Heisenberg Uncertainty Relations can be Replaced by Stronger Ones

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ABSTRACT: Two uncertainty relations, one related to the probability density current and the other one related to the probability density, are derived and discussed. Both relations are stronger than the Heisenberg uncertainty relations. Their generalization to the multidimensional case and to the mixed states is also discussed. © 2008 Wiley Periodicals, Inc. Int J Quantum Chem 109: 1626–1630, 2009

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1. Introduction

Uncertainty relations, one of the fundamental results of quantum mechanics, have been studied in a large number of articles (see e.g., [1–6]; for a detailed review, see [7]). The standard approach to their derivation is based on the wave function ψ. It is shown below that the approach based on the probability density current and probability density yields uncertainty relations that are stronger than the corresponding Heisenberg uncertainty relation.

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2. One-Dimensional Case

By analogy with continuum mechanics, it is possible to introduce in quantum mechanics not only the probability density ρ but also the probability density current j related to the "velocity" v

$$j = \rho v. \tag{1}$$

The quantities $\rho \geq 0$ and v can be expressed in terms of two real functions $s_1 = s_1(x,t)$ and $s_2 = s_2(x,t)$ as follows

$$\rho = \mathrm{e}^{-2s_2/\hbar}, \tag{2}$$

$$v = \frac{1}{m}\frac{\partial s_1}{\partial x}, \tag{3}$$

where x is the coordinate, t denotes time, and m is the mass. Then, by introducing the wave function ψ

$$\psi = e^{(is_1 - s_2)/\hbar}, \tag{4}$$

we can get two basic formulas of quantum mechanics

$$\rho = |\psi|^2 \tag{5}$$

and

$$j = \frac{\hbar}{2mi}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right), \tag{6}$$

where the star denotes the complex conjugate. It is seen that instead of ρ and j, the state of the quantum mechanical system can be described by the functions s_1 and s_2 or the wave function ψ [8–10].

It is assumed in this article that the probability density ρ has the properties

$$\int_{-\infty}^{\infty} \rho dx = 1 \tag{7}$$

and

$$\lim_{x \to \pm\infty} \rho(x) = 0. \tag{8}$$

Taking into account that the mean value

$$\left\langle \frac{\partial s_2}{\partial x} \right\rangle = \int_{-\infty}^{\infty} \psi^* \frac{\partial s_2}{\partial x} \psi dx = \int_{-\infty}^{\infty} \frac{\partial s_2}{\partial x} \rho dx = -\frac{\hbar}{2} \int_{-\infty}^{\infty} \frac{\partial \rho}{\partial x} dx \tag{9}$$

equals zero it can easily be shown that $\langle (\Delta p)^2 \rangle$ appearing in the Heisenberg uncertainty relation

$$\langle (\Delta x)^2 \rangle \langle (\Delta p)^2 \rangle \geq \hbar^2/4 \tag{10}$$

can be written as the sum of two quantities

$$\langle (\Delta p_1)^2 \rangle = \left\langle \left(\frac{\partial s_1}{\partial x} \right)^2 \right\rangle - \left\langle \frac{\partial s_1}{\partial x} \right\rangle^2 \tag{11}$$

and

$$\langle (\Delta p_2)^2 \rangle = \left\langle \left(\frac{\partial s_2}{\partial x} \right)^2 \right\rangle \tag{12}$$

that are greater than or equal to zero. The first quantity $\langle (\Delta p_1)^2 \rangle$ depends on $(\partial s_1/\partial x)$ and ρ and can be different from zero for the nonzero probability density current j only. The second quantity $\langle (\Delta p_2)^2 \rangle$ depends only on the form of the wave packet given by s_2 and is independent of j. Therefore, the separation of $\langle (\Delta p)^2 \rangle$ into two parts given above has a good physical meaning. An analogous separation was discussed also in [11] within the framework of one-dimensional stochastic mechanics.

Now we can use the Schwarz inequality $(u, u)(v, v) \geq |(u, v)|^2$, where the inner product is defined as the integration over all x. For the functions $u = (x - \langle x \rangle)\sqrt{\rho}$ and $v = (\partial s_1/\partial x - \langle \partial s_1/\partial x \rangle)\sqrt{\rho}$ we get the first uncertainty relation

$$\langle (\Delta x)^2 \rangle \langle (\Delta p_1)^2 \rangle \geq \left\langle (x - \langle x \rangle) \left(\frac{\partial s_1}{\partial x} - \left\langle \frac{\partial s_1}{\partial x} \right\rangle \right) \right\rangle^2. \tag{13}$$

Equation (13) was also derived within the framework of Nelson's stochastic mechanics [11].

The second uncertainty relation can be obtained by putting $u = (x - \langle x \rangle)\sqrt{\rho}$ and $v = (\partial s_2/\partial x)\sqrt{\rho}$ with the result

$$\langle (\Delta x)^2 \rangle \langle (\Delta p_2)^2 \rangle \geq \hbar^2/4. \tag{14}$$

Equation (14) is known for example from [12], see also the stochastic variational approach to the minimum uncertainty states [13]. Another discussion of Eq. (14) can be found in [8–10].

We see that the Heisenberg uncertainty relation (10) can be replaced by two more detailed uncertainty relations (13) and (14) for the information carried by the functions s_1 (information related to the probability density current j describing the motion in space) and s_2 (information related to the probability density ρ describing the form of the wave packet). For real wave functions ψ, corresponding to $s_1 = 0$, Eq. (13) gives trivial result $0 = 0$, and Eq. (14) becomes the Heisenberg uncertainty relation (10). In a general case, the uncertainty relations (13) and (14) are stronger than the Heisenberg uncertainty relation (10).

3. Multi-Dimensional Case

We consider the N-dimensional space with the coordinates $\mathbf{x} = (x_1, \ldots, x_N)$ and the probability density $\rho \geq 0$ given by the wave function ψ

$$\rho(\mathbf{x}, t) = |\psi(\mathbf{x}, t)|^2. \tag{15}$$

It is assumed that this probability density fulfills the boundary conditions

$$\rho|_{x_m=-\infty}^{\infty} = 0, \quad m = 1, \ldots, N \tag{16}$$

and the standard normalization condition

$$\int \rho(\mathbf{x},t)d\tau = 1, \quad d\tau = dx_1 \ldots dx_N, \tag{17}$$

where the integration is carried out over the whole space.

The mean values of the coordinates are defined as

$$\langle x_m \rangle = \int x_m \rho d\tau. \tag{18}$$

The $N \times N$ covariance matrix $(\Delta X)^2$ is given by the equation

$$(\Delta X)^2_{mn} = \int (x_m - \langle x_m \rangle)(x_n - \langle x_n \rangle)\rho d\tau. \tag{19}$$

Assuming that c_m are arbitrary complex numbers it can easily be verified that this matrix is positive semidefinite

$$\sum_{m,n=1}^{N} c_m^* (\Delta X)^2_{mn} c_n = \int \left| \sum_{m=1}^{N} c_m (x_m - \langle x_m \rangle) \right|^2 \rho d\tau \geq 0. \tag{20}$$

Analogously to Section 2, the wave function ψ is written in the form

$$\psi = e^{(is_1 - s_2)/\hbar}, \tag{21}$$

where $s_1 = s_1(x_1, \ldots, x_N, t)$ and $s_2 = s_2(x_1, \ldots, x_N, t)$ are real functions. The functions s_1 and s_2 give the probability density ρ

$$\rho = |\psi|^2 = e^{-2s_2/\hbar} \tag{22}$$

and the probability density current

$$j_k = \frac{\hbar}{2mi}\left(\psi^* \frac{\partial \psi}{\partial x_k} - \psi \frac{\partial \psi^*}{\partial x_k}\right) = \frac{1}{m}\frac{\partial s_1}{\partial x_k}\rho. \tag{23}$$

Further, we calculate the mean value of the momentum operator $\hat{p}_m = -i\hbar(\partial/\partial x_m)$, which must be real

$$\langle \hat{p}_m \rangle = \int \psi^* \hat{p}_m \psi d\tau = \int \frac{\partial s_1}{\partial x_m}\rho d\tau + i\int \frac{\partial s_2}{\partial x_m}\rho d\tau = \int \frac{\partial s_1}{\partial x_m}\rho d\tau = \left\langle \frac{\partial s_1}{\partial x_m} \right\rangle. \tag{24}$$

Similarly, we get

$$\langle \hat{p}_m \hat{p}_n \rangle = \int (\hat{p}_m \psi)^* (\hat{p}_n \psi) d\tau = \int \left(\frac{\partial s_1}{\partial x_m}\frac{\partial s_1}{\partial x_n} + \frac{\partial s_2}{\partial x_m}\frac{\partial s_2}{\partial x_n} \right) \rho d\tau \tag{25}$$

and

$$\begin{aligned} (\Delta P)^2_{mn} &= \int [(\hat{p}_m - \langle \hat{p}_m \rangle)\psi]^* (\hat{p}_n - \langle \hat{p}_n \rangle)\psi d\tau \\ &= \langle \hat{p}_m \hat{p}_n \rangle - \langle \hat{p}_m \rangle \langle \hat{p}_n \rangle \\ &= \int \left(\frac{\partial s_1}{\partial x_m}\frac{\partial s_1}{\partial x_n} + \frac{\partial s_2}{\partial x_m}\frac{\partial s_2}{\partial x_n} \right) \rho d\tau \\ &\quad - \int \frac{\partial s_1}{\partial x_m}\rho d\tau \int \frac{\partial s_1}{\partial x_n}\rho d\tau. \end{aligned} \tag{26}$$

Analogously to the matrix $(\Delta X)^2$, it can be shown that the matrix $(\Delta P)^2$ is positive semidefinite.

It can be verified that both matrices appearing in Eq. (26)

$$(\Delta P_1)^2_{mn} = \int \frac{\partial s_1}{\partial x_m}\frac{\partial s_1}{\partial x_n}\rho d\tau - \int \frac{\partial s_1}{\partial x_m}\rho d\tau \int \frac{\partial s_1}{\partial x_n}\rho d\tau \tag{27}$$

and

$$(\Delta P_2)^2_{mn} = \int \frac{\partial s_2}{\partial x_m}\frac{\partial s_2}{\partial x_n}\rho d\tau, \tag{28}$$

$$(\Delta P_1)^2 + (\Delta P_2)^2 = (\Delta P)^2 \tag{29}$$

are positive semidefinite, too. The matrix $(\Delta P_1)^2$ depends on $(\partial s_1/\partial x_m)$ and ρ (i.e., s_2) and can be different from zero for the nonzero probability density current $\mathbf{j} = (j_1, \ldots, j_N)$ only [see Eq. (23)]. The second matrix $(\Delta P_2)^2$ depends only on the form of the wave packet given by s_2 and is independent of $\mathbf{j}$. Therefore, the separation of $(\Delta P)^2$ into two parts given by Eqs. (27)–(29) has a good physical meaning.

Now, we define a correlation matrix G

$$G_{mn} = \int (x_m - \langle x_m \rangle) \left(\frac{\partial s_1}{\partial x_n} - \left\langle \frac{\partial s_1}{\partial x_n} \right\rangle \right) \rho d\tau \tag{30}$$

and create a new $2N \times 2N$ matrix M

$$M = \begin{pmatrix} (\Delta X)^2 & G^T \\ G & (\Delta P_1)^2 \end{pmatrix}, \tag{31}$$

where the superscript T denotes the transposition. Using similar arguments as in case of the matrix

$(\Delta X)^2$, it can be shown that the matrix M is positive semidefinite. Further, we make use of a general result valid for $N \times N$ matrices A, B, C, and D, where D is a regular matrix having the property $\det(D) \neq 0$ and 1 denotes the $N \times N$ unity matrix

$$\begin{pmatrix} 1 & -BD^{-1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} A - BD^{-1}C & 0 \\ C & D \end{pmatrix} \quad (32)$$

leading to

$$\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(A - BD^{-1}C)\det(D). \quad (33)$$

Applying this equation to the matrix M given by Eq. (31), the first multidimensional uncertainty relation for the matrices $(\Delta X)^2$ and $(\Delta P_1)^2$ is obtained

$$\det(M) = \det\{(\Delta X)^2(\Delta P_1)^2 - G^T[(\Delta P_1)^2]^{-1}G(\Delta P_1)^2\} \geq 0. \quad (34)$$

In the one-dimensional form, Eq. (34) leads to Eq. (13).

Further, we replace the function s_1 by s_2 and repeat the discussion made in the preceding paragraph. Taking into account the equation

$$\left\langle \frac{\partial s_2}{\partial x_m} \right\rangle = \int \frac{\partial s_2}{\partial x_m} \rho d\tau = -\frac{\hbar}{2} \int \frac{\partial \rho}{\partial x_m} d\tau = -\frac{\hbar}{2} \int \rho|_{x_m=-\infty}^{\infty} d\tau' = 0, \quad (35)$$

where $d\tau' = dx_1 \cdots dx_{m-1}dx_{m+1} \cdots dx_N$, the matrix element G_{mm} can be replaced by G'_{mm}

$$G'_{mm} = \int (x_m - \langle x_m \rangle) \frac{\partial s_2}{\partial x_m} \rho d\tau. \quad (36)$$

Performing here the integration by parts in the variable x_m, assuming that $[(x_m - \langle x_m \rangle)\rho]_{x_m=-\infty}^{\infty} = 0$ and using Eqs. (17), (18) we get

$$G'_{mm} = -\frac{\hbar}{2} \int [(x_m - \langle x_m \rangle)\rho]_{x_m=-\infty}^{\infty} d\tau' + \frac{\hbar}{2} \int \rho d\tau = \frac{\hbar}{2}. \quad (37)$$

By using Eqs. (16)–(18) we get similarly

$$G'_{mn} = \int (x_m - \langle x_m \rangle) \frac{\partial \rho}{\partial x_n} d\tau = \int (x_m - \langle x_m \rangle)\rho|_{x_n=-\infty}^{\infty} d\tau'' = 0, \quad m \neq n, \quad (38)$$

where $d\tau'' = dx_1 \cdots dx_{n-1}dx_{n+1} \cdots dx_N$. Equation (33) applied to the matrix

$$M' = \begin{pmatrix} (\Delta X)^2 & \hbar/2 \\ \hbar/2 & (\Delta P_2)^2 \end{pmatrix} \quad (39)$$

then yields the second multidimensional uncertainty relation

$$\det\left[(\Delta X)^2(\Delta P_2)^2 - \frac{\hbar^2}{4}\right] \geq 0 \quad (40)$$

or, in the one-dimensional form, Eq. (14).

The third uncertainty relation can be obtained by replacing $(\Delta P_2)^2$ in the matrix M' by $(\Delta P)^2 = (\Delta P_1)^2 + (\Delta P_2)^2$. The resulting matrix remains positive semidefinite, and Eq. (40) then leads to the multidimensional uncertainty relation

$$\det\left[(\Delta X)^2(\Delta P)^2 - \frac{\hbar^2}{4}\right] \geq 0 \quad (41)$$

which is known for example from [3–7]. The one-dimensional form of this relation is the Heisenberg uncertainty relation (10).

There is one important difference between the uncertainty relation (41) and the uncertainty relations (34) and (40). The uncertainty relation (41) is based on using the wave function ψ (see [3–7]). In contrast to it, the uncertainty relations (34) and (40) are based on using the probability density current and probability density. Because of Eq. (29), these uncertainty relations are in general stronger than the uncertainty relation (41).

Discussion of the multidimensional uncertainty relations (34) and (40) can be found also in [14].

4. Generalization to Mixed States

Finally, we note that the uncertainty relations (34), (40), and (41) can be generalized to mixed states when the system can be found in the states described with the probabilities w_j by the wave function $\psi_j(\mathbf{x}, t)$, $j = 1, 2, 3, \ldots$. The density matrix for such a system can be written as $\sum_j |\psi_j\rangle w_j \langle\psi_j|$. The matrices $(\Delta X)^2$, $(\Delta P_1)^2$, $(\Delta P_2)^2$, and G can be then defined as

$$(\Delta X)^2_{mn} = \sum_j w_j \int \psi_j^*(x_m - \langle x_m \rangle)(x_n - \langle x_n \rangle)\psi_j d\tau, \quad (42)$$

where

$$\langle x_m \rangle = \sum_j w_j \int \psi_j^* x_m \psi_j d\tau, \tag{43}$$

$$(\Delta P_1)^2_{mn} = \sum_j w_j \int \psi_j^* \frac{\partial s_{1j}}{\partial x_m} \frac{\partial s_{1j}}{\partial x_n} \psi_j d\tau - \sum_j w_j \int \psi_j^* \frac{\partial s_{1j}}{\partial x_m} \psi_j d\tau \sum_k w_k \int \psi_k^* \frac{\partial s_{1k}}{\partial x_n} \psi_k d\tau, \tag{44}$$

$$(\Delta P_2)^2_{mn} = \sum_j w_j \int \psi_j^* \frac{\partial s_{2j}}{\partial x_m} \frac{\partial s_{2j}}{\partial x_n} \psi_j d\tau \tag{45}$$

and

$$G_{mn} = \sum_j w_j \int \psi_j^* (x_m - \langle x_m \rangle) \left(\frac{\partial s_{1j}}{\partial x_n} - \left\langle \frac{\partial s_{1j}}{\partial x_n} \right\rangle \right) \psi_j d\tau. \tag{46}$$

Here, $\psi_j = \mathrm{e}^{(is_{1j} - s_{2j})/\hbar}$, s_{1j} and s_{2j} are real functions and $\sum_j w_j = 1$.

It can easily be shown that the uncertainty relations (34), (40), and (41) are valid also in this case.

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