On statistical mechanics in noncommutative spaces.

S. A. Alavi

Department of Physics, Sabzevar university of Tarbiat Moallem, Sabzevar, P. O. Box 397, Iran
and
Sabzevar House of Physics, Sabzevar, Iran.

Abstract

We study the formulation of quantum statistical mechanics in noncommutative spaces. We construct microcanonical and canonical ensemble theory in noncommutative spaces. We consider for illustration some basic and important examples in the framework of noncommutative statistical mechanics: (i). An electron in a magnetic field. (ii). A free particle in a box. (iii). A linear harmonic oscillator.

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Introduction.

To study quantum mechanical systems composed of indistinguishable entities, as most physical systems are, one finds that it is advisable to rewrite the ensemble theory in a language that is more natural to a quantum-mechanical treatment, namely the language of the operators and the wave functions[1]. Once we set out to study these systems in detail, we encounter a stream of new and altogether different physical concepts. In particular, we find that the behavior of even a noninteracting system, such as the ideal gas, departs considerably from the pattern set by the so-called classical treatments. In the presence of interactions the pattern becomes still more complicated.

Recently there have been notable studies on the formulation and possible experimental consequences of extensions of the usual physical theories in the noncommutative spaces[2]. The study on noncommutative spaces is much important for understanding phenomena at short distances beyond the present test of different physical theories. For a manifold parameterized by the coordinates $x_i$, the noncommutative relations can be written as:

$$[\hat{x}_i, \hat{x}_j] = i\theta_{ij}, \quad [\hat{x}_i, \hat{p}_j] = i\delta_{ij}, \quad [\hat{p}_i, \hat{p}_j] = 0,$$

(1)

where $\theta_{ij}$ is an antisymmetric tensor which can be defined as $\theta_{ij} = \frac{1}{2}\epsilon_{ijk}\theta_k$. In this paper we study the formulation of quantum statistics, namely the quantum-mechanical ensemble theory, the density matrix, etc., in a noncommutative space and the new features that arise.
Perturbation aspects of noncommutative dynamics.

NCQM is formulated in the same way as the standard quantum mechanics SQM (quantum mechanics in commutative spaces), that is in terms of the same dynamical variables represented by operators in a Hilbert space and a state vector that evolves according to the Schroedinger equation:

\[ i \frac{d}{dt} |\psi\rangle = H_{nc} |\psi\rangle, \]  

(2)

we have taken into account \( \hbar = 1 \). \( H_{nc} \equiv H_\theta \) denotes the Hamiltonian for a given system in the noncommutative space. In the literature two approaches have been considered for constructing the NCQM:

a) \( H_\theta = H \), so that the only difference between SQM and NCQM is the presence of a nonzero \( \theta \) in the commutator of the position operators i.e. Eq.(1).

b) By deriving the Hamiltonian from the moyal analog of the standard Schroedinger equation:

\[ i \frac{\partial}{\partial t} \psi(x, t) = H(p = \frac{1}{i} \nabla, x) \ast \psi(x, t) \equiv H_\theta \psi(x, t), \]  

(3)

where \( H(p, x) \) is the same Hamiltonian as in the standard theory, and as we observe the \( \theta \)-dependence enters now through the star product [3]. In [4], it has been shown that these two approaches lead to the same physical theory. Since the noncommutativity parameter if it is non-zero, should be very small compared to the length scales of the system, one can always treat the noncommutativity effects as some perturbations of the commutative counterpart.

For the Hamiltonian of the type:

\[ H(\hat{p}, \hat{x}) = \frac{\hat{p}^2}{2m} + V(\hat{x}). \]  

(4)

The modified Hamiltonian \( H_\theta \) can be obtained by a shift in the argument of the potential [5]:

\[ x_i = \hat{x}_i + \frac{1}{2} \theta_{ij} \hat{p}_j \quad \hat{p}_i = p_i. \]  

(5)

which lead to

\[ H_\theta = \frac{p^2}{2m} + V(x_i - \frac{1}{2} \theta_{ij} p_j). \]  

(6)

The variables \( x_i \) and \( p_i \) now, satisfy in the same commutation relations as the usual case:

\[ [x_i, x_j] = [p_i, p_j] = 0 \quad [x_i, p_j] = \delta_{ij}. \]  

(7)

Now we discuss the perturbation aspects of noncommutative dynamics. Using

\[ U(x + \Delta x) = U(x) + \sum_{n=1}^{\infty} \frac{U^{(n)}(x)}{n!}(\Delta x)^n, \]  

(8)
and Eq.(6) we have:
\[ H_{nc} = \frac{p^2}{2m} + V(x_i) + \sum_{n=1}^{\infty} \frac{V(n)(x_i)}{n!}(\Delta x_i)^n, \]  
(9)
where \( \Delta x_i = -\frac{1}{2} \theta \epsilon_{ij} p_j \) and \( H = \frac{p^2}{2m} + V(x) \) is the Hamiltonian in ordinary (commutative) space. To the first order we have:
\[ H_{nc} \equiv H_\theta = \frac{p^2}{2m} + V(x_i) + \Delta x_i \partial V/\partial x_i = H + \Delta x_i \partial V/\partial x_i = H + \theta H_I. \]  
(10)

We can use perturbation theory to obtain the eigenvalues and eigenfunctions of \( H_{nc} \):
\[ E_n = E_n^0 + \Delta E_n^0 = E_n^0 + \theta E_n^{(1)} + \theta^2 E_n^{(2)} + \ldots, \]  
(11)
\[ \hat{\phi}_n = \phi_n + \sum_{k \neq n} C_{nk}(\theta) \phi_k. \]  
(12)
where:
\[ C_{nk}(\theta) = \theta C_{nk}^{(1)} + \theta^2 C_{nk}^{(2)} + \ldots \]  
(13)
To the first order in perturbation theory we have:
\[ \theta E_n^{(1)} = \langle \phi_n | \theta H_I | \phi_n \rangle, \]  
(14)
\[ \hat{\phi}_n = \phi_n + \theta \sum_{k \neq n} C_{nk}^{(1)} \phi_k, \]  
(15)
\[ \theta C_{nk}^{(1)} = \frac{\langle \phi_k | \theta H_I | \phi_n \rangle}{E_n^0 - E_k^0}, \]  
(16)
where \( E_n^0 \) and \( \phi_n \) are the nth eigenvalue and eigenfunction of the Hamiltonian \( H \). \( E_n \) and \( \hat{\phi}_n \) are the nth eigenvalue and eigenfunction of \( H_{nc} \).

The density operator in noncommutative spaces.

Using the orthonormal functions \( \hat{\phi}_n \), an arbitrary wave function in a noncommutative space can be written as:
\[ \hat{\psi}^k(t) = \sum_n \hat{\alpha}_n^k(t) \hat{\phi}_n \]  
(17)
where:
\[ \hat{\alpha}_n^k(t) = \int \hat{\phi}_n^* \hat{\psi}^k(t) d\tau \]  
(18)
The time variation of these coefficients will given by:
where $\hat{H}_{nm} = \int \hat{\phi}_n^{*} \hat{H} \hat{\phi}_m$. We now introduce the density operator $\hat{\rho}(t)$, in a noncommutative space by the matrix elements:

$$\hat{\rho}_{nm}(t) = \frac{1}{n} \sum_{k=1}^{n} [\hat{a}_n^k(t) \hat{a}_m^{k*}(t)]$$

Clearly the matrix element $\hat{\rho}_{nm}(t)$, is the ensemble average of the quantity $a_m(t) a_n^{*}(t)$, which as a rule varies from member to member in the ensemble. We shall now determine the equation of motion for the density matrix $\hat{\rho}_{mn}(t)$:

$$i\hbar \frac{\partial}{\partial t} \hat{\rho}_{mn}(t) = \frac{1}{n} \sum_{k=1}^{n} [i\hbar \frac{\partial}{\partial t} \hat{a}_n^k(t)] \hat{a}_m^{k*}(t) + i\hbar [\frac{\partial}{\partial t} \hat{a}_m^{k*}(t)] \hat{a}_n^k(t)$$

It can be written in the following form:

$$\frac{1}{n} \sum_{k=1}^{n} [\hat{H}_{m \ell} \hat{a}_n^k(t) \hat{a}_m^{k*}(t)] - \sum_{k=1}^{n} \sum_{\ell} [\hat{H}_{m \ell} \hat{a}_n^k(t) \hat{a}_m^{k*}(t)] = (\hat{H} \hat{\rho} - \hat{\rho} \hat{H})_{mn}$$

Using the commutator notation, it can be written as:

$$i\hbar \dot{\hat{\rho}} = [\hat{H}, \hat{\rho}]$$

Now, we consider the expectation value of a physical quantity $G$, in a noncommutative space which is dynamically represented by an operator $\hat{G}$. This will naturally be determined by the double averaging process:

$$< \hat{G} >= \frac{1}{n} \sum_{k=1}^{n} \int \hat{\psi}^k \hat{\psi}^k G d\tau$$

or:

$$< \hat{G} >= \frac{1}{n} \sum_{k=1}^{n} \sum_{\ell} \hat{a}_n^{k*} \hat{a}_m^k \hat{G}_{nm}$$

where:

$$\hat{G}_{nm} = \int \hat{\phi}_n^{*} \hat{G} \hat{\phi}_m d\tau$$

Introducing the density matrix $\hat{\rho}$, it takes a particularly neat form:

$$< \hat{G} >= \sum_{m,n} \hat{\rho}_{nm} \hat{G}_{nm} = \sum_{m} (\hat{\rho} \hat{G})_{mm} = Tr(\hat{\rho} \hat{G})$$
We note that if the original wave functions $\hat{\psi}_k$, were not normalized then the expectation value $\langle \hat{G} \rangle$ would be given by the formula

$$
\langle \hat{G} \rangle = \frac{\text{Tr}(\hat{\rho}\hat{G})}{\text{Tr}(\hat{\rho})}
$$

(28)

The interesting point is that the equations (23) and (28) are the same as the commutative case with quantities replaced by their noncommutative counterparts.

Statistics of the various ensembles.

The microcanonical ensemble.

The construction of the microcanonical ensemble is based on the premise that the systems constituting the ensemble are characterized by a fixed number of particles $N$, a fixed volume $V$ and an energy lying within the interval $(E - \Delta, E + \Delta)$, where $\Delta \ll E$. The total number of distinct microstates accessible to a system is then denoted by the symbol $\Gamma(N, V, E; \Delta)$ and by assumption, any of these microstates is just as likely to occur as any other.

Accordingly, the density matrix $\hat{\rho}_{mn}$ (which in the energy representation must be a diagonal matrix) will be of the form $\hat{1}/\Gamma$, for each of the accessible states and 0, for all other states.

We note that $\hat{\rho}$ is independent of energy (energy eigenstates) and the volume $V$, so it does not depend on space coordinates. It means that the noncommutativity of space has no effects on $\hat{\rho}$ in microcanonical ensemble.

The dynamics of the system determined by the expression for its entropy, which in turn is given by:

$$
S = k \ln \Gamma
$$

(29)

which as mentioned above remains unchanged in noncommutative spaces.

The canonical ensemble.

In this ensemble the macrostate of a member system is defined through the parameters $N$, $V$ and $T$: the energy $E$ now becomes a variable quantity. The probability that a system, chosen at random from the ensemble, possesses an energy $E$, is determined by the Boltzmann factor $\exp(-\beta E)$, where $\beta = \frac{1}{kT}$.

The density matrix in the energy representation is therefore takes as:

$$
\hat{\rho}_{mn} = \hat{\rho}_n \delta_{mn}
$$

(30)

where:

$$
\hat{\rho}_n = c e^{-\beta E_n}; \quad n = 0, 1, 2, ...
$$

(31)
Here $E_n$ are the energy eigenvalues in noncommutative space (Eq. 11), and the constant $c$ is given by:

$$c = \frac{1}{\sum_n e^{\beta E_n}} = \frac{1}{\hat{Q}_N(\beta)}$$

(32)

where $\hat{Q}_N(\beta)$, is the partition function of the system in noncommutative space. The density operator in the canonical ensemble may be written as:

$$\hat{\rho} = \sum_n \hat{\phi}_n \frac{1}{\hat{Q}_N(\beta)} e^{-\beta E_n} \langle \hat{\phi}_n | =$$

$$\frac{1}{\hat{Q}_N(\beta)} e^{-\beta \hat{H}} \sum_n | \hat{\phi}_n \rangle \langle \hat{\phi}_n | = \frac{e^{-\beta \hat{H}}}{Tr(e^{-\beta \hat{H}})}$$

(33)

Then the expectation value of a physical quantity $G$, in a noncommutative space is given by:

$$\langle \hat{G} \rangle_N = Tr(\hat{\rho} \hat{G}) = \frac{Tr(\hat{G} e^{-\beta \hat{H}})}{Tr(e^{-\beta \hat{H}})}$$

(34)

Examples.

(i). An electron in a magnetic field.

The Hamiltonian of the system has the following form:

$$\hat{H} = -\mu_B (\vec{\sigma} \cdot \vec{B})$$

(35)

where $\mu_B = \frac{e \hbar}{2mc}$. The Hamiltonian is space independent, so there is no corrections due to the noncommutativity of space on the statistical (Thermodynamical) properties of this system.

(ii). A free particle in a box.

Let us consider the motion of a particle with charge $e$ and mass $m$ in the presence of a magnetic field produced by a vector potential $\vec{A}$. The lagrangian is as follows:

$$L = \frac{1}{2} m V^2 + \frac{e}{c} \vec{A} \cdot \vec{V} - V(x, y)$$

(36)

where $V_i = h_i q_i$ (no summation, $i = 1, 2, 3$), are the components of the velocity of the particle and $h_i (i = 1, 2, 3)$ are the scale factors. $V(x, y)$ describes aditional interactions (impurities). For the case of a free particle $V(x, y) = 0$. In the absence of $V$ the quantum spectrum consists of the well-known Landau levels. In the strong magnetic field limit only the lowest Landau level is relevant. But the large $B$ limit corresponds to small $m$, so setting the mass to zero effectively
projects onto the lowest Landau level. In the chosen gauge $\vec{A} = (0, h_1 q_1 B)$ and in that limit, the Lagrangian (36) takes the following form:

$$L' = \frac{e}{c} B h_1 h_2 q_1 q_2 - V(x, y)$$

(37)

which is of the form $pq - H(p, q)$, and suggests that $\frac{e}{c} B h_1 q_1$ and $h_2 q_2$ are canonical conjugates, so we have:

$$[h_1 q_1, h_2 q_2] = -i \frac{hc}{eB}$$

(38)

which can be written in general form:

$$[h_i q_i, h_j q_j] = i \theta_{ij}$$

(39)

which is the fundamental space-space noncommutativity relation in a general noncommuting curvilinear coordinates. The cartesian, circular cylindrical and spherical polar coordinates are three special cases [6].

So a free particle in a noncommutative space is equal to a particle in commutative space but in the presence of a magnetic field. The Hamiltonian of a particle in a magnetic field is:

$$H = \frac{1}{2m} (\vec{p} - \frac{q}{c} \vec{A})^2$$

(40)

On the other hand let us introduce the noncommutativity to momentums instead of space coordinates:

$$[\hat{x}_i, \hat{x}_j] = 0 \quad [\hat{x}_i, \hat{p}_j] = i \delta_{ij} \quad [\hat{p}_i, \hat{p}_j] = i \theta_{ij}$$

(41)

one can easily show that there is a transformation:

$$\hat{p}_i = p_i + \frac{1}{2} \theta_{ij} x_j \quad \hat{x}_i = x_i$$

(42)

where the new variables $p_i$ and $x_i$ satisfy the standard commutation relations (7). We note that (42) is the same as $p_i \rightarrow p_i - \frac{1}{2} \theta_{ij} x_j$ with $A_i = -\frac{1}{2} \theta_{ij} x_j$.

Now the Hamiltonian of a free particle in a noncommutative space is:

$$H = \frac{1}{2m} \hat{p}^2 =$$

$$\left( p_i + \frac{1}{2} \theta_{ij} x_j \right)^2 = p_i^2 + \theta_{ij} p_i x_j + O(\theta^2) = p_i^2 - \frac{1}{2} \vec{L} \cdot \vec{\theta} + O(\theta^2)$$

(43)

where $L_k = \epsilon_{ijk} x_i p_j$. Since for a free particle $\vec{L} = 0$, so to the first order there is no corrections on the Hamiltonian and therefore there is no corrections due to noncommutativity of space on the statistical(Thermodynamical) properties
of this system.

(iii). A harmonic oscillator.

The case of a linear harmonic oscillator is irrelevance, because there is only one space variable. In the case of harmonic oscillator in higher dimensions for instance spherical harmonic oscillator, the corrections on the Hamiltonian due to noncommutativity of space is given by:

\[ H_I = \frac{\partial V}{\partial x_i} \Delta x_i = -\frac{1}{2} \theta_{ij} \frac{\partial V}{\partial x_i} p_j \]  \hspace{1cm} (44)

where:

\[ V = \frac{1}{2} m \omega^2 \sum_{i=1}^3 x_i^2 \]  \hspace{1cm} (45)

We put \( \theta_3 = \theta \) and the rest of the \( \theta \) components to zero, which can be done by a rotation or by a redefinition of coordinates. So we have:

\[ H_I = -\frac{1}{2} \theta_{ij} (m \omega^2 x_i) p_j = \frac{1}{4} m \omega^2 \epsilon_{ijk} x_i p_j \theta_k = -\frac{1}{4} \bar{L} \cdot \bar{\theta} = \frac{1}{4} L_z \theta \]  \hspace{1cm} (46)

For a spherical harmonic oscillator the unperturbed(commutative) eigenfunctions are given by:

\[ \phi_{nlm}(r \theta \phi) \propto r^{\ell+1} e^{-\frac{\alpha r^2}{2}} L_n^{\frac{\ell+1}{2}} (\alpha r^2) Y_{\ell m}(\theta \phi) \]  \hspace{1cm} (47)

where \( L_n^{\frac{\ell+1}{2}} (\alpha r^2) \) are Laguerre’s functions. Using Eqs.(14) and (31), one can easily derive the energy eigenvalues in noncommutative space and so the density operator \( \hat{\rho} \) and the partition function \( \hat{Q}_N(\beta) = \sum_n e^{-\beta E_n} \). The thermodynamical properties of the system can be done straightforwardly using partition function.

We have:

\[ E_n^1 = \langle \phi_{nlm} | H_I | \phi_{nlm} \rangle = \frac{1}{4} m \theta \]  \hspace{1cm} (48)

So:

\[ \hat{Q}_N(\beta) = e^{-\frac{4}{m \theta} Q_N(\beta)} \]  \hspace{1cm} (49)

The Helmholtz free energy is given by:

\[ \hat{A} = \frac{k + \beta}{4} m \theta + A \]  \hspace{1cm} (50)

Whence we obtain:

\[ \hat{S} = -\frac{\partial \hat{A}}{\partial T} = \frac{k \beta}{4} m \theta + S \]  \hspace{1cm} (51)

\[ \hat{U} = \frac{k + \beta}{2} m \theta + U \]  \hspace{1cm} (52)
\[ \hat{C} = \frac{k\beta}{2} m\theta + C \]  

(53)

where \( \hat{S}, \hat{U} \) and \( \hat{C} \) are the entropy, the enternal energy and the specific heat of the system in noncommutative space and \( S, U \) and \( C \) are their counterpart in the commutative case.

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