Eigenstates of Harmonic Oscillator as the States of Maximal Quantropy

D.Lalovic, D.Davidovic, N.Bijedic and S.Zekovic
Institute for Nuclear Sciences "B.Kidric", Vinca, 11001 Beograd, Yugoslavia.

A new definition of entropy for a quantum mechanical state is introduced. On the basis of this definition a new physical quantity, named quantropy, is introduced. It is shown that the eigenstates of harmonic oscilator are the states of maximal quantropy.

1. Introduction

Quantum mechanics is a statistical theory and, cosequently, it has some properties which are common to all statistical theories. But there are also some fundamental differences between quantum mechanics and other statistical theories. One of such differences reflects in the fact that entropy, which is one of the fundamental concepts in all statistical theories, plays no any role in the standard form of quantum mechanics. Namely, in the standard form of quantum mechanics entropy S of a given state is given by the expression $S = - \mathrm{Tr}\ (\hat{\rho}\ \ln\ \hat{\rho}\ )$, where $\hat{\rho} = |g\rangle\langle g|$ is a density matrix (note that we are considering only pure states). Since the eigenvalues of $\hat{\rho}$ are 0 and 1, entropy is zero for every pure state. Thus here we have an awkward situation, not present in other statistical theories, that we must ascribe zero entropy to a state, in spite of the fact that the state is not described deterministically. This fact one might accept simply as one of the peculiarities of quantum mechanics. However, having in mind that entropy is one of the most profound concepts in our conceiving of nature, we find it worth to make an effort in order to get a deeper insight in possible role of entropy in quantum mechanics. The present paper is devoted to such an analysis. The organization of the paper is the following. In Part 2. we introduce a new definition of entropy of a quantum mechanical state, which ascribes a non-zero entropy to pure states. We then discuss possible role of this entropy in determining of stationary states, in analogy with the corresponding role of entropy in classical statistical physics, and we point out the need of introducing a new physical quantity, which we name quantropy. In Part 3. we show that eigenstates of harmonic oscilator are states of maximal quantropy.

2. A New Definition of Entropy in Quantum Mechanics

If we want to attribute to entropy some non-trivial role in quantum mechanics it is evident that we need a new definition of entropy, different from that of the standard quantum mechanics. If we want the role of entropy in quantum mechanics to be similar to the role of entropy in classical statistical physics, then it seems natural to look for a definition of entropy in quantum mechanics which would be as close as possible to the definition of entropy in classical statistical mechanics. In the latter theory entropy can be defined by the following expression[1)]

$$S = -\iint f(q,p) \ln 2\pi\hbar f(q,p)\, dq\, dp \qquad (1)$$

where f(q,p) is probability distribution function in phase space. For simplicity, in the present paper we shall work in one dimension, and we shall put $\hbar = 1$. It is evident that a definition of entropy in quantum mechanics, in close analogy with (1), is possible only if we can get a complete description of a quantum mechanical state by a non-negative function f(q,p) in phase space. Such a description, though unusual, is possible in the following way. If we represent matrix in some basis then diagonal matrix elements are non-negative quantities. But there are off-diagonal matrix elements, which are complex numbers in the general case. They can not be ignored because they carry a part of the information about the state of a system not contained in diagonal matrix elements. But there is one basis with a special property such that all off-diagonal matrix elements of the density matrix, represented in this basis, can be expressed as linear combinations of diagonal matrix elements. In other words, in this representation off-diagonal matrix elements carry no any new information about a state which is not already contained in diagonal matrix elements. This means that density matrix in this representation is completely determined by its diagonal matrix elements. This special basis (which we shall call phase space representation) consists of minimal wave packets. In the coordinate representation they have the following form

$$\langle x \mid q,p \rangle = N \exp\{- b/2\ (x-q)^2 + ixp\} \tag{2}$$

where N is normalization factor. In the phase space representation diagonal matrix elements of the density matrix $\hat{\rho}$ which corresponds to a state g are given by the following expression

$$2\pi\ f(q,p) \equiv \langle q,p \,|\hat{\rho}|\, q,p \rangle = N^2 \iint g^*(x) g(x') F(x,x',q,p,b) dx' dx \tag{3}$$

where

$$F(x,x',q,p,b) = \exp\{ - b/2\ (x-q)^2 - b/2\ (x'-q)^2 + i(x - x')p \}$$

As we have already pointed out, the off-diagonal matrix elements can be expressed by the diagonal ones[2] so that a complete description of a state is given by the function f(q,p) defined by (3). We now can define entropy of a quantum mechanical state by the same expression as in classical statistical mechanics, i.e., by the expression (1).

We shall now analyse whether this entropy can play in quantum mechanics a role similar to the role played by entropy in classical statistical mechanics. As it is well known, in the latter theory, entropy, among other things, determines probability distribution function f(q,p) of a stationary state, through the principle of maximal entropy. This prinoiple states that in stationary state, probability distribution function f(q,p) of a system with Hamiltonian H(q,p) and with given avarage energy E

$$E = \iint f(q,p)\ H(q,p)\ dqdp \tag{4}$$

must be such that entropy is maximal, i.e., f(q,p) must be such that for small variations of f(q,p) variation of S must be zero

$$S = - \iint \ln f(q,p)\, \delta f(q,p)\ dqdp = 0 \tag{5}$$

The variations $\delta f(q,p)$ are subject to the following additional conditions

$$\iint \delta f(q,p)\, H(q,p)\, dqdp = 0 \qquad (6)$$

$$\iint \delta f(q,p)\, dqdp = 0 \qquad (7)$$

The important point to be noted here is that in the condition (4), through which the Hamiltonian of the system influences the solution of (5), the energy E is an external parameter, fixed from outside. This fact is the main reason why entropy in quantum mechanics (in spite of the fact that we now have a definition of entropy quite analogous to that of classical statistical mechanics) can not play same role in determining f(qp) as in classical statistical mechanics. Namely, energy of a stationary state in quantum mechanics is an internal parameter, which can not be fixed from outside. This means that in quantum mechanics we can not put a condition analogous to (4). Instead, we must include energy in the very process of variation, together with entropy. We have found that the simplest possibility is to vary quantity S/E instead of S alone. The quantity K = S/E we shall call quantropy and, in analogy with the principle of maximal entropy, we introduce the principle of maximal quantropy. This principle states that the function f(q,p), as given by (3), for a stationary state, must be such that quantropy is maximal (here we have in mind not only absolute maximum but local maxima also), i.e., we require

$$\delta K = S\,\delta E - E\,\delta S = 0 \qquad (8)$$

In terms of the variation $\delta f(q,p)$, relation (8) has the following form

$$\iint \{S\, H(q,p) + E \ln f(q,p)\}\, \delta f(q,p)\, dqdp = 0 \qquad (9)$$

The variation $\delta f(q,p)$ is subject to two additional conditions. One is identical to the condition (7) above, and second requires that $\delta f(q,p)$ must be such that $f(q,p) + \delta f(q,p)$ represents also a pure state. This condition, which shall be called pure state condition, stands instead of the condition (6). In the next section we shall apply the principle of maximal quantropy to the case of harmonic oscilator and we shall show that eigenstates of harmonic oscilator are the states of maximal quantropy.

3. Eigenstates of Harmonic Oscilator as the States of Maximal Quantropy

The main problem in finding functions $f(q,p)$ which satisfy extremality condition (9) is to satisfy pure state condition. Usually, this kind of problem is treated by the method of Lagrange multipliers. However, in our case it turns out that this method is difficult to apply. For this reason we shall ensure satisfying pure state condition by relying directly upon the definition (3) of the function $f(q,p)$. Namely, all possible variations of $f(q,p)$, which satisfy pure state condition, can be get by variations of $g(x)$ and b in (3). In this way, puting $\delta g(x) = e_1\, h(x)$, $\delta b = -\, e_2\, b$, where e_1 and e_2 are small parameters, and $h(x)$ is an arbitrary wave function, we get

$$\delta f(q,p) = \delta f_1(q,p) + \delta f_2(q,p)$$

where

$$\delta f_1(q,p) = 2e_1 \,\mathrm{Re} \iint g^*(x)\, h(x')\, F(x,x',q,p,b)\, dx'dx \qquad (10)$$

$$\delta f_2(q,p) = e_2 b \iint \left[(x-q)^2+(x'-q)^2\right] g^*(x) g(x') F(x,x',q,p,b) dx'dx \qquad (11)$$

In (10) and (11) we have omited normalisation factors.
We shall now show that, in the case of harmonic oscilator, the relation (9) is satisfied if the function $f(q,p)$ in (9) is that which corresponds to an eigenstate of harmonic oscilator, i.e., if $f(q,p)$ is the function which we get from (3) for some particular value of b, when for $g(x)$ we put an eigenfunction of harmonic oscilator. Since the small parameters e_1 and e_2 are independent, the relation (9) must be satisfied for $\delta F_1(q,p)$ and $\delta f_2(q,p)$ separately.

In order to simplify writing, we shall introduce some convenient notations. The Hamiltonian of harmonic oscilator we shall write in the form

$$H(q,p) = 1/2\,\omega\, (Q^2 + P^2) = 1/2\, \omega\, r^2 \qquad (12)$$

where we have introduced the notation

$$Q^2 = aq^2, \quad P^2 = 1/a\, p^2, \quad r^2 = Q^2 + P^2, \quad a = m\omega$$

Note that Q, P, and r are dimensionless variables. We also introduce a complex variable z

$$z = Q + iP = r\, e^{i\alpha}$$

Let us now calculate $\delta f_1(Q,P)$ and $\delta f_2(Q,P)$, as given by (10) and (11), for a particular value of b, b = a, and for g(x) which is an eigenfunction of harmonic oscilator, i.e.,

$$g(x) = g_n(x) = N \exp\{-1/2\, ax^2\}\, H_n(a^{1/2} x) \tag{13}$$

where N is a normalisation factor and H_n is Hermit polinomial. Further on we shall omit normalisation factors because they can be absorbed in parameters e_1 and e_2. The arbitrary wave function h(x) we shall develope in a series over harmonic oscilator eigenfunctions

$$h(x) = \Sigma \quad A_m\, g_m(x) \tag{14}$$

Now for $\delta f_1(Q,P)$ and $\delta f_2(Q,P)$ we get

$$\delta f_1 = 2e_1 \exp\{-1/2\, r^2\} \mathrm{Re}\{ \sum_{m \neq n} A_m\, r^{n+m}\, e^{i(m-n)} \} \tag{15}$$

$$\delta f_2 = e_2 r^n \exp\{-1/2\, r^2\}\, \mathrm{Re}\{ 1/4\, z^{n+2} + 1/2\, (2n+1) z^n +$$

$$+ n(n-1) z^{n-2} - r\cos\alpha\, (z^{n+1} + 2n z^{n-1}) + r^2 \cos^2\alpha\, z^n \} \tag{16}$$

Note that in calculating (15) and (16) we have taken into account condition (7). From (3) we can find the function f(Q,P), for b = a, which corresponds to the harmonic oscilator eigenfunction $g_n(x)$ and the result is

$$f_n(Q,P) = A\, r^{2n} \exp\{-1/2\, r^2\} \tag{17}$$

where A is a normalisation factor.

Using (17) and (12), one can easily check that (9) is satisfied for any δf_1 and δf_2 as given by (15) and (16).

If we wish to check that this extremum is maximum we must calculate $\delta^2 K'$ and see whwther this quantity is negative. This is a straightforward but rather lengthy procedure which we shall not present here, but the result is that this is indeed maximum. Since these are local maxima, it is interesting to see which state has greatest quantropy, i.e., which of these maxima is an absolute maximum. In order to answer this question we must calculate quantropy for harmonic oscilator eigenstate $g_n(x)$ as a function of n. The result is

$$K_n = 1/_\omega \ \{ \ln n!/n + C - (1/2 + 1/3 + \cdot \quad + 1/(n-1)) \}$$

for n = 1

$$K_0 = 1/_\omega \quad , \text{ for } n = 0$$

where C is Euler constant.
One can show that K_n is a descending function of n, so we have to compare only K_1 and K_0. Since $K_1 = C/_\omega \approx 0,58/_\omega$, we see that the ground state of harmonic oscilator has greatest quantropy.

4. Discussion

We have shown that eigenstates of harmonic oscilator represent local maxima of quantropy and that absolute maximum of quantropy corresponds to the ground state. This result is very interesting and there naturally arises the question whether the principle of maximal quantropy is a new general physical principle, or the present result is just an accident. At the present moment we are not able to answer this question. Even in the case of harmonic oscilator treated here there are some open questions. For instance, we have not shown that there are no other states, besides harmonic oscilator eigenstates, which satisfy relation (9) with harmonic oscilator Hamiltonian, though, intuitively, one feels that there should not be such states. These and some other important questions concerning quantropy will be subject of fourthcoming papers.

References

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