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Quantum systems at negative temperatures: a holomorphic approach based on coherent states

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Abstract. A quantum statistical formalism which accommodates both positive and negative temperatures is studied. The Dirac contour representation is used to extend the harmonic oscillator Hilbert space into a larger space which is suitable for the description of quantum systems at both positive and negative temperatures. The analytic continuation of various physical quantities into the negative temperature region is examined in detail. The formalism can be useful for the description of systems which are excited to higher states, and which decay into the lower states.

1. Introduction

The concept of negative temperatures has been known for a long time [1]. It is an interesting concept in itself, and it can also be useful in the description of systems that are excited to higher states and whose decay into the lower states is described through the negative temperature formalism. It is thus related to Glauber's inverted oscillator [2] which also describes such systems.

Although there has been a lot of work on the concept of negative temperatures in the context of classical thermodynamics, it has never really been properly introduced into quantum statistical mechanics. In a recent publication [3] we have pursued this idea. We have shown that a contour representation introduced by Dirac [4] extends rather naturally into a generalized contour representation that accomodates both the positive and negative temperature Hilbert spaces. It is the purpose of this paper to expand considerably our previous work and also to present the technical details associated with it.

In section 2 we discuss the Dirac contour representation at positive temperatures. Holomorphic representations have been used extensively in various areas of physics. They exploit the powerful theory of analytic functions in a quantum context. Examples include the Bargmann representation [5], other analytic representations in the context of coherent states [6–9] and in many-body theory [10], and conformal field theories (see e.g. [11]), etc. In this section we discuss the Dirac contour representation and its relationship to the more familiar representation of Bargmann. The results are interesting in their own right, regardless of the application to negative temperatures that we discuss later. For example, a similar formalism (at positive temperatures) has been used in [9] in an applied quantum optics context.

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In section 3 we extend the contour formalism so that we can describe both positive and negative temperatures. We define explicitly the Hilbert spaces associated with positive and negative temperatures and define creation and annihilation operators, number eigenstates, coherent states, etc. We thus provide a solid foundation for the description of quantum systems at negative temperatures. Although almost every textbook on thermodynamics introduces the concept of negative temperature, the foundations for a quantum formalism at negative temperatures (i.e. an explicit description of the Hilbert space, creation and annihilation operators at negative temperatures and their relation to their counterparts at positive temperatures, etc) have hitherto been missing. This is precisely the aim of section 3.

In section 4 we expand further these ideas. We study the harmonic oscillator formalism in the enlarged Hilbert space $\mathcal{H}_p \oplus \mathcal{H}_n$ that accomodates both positive and negative temperatures. We introduce the temperature reversal operator and explore deep connections between the positive and negative temperature parts of various operators and states. In particular we consider displacement operators and coherent states and show how the positive temperature parts are related to the negative temperature parts through analytic continuation.

We conclude in section 5 with a discussion of our results.

2. The Hilbert space $\mathcal{H}_p$ in the Dirac contour representation

Let $\mathcal{H}_p$ be the usual harmonic oscillator Hilbert space and $|N; p\rangle$ the number eigenstates,

$$\langle N; p|M; p\rangle = \delta_{NM} \tag{1}$$

$$\sum_{N=0}^{\infty} |N; p\rangle\langle N; p| = \mathbf{1}_p. \tag{2}$$

The index p (for positive temperatures) is used in conjuction with the usual notation in order to distinguish the states and operators associated with the Hilbert space $\mathcal{H}_p$ which are studied in this section, from their negative-temperature counterparts denoted with the index n which are associated with the Hilbert space $\mathcal{H}_n$ and which are studied in the next section. Let a_p and $a_p^\dagger$ be the usual annihilation and creation operators, respectively,

$$a_p|N; p\rangle = N^{1/2}|N-1; p\rangle \tag{3}$$

$$a_p^\dagger|N; p\rangle = (N+1)^{1/2}|N+1; p\rangle. \tag{4}$$

In the Dirac contour representation [4] of $\mathcal{H}_p$, the normalized eigenkets and eigenbras of the number operator $a_p^\dagger a_p$ are respectively represented as

$$|N; p\rangle \to (N!)^{-1/2} z^n \qquad \langle N; p| \to (N!)^{1/2} z^{-N-1} \tag{5}$$

where $N = 0, 1, 2, \ldots$. More generally, arbitrary normalized states in $\mathcal{H}_p$,

$$|f; p\rangle = \sum_N f_N |N; p\rangle \qquad \langle f; p| = \sum_N f_N^* \langle N; p| \qquad \sum_N |f_N|^2 = 1 \tag{6}$$

where, here and henceforth, all oscillator sums run from zero to infinity, are represented as

$$|f; p\rangle \to \sum_N f_N (N!)^{-1/2} z^N \equiv f_k^p(z) \tag{7}$$

$$\langle f; p| \to \sum_N f_N^* (N!)^{1/2} z^{-N-1} \equiv f_b^p(z) \tag{8}$$

where the indices k and b refer to ket and bra, respectively. The function $f_k^p(z)$ is a holomorphic function in the complex plane. In fact it is the same as the Bargmann representation of $|f; p\rangle$ which is known to be an analytic function of order $\rho \leqslant 2$ (and of type $\sigma \leqslant \frac{1}{2}$ if $\rho = 2$). The function $f_b^p(z)$ is the Borel transform of $f_k^p(z)$ and is clearly non-analytic.

Using the relation,

$$\oint_{C'} \frac{\mathrm{d}z}{2\pi \mathrm{i}} \frac{\exp(\zeta^* z)}{z^{N+1}} = \frac{(\zeta^*)^N}{N!} \tag{9}$$

where C' is an anticlockwise contour enclosing the origin, we prove the 'generalized Fourier transform' relation between $f_b^p(z)$ and $f_k^p(z)$,

$$\oint_C \frac{\mathrm{d}z}{2\pi \mathrm{i}} f_b^p(z) \exp(\zeta^* z) = [f_k^p(\zeta)]^* \tag{10}$$

under conditions of convergence which need to be specified on an individual basis, but which generally amount to the anticlockwise contour C enclosing the singularities of $f_b^p(z)$. The inverse formula is given by the Laplace transform,

$$f_b^p(z) = \frac{1}{z} \int_0^\infty \mathrm{d}t \, \mathrm{e}^{-t} \left[f_k^p \left(\frac{t}{z^*} \right) \right]^*. \tag{11}$$

In order to prove this we start from equation (7) which we rewrite as

$$f_k^p \left(\frac{t}{z^*} \right) = \sum_N f_N (N!)^{-1/2} \left(\frac{t}{z^*} \right)^N \tag{12}$$

where t is a real number. We then multiply both sides by e^{-t} and integrate for t taking values from 0 to ∞. Using the fact that

$$\int_0^\infty \mathrm{d}t \, \mathrm{e}^{-t} t^N = N! \tag{13}$$

we prove equation (11). The transformation (11) is of course known to be the inverse of equation (10) and here we gave an explicit proof in our own context. The scalar product of two states $|f; p\rangle$ and $|g; p\rangle$ is given by

$$\langle f; p | g; p \rangle = \oint_C \frac{\mathrm{d}z}{2\pi \mathrm{i}} f_b^p(z) g_k^p(z) = \sum_{N=0}^{\infty} f_N^* g_N. \tag{14}$$

As an example we consider the coherent state $|A; p\rangle$:

$$|A; p\rangle \to \exp(-\tfrac{1}{2}|A|^2 + Az) \tag{15}$$

$$\langle A; p| \to \exp(-\tfrac{1}{2}|A|^2)(z - A^*)^{-1} \qquad |z| > |A|. \tag{16}$$

We observe that the bra-state representation is valid only for $|z| > |A|$, an effect of which is that in contour integrations involving this state, such as those in equations (10) and (14), the point A must lie inside the contour C.

We next study the relationship between the Dirac contour representation and the more familiar Bargmann representation [5], in which the normalizable ket state $|f; p\rangle$ is also represented by the holomorphic function $f_k^p(z)$ but where its corresponding adjoint bra state $\langle f; p|$ is represented by the complex conjugate function $[f_k^p(z)]^*$. By inserting into equation (14) the relation,

$$g_k^p(z) = \int \frac{\mathrm{d}^2\zeta}{\pi} \exp(\zeta^* z - |\zeta|^2) g_k^p(\zeta) \tag{17}$$

which is valid for all holomorphic functions $g_k^p(z)$, and by making use of equation (10), we readily derive the alternative relation,

$$\langle f; p | g; p \rangle = \int \frac{\mathrm{d}^2\zeta}{\pi} \mathrm{e}^{-|\zeta|^2} [f_k^p(\zeta)]^* g_k^p(\zeta) \tag{18}$$

which is the usual relation for the inner product in the Bargmann representation.

An arbitrary operator Θ_p

$$\Theta_p \equiv \sum_{M,N=0}^{\infty} \Theta_{MN} |M;\, p\rangle\langle N;\, p| \tag{19}$$

is represented by the function

$$\Theta_p(z_1, z_2) = \sum_{M,N=0}^{\infty} \Theta_{MN} \left(\frac{N!}{M!}\right)^{1/2} \frac{z_1^M}{z_2^{N+1}}. \tag{20}$$

Its trace is given by the formula,

$$\begin{aligned}\operatorname{Tr}\Theta_p \equiv \sum_N \Theta_{NN} &= \sum_N \oint_{C_1}\oint_{C_2} \frac{\mathrm{d}z_1\,\mathrm{d}z_2}{(2\pi\mathrm{i})^2}\Theta_p(z_1, z_2)\frac{z_2^N}{z_1^{N+1}} \\ &= -\frac{1}{4\pi^2}\oint_{C_1}\oint_{C_2}\frac{\mathrm{d}z_1\,\mathrm{d}z_2}{z_1 - z_2}\Theta_p(z_1, z_2) \qquad C_2 < C_1\end{aligned} \tag{21}$$

where the integrations over z_1 and z_2 run anticlockwise around the contours C_1 and C_2 respectively, which encircle the origin. The summation over N converges to the quoted result if and only if $|z_1| > |z_2|$. This implies that the ring of the contour C_2 (defined as $r_{\min} \leqslant |z| \leqslant r_{\max}$, where $r_{\min}$ and $r_{\max}$ are the minimum and maximum distances respectively from the origin to points on the contour) lies wholly inside the ring of the contour C_1. This condition is denoted symbolically by $C_2 < C_1$. One may also readily check that formally we have that the mode of action of Θ_p on an arbitrary ket state $|g;\, p\rangle$ has the Dirac contour representation,

$$\Theta_p|g;\, p\rangle \to \oint_C \frac{\mathrm{d}z'}{2\pi\mathrm{i}}\Theta_p(z, z')g_k^p(z') \tag{22}$$

with a similar representation for $\langle f;\, p|\Theta_p$,

$$\langle f;\, p|\Theta_p \to \oint_C \frac{\mathrm{d}z'}{2\pi\mathrm{i}} f_b^p(z')\Theta_p(z', z). \tag{23}$$

Similarly, if $\Theta_{1;p}$ and $\Theta_{2;p}$ are two operators in $\mathcal{H}_p$ represented by the functions $\Theta_{1;p}(z_1, z_2)$ and $\Theta_{2;p}(z_1, z_2)$ respectively, it is easy to show that their product takes the form of a generalized convolution,

$$\Theta_{1;p}\Theta_{2;p} \to \oint_C \frac{\mathrm{d}z}{2\pi\mathrm{i}}\Theta_{1;p}(z_1, z)\Theta_{2;p}(z, z_2). \tag{24}$$

As examples we now consider the representations of the operators $\mathbf{1}_p$, a_p, $a_p^\dagger$, and $a_p^\dagger a_p$. For the unit operator $\mathbf{1}_p$, $\Theta_{MN} = \delta_{M,N}$ and equation (20) converges to $(z_2 - z_1)^{-1}$ when $|z_1| < |z_2|$. For $|z_1| \geqslant |z_2|$ the sum diverges. However, the latter case implies, for example, that the point z in equation (22) lies outside the contour C, and hence that the result is zero. In this sense we are, therefore, justified to say that for $|z_1| > |z_2|$, the Dirac contour representation of $\mathbf{1}_p$ is zero. We write accordingly,

$$\mathbf{1}_p \to (z_2 - z_1)^{-1}\theta(|z_2| - |z_1|) \tag{25}$$

where $\theta(x)$ is the unit step function; $\theta(x) \equiv 1$ for $x > 0$, and $\theta(x) \equiv 0$ for $x \leqslant 0$. Similarly we prove:

$$a_p \to (z_2 - z_1)^{-2}\theta(|z_2| - |z_1|) \tag{26}$$

$$a_p^\dagger \to z_1(z_2 - z_1)^{-1}\theta(|z_2| - |z_1|) \tag{27}$$

$$a_p^\dagger a_p \to z_1(z_2 - z_1)^{-2}\theta(|z_2| - |z_1|). \tag{28}$$

More generally we show that the following representations hold for arbitrary (integral) powers of the creation and destruction operators,

$$(a_p^\dagger)^M \to z_1^M (z_2 - z_1)^{-1}\theta(|z_2| - |z_1|) \tag{29}$$

$$(a_p)^N \to N!(z_2 - z_1)^{-N-1}\theta(|z_2| - |z_1|). \tag{30}$$

Use of equation (24) also yields the relations for normal-ordered and antinormal-ordered products,

$$(a_p^\dagger)^M (a_p)^N \to N! z_1^M (z_2 - z_1)^{-N-1}\theta(|z_2| - |z_1|) \tag{31}$$

$$(a_p)^N (a_p^\dagger)^M \to \left[\left(\frac{\mathrm{d}}{\mathrm{d}z_1}\right)^N \frac{z_1^M}{z_2 - z_1}\right]\theta(|z_2| - |z_1|). \tag{32}$$

The further use of equation (22) then also shows that,

$$(a_p^\dagger)^M (a_p)^N |g;\, p\rangle \to z^M \left(\frac{\mathrm{d}}{\mathrm{d}z}\right)^N g_k^p(z) \tag{33}$$

$$(a_p)^N (a_p^\dagger)^M |g;\, p\rangle \to \left(\frac{\mathrm{d}}{\mathrm{d}z}\right)^N z^M g_k^p(z). \tag{34}$$

It is seen that action of the operators $a_p^\dagger$ and a_p on ket states $|g;\, p\rangle$ within $\mathcal{H}_p$ is equivalent to multiplication by z and differentiation with respect to z, respectively, of the holomorphic function $g_k^p(z)$, i.e.

$$a_p^\dagger \to z \tag{35}$$

$$a_p \to \mathrm{d}/\mathrm{d}z \tag{36}$$

just as in the usual Bargmann representation. However, it is important to realize that the mode of action of $a_p^\dagger$ and a_p with respect to the bra states $\langle f;\, p|$ in terms of the corresponding *non-analytic* functions $f_b^p(z)$ cannot be so simply expressed.

In order to exemplify the use of the above formalism we now prove that the eigenkets of the number operators are indeed the number eigenstates:

$$\frac{1}{2\pi \mathrm{i}}\oint_C \frac{z_1}{(z_1 - z_2)^2} z_2^N (N!)^{-1/2}\,\mathrm{d}z_2 = N z_1^N (N!)^{-1/2}. \tag{37}$$

We also prove that the eigenkets of the annihilation operator are indeed the coherent states:

$$\frac{1}{2\pi \mathrm{i}}\oint_C (z_1 - z_2)^{-2} \exp[-\tfrac{1}{2}|A|^2 + A z_2]\,\mathrm{d}z_2 = A \exp[-\tfrac{1}{2}|A|^2 + A z_1]. \tag{38}$$

We also consider the thermal density operator in $\mathcal{H}_p$,

$$\rho_p^{\mathrm{th}}(\beta) \equiv (1 - \mathrm{e}^{-\beta}) \exp(-\beta a_p^\dagger a_p) \qquad \beta \geqslant 0. \tag{39}$$

Its Dirac contour representation is

$$\rho_p^{\mathrm{th}}(\beta; z_1, z_2) = \frac{1 - \mathrm{e}^{-\beta}}{z_2 - \mathrm{e}^{-\beta} z_1}\theta(|z_2| - \mathrm{e}^{-\beta}|z_1|). \tag{40}$$

For later purposes we also consider the 'entropy operator':

$$V_p(\beta_p) \equiv \rho_p^{\mathrm{th}} \ln \rho_p^{\mathrm{th}} = \sum_{N=0}^{\infty} (1 - \mathrm{e}^{-\beta_p})\mathrm{e}^{-N\beta_p}[-N\beta_p + \ln(1 - \mathrm{e}^{-\beta_p})]|N;\, p\rangle\langle N;\, p|. \tag{41}$$

The trace of this operator with a minus sign, is the von Neumann entropy of the thermal density matrix. In the Dirac contour representation V_p is represented by the function:

$$V_p(\beta_p; z_1, z_2) = (1 - e^{-\beta_p}) \left[-\frac{\beta_p z_1 e^{-\beta_p}}{[z_2 - z_1 e^{-\beta_p}]^2} + \frac{\ln(1 - e^{-\beta_p})}{z_2 - z_1 e^{-\beta_p}} \right] \theta(|z_2| - e^{-\beta_p}|z_1|). \tag{42}$$

We next consider squeezed states defined as

$$|A; r, \theta\rangle = S(r, \theta)|A\rangle \tag{43}$$

$$S(r, \theta) = \exp[-\tfrac{1}{4} r e^{-i\theta} (a^\dagger)^2 + \tfrac{1}{4} r e^{i\theta} a^2] \tag{44}$$

where $S(r, \theta)$ is the squeezing operator. It is easy to show that

$$\langle z^* | A; r, \theta\rangle = (1 - |\sigma|^2)^{1/4} \exp[\alpha z^2 + \beta z + \gamma - \tfrac{1}{2}|z|^2] \tag{45}$$

$$\sigma = -\tanh(\tfrac{1}{2} r) e^{-i\theta} \tag{46}$$

$$\alpha = \tfrac{1}{2}\sigma \tag{47}$$

$$\beta = A(1 - |\sigma|^2)^{1/2} \tag{48}$$

$$\gamma = -\tfrac{1}{2}\sigma^* A^2 - \tfrac{1}{2}|A|^2. \tag{49}$$

We can now evaluate $f_k^p(z)$:

$$f_k^p(z) = (1 - |\sigma|^2)^{1/4} \exp[\alpha z^2 + \beta z + \gamma] \tag{50}$$

and use equation (11) (in conjunction with equation (3.322.2) of [12]) to get

$$\begin{aligned} f_b^p(z) = {} & i \left(\frac{\pi}{2\sigma^*} \right)^{1/2} (1 - |\sigma|^2)^{1/4} \exp\left[-\frac{1}{2}|A|^2 - \frac{1}{2\sigma^*}(A^*)^2 + \frac{A^*}{\sigma^*} z (1 - |\sigma|^2)^{1/2} - \frac{z^2}{2\sigma^*} \right] \\ & \times \left\{ 1 - \Phi\left[\frac{i A^* (1 - |\sigma|^2)^{1/2}}{(2\sigma^*)^{1/2}} \right] \right\} \end{aligned} \tag{51}$$

where Φ is the error function. This result is valid for $\Re(-\frac{z^2}{2\sigma^*}) > 0$.

3. The Hilbert space $\mathcal{H}_n$ and its synthesis with the Hilbert space $\mathcal{H}_p$

In section 2 we used functions of the type (7) for the bra representations of states and functions of the type (6) for the ket representations. Of course, it could be the other way around, i.e. we could equally well use functions of the type (6) for the bra representations and functions of the type (7) for the ket representations. We present this in this section and get another Hilbert space $\mathcal{H}_n$ which by itself is the same as $\mathcal{H}_p$ and has no novel features; however, in conjuction with $\mathcal{H}_p$ it has several novel properties which will lead to its interpretation as the Hilbert space for the harmonic oscillator at negative temperatures.

The Hilbert space $\mathcal{H}_n$ is spanned by the number eigenstates $|N; n\rangle$ which obey relations analogous to equations (1) and (2) with the index p replaced by n. The annihilation and creation operators a_n and $a_n^\dagger$ obey relations analogous to equations (3) and (4). In the Dirac contour representation the number eigenstates in $\mathcal{H}_n$ are represented as:

$$|N; n\rangle \to (N!)^{1/2} z^{-N-1} \qquad \langle N; n| \to (N!)^{-1/2} z^N. \tag{52}$$

Arbitrary states $|f; n\rangle$ and $\langle f; n|$ in $\mathcal{H}_n$ have analogous expansions to that in equation (6) for $\mathcal{H}_p$, and have the corresponding Dirac contour representations,

$$|f; n\rangle \to \sum_N f_N (N!)^{1/2} z^{-N-1} \equiv f_k^n(z) \tag{53}$$

$$\langle f; n| \to \sum_N f_N^* (N!)^{-1/2} z^N \equiv f_b^n(z). \tag{54}$$

The scalar product is given by equation (14). It is clear that the overlap of any state in $\mathcal{H}_n$ with any state in $\mathcal{H}_p$ is identically zero.

We next consider general operators in $\mathcal{H}_p \oplus \mathcal{H}_n$,

$$\Theta \equiv \sum_{M,N} A_{MN}|M;\,p\rangle\langle N;\,p| + \sum_{M,N} B_{MN}|M;\,n\rangle\langle N;\,p| + \sum_{M,N} C_{MN}|M;\,p\rangle\langle N;\,n| + \sum_{M,N} D_{MN}|M;\,n\rangle\langle N;\,n|. \tag{55}$$

They are represented by the function

$$\Theta(z_1,z_2) = \sum_{M,N} A_{MN}\left(\frac{N!}{M!}\right)^{1/2}\frac{z_1^M}{z_2^{N+1}} + \sum_{M,N} B_{MN}\frac{(M!N!)^{1/2}}{z_1^{M+1}z_2^{N+1}} + \sum_{M,N} C_{MN}\frac{z_1^M z_2^N}{(M!N!))^{1/2}} + \sum_{M,N} D_{MN}\left(\frac{M!}{N!}\right)^{1/2}\frac{z_2^N}{z_1^{M+1}}. \tag{56}$$

The analogues of equations (25)–(28) are,

$$\mathbf{1}_n \to (z_1-z_2)^{-1}\theta(|z_1|-|z_2|) \tag{57}$$

$$a_n \to z_2(z_1-z_2)^{-1}\theta(|z_1|-|z_2|) \tag{58}$$

$$a_n^\dagger \to (z_1-z_2)^{-2}\theta(|z_1|-|z_2|) \tag{59}$$

$$a_n^\dagger a_n \to z_2(z_1-z_2)^{-2}\theta(|z_1|-|z_2|). \tag{60}$$

Comparison of equations (25), (26) and (28) with (57), (59) and (60) shows,

$$J \equiv \mathbf{1}_p - \mathbf{1}_n \to (z_2-z_1)^{-1} \tag{61}$$

$$a \equiv a_p + a_n^\dagger \to (z_2-z_1)^{-2} \tag{62}$$

$$a_p^\dagger a_p + a_n a_n^\dagger \to z_1(z_2-z_1)^{-2}. \tag{63}$$

In order to analytically continue the operator $a_p^\dagger$ of equation (27) with the operator a_n of equation (58) we need to introduce first an 'extended' destruction operator $\tilde{a}_n$,

$$\tilde{a}_n \equiv a_n + |0;\,p\rangle\langle 0;\,n|. \tag{64}$$

Using equations (56) and (58) we see that the operator $\tilde{a}_n$ is represented by the function:

$$\tilde{a}_n \to z_1\,(z_1-z_2)^{-1}\,\theta\,(|z_1|-|z_2|) \tag{65}$$

and combining this with equation (27) we get

$$b^\dagger \equiv a_p^\dagger - \tilde{a}_n \to z_1\,(z_2-z_1)^{-1}\,. \tag{66}$$

Equations (62) and (66) show that as we cross the boundary $|z_1| = |z_2|$ (e.g. as the point z passes through the contour C in equation (22)), the transition $a_p \to a_n^\dagger$, $a_p^\dagger \to -\tilde{a}_n$ takes place for the individual creation and destruction operators. The corresponding transition for an arbitrary function $f(a_p, a_p^\dagger)$ is, however, more subtle and is not simply obtained by making the above transition for each individual operator, i.e. $f(a_p, a_p^\dagger) \nrightarrow f(a_n^\dagger, -\tilde{a}_n)$, as is already apparent from equations (61) and (63).

We next introduce the complex conjugates of the operators a and $b^\dagger$ in equations (62) and (66) correspondingly:

$$a^\dagger = a_p^\dagger + a_n \tag{67}$$

$$b = a_p - \tilde{a}_n^\dagger = a_p - a_n^\dagger - |0;\,n\rangle\langle 0;\,p|. \tag{68}$$

They are represented by the functions:

$$a^\dagger \to z_1(z_2-z_1)^{-1}\theta(|z_2|-|z_1|)+z_2(z_1-z_2)^{-1}\theta(|z_1|-|z_2|) \tag{69}$$

$$b \to (z_2-z_1)^{-2}\epsilon(|z_2|-|z_1|)-\frac{1}{z_1z_2} \tag{70}$$

where $\epsilon(x)=1$ if $x>1$ and $\epsilon(x)=-1$ if $x<1$. We easily see that:

$$[a,a^\dagger]=[b,b^\dagger]=\mathbf{1}_p-\mathbf{1}_n=J \tag{71}$$

$$[a,b^\dagger]=[b,a^\dagger]=\mathbf{1}_p+\mathbf{1}_n=\mathbf{1} \tag{72}$$

$$[a,b]=|0;n\rangle\langle 1;p|-|1;n\rangle\langle 0;p| \tag{73}$$

$$[a^\dagger,b^\dagger]=-|1;p\rangle\langle 0;n|+|0;p\rangle\langle 1;n| \tag{74}$$

where $\mathbf{1}$ is the operator in the total Hilbert space $\mathcal{H}$:

$$\mathbf{1}_p+\mathbf{1}_n=\mathbf{1}\to(z_2-z_1)^{-1}\epsilon(|z_2|-|z_1|). \tag{75}$$

It is easy to prove that

$$J^2=\mathbf{1} \tag{76}$$

$$a^\dagger a=a_p^\dagger a_p+a_n a_n^\dagger \tag{77}$$

$$b^\dagger b=a_p^\dagger a_p+\tilde{a}_n\tilde{a}_n^\dagger=a^\dagger a+|0;p\rangle\langle 0;n|. \tag{78}$$

More generally we prove

$$(a_n)^N\to(z_2)^N(z_1-z_2)^{-1}\theta(|z_1|-|z_2|) \tag{79}$$

$$(a_n^\dagger)^N\to(N!)(z_1-z_2)^{-N-1}\theta(|z_1|-|z_2|). \tag{80}$$

Comparing equations (30) and (80) we see that

$$(a_p)^N-(-a_n^\dagger)^N\to(N!)(z_1-z_2)^{-N-1}. \tag{81}$$

Note, however, that equations (29) and (79) show that a_n^N is not the analytic continuation of $(a_p^\dagger)^N$.

The thermal density operator $\rho_n^{\mathrm{th}}(\beta)$ in $\mathcal{H}_n$, with $\beta\geqslant 0$, is defined exactly as in equation (39), but with $a_p\to a_n$. Its Dirac contour representation is given by,

$$\rho_n^{\mathrm{th}}(\beta;z_1,z_2)=\frac{1-\mathrm{e}^{\beta}}{z_2-\mathrm{e}^{\beta}z_1}\theta(-|z_2|+\mathrm{e}^{\beta}|z_1|). \tag{82}$$

We see clearly that equation (82) represents the analytic continuation of equation (40), defined in $\mathcal{H}_p$, into what in $\mathcal{H}_p$ is the '*forbidden region*' $\beta<0$ and $|z_2|<\mathrm{e}^{-\beta}|z_1|$. Whereas the region $\beta<0$ is forbidden within either $\mathcal{H}_p$ or $\mathcal{H}_n$ alone, the enlarged space $\mathcal{H}_p\oplus\mathcal{H}_n$ allows a precise and meaningful framework for a description of negative temperatures.We now define the generalized thermal density operator $\rho^{\mathrm{th}}(\beta)$, for all real values of β,

$$\rho^{\mathrm{th}}(\beta)=\begin{cases}\rho_p^{\mathrm{th}}(\beta) & \beta>0\\ \rho_n^{\mathrm{th}}(-\beta) & \beta<0\end{cases} \tag{83}$$

within $\mathcal{H}_p\oplus\mathcal{H}_n$. We stress again that whereas in either $\mathcal{H}_p$ or $\mathcal{H}_n$ alone only the operators $\rho_p^{\mathrm{th}}(\beta)$ and $\rho_n^{\mathrm{th}}(\beta)$, respectively, with $\beta>0$, are meaningful, within $\mathcal{H}_p\oplus\mathcal{H}_n$ the extended $\rho^{\mathrm{th}}(\beta)$ is meaningful. Its Dirac contour representation is given by,

$$\rho^{\mathrm{th}}(\beta;z_1,z_2)=\frac{1-\mathrm{e}^{-\beta}}{z_2-\mathrm{e}^{-\beta}z_1}\theta[\beta(|z_2|-\mathrm{e}^{-\beta}|z_1|)]. \tag{84}$$

We next prove analogous results to those given above for the entropy operator. The counterpart at negative temperatures of the operator given by equation (42) is

$$V_n(\beta_n) \equiv \rho_n^{\text{th}} \ln \rho_n^{\text{th}} = \sum_{N=0}^{\infty} (1 - \mathrm{e}^{-\beta_n})\mathrm{e}^{-N\beta_n}[-N\beta_n + \ln(1 - \mathrm{e}^{-\beta_n})]|N; n\rangle\langle N; n| \tag{85}$$

where $\beta_n \geqslant 0$. In the Dirac contour representation V_n is represented by the function:

$$\begin{aligned} V_n(\beta_n; z_1, z_2) &= (1 - \mathrm{e}^{-\beta_n}) \left[-\frac{\beta_n z_2 \mathrm{e}^{-\beta_n}}{[z_1 - z_2\mathrm{e}^{-\beta_n}]^2} + \frac{\ln(1 - \mathrm{e}^{-\beta_n})}{z_1 - z_2\mathrm{e}^{-\beta_n}} \right] \theta(|z_1| - \mathrm{e}^{-\beta_n}|z_2|) \\ &= (1 - \mathrm{e}^{\beta_n}) \left[\frac{\beta_n z_1 \mathrm{e}^{\beta_n}}{[z_2 - z_1\mathrm{e}^{\beta_n}]^2} + \frac{\ln(\mathrm{e}^{\beta_n} - 1)}{z_2 - z_1\mathrm{e}^{\beta_n}} \right] \theta(|z_1|\mathrm{e}^{\beta_n} - |z_2|). \end{aligned} \tag{86}$$

Comparing equations (42) and (86) we see that equation (86) is the analytic continuation of equation (42) into the forbidden region. Hence, we define the operator,

$$V(\beta; z_1, z_2) = \begin{cases} V_p(\beta_p = \beta; z_1, z_2) & \beta > 0 \\ V_n(\beta_n = -\beta; z_1, z_2) & \beta < 0 \end{cases} \tag{87}$$

within the extended Hilbert space $\mathcal{H}$. Its Dirac contour representation is the function

$$V(\beta; z_1, z_2) = (1 - \mathrm{e}^{-\beta}) \left[-\frac{\beta z_1 \mathrm{e}^{-\beta}}{[z_2 - z_1 \exp(-\beta)]^2} + \frac{\ln|(1 - \mathrm{e}^{-\beta})|}{z_2 - z_1 \exp(-\beta)} \right] \theta(\beta(|z_2| - \mathrm{e}^{-\beta}|z_1|)). \tag{88}$$

4. The harmonic oscillator formalism in $\mathcal{H}$

We consider the position and momentum operators in $\mathcal{H}$:

$$x = x_p + x_n = 2^{-1/2}(a^\dagger + a) \tag{89}$$

$$p = p_p - p_n = 2^{-1/2}\mathrm{i}(a^\dagger - a) \tag{90}$$

where x_p, p_p and x_n, p_n are the position and momentum operators in $\mathcal{H}_p$ and $\mathcal{H}_n$ correspondingly. We easily show

$$[x, p] = \mathrm{i}J \tag{91}$$

where J is the operator of equation (61). The eigenstates of x_p and x_n are $|x; p\rangle$ and $|x; n\rangle$ correspondingly. In terms of them we can write the resolutions of the identity:

$$\int \mathrm{d}x\, |x; p\rangle\langle x; p| = \pi_p \tag{92}$$

$$\int \mathrm{d}x\, |x; n\rangle\langle x; n| = \pi_n \tag{93}$$

where π_p and π_n are projection operators onto the Hilbert spaces $\mathcal{H}_p$ and $\mathcal{H}_n$, denoted in the previous section as $\mathbf{1}_p$ and $\mathbf{1}_n$ correspondingly:

$$\pi_p = \mathbf{1}_p = \sum_{N=0}^{\infty} |N; p\rangle\langle N; p| \tag{94}$$

$$\pi_n = \mathbf{1}_n = \sum_{N=0}^{\infty} |N; n\rangle\langle N; n|. \tag{95}$$

We also introduce the ‘temperature reversal’ operator,

$$T = \sum_{N=0}^{\infty} |N;\, p\rangle\langle N;\, n| + \sum_{N=0}^{\infty} |N;\, n\rangle\langle N;\, p|$$
$$= \int \mathrm{d}x\, |x;\, p\rangle\langle x;\, n| + \int \mathrm{d}x\, |x;\, n\rangle\langle x;\, p| \tag{96}$$

which, acting on a state in $\mathcal{H}_n$, changes it into its counterpart in $\mathcal{H}_p$; and vice versa. We easily see that

$$T = T^\dagger \qquad T^2 = \mathbf{1} \tag{97}$$
$$T\pi_p T^\dagger = \pi_n \qquad TJ + JT = 0 \tag{98}$$
$$Ta_p T^\dagger = a_n \qquad Ta_p^\dagger T^\dagger = a_n^\dagger \tag{99}$$
$$Ta_n T^\dagger = a_p \qquad Ta_n^\dagger T^\dagger = a_p^\dagger \tag{100}$$
$$TaT^\dagger = a^\dagger \qquad Ta^\dagger T^\dagger = a. \tag{101}$$

We next consider the displacement operator,

$$D(A) = \exp[Aa^\dagger - A^* a] = D_p(A)\pi_p + D_n(-A^*)\pi_n \tag{102}$$

where

$$D_p(A) \equiv \exp[Aa_p^\dagger - A^* a_p] \tag{103}$$
$$D_n(A) \equiv \exp[Aa_n^\dagger - A^* a_n]. \tag{104}$$

It is easy to prove the following relations for the effect on the displacement operators of temperature reversal,

$$TD(A)T^\dagger = D(-A^*) \tag{105}$$
$$TD_p(A)T^\dagger = D_n(A) \tag{106}$$
$$TD_n(A)T^\dagger = D_p(A). \tag{107}$$

We can also easily prove the compound relation:

$$D(A)D(B) = D(A+B)\exp[\tfrac{1}{2}(AB^* - A^*B)J]$$
$$= \pi_p D_p(A+B)\exp[\tfrac{1}{2}(AB^* - A^*B)] + \pi_n D_n(A+B)\exp[-\tfrac{1}{2}(AB^* - A^*B)]. \tag{108}$$

The mode of action of the displacement operator on the annihilation and creation operators is given by

$$D(A)aD^\dagger(A) = a - AJ = (a_p - A\pi_p) + (a_n^\dagger + A\pi_n) \tag{109}$$
$$D(A)a^\dagger D^\dagger(A) = a^\dagger - A^* J = (a_p^\dagger - A^*\pi_p) + (a_n + A^*\pi_n). \tag{110}$$

Using equation (55) and the known result [13],

$$\langle M|D(A)|N\rangle = \left[\frac{N!}{M!}\right]^{1/2} A^{M-N} \exp\left(-\frac{1}{2}|A|^2\right) L_N^{M-N}(|A|^2) \tag{111}$$

where L_N^{M-N} are Laguerre polynomials, we prove that the displacement operators are represented by the following functions in the Dirac contour representation,

$$D_p(A) \to \exp\left[-\frac{1}{2}|A|^2 + Az_1\right] \frac{1}{z_2 - z_1 + A^*} \qquad |z_2| > |z_1 - A^*| \tag{112}$$
$$D_n(A) \to \exp\left[-\frac{1}{2}|A|^2 - A^* z_2\right] \frac{1}{z_1 - z_2 - A} \qquad |z_2| < |A| \qquad |z_2 + A| < |z_1|. \tag{113}$$

By acting with $D_p(A)$ on the ket vacuum we get coherent states:

$$D_p(A)|0;\,p\rangle \equiv |A;\,p\rangle \to \oint_C \frac{\mathrm{d}z_2}{2\pi\mathrm{i}} \exp\left[-\frac{1}{2}|A|^2 + Az_1\right] \frac{1}{z_2 - z_1 + A^*}$$
$$= \exp\left[-\frac{1}{2}|A|^2 + Az_1\right] \tag{114}$$

where the point $z_1 - A^*$ is inside the contour C in the z_2-plane, in agreement with the inequality in equation (112). This result is in agreement with equation (15) for coherent states. Similarly, by acting with $D_p(A)$ on the bra vacuum we get

$$\langle 0;\,p|D_p(A) = \langle -A;\,p| \to \oint_C \frac{\mathrm{d}z_1}{2\pi\mathrm{i}} \exp\left(-\frac{1}{2}|A|^2 + Az_1\right) \frac{1}{z_1(z_2 - z_1 + A^*)}$$
$$= \exp\left(-\frac{1}{2}|A|^2\right) \frac{1}{z_2 + A^*} \tag{115}$$

where in the z_1-plane the origin is inside the contour C and the point $z_2 + A^*$ is outside the contour C, in agreement with the inequality in equation (112). This result agrees with equation (16). Similar results can be given for $|A; n\rangle$ and $\langle A; n|$.

Resolutions of the identity in terms of the coherent states are:

$$\int \frac{\mathrm{d}^2 A}{\pi} |A;\,p\rangle\langle A;\,p| = \pi_p \tag{116}$$

$$\int \frac{\mathrm{d}^2 A}{\pi} |A;n\rangle\langle A;n| = \pi_n. \tag{117}$$

From these equations we get

$$\int \frac{\mathrm{d}^2 A}{\pi} |A;\,p\rangle\langle A;\,p| + \int \frac{\mathrm{d}^2 A}{\pi} |A;n\rangle\langle A;n| = \mathbf{1} \tag{118}$$

$$\int \frac{\mathrm{d}^2 A}{\pi} |A;\,p\rangle\langle A;\,p| - \int \frac{\mathrm{d}^2 A}{\pi} |A;n\rangle\langle A;n| = J. \tag{119}$$

5. Discussion

The concept of negative temperature has been studied extensively in the context of classical thermodynamics. In this paper (and in [3]) we have studied this concept in the context of quantum statistical mechanics. We have introduced explicitly a Hilbert space and related creation and annihilation operators for negative temperatures, and studied them in relation to their counterparts at positive temperatures.

In section 2 we have discussed the standard harmonic oscillator (at positive temperatures) in the Dirac contour representation. This representation is interesting even if we are studying positive temperatures only; but it is also well suited for generalizations to negative temperatures. In section 3 we have introduced explicitly the Hilbert space for negative temperatures, and have studied its properties. In section 4 we have extended further the formalism and studied rather fully the properties of operators in the enlarged Hilbert space $\mathcal{H}_p \oplus \mathcal{H}_n$. These properties reveal deep connections between positive and negative temperatures.

From a more physical point of view negative temperatures can be useful in the description of systems that are excited to higher states and which decay into lower states (e.g. Glauber's inverted oscillator [2]). If we try to describe these physical situations confining ourselves only to the positive temperature Hilbert space, we arrive at non-normalizable wavefunctions which indicate precisely the fact that the Hilbert space is too small for the problem under consideration. From this point of view the concept of negative temperature provides the necessary enlargement of the Hilbert space.

It is perhaps relevant to explain briefly the route that we followed in arriving at these concepts. In [14] we have introduced generalized temperature-dependent P and Q representations in terms of thermal coherent states. We have noted that such generalized P and Q representations formally represent the analytic continuation of each other to negative temperatures. However, such a comment can only be made rigorous within an appropriate formalism for negative temperatures. The present work provides just such a rigorous foundation for our earlier work. An alternative and simpler proof of the continuation between P and Q representations as we go from positive to negative temperatures can now be given, which relies on the above mapping $a_p \leftrightarrow a_n^\dagger$, $a_p^\dagger \leftrightarrow -\tilde{a}_n$ between $\mathcal{H}_p$ and $\mathcal{H}_n$, and on the well known result that the P and Q representations of a given operator are related, respectively, to its antinormal- and normal-ordered forms.

In summary, we have shown that the Dirac contour representation easily and elegantly accommodates an extended Hilbert space suitable for the description of quantum physics at negative temperatures. In future publications we intend to demonstrate that the formalism can usefully be applied to specific problems of topical interest in quantum optics, quantum electronics, and solid-state optoelectronics.

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