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Entropy in Quantum Statistics

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The state and entropy of quantum mechanical systems are considered for non-orthogonal representations of the wave function. It is shown that there follow from the general formulas, on the one hand, the expressions of classical statistics, and, on the other, the well-known results of quantum statistics.

WHEN one speaks of quantum theory, the word "statistics" must be understood in two different senses. Quantum theory is statistical in itself; the wave function, in particular, has a statistical meaning. The statistical aggregates which correspond to these can, in the terminology of D. I. Blokhintsev, be called "pure" ensembles. But side by side with these "pure" statistics, there exist statistics of another type, which come into force whenever the wave function itself is random. Under the term "quantum statistics", we shall denote the latter, i.e., statistics which are concerned with the study of "mixed" ensembles. At the same time we shall associate with quantum statistics not only statistical physics of equilibrium processes, i.e., statistical thermodynamics, but also the quantum statistics of non-equilibrium states, although the latter has not yet been developed at the present time.

Contemporary quantum statistics, which is confined to statistical thermodynamics, operates with a statistical collection of wave functions, such that the separate representations of the wave function, which are the eigenfunctions of the energy, are mutually orthogonal. For such a collection there are formulas which determine the entropy.

It is natural to raise the question as to what is the entropy of an arbitrary statistical aggregate of wave functions, in other words, an arbitrary system on which a complete determination has not been fully carried out, i.e., an arbitrary mixed ensemble. The desired formula must undergo transition to the formula of classical statistics under appropriate conditions, and must also become the known formula in quantum statistical thermodynamics for orthogonal representations of the wave function.

1. Consider a sequence of possible representations of the wave function: $\psi_1(x), \psi_2(x), \ldots$ (x denotes the totality of arguments $x_1, \ldots, x_r$, which can also be discrete). Furthermore, let w_1 be the known probability associated with $\psi_1(x)$, w_2 that associated with $\psi_2(x)$, etc., i.e., we have the probabilities

$$w_i = \mathrm{P}\{\psi(x) = \psi_i(x)\}, \quad i = 1, 2, \ldots .$$

In such a case we shall say that the scheme

$$\begin{pmatrix} \psi_1(x) & \psi_2(x) & \ldots \\ w_1 & w_2 & \ldots \end{pmatrix} \tag{1}$$

is given.

The wave function $\psi(x)$ can sometimes be represented as a function of some continuous set of functions. In the arbitrary case, $\psi(x)$ is a random function, and as such can be completely described by the known statistical characteristics of random functions, e.g., by an infinite sequence of moment functions:

$$\mathrm{M}\,\psi(x), \quad \mathrm{M}\,\psi(x_1)\psi(x_2), \quad \mathrm{M}\,\psi(x_1)\psi^*(x_2), \tag{2}$$
$$\mathrm{M}\,\psi(x_1)\psi(x_2)\psi(x_3), \quad \mathrm{M}\,\psi(x_1)\psi(x_2)\psi^*(x_3), \ \ldots$$

(here M is the mathematical expectation).

From the very beginning, there arises the question of the role played by these or other moment functions, and whether they are all important in the description of the physical object (the mixed quantum ensemble). In this connection, the following postulate is far from trivial: there is no moment function of the set (2) except $\mathrm{M}\,\psi(x)\psi^*(x') = \rho(x, x')$, that has absolutely no significance.

If we fix $\rho(x, x')$ and vary the other moment functions, then the random wave function will invariably describe the same physical object. There is an analogous situation in electrodynamics, where the different four component vector potentials $\mathbf{A}_1$ and $\mathbf{A}_2$ describe the same field, if the difference $\mathbf{A}_1 - \mathbf{A}_2$ is the gradient of some function, or, in quantum mechanics, if it is given by the multiplication of the wave function by a number of unit absolute value. The reason for this circumstance must be sought in what follows. "The state matrix" $\psi(x)\psi^*(x')$ plays, in quantum mechanics, the role of the probability density distribution (thus, for $x = x'$, we have an exact probability density distribution, but in reduced space). If the distribution density is random, then in all probable problems only the mathematical expectation of the distribution density has significance --- which is equivalent to the linearity‘ of the mathematical apparatus of quantum mechanics. Thus, both the postulate which has been stated, and the linearity of the mathematical apparatus have as their fundamental basis the("pure") statistics of quantum theory.

Instead of the system (1) we could also have chosen any other scheme

$$\begin{pmatrix} \psi_1'(x) & \psi_2'(x)\ldots \\ w_1' & w_2' \ldots \end{pmatrix}, \tag{3}$$

for which

$$\sum_i w_i'\psi_i'(x)\psi_i'^*(x') = \sum_i w_i\psi_i(x)\psi_i^*(x').$$

Such schemes, which equally describe the same physical object, we shall call equivalent.

To each quantum-statistical system, and to the density matrix describing it, there corresponds an infinite set of equivalent schemes which represent the given physical object. Among these, the basic role is played by those schemes with orthogonal representations, i.e., the schemes

$$\begin{pmatrix} \varphi_1(x) & \varphi_2(x) & \cdots \\ p_1 & p_2 & \cdots \end{pmatrix}, \tag{4}$$

for which

$$\int \varphi_i(x)\varphi_j^*(x)\,dx = \delta_{ij}\,. \tag{5}$$

Let an arbitrary non-orthogonal scheme be given. We attempt to find an equivalent scheme with orthogonal representations. This problem is equivalent to the problem of reducing the Hermitian matrix

$$\rho(x, x') = \sum_i w_i\psi_i(x)\,\psi_i^*(x') \tag{6}$$

to diagonal form by a unitary transformation. The latter can be found for an arbitrary matrix (6), as long as this matrix is Hermitian. As usual, this transformation is found by the solution of the equation

$$\rho\varphi = \lambda\varphi, \tag{7}$$

or, for a continuous coordinate x,

$$\int \rho(x,\ x')\varphi_m(x')\,dx' = \lambda_m\varphi_m(x). \tag{7a}$$

For a discrete spacing x, the integrals in Eqs. (5), (7a) and also in many of the following equations, must be replaced by summations.

The matrix $\phi_m(x)$ will also be the matrix of the desired unitary transformation. In the new representation, the density matrix will have the diagonal form

$$\rho_{mn} = \iint \varphi_m^*(x)\,\rho(x,\ x')\,\varphi_n(x')\,dx\,dx' = \lambda_m\,\delta_{mn}.$$

The inverse transformation is written in the form

$$\begin{aligned} \rho(x,\ x') &= \sum \varphi_m(x)\,\rho_{mn}\,\varphi_n^*(x') \\ &= \sum \lambda_m\varphi_m(x)\,\varphi_m^*(x'), \end{aligned} \tag{8}$$

whence it is evident that $\rho(x, x')$ is the density matrix of the scheme

$$\begin{pmatrix} \varphi_1(x) & \varphi_2(x) & \cdots \\ \lambda_1 & \lambda_2 & \cdots \end{pmatrix}, \tag{9}$$

which, by virtue of Eqs. (6) and (8) is equivalent to the scheme (1). The orthogonality of this scheme, i.e., Eq. (5), follows from the unitary property of the matrix $\phi_m(x)$.

As a consequence of the invariance of the trace of a matrix for a unitary transformation, we have

$$\sum \lambda_m = \mathrm{Tr}\rho = \int \rho(x,\ x)\,dx = 1. \tag{10}$$

It remains only to prove the non-negative character of the λ_m, i.e., that λ_m can actually play the role of a probability.

The density matrix is always positive definite, since, for an arbitrary function $f(x)$,

$$\begin{aligned} &\iint \rho(x,\ x')f(x)f^*(x')\,dx\,dx' \\ &= \sum_i \omega_i \left|\int \psi(x)f(x)\,dx\right|^2 \geqslant 0. \end{aligned} \tag{11}$$

It then follows that all the λ_m are non-negative; this can easily be established by setting $f(x) = \phi_m^*(x)$ in Eq. (11) (in this case the left hand side of Eq. (11) reduces to λ_m).

We now discuss the problem of the uniqueness of the scheme of orthogonal representations. Linear algebra furnishes the information that the decomposition of the density matrix into orthogonal representations can have a unique form if, and only if, there are no duplicates among the eigenvalues λ_1, $\lambda_2, \ldots$. On the other hand, suppose that there is degeneracy. Let $\Lambda_1, \Lambda_2, \ldots$ be the collection of different values which occur among the $\lambda_1, \lambda_2, \ldots$, and let $l_1, l_2, \ldots$ be the corresponding multiplicity (Λ_j occurs among the λ_j just l_j times). In such notation, Eq. (10) can be written

$$\sum_j l_j \Lambda_j = 1.$$

To each Λ_j there will correspond l_j orthogonal functions

$$\varphi_{j1}, \ldots, \varphi_{jl_j} \quad \left(\int \varphi_{jm}(x) \overset{*}{\varphi}_{jn}(x)\, dx = \delta_{mn}\right). \tag{12}$$

However, the set of functions (12) is not uniquely determined; it is possible to replace it by any other set obtained from Eq. (12) by means of the application of a unitary transformation. Only the linear manifold remains invariant in all these transformations:

$$[\varphi_{j1}, \ldots, \varphi_{jl_j}] \equiv \mu_1 \varphi_{j1} + \ldots + \mu_{l_j} \varphi_{jl_j} \tag{13}$$

($\mu_1, \ldots, \mu_{l_j}$ arbitrary numbers), and also the sphere $|\mu_1|^2 + \ldots + |\mu_{l_j}|^2 = 1$ is invariant.

In the case of degeneracy ($l_j > 1$), the selection of any preferred system of representations has no meaning, and even the requirement of orthogonality cannot lead to such a system. Avoiding unjustified multivaluedness, and not wanting to redefine the object (i.e., to speak of it somewhat unnecessarily) we shall here characterize the object by a designation which describes its linear manifold (or sphere)

$$[\psi_1(x), \ldots, \psi_s(x)]. \tag{14}$$

The quantum statistical state that is described by Eq. (14) is a generalization of the state which is described by the individual wave function $\psi(x)$. Choosing a state of type (14) as a possible representation, we get the equivalent scheme

$$\begin{pmatrix} [\varphi_{11}(x), \ldots, \varphi_{1l_1}(x)] & [\varphi_{21}(x), \ldots, \varphi_{2l_2}(x)] & \cdots \\ P_1 & P_2 & \cdots \end{pmatrix} \quad (P_j = l_j \Lambda_j). \tag{15}$$

This scheme is fundamental in this sense, that each quantum-statistical state (each scheme) reduces to it single-valuedly, and conversely, to the different states (density matrices) there correspond different fundamental schemes, i. e., there exists a one-to-one correspondence. The different representations of Eq. (15)(for example, $[\phi_{j1}, \ldots, \phi_{jl_j}]$ and $[\phi_{k1}, \ldots, \phi_{kl_k}]$, $j \neq k$) are mutually orthogonal. The linear manifolds are orthogonal if their elements are orthogonal :

$$\int \varphi_{j\alpha} \overset{*}{\varphi}_{k\beta} = 0, \quad \alpha = 1, \ldots, l_j,$$

$$\beta = 1, \ldots, l_k \quad (j \neq k).$$

If there is no degeneracy, the form of Eq. (15) can also be used formally, since, in the case of a single function, $[\phi(x)]$ coincides with $\phi(x)$.

2. We proceed to a consideration of the entropy, by which we understand, in keeping with references 1 and 2, a quantity which characterizes the indefiniteness (neginformation), or statistical dispersion, of a given state. Following the custom established in information theory, we shall denote dimensionless entropy by H. Then the ordinary entropy, which has the dimensions of energy/degree, will be given by

$$S = kH,$$

where k is the Boltzmann constant.

We shall denote by A_i an event which consists of the identification of $\phi_i(x)$ with one of the scheme (1), $i = 1, 2, \ldots$. If the events A_1, $A_2, \ldots$ are mutually exclusive, then, by the

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[1] *The Theory of the Transmission of Electrical Signals in the Presence of Interference*, Collected Translations under the editorship of N. A. Zheleznov, Moscow, 1953

[2] R. L. Stratonovich, J. Exper. Theoret. Phys. USSR 28, 409 (1955); Soviet Phys 1, 254 (1955)

general formula which appears in reference 2, the entropy of the system is equal to

$$H = -\sum_i P(A_i) \ln \frac{P(A_i)}{Q(A_i)}, \tag{16}$$

where $P(A_i)$ and $Q(A_i)$ are the probability and abstract "volume" of the event A_i.

Making use of the independence of the "volumes" of the events of the probability distribution, we determine $Q(A_i)$. We recall that the entropy of a "determined" (in the sense of the absence of "mixed statistics") quantum state, which is described by the wave function $\psi_i(x)$, is equal to zero. Substituting $w_i = 1$, $w_j = 0$ $(j \neq 1)$ in Eq. (16) and equating this expression to zero, we obtain $Q(A_i) = 1$. We can carry out such a procedure for different i, so that

$$H = -\sum_i w_i \ln w_i. \tag{17}$$

This well-known formula is correct when the events $A_1, A_2, \ldots$ are mutually exclusive.

It is a characteristic feature of quantum theory that a system described by the wave function ψ_i will be found in the state of ψ_j with the probability

$$P_{ij} = \left| \int \psi_i \psi_j^* dx \right|^2. \tag{18}$$

Therefore, if $P_{ij} \neq 0$, a duality exists in regard to the incompatibility of the events A_i and A_j $(i \neq j)$: on the one hand, they appear to be incompatible since the function ψ_j is not obtained if the function $\psi_i \neq \psi_s$ is obtained (and conversely); on the other hand, the probability of locating (by measurement) in the state ψ_j the system, which is described by the function ψ_i, is different from zero. If by A_i we understand the appearance of the system in the physical state ψ_i, then in the well-known sense the probability of the joint event $A_i A_j$ is equal to P_{ij}. According to quantum theory, knowing the wave function, it is impossible (without measurement of this function) to carry further the precise identification of the state of the system. This prevents the separation of each event A_i into arbitrary elementary sub-events (for example, into $A_i A_j$ and $A_i - A_i A_j$) for the purpose of defining the entropy analogous to Eq. (16) by summing over the elementary events.

If, to one physical state, one can refer different wave functions, (of course, with different probabilities), then, consequently, in the description of the state by wave functions there takes place a certain redefinition (over describing). In the introduction of mixed statistics, which describe the one mathematical object (the density matrix of the fundamental scheme) by many different equivalent schemes, we frequently remove this redefinition and in this sense the quantum description approximates the classical. Therefore, the solution of the difficulty in the definition of the entropy of a non-orthogonal scheme, arising as a consequence of the redefinition, must be sought in the idea equivalence set forth in Sec. 1.

We substitute for the original scheme (1) the equivalent orthogonal scheme (9). For orthogonal representations, the events $A_1, A_2, \ldots$ are mutually exclusive in both senses, and therefore Eq. (17) is applicable. Equivalent schemes which describe one and the same object must have identical entropy; therefore, the entropy of the nonorthogonal scheme (1) is equal to

$$H = -\sum_m \lambda_m \ln \lambda_m, \tag{19}$$

where λ_m are the eigenvalues of the density matrix (8).

For example, we consider the scheme

$$\begin{pmatrix} \psi_1(x) & \psi_2(x) \\ w_1 & w_2 \end{pmatrix},$$

which consists of two nonorthogonal representations. When $\psi_1 \neq \psi_2$, $w_1 \neq 0, 1$, there is an additional indefiniteness in the system; consequently,

$$H > 0.$$

But since, as a consequence of the nonorthogonality , the states ψ_1 and ψ_2 represent in known degree one and the same object, but the entropy will be less than for the completely different states, i.e.,

$$H < -w_1 \ln w_1 - w_2 \ln w_2.$$

Actually, interpolation according to Eq. (19) in the intermediate case, when $0 < P_{12} < 1$, gives

$$H = -\lambda_1 \ln \lambda_1 - \lambda_2 \ln \lambda_2,$$

where

$$\lambda_{1,2} = \frac{w_1 + w_2}{2} \pm \sqrt{\left(\frac{w_1 - w_2}{2}\right)^2 - P_{12} w_1 w_2}.$$

When degeneracy of the eigenvalues occurs, Eq. (19) can be written in the form

$$H = -\sum_j l_j \Lambda_j \ln \Lambda_j.$$

The quantity $l_j \Lambda_j = P_j$ is nothing else than the probability of obtaining the jth linear manifold [state of type (14)]. Therefore, in complete correspondence with Eq. (16), we have

$$H = -\sum_j P_j \ln (P_j / Q_j), \qquad (20)$$

where Q_j is the abstract "volume" of the event which consists of the obtaining of the jth linear manifold, and is equal to the weight l_j ot the latter.

Eqs. (19) and (20) can be written in matrix form:

$$H = -\operatorname{Tr} \lambda \ln \lambda \quad (\lambda = \| \lambda_{mn} \| = \| \lambda_m \delta_{mn} \|),$$

or in the arbitrary representation

$$H = -\operatorname{Tr} \rho \ln \rho. \qquad (21)$$

From such a form of description, and especially from the form $H = -\ln \rho$, it is evident that the entropy of a quantum-statistical system is a direct generalization of the classical entropy.

3. We have shown that the formulas introduced for corresponding conditions lead to formulas for the entropy of "classical" statistics.

If the quantum system (which does not consist of identical particles) does not have a cyclic or spin degree of freedom, and the coordinates x are continuous, then its density matrix can be written in the form

$$\rho(x, x') = \int w\left(\frac{x + x'}{2}, p\right) \qquad (22)$$

$$\times \exp \{ip(x - x')/\hbar\}\, dp,$$

where $w(q, p)$ is the normalized "probability density" in phase space:

$$\int w(q, p)\, dq\, dp = 1.$$

However, each function $w(q, p)$, being transformed according to Eq. (22), yields the function $\rho(x, x')$ which becomes a sort of density matrix, since the condition of positive definiteness of the matrix $\rho(x, x')$ can be violated. The quantum "probability density" $w(q, p)$ satisfies the condition

$$\iiint w\left(\frac{x + x'}{2}, p\right) e^{ipx/\hbar} f(x) \qquad (23)$$

$$\times\, [e^{ipx'/\hbar} f(x')]^* \, dx dx' dp \geqslant 0$$

for an arbitrary function $f(x)$. The inequality in Eq. (23) is a precise, although not clear, mathematical formulation of the Heisenberg uncertainty principle.

From the quantum formula (19) we derive an expression for the entropy under the condition of the applicability of the classical approximation, when

$$p_{0i} q_{0i} \gg h, \qquad (24)$$
$$\frac{1}{p_{0i}} \sim \frac{1}{w} \frac{\partial w}{\partial p_i}; \quad \frac{1}{q_{0i}} \sim \frac{1}{w} \frac{\partial w}{\partial q_i} \quad (i = 1, \ldots, r).$$

For this purpose, we consider Eq. (7a), where we represented the density matrix in the form (22). We choose the interval

$$\tilde{\lambda}_j < \lambda_m < \tilde{\lambda}_j + \Delta\lambda, \qquad (25)$$

in which l_j coincides with the eigenvalues ($m = m_j + 1, \ldots, m_j + l_j$). When $\Delta\lambda$ is sufficiently small, all the eigenvalues entering into Eq. (25) can be replaced by $\tilde{\lambda}_j$. Therefore, for the eigenfunctions which correspond to the λ_m, we have

$$\int \rho(x, x') \varphi_m(x')\, dx' \approx \tilde{\lambda}_j \varphi_m(x). \qquad (26)$$

An arbitrary linear combination of eigenfunctions satisfies the same equation. In particular,

$$\int \rho(x, x') \tilde{\varphi}_s(x')\, dx' \approx \tilde{\lambda}_j \tilde{\varphi}_s(x); \qquad (27)$$
$$\tilde{\varphi}_s(x) = \sum_{k=1}^{l_j} c_{sk} \varphi_{m_j + k}(x) \quad (s = 1, \ldots, l_j).$$

The transformation from Eq. (7a) to (27) is a transformation to an approximately equivalent scheme. We choose $\| c_{sk} \|$ in such a fashion that each function $\phi_s(x)$ maintains a harmonic factor which rapidly decreases relative to the other (amplitude) factor:

$$\tilde{\varphi}_s(x) = \varphi_s^0(x) \exp\{ik_s x\}; \tag{28}$$

$$k_s \gg \frac{1}{\varphi_s^0} \frac{\partial}{\partial x} \varphi_s^0; \tag{29}$$

and that $\phi_s^0(x)$, nonetheless, be appreciably different from zero only in a small (in comparison with q_{oi}) region near some point q_s. The existence of such a selection, together with the condition for the smallness of $\Delta\lambda$ is valid only for the actual fulfilling of the inequality (24).

Substituting Eq. (28) into Eq. (27) and writing $p_s = k_s\hbar$, we find

$$\int w\left(\frac{x+x'}{2}, p\right) \exp\{i(p-p_s) \times (x-x')/\hbar\} \varphi_s^0(x')\, dp\, dx' \approx \tilde{\lambda}_j \varphi_s^0(x). \tag{30}$$

We make valid use of the equation

$$\int F(x', y') \exp\{i(y-y') \times (x-x')/\hbar\}\, dx'dy' \approx h^r F(x,y), \tag{31}$$

as can easily be seen from

$$\int F(x', y') \exp\{i(y-y')(x-x')/\hbar\}\, dy'$$
$$= F(x', y) \int \exp\{i\eta(x'-x)/\hbar\} \mu(\eta)\, d\eta$$
$$= F(x', y)(2\pi\hbar)^r \delta_\varepsilon(x'-x),$$

under the condition

$$\left(F \Big/ \frac{\partial F}{\partial x_i}\right)\left(F \Big/ \frac{\partial F}{\partial y_i}\right) \gg h. \tag{32}$$

Here $\eta = y' - y$, $\mu(\eta) = F(x', y+\eta)/F(x', y)$ [i.e., $\mu(\eta) \sim 1$ for $\eta \lesssim F/[\partial F/\partial y]$):

$$\delta_\varepsilon(x'-x) = \prod_{i=1}^{r} \delta_{\varepsilon_i}(x_i' - x_i);$$

$\delta_{\epsilon i}(x_i' - x_i)$ is a function which approximates the δ function, and which has the equivalent width

$$\varepsilon_i \sim \hbar \frac{1}{F} \frac{\partial F}{\partial y_i}.$$

For $F = w\phi_s^0$, Eq. (32) is satisfied as a consequence of Eqs. (24) and (29) (since $p_{oi} \sim k_s\hbar = p_s$); therefore, Eq. (31) can be applied for the calculation of the left hand side of Eq. (30). As a result, we obtain from Eq. (30)

$$\tilde{\lambda}_j \varphi_s^0(x) \approx h^r w(x, p_s) \varphi_s^0(x)$$
$$\approx h^r w(q_s, p_s) \varphi_s^0(x)$$

or

$$\tilde{\lambda}_j \approx h^r w(q_s, p_s). \tag{33}$$

In replacing x by q_s, use is made of the fact that $\phi_s^0(x)$ differs significantly from zero only in the region close to q_s.

In taking various s, we shall get different points q_s, p_s $(s = 1, \ldots, l_j)$, but for all these points,

$$h^r w(q_1, p_1) \approx \ldots \approx h^r w(q_{l_j}, p_{l_j}) \approx \tilde{\lambda}_j.$$

Considering this, we have

$$H = -\sum \lambda_m \ln \lambda_m \tag{34}$$
$$\approx -\sum_j \tilde{\lambda}_j \sum_{s=1}^{l_j} \ln h^r w(q_s, p_s).$$

Let $L(q, p)$ be an arbitrary function and let L be the corresponding operator*. According to the correspondence principle, when the classical approximation is applied,

$$\bar{\mathrm{L}} = \mathrm{Tr}(\rho \mathrm{L}) \approx \int L(q, p) w(q, p)\, dq\, dp, \tag{35}$$

But

$$\mathrm{Tr}(\rho \mathrm{L}) = \sum \lambda_m (\varphi_m^* \mathrm{L} \varphi_m) \tag{35a}$$
$$\approx \sum_j \tilde{\lambda}_j \sum_{s=1}^{l_j} (\tilde{\varphi}_s^* \mathrm{L} \tilde{\varphi}_s).$$

We then have

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* We note, without proof, that the following relation holds:

$$\mathrm{L} = \frac{1}{h^r} \int L\left(\frac{x+x'}{2}, p\right) \exp\{ip(x-x')/\hbar\}\, dp.$$

$$\sum_j \tilde{\lambda}_j \sum_{s=1}^{l_j} L(q_s, p_s) \tag{36}$$

$$\approx \int w(q, p)\, L(q, p)\, dq\, dp.$$

If we put $L(q, p) = \ln h^r w$ then, from Eqs. (34) and (36), we get

$$H \approx -\int w(q, p) \ln [h^r w(q, p)]\, dq\, dp \tag{37}$$

(r = number of degrees of freedom). This formula, which differs from the usual formula

$$H = -\int w \ln w\, dq\, dp$$

(in which an additive constant is undetermined), by a constant $r \ln h$, is identical with the exact formula given in reference 2. The considerations of this latter work, which lead to formulas containing Planck's constant, are verified in the same way.

One can arrive at Eq. (37) by a different sort of demonstration, namely, that the density matrix is the operator for the "physical quantity" $h^r w(q, p)$ with subsequent use of Eq. (35) for $L = \ln \rho$. From the considerations set forth above, it is evident that we can take as one of the possible schemes in the classical approximation, the scheme which consists of functions localized in the neighborhood of the point in phase space. The latter scheme is far more graphic from the point of view of the calssical representation.

When the system consists of identical particles, i.e., particles which obey the Bose or Fermi statistics, specific differences appear from the case considered earlier. For M identical particles, each of which has n degrees of freedom ($r = nM$) the denisty matrix, instead of (22), has the form

$$\rho(x_1, \ldots, x_M; x'_1, \ldots, x'_M) = C \sum_\alpha \varkappa_\alpha r(x_1, \ldots, x_M; x'_{\alpha_1}, \ldots, x'_{\alpha_M}), \tag{38}$$

where

$$r(x_1, \ldots, x_M; x_1, \ldots, x'_M) = \int \cdots \int w\left(\frac{x_1 + x'_1}{2}, \ldots, \frac{x_M + x'_M}{2}; p_1, \ldots, p_M\right)$$

$$\times \exp\left\{\frac{i}{\hbar} [p_1(x_1 - x'_1) + \ldots + p_M(x_M - x'_M)]\right\} dp_1, \ldots, dp_M.$$

The $\alpha_1, \ldots, \alpha_M$ are some permutation of the numbers $1, 2, \ldots, M$; $\sum_\alpha$ is the sum over all $M!$ such permutations, $\kappa_\alpha = 1$ for bosons and $\kappa_\alpha = (-1)^{p_\alpha}$ for fermions (p_α is the number of transpositions of the permutation $\alpha_1, \ldots, \alpha_M$); C is a normalizing constant. The density of distribution w for identical particles we shall of course assume to be symmetric.

Under the condition of applicability of the classical approximation (24), the functions $r(x_1, \ldots; x'_1, \ldots)$ are significantly different from zero only for nearly identical values of the primed and unprimed arguments:

$$r(x_1, \ldots; x'_1, \ldots) = \tilde{r}(x_1, \ldots, x_M)\, \delta_{\varepsilon_1}(x_1 - x'_1) \ldots \delta_{\varepsilon_M}(x_M - x'_M), \quad (\varepsilon \sim \hbar/p_0).$$

From this it follows that for $x_1 = x'_1, \ldots, x_M = x'_M$, $x_\alpha - x_\beta \gg \epsilon$ ($\alpha \neq \beta$) we can take into consideration only one of the terms of the sum (38), for which

$$\rho(x_1, \ldots, x_M; x_1, \ldots, x_M) \approx Cr(x_1, \ldots, x_M; x_1, \ldots, x_M).$$

Neglecting the integral over volumes where the arguments reduce to distances of the order of ϵ ($\epsilon \ll q_0$) and where this equality is invalid, we have

$$\int \rho(x_1, \ldots, x_M; x_1, \ldots, x_M)\, dx_1 \ldots dx_M \approx C \int r(x_1, \ldots, x_M; x_1, \ldots, x_M)\, dx_1 \ldots dx_M = C,$$

from which

$$C \approx 1. \tag{39}$$

We shall take the local wave function $\tilde{\psi}_{q_1 \ldots q_M p_1 \ldots p_M}(x_1, \ldots, x_M)$ which corresponds to this case, when one particle is close to the point (q_1, p_1), another close to (q_2, p_2) and so forth:

$$\tilde{\psi}_{q_1 \ldots q_M p_1 \ldots p_M}(x_1, \ldots, x_M) = C' \sum_\beta \varkappa_\beta \psi^0_{q_1 \ldots q_M}(x_{\beta_1}, \ldots, x_{\beta\beta_M}) \times \exp\left\{\frac{i}{\hbar}(p_1 x_{\beta_1} + \ldots + p_M x_{\beta M})\right\}. \tag{40}$$

Here C' is the normalizing constant, $\psi^0_{q_1 \ldots q_M}(x_1, \ldots, x_M)$ is a slowly changing function (in comparison with the harmonic factor) which differs appreciably from zero only for $x_1 \sim q_1, \ldots, x_M \sim q_M$.

We apply the operator ρ to Eq. (40). Taking into account Eq. (38), and changing the signs of the transformed integrations, we get

$$\begin{aligned}\rho\tilde{\psi} &= M!C'C\sum_{\gamma} \varkappa_\gamma \int w\left(\frac{x_1 + x_1'}{2}, \ldots, \frac{x_M + x_M'}{2}; p_1', \ldots, p_M'\right) \psi^0 (x_{\gamma_1}', \ldots) \\ &\quad \times \exp\left\{\frac{i}{\hbar}[p_1'(x_1 - x_1') + p_1 x_{\gamma_1}' + \ldots]\right\} dx_1' \ldots dp_1' \ldots \\ &= M!C'C\sum_{\gamma} \varkappa_\gamma \exp\left\{\frac{i}{\hbar}(p_1 x_{\gamma_1} + \ldots)\right\} \int w\left(\frac{x_1 + x_1'}{2}, \ldots; p_1', \ldots\right) \psi^0 (x_{\gamma_1}', \ldots) \\ &\quad \times \exp\left\{\frac{i}{\hbar}[(p_1' - p_{\sigma_1})(x_1 - x_1') + \ldots]\right\} dx_1' \ldots dp_1' \ldots,\end{aligned}$$

where $\sigma_1, \ldots, \sigma_M$ are permutations inverse to $\gamma_1, \ldots, \gamma_M$ $(\gamma_{\sigma i} = i)$. Applying Eq. (31) we then obtain

$$\begin{aligned}\rho\tilde{\psi} &\approx M!C'h^r \sum_{\gamma} \varkappa_\gamma \exp\left\{\frac{i}{\hbar}(p_1 x_{\gamma_1} + \ldots)\right\} \\ &\quad \times w(x_1, \ldots; p_{\sigma_1}, \ldots)\, \psi^0_{q_1} \ldots (x_{\gamma_1}, \ldots) \\ &\approx M!\, h^r C' \sum_{\gamma} \varkappa_\gamma \exp\left\{\frac{i}{\hbar}\, p_1 x_{\gamma_1} + \ldots)\right\} \\ &\quad \times w(q_{\sigma_1}, \ldots; p_{\sigma_1}, \ldots)\, \psi^0_{q_1} \ldots (x_{\gamma_1}, \ldots)\end{aligned}$$

or, considering the symmetry of the density function,

$$\rho\tilde{\psi}_{q_1 \ldots p_1, \ldots}(x_1, \ldots) \tag{41}$$

$$\approx M!\, h^r w(q_1, \ldots; p_1 \ldots)\, \tilde{\psi}_{q_1 \ldots p_1 \ldots}(x_1, \ldots).$$

Taking into account the equality thus obtained or the relation stemming from it

$$(\tilde{\psi}^*_{q_1 \ldots p_1 \ldots}\, \rho\tilde{\psi}_{q_1 \ldots p_1 \ldots}) \tag{42}$$

$$\approx M!\, h^r w(q_1, \ldots; p_1, \ldots),$$

we conclude that the denisty matrix is the operator of the "physical quantity" $M!\,h^r w(q_1 \ldots; p_1, \ldots)$. Furthermore, the functions ln $\times[M!\,h^r w(q_1, \ldots; p_1, \ldots)]$ correspond to the operator ln ρ and, as a consequence of Eqs. (21), (35), and (35a), we have

$$H \approx -\int w(q, p) \ln [M!\, h^r w(q, p)]\, dq\, dp, \tag{43}$$

$$[q = (q_1, \ldots, q_r);$$

$$p = (p_1, \ldots, p_r); \quad r = nM].$$

A similar formula was obtained in reference 2 as the formula which determines the configurational neginformation, which coincides with the actual neginformation for essentially indistinguishable particles. Thus the quantum consideration verifies the conclusions of the previous work.

4. In those cases in which a scheme of type (1) is not assigned, but some information Γ of another kind is available concerning the quantum-statistical system, the density matrix can be determined by use of the following principal of maximum neginformation: since nothing is known about the system except Γ, then the desired density matrix must have the maximum neginformation (entropy) of all density matrices consisting with Γ.

The choice of another density matrix which has a smaller neginformation would have implied a fixing of some additional information in addition to Γ. Thus the problem of the search for an unknown density matrix reduces to the conventional extremal problem for expressions which determine the entropy. We note that the principle just demonstrated does not appear as a consequence of the second law of thermodynamics, since it is far wider than the latter and is suitable for investigation of density matrices for nonequilibrium states, i.e., it emerges from the framework of statistical thermodynamics. If we choose the condition $E \leqq \mathrm{H} \leqq E + \Delta E$ for Γ (H is the Hamiltonian of the system), then the solution of the extremal problem leads to the quantum microcanonical distribution. However, in physical problems, there cannot be complete certainty that the energy for any other physical quantity does not exceed the limits of some interval. It is more accurate to use for the condition on Γ the fixing of the phenomenological parameters: $\mathscr{L}_1, \ldots, \mathscr{L}_m$. But in the transition from the phenomenological picture to dynamic, there corresponds a statistical mean to the phenomenological parameters. From this point of view it is more accurate to put the conditions Γ in the form: $\overline{L}_1 = \mathscr{L}_1, \ldots, \overline{L}_m = \mathscr{L}_m$. Then the variational problem will have the form

$$\delta \operatorname{Tr}(\rho \ln \rho) = 0 \tag{44}$$

for the conditions

$$\operatorname{Tr}\rho = 1;\ \operatorname{Tr}(\rho L_1) = \mathscr{L}_1; \ldots; \tag{45}$$

$$\operatorname{Tr}(\rho L_m) = \mathscr{L}_m.$$

To these conditions, generally speaking, one would have to add the condition of positive definiteness and Hermitian character of the function ρ. However, functions which are not positive definite, have less (and even negative) entropy; therefore,their inclusion in the class of functions of comparison cannot change the result. Since we do not introduce the Hermitian condition, we also broaden the class of the functions of comparison. If the extremal of this expanded class is Hermitian (which is fulfilled, as is easy to prove), then it will be simultaneously an extremal for the much narrower class of Hermitian functions of comparison.

Solving Eqs. (44) and (45) with the help of Lagrangian multipliers and bearing in mind that, in general,

$$\delta \operatorname{Tr}(\rho^k) = \operatorname{Tr}(k\rho^{k-1}\delta\rho),$$

we find

$$\operatorname{Tr}[(\ln \rho + \gamma_0 + \gamma_1 L_1 + \ldots + \gamma_m L_m + 1)\delta\rho] = 0,$$

whence

$$\rho = \exp\{\gamma - \gamma_1 L_1 - \ldots - \gamma_m L_m\}, \tag{46}$$

where $\gamma_1, \ldots, \gamma_m$ and $\gamma = -\gamma_0 - 1$ are defined by Eq. (45).

When $m = 1$, $L_1 = H$, the density matrix (46) coincides with the quantum canonical distribution, which is usually hypothesized[3] or derived from the (hypothesized in its turn) microcanonical distribution[4].

Starting out from the framework of statistical thermodynamics, it is possible to put for $L_1, \ldots, L_m$ non-equilibrium distribution of energy, density, current, etc., and to obtain the density matrices which describe such systems. Thus, furnishing a basis for the analytic use of the principal of maximum neginformation, the formula of quantum entropy is shown to be useful in the quantum statistical theroy of nonequilibrium processes.

Translated by R. T. Beyer
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[3] M. A. Leontovich, Statistical Physics GITTL, Moscow-Leningrad, 1944

[4] A. Ia. Khinchin, *Mathematical Foundations of Quantum Statistics,* Dover, New York, 1949