, given by relations (17) and (18), exactly coincides with the result of the procedure proposed in [9], proceeding from the definition of \( L \) as the upper bound of inequality (16).

Another way of finding a smooth form of the boundary, \( B(N_{\text{eff}}) \), can be chosen by substituting \( L \) by the value of \( \tilde{L}' \) corresponding to \( \min_{\tilde{L}} B(N_{\text{eff}}, \tilde{L}) \). The thus obtained curve has the advantage that it is wholly located in the physical domain and is tangent to the strict boundary at individual points. Unfortunately, at large \( s \) this method does not lead to analytical formulas.

Finally, according to the above mentioned property of equivalence of the direct and the inverse problems, the domain of physically realizable states can be represented as inequality to the largest possible value of \( N_{\text{eff}} \) at given \( \Delta x \Delta q \). On the basis of (17),

\[
\Delta x \Delta q \geq \frac{s + 2 \tilde{L}(N_{\text{eff}})}{2(s + 2)}. \tag{18}
\]
(18) it gives the analytical expression

\[ N_{\text{eff}} \leq \frac{1}{2\Delta x \Delta q} \frac{\Gamma \left( (s+2)\Delta x \Delta q + s/2 + 1 \right)}{(s+1)!\Gamma \left( (s+2)\Delta x \Delta q - s/2 \right)}. \]  

(19)

The introduction of the concept of “packing coefficient” \( C(s, N_{\text{eff}}) \) (whose explicit form is not described by simple analytical formula) permits to rearrange relations (14) and (18) into the form similar to (2). The point of such transformation is that thus the main dependence of generalized uncertainty relation on problems parameters is emphasized whereas \( C(s, N_{\text{eff}}) \) plays role of correction factor with comparatively weak dependence on \( N_{\text{eff}} \).

The method of obtaining the approximate expression for the physical domain boundary supposes itself that the approximation (18) should tend to the exact formula (14) with increasing \( \mathcal{L} \) (and, thus \( N_{\text{eff}} \) as well). Really, exactly in the limit of \( \mathcal{L} \gg 1 \) the substitution of a discrete value of \( \mathcal{L} \) by a continuous value of \( \hat{\mathcal{L}} \) slightly effects the weights of individual states in (13). However, even at small \( N_{\text{eff}} \gtrsim 1 \) the approximate relations (18) and (19) turn to be in a very good accord with the rigorous inequality (14). The reason for this is the above mentioned local behavior of \( B(\hat{\mathcal{L}}) \).

The said is illustrated by plots of exact and approximate dependencies of \( C(s, N_{\text{eff}}) \) given in the Fig. 1 for some values of \( s \). From this figure it is seen that insignificant discrepancies between (14) and (18) only take place near \( N_{\text{eff}} \approx 1 \) and they are the more pronounced, the greater the problem dimension \( s \). Accordingly, as \( s \) is increased, thus approximate relation approaches the rigorous one evenly closely at larger values of \( N_{\text{eff}} \).

Comparing inequalities (2) and (18), it can be easily shown that (2) is an asymptotic form of (18) (and, consequently, (14)) at \( N_{\text{eff}} \to \infty \), but at \( s > 1 \) a good approximation of (2) to (14) is only attained at large \( N_{\text{eff}} \). At the same time, the refined form of the uncertainty relation (14) correctly describes all range of values of \( N_{\text{eff}} \) and, in particular, the ultimate case of pure states

\[ C(s, N_{\text{eff}} = 1) = 1, \quad (\Delta x \Delta q)|_{N_{\text{eff}} = 1} \geq \left( \frac{1}{2} \right)^s. \]

The coincidence of the asymptotic form of packing coefficient \( C(s, N_{\text{eff}} \gg 1) \) with formula (7) justifies the use in [5], when proving (2), of assumption that the Wigner function is nonnegative for the density matrix in the state with minimal uncertainty.

4. Discussion

At a qualitative level, the treatment of standard uncertainty relation as a requirement for phase space quantization in wave mechanics is rather frequently occurred in the literature on physics (see, for example [11]). Therefore, it can serve, in some way, as an argument in substantiating the postulate of statistical mechanics on the number of cells in phase space of the system:

\[ \frac{\mathcal{V}_p(E)}{N} = (2\pi)^s, \]  

(20)
where $\mathcal{V}_p(E)$ is the phase volume of the system with given energy $E$ and $N$ is the number of levels with energies not exceeding $E$ (detailed definitions can be found in [4]).

The results of [1-3, 5, 9] and the present paper open up the possibility of quantitative comparison of relations (2), (14) and (20).

First of all their similarity lies in the fact that the quantities of the same physical nature enter into the right- and the left-hand sides of expressions (2) and (20) by identical manner. But the differences between (2) and (20) are far more essential and there is nothing strange about it, if we take into account the way in which the concepts of the phase volume and the number of states are introduced in both cases.

The postulate given by (20) specifies the relation between energetic structure of the quantum system and the phase space which can be associated with this system in the quasi-classical approximation [4]. Such a relation is assumed to be universal and independent of a particular Hamiltonian of the system. Formula (20) describes system as a whole and has no connection to its particular physical state.

On the contrary, inequalities (2), (14) refer just to the physical state of quantum system. Like Eq. (20), they are explicitly associated with neither the kind of Hamiltonian nor the structure of energy levels. The only limitation is that since the basic functions of expansion (9) form a complete set, the wave-packets, satisfying the condition of minimum uncertainty for mixed states, can be constructed only for Hamiltonians whose eigenfunctions also form a complete orthonormal basis. This holds, in particular, for the simplest system of noninteracting particles in a free space. In general, however, the eigenstates of density operator are not the states with constant energy and, thus, the state with minimum uncertainty will not be stationary. The exception is the case of multidimensional harmonic oscillator.

It is clear from the said that the quantities $\Delta v_p$ and $\mathcal{V}_p$, respectively, in Eq. (2), (14) and (20) not only do not coincide numerically with one another (even for oscillator), but also have a different operational meaning. A similar statement in general case is true for the quantities $N_{\text{eff}}$ and $N$ as well. So there is nothing surprising in the fact that relation (2) has the form of inequality, while (20) — equality. Possibly, a better correlation between (2) and (20) can be attained by using other, alternative formulations of the uncertainty principle [9].

It would be worth to draw attention to one more difference between (2) and (20). In the postulate given by (20), the phase space volume of any quantum cell is constant and varies with change of dimensionality in a strictly definite way — as $(\text{const})^s$. On the contrary, in the generalized uncertainty relation (14), the minimal specific phase volume (i.e. the volume per one effective pure state of the system) depends on the value of $N_{\text{eff}}$. As seen from Fig. 1, the quantity $C(s, N_{\text{eff}})$ is less than unity and monotonically decreases with increasing $N_{\text{eff}}$. It means that as the number of pure states involved in the statistical mixture for $\rho(X, X')$ raises, there is a gain in the packing density of states.

In the paper [5] it was also noted the effect of increasing packing with augment of
the configurational space dimension \( s \), that is expressed by the inequality
\[
C(ks) \leq C(s)^k, \quad (k \geq 1).
\]
From (19) one can easily see that an analogous relation for the coefficients \( C(s, N_{\text{eff}}) \) in the general case does not hold and this property of packing is asymptotic, i.e. in each particular case \((s, k)\) it takes place beginning with sufficiently large \( N_{\text{eff}} \). The reason for this should be sought in the peculiarities of behavior of degeneration multiplicity \( g_s(\|n\|) \) as a function of \( \|n\| \) and \( s \). It is natural to suppose that the decrease in the coefficient \( C(s) \) with increasing \( s \) is due to the rapid growth of the value of \( g_s \), and for different dimensions it would be proper to compare the packing at equal values of the parameter \( \mathcal{C} \) rather than \( N_{\text{eff}} \).

In this context, it is interesting to consider the case of the density matrix (9) with equal weights of all pure states \( a_{n,n'} = \delta_{n,n'}/N \) involved, that somewhat resembles the definition of \( N \) in (20). For this situation all methods of determining \( N_{\text{eff}} \) gives \( N_{\text{eff}} = N \) and, although the minimum of uncertainty relation (14) for such a system is slightly exceeded, both the above properties of the packing coefficient are fulfilled.

In conclusion, it is necessary to discuss also the question of what physical meaning is attributed to the arguments (coordinates) entering into the density matrix \( \rho(X,X') \). These may be either the coordinates of one particle in the real three-dimensional space or the coordinates of several particles in the configurational space or both at once. The above solution for the density matrix in the state with minimal uncertainty is invariant under any permutation of its arguments \((x_i \Leftrightarrow x_j)\). For the real coordinates of one particle it means that the corresponding wave-packet possesses some rotational symmetry in three-dimensional space. But when arguments being interchanged correspond to several particles it is necessary to take into account the properties of their permutational symmetry. For indistinguishable identical particles the state with such a symmetry can only be realized in the case when these particles follow the Bose statistics. On the contrary, identical particles with Fermi statistics can not be described by a density matrix of the form of (9) with the coefficients given by (13). The state with minimal uncertainty for fermions should be sought from the very beginning in the class of wavefunctions antisymmetrized in permutations of arguments, which, naturally, should lead to a result drastically different from (14).

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Figure caption

Fig. 1. The packing coefficient $C(s, N_{\text{eff}})$ vs. the effective number of pure states in statistical mixture (9) for dimensions $s = 1, 2, 3$. Solid line — strict inequality (14), dotted line — approximation (18), dashed line — the asymptotic value $C(s)$ for $N_{\text{eff}} \gg 1$ (7).