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# ENTROPY OF THE DISTRIBUTION OF DYNAMIC VARIABLES

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**Abstract**

**Full Text**

**PHYSICS**

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## **ENTROPY OF THE DISTRIBUTION OF DYNAMIC VARIABLES**

In works <sup>(1,2)</sup> the concept of the entropy of a random variable (see, for example, <sup>(3,4)</sup>) was applied to characterize the degree of delocalization of an electron in a stationary state of an atomic-molecular system. In the present work the concept of the entropy of the state of a quantum system is applied to describe probability distributions of arbitrary dynamic variables and is illustrated by the example of the harmonic oscillator.

Considering a certain state of a system  $\psi(x)$ , we generally do not have exact information about the magnitude of the dynamic variable  $L$ , but can calculate only the probability of detecting the value  $L$  in some interval  $dL$  under one or another set of specific measurements:

$$w(L) dL = |c(L)|^2 dL, \quad (1)$$

where

$$c(L) = \int \psi^*(x, L) \psi(x) dx. \quad (2)$$

To characterize the diversity of possible values of  $L$ , it is expedient to introduce the concept of entropy

$$H_L = - \int w(L) \ln w(L) dL \quad (3)$$

as a measure of the deficiency of information about the given state of the system or, in other words, as a measure of the uncertainty described by the distribution  $w(L)$ .\*

The entropy of continuous distributions of  $L$  defined in this way has the dimension of the logarithm of  $L^{-1}$  and therefore is defined only up to an additive constant depending on the choice of the system of units. Differences of entropies of distributions of any dynamic variable, of course, will not depend on the system of units. In order to avoid the logarithm of the dimensional quantity  $w(L)$

in the expression for entropy (1), the variables  $L$  must be regarded as dimensionless, i.e., referred to some unit of this variable. For discrete distributions,  $w(L_i)$  is a dimensionless quantity, which makes it possible to regard the entropy as an unambiguous characteristic. The entropy of a certain probability distribution has a number of general properties. For the distribution of discrete quantities they are formulated in works <sup>(5)</sup>.

The maximum of entropy corresponds to the most uncertain distribution ( $w(L)$  does not depend on  $L$ ). The minimum value for discrete quantities is equal to zero and is attained under complete certainty, i.e., in the case where the probability  $w(L)$  is equal to unity at some one specific value  $L = L_i$  and is equal to zero for all  $L \neq L_i$ . The range of change of entropy for continuous distributions  $w(L)$  is different. Under complete uncertainty of the distribution it is maximal (in the infinite limits  $H \rightarrow +\infty$ ). In passing to complete certainty, the value of the entropy of the dis—

\* For definiteness we use natural logarithms.

of the distribution tends to  $-\infty$ . This is easy to show by substituting the value of the delta function  $\delta(L - L_i)$  for  $w(L)$  in (3).

The study of the entropies of distributions of various dynamical variables in one and the same state, and the establishment of the relation between them as a function of the state of the system, will make it possible to approach the consideration of a number of phenomena from another, somewhat unusual, point of view. In this respect, the study of the relation between the entropies of distributions of canonically conjugate quantities and, in particular, between the entropies of distributions of coordinates and momenta, is of substantial interest. Investigations in this direction should not be limited only to stationary states. The consideration of nonstationary states will make it possible to investigate the time behavior of entropy. In addition, it will be necessary subsequently to clarify the influence on the entropy of dynamical variables of various kinds of internal interactions in isolated quantum systems, as well as of external actions on nonclosed systems, and to investigate reversible and irreversible changes.

As an example of the effectiveness of introducing the concept of entropy for characterizing various stationary states of quantum systems, let us consider several questions connected with the values of the entropies of the coordinate and momentum distributions of a quantum harmonic oscillator. At the same time, for comparison, we shall consider the corresponding entropies of a classical harmonic oscillator.

Using the form of the wave functions of the harmonic oscillator for the zeroth and first energy levels <sup>(6)</sup>, it is not difficult to obtain, according to (3), the following values of the entropies  $H_q$  for coordinates and of the entropies  $H_p$  for momenta:

$$H_q^0 = \frac{1}{2} \ln \frac{\pi e h}{\mu \omega} = \frac{1}{2} \ln \pi e + \frac{1}{2} \ln h - \frac{1}{4} \ln \mu - \frac{1}{4} \ln k; \quad (4)$$

$$H_p^0 = \frac{1}{2} \ln \pi e h \mu \omega = \frac{1}{2} \ln \pi e + \frac{1}{2} \ln h + \frac{1}{4} \ln \mu + \frac{1}{4} \ln k; \quad (5)$$

$$H_q^1 = H_q^0 + 0,270; \quad (6)$$

$$H_p^1 = H_p^0 + 0,270; \quad (7)$$

$$H_q^\nu = H_q^0 + \int_{-\infty}^{\infty} f_\nu(z) dz; \quad (8)$$

$$H_p^\nu = H_p^0 + \int_{-\infty}^{\infty} f_\nu(z) dz. \quad (9)$$

In formulas (4)–(9) the values  $\mu$ ,  $k$ , and  $h$  are dimensionless, i.e., computed with respect to the units of mass, quasi-elastic constant, and action, for example, in the CGS system. Thus it is again established that the values of entropy are determined only up to an additive constant. The true meaning is possessed not by the entropy values themselves, but by their differences.

From comparison of (6)–(9) with (4) and (5), it follows that the term depending on the properties of the given oscillator ( $\mu$  and  $k$ ) is the same for all energy levels. When the level number of the oscillator is increased ( $0 \rightarrow \nu$ ), the entropy and, consequently, the uncertainty of the corresponding distributions changes by the constant quantity

$$\int_{-\infty}^{\infty} f_\nu(z) dz,$$

which does not depend on the properties of the oscillator. In formulas (6) and (7) the integration is elementary, and the result obtained shows that, in passing from the level  $\nu = 0$  to the level  $\nu = 1$ , the entropies  $H_q$  and  $H_p$  increase. The same result is naturally to be expected also in passing to higher levels. Consequently, for the lower bound of the sum of entropies

for the entropies  $H_q$  and  $H_p$  of a harmonic oscillator we have

$$H_q^\nu + H_p^\nu \geq \ln \pi e h. \quad (10)$$

Apparently, this relation for the sum of the entropies (10) has a general character.

The entropies of the distributions depend essentially on the properties of the oscillator. As  $\mu \rightarrow \infty$ , the entropy  $H_q \rightarrow -\infty$ , while  $H_p \rightarrow \infty$ , i.e., the coordinates of heavy oscillators are completely determined, and their momenta completely undetermined. An analogous result holds for  $k \rightarrow \infty$ . As  $\mu \rightarrow 0$  or  $k \rightarrow 0$  (free particles), the entropy  $H_q \rightarrow \infty$ , and the entropy  $H_p \rightarrow -\infty$ ; all coordinates of such oscillators are equally probable, while the momenta are completely determined. In all cases, the main significance lies in estimating the change of entropy when one or another parameter of the system under consideration is changed. Thus, for example, increasing the mass of an oscillator from  $\mu_1$  to  $\mu_2$ , with the same value of the quasi-elastic constant  $k$ , leads to a decrease in the coordinate entropy equal to  $H_q(\mu_2) - H_q(\mu_1) = -\frac{1}{4} \ln \mu_2/\mu_1$  ( $dH_2 = -\frac{1}{4} d\mu/\mu$ ), and to an increase of the momentum entropy by the same amount. These changes in entropy are identical for all oscillatory levels.

From the form of the eigenfunctions of the harmonic oscillator in the coordinate and momentum representations, in the most general case it follows (see, for example, formulas (4)–(9)) that the difference between the coordinate and momentum entropies does not depend on the level number  $\nu$  and is determined only by the parameters of the oscillator:

$$H_p^\nu - H_q^\nu = \ln \mu \omega = \frac{1}{2} \ln \mu k. \quad (11)$$

As the product  $\mu k$  increases, the difference between the uncertainties of momentum and coordinate increases. It should be noted that, unlike (4)–(9), expression (11) does not contain the constant  $h$  and, consequently, it must be fully valid in classical theory as well.

If we make use of the uncertainty relation for the canonically conjugate coordinates and momenta of a harmonic oscillator [6]

$$\Delta q \Delta p = (\nu + \frac{1}{2})h \quad (12)$$

and of the fact [4] that, for a given value of the entropy, a Gaussian distribution has the smallest dispersion, it is not difficult to obtain an upper bound for the sum of the entropies of coordinates and momenta:

$$H_q^\nu + H_p^\nu \leq \ln 2\pi e h (\nu + \frac{1}{2}). \quad (13)$$

Comparing (11) and (13), one can find the upper bound of  $H_q^\nu$  and  $H_p^\nu$  separately:

$$H_q^\nu \leq \frac{1}{2} \ln \frac{2\pi e}{\mu \omega} (\nu + \frac{1}{2})h = H_q^0 + \frac{1}{2} \ln 2(\nu + \frac{1}{2}); \quad (14)$$

$$H_p^\nu \leq \frac{1}{2} \ln 2\pi e \mu \omega (\nu + \frac{1}{2}) h = H_p^0 + \frac{1}{2} \ln 2(\nu + \frac{1}{2}). \quad (15)$$

For  $\nu = 0$  the distributions in coordinates and momenta are Gaussian, and therefore, in complete agreement with the exactly calculated values (4) and (5), the equality sign must stand in (14) and (15). For the level  $\nu = 1$  we also obtained in (6) and (7) exact values of the entropies. The true excess over the corresponding entropies for the 0 levels is equal to 0.270. This number is approximately half as large as the number  $\ln \sqrt{3}$  entering into (14) and (15). As  $\nu$  increases, the upper bound for the entropies rises, though for large  $\nu$  very slowly.

Let us now calculate the entropies of coordinates and momenta for a classical harmonic oscillator with a given energy  $E$ . In the classical case—

whereas the distribution of coordinates and momenta is given by formulas (7)

$$w(q) dq = \frac{1}{\pi} \sqrt{\frac{k}{2E}} \frac{dq}{\sqrt{1 - \frac{q^2}{2E}k}}, \quad (16)$$

$$w(p) dp = \frac{1}{\pi} \sqrt{\frac{1}{2E\mu}} \frac{dp}{\sqrt{1 - \frac{p^2}{2E\mu}}}. \quad (17)$$

In contrast to the quantum distributions, the classical distribution over coordinates does not depend on the mass of the oscillator, while the distribution over momenta does not depend on its quasi-elastic constant.

The entropies of the coordinate and momentum distributions of the classical harmonic oscillator are equal to:

$$H_q^E = \frac{1}{2} \ln \frac{\pi^2 E}{\mu \omega^2}; \quad (18)$$

$$H_p^E = \frac{1}{2} \ln \pi^2 E \mu. \quad (19)$$

Let us compare the formulas obtained with the corresponding expressions for the quantum oscillator. The difference of entropies  $H_q^E - H_p^E$  is determined, as in the case of the quantum oscillator, by equality (11). Setting  $E = \hbar \omega (\nu + 1/2)$  in the classical formulas (18)–(19), it is not difficult to see that the dependence of the entropy of the coordinate and momentum distributions on  $\mu$  and  $\omega$  is the same in the classical and quantum cases. In absolute magnitude, however, the uncertainty of the coordinates and momenta of the classical oscillator is greater than for the quantum oscillator by an amount that does not depend on the properties of the oscillator.

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*Note: Figure translations are in progress. See original paper for figures.*

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