Statistical mechanics of quasianti-Hermitian quaternionic systems.

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We study the statistical mechanics of quasianti-Hermitian quaternionic systems with constant number of particles in equilibrium. We show that the explicit knowledge of the metric operator is not necessary for study the thermodynamic properties of the system. We introduce a toy model where the physically relevant quantities are derived. We derive the energy fluctuation from which we observe that for large \( N \) the relative r.m.s fluctuation in the values of \( E \) is quite negligible. We also study the negative temperature for such systems. Finally two physical examples are discussed.

1 Introduction

Non-Hermitian Hamiltonians are currently an active field of research, motivated by the necessity to understand the mathematical properties of their subclasses, namely the pseudo-Hermitian and pseudoanti-Hermitian Hamiltonian. Also, to investigate the existence of a suitable similarity transformation that maps such Hamiltonians to an equivalent Hermitian form is important from a physical point of view. A consistent theory of quantum mechanics demands a certain inner product that ensures the associated norm to be positive definite. In this direction there have been efforts to look for non-Hermitian Hamiltonians which have a real spectrum such that the accompanying dynamics is unitary.

The interest in non-Hermitian Hamiltonians was stepped up by a conjecture of Bender and Boettcher [1] that PT-symmetric Hamiltonians could possess real bound-state eigenvalues. Subsequently, Mostafazadeh [2] showed that the concept of PT symmetry has its roots in the theory of pseudo-Hermitian operators. He pointed out that the reality of the spectrum is ensured [3] if the Hamiltonian \( H \) is Hermitian with respect to a positive-definite inner product \( \langle . , . \rangle_+ \) on the Hilbert space \( \mathcal{H} \) in which \( H \) is acting [4].

In the pseudo-Hermitian representation of quantum mechanics, a quantum system is determined by a triplet \((\mathcal{H}, H, \eta)\) where \( \mathcal{H} \) is an auxiliary Hilbert space,
$H : H \rightarrow H$ is a linear (Hamiltonian) operator with a real spectrum and a complete set of eigenvectors, and $\eta : H \rightarrow H$ is a linear, positive-definite, invertible (metric) operator fulfilling the pseudo-Hermiticity condition:

$$H^\dagger = \eta \eta^{-1}H\eta, \quad \eta_+ = \eta^\dagger_+ > 0$$

The condition that the metric must be positive definite (quasi Hermiticity) is necessary for compatibility of models with the postulates of quantum mechanics [5].

The physical Hilbert space $H_{phys}$ of the system is defined as the complete extension of the span of the eigenvectors of $H$ endowed with the inner product

$$<.,.>:=<.\mid \eta .>$$

where $<.,.>$ is the defining inner product of $H$, and the observables are identified with the self-adjoint operators acting in $H_{phys}$, alternatively $\eta$-pseudo-Hermitian operators acting in $H$, [3,6].

The foundations of quaternionic quantum mechanics (QQM) were laid by Finkelstein et al., in the 1960’s [7]. A systematic study of QQM is given in [8], which also contains an interesting list of open problems.

It is worth mentioning that while in both QQM and CQM (complex quantum mechanics) theories, observables are associated with self-adjoint (or Hermitian) operators, the Hamiltonians are Hermitian in CQM, but they are anti-Hermitian in QQM, and the same happens for the symmetry generators, like the angular momentum operators.

On the other hand as we mentioned earlier theoretical framework of CQM has been extended and generalized by introducing the pseudo-Hermitian operators. By the same motivation if one wishes to extend and generalize the theoretical framework of standard quaternionic Hamiltonians and symmetry generators, one needs to introduce and study the pseudo-anti-Hermitian quaternionic operators.

Moreover, the theory of open quantum systems can be obtained, in many relevant physical situations, as the complex projection of quaternionic closed quantum systems [9].

Experimental tests on QQM were proposed by Peres [10] and carried out by Kaiser et al. [11] searching for quaternionic effects manifested through non-commuting scattering phases when a particle crosses a pair of potential barriers. See also [12]. A review of the experimental status of QQM can be found in [13].

By definition a quaternionic linear operator $H$ is said to be ($\eta$-)pseudoanti-Hermitian if a linear invertible Hermitian operator $\eta$ exists such that $\eta H \eta^{-1} = -H^\dagger$. If $\eta$ is positive definite, $H$ is said quasianti-Hermitian.
2 pseudoanti-Hermitian quaternionic systems.

A quaternion is usually expressed as $q = q_0 + iq_1 + jq_2 + kq_3$ where $q_{0,1,2,3} \in \mathbb{R}$ and $i^2 = j^2 = k^2 = ijk = -1, ij = -ji = k$, and with an involutive anti-automorphism (conjugation) such that, $q \rightarrow \overline{q} = q_0 - iq_1 - jq_2 - kq_3$.

The density matrix $\rho_\psi$ associated with a pure state $\psi$ belonging to a quaternionic $n$-dimensional right Hilbert space $Q^n$ is defined by : $\rho_\psi = |\psi\rangle \langle \psi|$ and is the same for all normalized ray representatives[14].

Denoting by $Q^\dagger$ the adjoint of an operator $Q$ with respect to the pseudo-inner product $(.,.)_\eta = (\eta . .)$, (where $(.,.)$ represent the standard quaternionic inner product in the space $Q^n$). We have

$$Q^\dagger = \eta^{-1}Q^\dagger\eta$$

so that for any $\eta$-pseudo-Hermitian operator i.e., satisfying the relation

$$\eta Q \eta^{-1} = Q^\dagger$$

one has, $Q = Q^\dagger$. These operators constitute the physical observables of the system. If $Q$ is $\eta$-pseudo-Hermitian, Eq.(4) immediately implies that $\eta Q$ is Hermitian, so that the expectation value of $Q$ in the state $|\psi\rangle$ with respect to the pseudo-inner product $(.,.)_\eta = (\eta . .)$ can be obtained[14]:

$$<\psi | \eta Q | \psi > = ReTr(|\psi\rangle \langle \eta Q | \eta \rangle) = ReTr(\rho Q)$$

where $\rho = |\psi\rangle \langle \psi | \eta$.

More generally, if $\rho$ denotes a generic quaternionic (Hermitian, positive definite) density matrix, we can associate it with a generalized density matrix $\tilde{\rho}$ by means of a one-to-one mapping in the following way:

$$\tilde{\rho} = \rho \eta$$

and obtain $<Q >_\eta = ReTr(\tilde{\rho}Q)[14]$. Note that $\tilde{\rho}$ is $\eta$-pseudo-Hermitian:

$$\tilde{\rho}^\dagger = \eta \rho = \eta \tilde{\rho} \eta^{-1}$$

Let us then consider the space of quaternionic quasi-Hermitian density matrices, that is the subclass of $\eta$-pseudo-Hermitian density matrices with a positive $\eta$. Thus, an (Hermitian) operator $\Theta$ exists such that $\eta = \Theta^2$, and the $\eta$-pseudo-Hermitian density matrices are positive definite. Then the inner product $(.,.)_\eta = (\eta . .)$ introduced in the Hilbert space is positive and the usual requirements for a proper quantum measurement theory can be maintained.

The most general 2-dimensional complex positive $\eta$ operator is given by :

$$\eta = \Theta^2 = \begin{pmatrix} x^2 + |z|^2 & (x+y)z \\ (x+y)z^* & y^2 + |z|^2 \end{pmatrix}$$
where $x, y \in R$, $z \in C$ and $xy \neq |z|^2$ [14]. The choice of complex metric operators can be justified as follows: it is shown in [14] that the complex projections of time-dependent $\eta$-quasianti-Hermitian quaternionic Hamiltonian dynamics are complex stochastic dynamics in the space of complex quasi-Hermitian density matrices if and only if a quasistationarity condition is fulfilled, i.e., if and only if $\eta$ is an Hermitian positive time-independent complex operator.

Now let $H$ describes an ensemble of a huge but fixed number of independent particles. In what follows we study the statistical description of the system in equilibrium. The state of the system is characterized by a density matrix $\rho$ which can be written in energy representation as

$$\rho = \sum_n W_n |n\rangle\langle n|, \quad Tr\rho < \infty$$

(8)

In equilibrium, the density matrix operator is solution of Bloch equation:

$$\frac{\partial \rho}{\partial \beta} = -H\rho$$

(9)

with initial condition $\rho(0) = 1$ and $\beta = \frac{1}{kT}$, $k$ is the familiar Boltzmann constant. Its formal solution $\rho = e^{-\beta H}$ fixes the coefficients to be $W_n = \exp(-\beta E_n)$. Normalization factor of the density matrix depends on the inverse temperature $\beta$ and is called partition function.

$$Z = Tr\rho$$

(10)

It plays an important role in thermodynamics of the system because it allows direct computation of thermodynamic quantities.

Using the definition of the expectation value of an operator in quasianti-Hermitian picture i.e., Eq.(5) one can show that:

$$Z = \sum_n \langle n|\rho|n\rangle = \sum_n \langle \tilde{n}|\tilde{\rho}|\tilde{n}\rangle = \tilde{Z}$$

(11)

where $|\tilde{n}\rangle$, $\tilde{\rho}$ and $\tilde{Z}$ are energy eigenkets, density operator and partition function in quasianti-Hermitian quaternionic picture respectively. This means that the partition function is the same in both cases. So we can derive the thermodynamic properties of a physical system in equilibrium in pseudoanti-Hermitian quaternionic picture without explicit knowledge of the metric operator $\Theta$.

On the other hand Bloch equation (9) resembles Schrödinger equation for evolution operator in QQM. The link can be established by the substitution $\beta \rightarrow t$. Working in quasianti-Hermitian picture the equation (9) reads:

$$\frac{\partial \tilde{U}}{\partial t} = -\tilde{H}\tilde{U}. \quad \tilde{U}(0) = 1$$

(12)
where we defined $\tilde{U}(t) = \tilde{\rho}(t)$. In quasi-Hermitian picture. In x-representation, we have

$$\tilde{\rho}(x_1, x_2) \mid_{\beta=\tilde{t}} = \tilde{U}(x_1, x_2; t) = \langle x_1 \mid e^{-\tilde{H}t} \mid x_2 \rangle \equiv G(x_1, x_2; t). \quad (13)$$

the propagator (13) is of fundamental importance because it allows to compute partition function ($Z = \int G(x_1, x_2; -\beta)dx$) with use of standard techniques. The analogous equations in the case of pseudo-Hermitian Hamiltonian have been derived in [15].

3 Statistical mechanics of quasianti-Hermitian quaternionic systems. A Toy model.

We consider an ensemble of systems each consisting of $N$ distinguishable particles without mutual interaction. The partition function can be written as follows:

$$Z = (Z_1)^N \quad (14)$$

where $Z_1$ may be regarded as the partition function of a single particle in the system. In the quasianti-Hermitian quaternionic picture, the subsystem is described by the following most general Hamiltonian:

$$H = \begin{pmatrix} a & c \\ d & b \end{pmatrix}$$

Here $a, b$ and $c$ are three arbitrary quaternion. The requirement that the Hamiltonian be pseudoanti-Hermitian quaternionic with respect to $\eta$ i.e. $\eta H \eta^{-1} = -H^\dagger$ gives: $a^* = -a, b^* = -b$ and $d = -\frac{\alpha}{\gamma} c^*$, where $\eta$ is given by:

$$\eta = \Theta^2 = \begin{pmatrix} \alpha & 0 \\ 0 & \gamma \end{pmatrix}$$

where we have chosen $z = 0, x^2 = \alpha$ and $y^2 = \gamma$ in the matrix $\eta$ introduced in section 2. The energy levels of the system may depend on the external parameters e.g. on the volume in which the particle is confined. We shall find the partition function by solving the Eq.(12). By separating the Hamiltonian into its diagonal and non-diagonal part we have

$$H = H_0 + H' \quad (15)$$

where:

$$H_0 = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}, \quad H' = \begin{pmatrix} 0 & c \\ -\frac{\alpha}{\gamma} c^* & 0 \end{pmatrix}$$

5
Let us introduce the following transformation:

\[ U_0(t) = \exp(-H_0 t) \]  

we also define a new operator in the interaction picture as follows:

\[ U_I(t) = U_0^\dagger(t) U(t) U_0(t) \]  

Then Eq.(12) changes into the following form:

\[ \frac{\partial U_I}{\partial t} = -H'_I(t) U_I(t), \quad U_I(0) = 1 \]  

where \( H'_I(t) = U_0(t)^\dagger H' U_0(t) \). One can find the solution iteratively by integrating both sides of the equation.

\[ U_I(t) = 1 - \int_0^t dt' H_I(t') + \int_0^t dt' \int_0^{t'} dt'' H'_I(t') H'_I(t'') + ... \]  

where we have neglected the higher order terms, then we have:

\[ U_I(t) \sim \left( 1 + \frac{\alpha}{\gamma} \frac{c^2}{a-b} t - \frac{\alpha}{\gamma} \frac{c^2}{(a-b)^2} (e^{(a-b)t} - 1) \right. \]

\[ \left. - \frac{\beta}{\gamma} \frac{d}{a-b} (e^{-(a-b)t} - 1) \right) \frac{e^{-a\beta}}{1 - \frac{\alpha}{\gamma} \frac{c^2}{a-b} t - \frac{\alpha}{\gamma} \frac{c^2}{(a-b)^2} (e^{-(a-b)t} - 1)} \]  

The approximate value of the partition function is as follows:

\[ Z_1(\beta) = \text{Tr}(U_0(t) U_I(t)) |_{t \rightarrow \beta} \sim e^{-a\beta} + e^{-b\beta} - \frac{\alpha}{\gamma} \frac{c^2}{a-b} \beta (e^{-b\beta} - e^{-a\beta}) \]  

Now the calculation of the thermodynamic quantities is straightforward. For the Helmholtz free energy of the system we have:

\[ A = -NkT \ln Z_I = -\frac{N}{\beta} \ln Z_1 = -\frac{N}{\beta} \ln [e^{-a\beta} + e^{-b\beta} - \frac{\alpha}{\gamma} \frac{c^2}{a-b} \beta (e^{-b\beta} - e^{-a\beta})] \]  

The entropy of the system is:

\[ S = Nk \ln [e^{-a\beta} + e^{-b\beta} - \frac{\alpha}{\gamma} \frac{c^2}{a-b} \beta (e^{-b\beta} - e^{-a\beta})] + \frac{Nk\beta}{(a-b) + \frac{\alpha}{\gamma} c^2 \beta} e^{\beta b} + [b(a-b) + \frac{\alpha}{\gamma} c^2 - \frac{\alpha}{\gamma} c^2 \beta b] e^{\beta a} \]  

\[ \frac{[a(a-b) - \frac{\alpha}{\gamma} c^2 + \frac{\alpha}{\gamma} c^2 \beta a] e^{\beta b} + [b(a-b) + \frac{\alpha}{\gamma} c^2 - \frac{\alpha}{\gamma} c^2 \beta b] e^{\beta a}}{[(a-b) + \frac{\alpha}{\gamma} c^2 \beta] e^{\beta b} + [(a-b) - \frac{\alpha}{\gamma} c^2 \beta] e^{\beta a}} \]
The internal energy of the system is given by:

\[ U = N \frac{e^{\beta b}[a(b - b + \frac{\alpha}{\beta}c^2 \beta) - \frac{\alpha}{\beta}c^2] + e^{\beta a}[b(a - b - \frac{\alpha}{\beta}c^2 \beta) + \frac{\gamma}{\beta}b^2]}{e^{\beta b}[a - b + \frac{\alpha}{\beta}c^2 \beta] + e^{\beta a}[a - b - \frac{\alpha}{\beta}c^2 \beta]} \]  

(23)

The specific heat per particle \( C_V \) which describes how the temperature changes when the heat is absorbed while volume \( V \) of the system remains unchanged is given by:

\[ C_V = \frac{1}{N} \left( \frac{\partial U}{\partial \beta} \right)_V = -\frac{\beta^2 k}{N} \left( \frac{\partial U}{\partial \beta} \right) = \]

\[ \frac{\beta^2 k - e^{\beta(a+b)}\{(a-b)^2[(a-b)^2 - (\frac{\alpha}{\beta}c^2 \beta)^2 - 4(\frac{\gamma}{\beta}c^2)^2] + 2(\frac{\alpha}{\beta}c^2)^2[\gamma c^2 a^2 + e^{2\beta b}]\}}{N} \]

\[ \frac{\{e^{\beta b}[a - b + \frac{\alpha}{\beta}c^2 \beta] + e^{\beta a}[a - b - \frac{\alpha}{\beta}c^2 \beta]\}^2}{(24)} \]

The pressure of the system is as follows:

\[ P = -(\frac{\partial A}{\partial V})_\beta = N \frac{[-(a-b)^2a' - \frac{\alpha}{\beta}c^2(\beta(a-b) + 1)a' + \frac{\gamma}{\beta}c^2b' + 2\frac{\alpha}{\beta}c(a-b)c']}{[(a-b)^2 + \frac{\alpha}{\beta}c^2(b(a-b))e^{-a\beta}]} e^{-a\beta} + \]

\[ \frac{N}{[(a-b)^2 + \frac{\alpha}{\beta}c^2(a-b)]} e^{-a\beta} + [(a-b)^2 - \frac{\alpha}{\beta}c^2(a-b)] e^{-b\beta} \]

(25)

where the prime symbol represents the derivative with respect to the volume, \( a' = \frac{\partial a}{\partial V} \).

### 4 Energy fluctuation.

We first write down the expression for the mean energy:

\[ U = \langle E \rangle = \frac{\sum_r E_r g_r \exp(-\beta E_r)}{\sum_r g_r \exp(-\beta E_r)} \]  

(26)

where \( g_r \) is the multiplicity of a particular energy level \( E_r \). By differentiating the expression of the mean energy with respect to the parameter \( \beta \), we obtain:

\[ \frac{\partial U}{\partial \beta} = -\{\langle E^2 \rangle - \langle E \rangle^2\} \]  

(27)

whence it follows that:

\[ \langle (\Delta E)^2 \rangle = \langle E^2 \rangle - \langle E \rangle^2 = -\frac{\partial U}{\partial \beta} = kT^2 \left( \frac{\partial U}{\partial T} \right) = kT^2 C_V \]  

(28)
So, for the relative root-mean-square fluctuation in \( E \), we have:

\[
\frac{\sqrt{\langle (\Delta E)^2 \rangle}}{\langle E \rangle} = \frac{\sqrt{kT^2C_V}}{U} = \frac{1}{\sqrt{N}} \beta \sqrt{k f(a, b, c, \alpha, \beta, \gamma)} \propto \frac{1}{\sqrt{N}}
\]

(29)

where \( f(a, b, c, \alpha, \beta, \gamma) \) is the numerator of Eq.(24) and \( g(a, b, c, \alpha, \beta, \gamma) \) is the numerator of Eq.(23). As we observe it is \( O(N^{-\frac{1}{2}}) \), \( N \) being the number of particles in the system. Consequently, for large \( N \) (which is true for every statistical system), the relative r.m.s. fluctuation in the values of \( E \) is quite negligible. Thus for all practical purposes, a system in the canonical ensemble in pseudoanti-Hermitian quaternionic picture, has an energy equal to or almost equal to the mean energy \( U \); the situation is therefore practically the same as in the microcanonical ensemble.

5 Negative temperature.

Let us consider our system from the combinatorial point of view. The question then arises: in how many different ways, can our system attain a state of energy \( E \)? This can be tackled in precisely the same way as the problem of the random walk. Let \( N_+ \) be the number of particles with energy \( E_+ \) and \( N_- \) with energy \( E_- \); then

\[
E = E_+ N_+ + E_- N_-, \quad N = N_+ + N_-
\]

(30)

Solving for \( N_+ \) and \( N_- \), we obtain:

\[
N_+ = \frac{E - NE_-}{E_+ - E_-}, \quad N_- = \frac{E - NE_+}{E_+ - E_-}
\]

(31)

The desired number of ways is then given by the expression:

\[
\Omega(N, E) = \frac{N!}{N_+!N_-!} = \frac{N!}{(E-NE_+)/(E_+ - E_-)}(E-NE_-)/(E_+ - E_-)
\]

(32)

whence we obtain for the entropy of the system:

\[
S(N, E) = k \ln \Omega \approx
\]

\[
k[N \ln N - \frac{E - NE_+}{E_+ - E_-} \ln\left(\frac{E - NE_+}{E_+ - E_-}\right) - \frac{E - NE_-}{E_+ - E_-} \ln\left(\frac{E - NE_-}{E_+ - E_-}\right)]
\]

(33)

The temperature of the system is then given by:

\[
\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_N = \frac{k}{E_+ - E_-} \ln\left(-\frac{E - NE_-}{E - NE_+}\right)
\]

(34)

from Eq.34, we note that so long as \( E < \frac{N}{2}(E_+ + E_-) \), \( T > 0 \). However the same equation tells us that if \( E > \frac{N}{2}(E_+ + E_-) \), then \( T < 0 \). Let us examine the matter
a little more closely. For this purpose we consider as well the variation of the entropy $S$ with the energy $E$. We note that for $E = NE_-$, both $S$ and $T$ vanish. As $E$ increase, they too increase until we reach the special situation where $E = \frac{N}{2}(E_+ + E_-)$. The entropy is then seen to have attained its maximum value $S = Nk\ln 2$, while the temperature has reached an infinite value. Throughout this range, the entropy was a monotonically increasing function of energy, so $T$ was positive. Now as $E$ equals $\frac{N}{2}(E_+ + E_-)$, $(\frac{dS}{dE})$ becomes $0-$ and $T$ becomes $-\infty$. With a further increase in the value of $E$, the entropy monotonically decreases; as a result, the temperature continues to be negative, though its magnitude steadaying decreases. Finally, we reach the largest value of $E$, namely $NE_+$, where the entropy is once again zero and $T = -0$.

6 Physical examples.

6.1 A spin one half system in a constant quasianti-Hermitian quaternionic potential.

We now consider a two-level quantum system with a quasianti-Hermitian quaternionic Hamiltonian $H = H_\alpha + jH_\beta$. $H_\alpha$ denotes the free complex anti-Hermitian Hamiltonian describing a spin half particle in a constant magnetic field[14].

$$H_\alpha = \frac{\omega}{2} \left( \begin{array}{cc} i & 0 \\ 0 & -i \end{array} \right)$$

and $jH_\beta$ is a purely quasianti-Hermitian quaternionic constant potential :

$$jH_\beta = \left( \begin{array}{cc} 0 & j\frac{x}{v} \\ j\frac{x}{v} & 0 \end{array} \right)$$

$v, x \neq 0 \in \mathbb{R}$.

We note that $H = H_\alpha + jH_\beta$ is $\eta'$-quasianti-Hermitian quaternionic i.e., $
\eta' H \eta'^{-1} = -H^\dagger$, where :

$$\eta' = \left( \begin{array}{cc} x^2 & 0 \\ 0 & 1 \end{array} \right)$$

The eigenvalues and the corresponding biorthonormal eigenbasis of the quaternionic Hamiltonian $H$ are[16]:
\[ iE_{\pm} = i(\frac{\omega}{2} \pm v) \]  

and:

\[ |\psi_{\pm}\rangle = \left( \frac{\pm i}{j} \right) \frac{1}{\sqrt{2}}, \quad |\phi_{\pm}\rangle = \left( \frac{\pm xi}{j} \right) \frac{1}{\sqrt{2}} \]

We note that the metric \( \eta' \) is a special case of our metric and can be obtained by substituting \( \alpha = x^2 \) and \( \gamma = 1 \). We also note that the Hamiltonian \( H \) is a special case of our general Hamiltonian and can be obtained by substituting \( a = i \frac{\omega}{2}, b = -i \frac{\omega}{2}, c = j \frac{v}{2} \) and \( d = -\frac{\omega}{2} c^* \). So the thermodynamic properties of this system can be obtained straightforwardly from equations (21-25), for instance we have:

\[
S = Nk \ln[2(\cosh \frac{\omega}{2} - \frac{v^2}{2} \sinh \frac{\omega}{2})]
+ Nk\beta \omega^2 \sin \frac{\omega}{2} \tan \frac{\omega}{2} + 2v^2 \sinh \frac{\omega}{2} \tan \frac{\omega}{2}
\]

\[
U = N \omega^2 \sin \frac{\omega}{2} \tan \frac{\omega}{2} + 2v^2 \sinh \frac{\omega}{2} \tan \frac{\omega}{2} \]

(36) \hspace{2cm} (37)

Moreover the negative temperature discussed in previous section is applicable to this system which we study now.

Let \( N_+ \) be the number of particles with energy \( E_+ = \frac{\omega}{2} + v \) and \( N_- \) with energy \( E_- = \frac{\omega}{2} - v \), then we have:

\[ E = E_+ N_+ + E_- N_-, \quad N = N_+ + N_- \]  

(38)

The number of ways this system can attain a state of energy \( E \) is given by:

\[
\Omega(N, E) = \frac{N!}{N_+!N_-!} = \frac{N!}{(-\frac{E - N(\frac{\omega}{2} + v)}{2v})!(\frac{E - N(\frac{\omega}{2} - v)}{2v})!} \]

(39)

whence we obtain for the entropy of the system:

\[
S(N, E) = k \ln \Omega \approx
k[N \ln N + \frac{E - N(\frac{\omega}{2} + v)}{2v} \ln(-\frac{E - N(\frac{\omega}{2} + v)}{2v}) - \frac{E - N(\frac{\omega}{2} - v)}{2v} \ln(\frac{E - N(\frac{\omega}{2} - v)}{2v})]
\]

(40)

The temperature of the system is then given by:

\[
\frac{1}{T} = \left( \frac{\partial S}{\partial E} \right)_N = -\frac{k}{2v} \ln(-\frac{E - N(\frac{\omega}{2} - v)}{E - N(\frac{\omega}{2} + v)}) \]

(41)
We note that so long as \( E < \frac{N}{2} \omega \), \( T > 0 \). However if \( E > \frac{N}{2} \omega \), then \( T < 0 \).

Now we consider as well the variation of the entropy \( S \) with the energy \( E \). We note that for \( E = N ( \frac{v}{2} - \nu ) \), both \( S \) and \( T \) vanish. As \( E \) increase, they too increase until we reach the special situation where \( E = \frac{N}{2} \omega \). The entropy is then seen to have attained its maximum value \( S = N k \ln 2 \), while the temperature has reached an infinite value. Throughout this range, the entropy was a monotonically increasing function of energy,so \( T \) was positive. Now as \( E \) equals \( \left[ \frac{N}{2} \omega \right] + \), \( \left( \frac{\delta S}{\delta E} \right) \) becomes \( 0^- \) and \( T \) becomes \( -\infty \). With a further increase in the value of \( E \), the entropy monotonically decreases; as a result, the temperature continues to be negative, though its magnitude steadly decreases. Finally, we reach the largest value of \( E \), namely \( N ( \frac{v}{2} + \nu ) \), where the entropy is once again zero and \( T = -0 \).

As we mentioned earlier the physical system is a spin half particle in the quaternionic potential. How to produce in laboratory quaternionic potentials has been investigated by Peres, McKellar, Brumby and others [10,11,12,17,18]. This system is the quasianti-Hermitian quaternionic analogue of the ordinary(Hermitian) magnetic system i.e., a system composed of spin half particles in a constant magnetic field which is a famous system showing negative temperature discussed in the text books, see e.g.,[20]. Each dipole has a choise of two energy \( E_- = -\mu H \) and \( E_+ = +\mu H \).

### 6.2 Optimal entanglement generation.

The next system we will study is composed of two C qubits A and B, parametrized by the Bloch vectors \( \vec{a} \equiv (a_1, a_2, a_3) \) and \( \vec{b} \equiv (b_1, b_2, b_3) \), respectively. The most general Hamiltonian for two qubits (in the interaction picture) can be written as:

\[
H = \sum_i \zeta_i \sigma_i^A \otimes \sigma_i^B \tag{42}
\]

where the parameters \( \zeta_1, \zeta_2 \) and \( \zeta_3 \) are constant if there is no free evolution for individual qubits. Assume now we have initially two complex pure states, with Bloch vectors \( \vec{a} \equiv (1, 0, 0) \) and \( \vec{b} \equiv (0, 1, 0) \), respectively. We also assume some interaction associated with the following parameters :

\[
\zeta_3 = 1, \zeta_1 = \zeta_2 = 0 \tag{43}
\]

It is shown in [19] that the corresponding anti-Hermitian quaternionic Hamiltonian has the following form:

\[
H(t) = \begin{pmatrix}
-2je^{-i\phi} & 0 \\
0 & 0
\end{pmatrix}, \phi \in R
\]
It is easy to check that the Hamiltonian is anti-Hermitian quaternionic with respect to $\eta$ given in section 3.

Again we note that this Hamiltonian is a special case of our general Hamiltonian and can be obtained by substituting $a = \frac{\sqrt{2}j e^{-i\phi}}{e^{\frac{i\phi}{2}}} = b = 0$ and $c = 0$, so its thermodynamic properties can be obtained from equations (21-25) by substitution the values of $a, b$ and $c$.

We know that any two-level system can be used as a qubit. Several physical implementations which approximate two-level systems to various degrees were successfully realized. The following are three examples of physical implementations of qubits (the choices of basis are by convention only).

1). Optical lattices (Atomic spin), $|0\rangle$: up; $|1\rangle$: down.
2). Josephson junction (Superconducting charge qubit), $|0\rangle$: Uncharged superconducting island ($Q=0$); $|1\rangle$: Charged superconducting island ($Q=2e$, one extra Cooper pair).
3). Quantum dot (Dot spin), $|0\rangle$: up; $|1\rangle$: down.

7 Conclusion.

We have studied the statistical mechanics of quasianti-Hermitian quaternionic systems in equilibrium in the framework of canonical ensemble. We derive all the physically relevant quantities without explicit calculation of the metric operator or the spectrum of the Hamiltonian. We derive the energy fluctuation from which we observe that for large $N$, the relative r.m.s fluctuation in the values of $E$ is quite negligible. We also study the negative temperature for such systems. Two physical examples are discussed.

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