PHYSICAL REVIEW A

ATOMIC, MOLECULAR, AND OPTICAL PHYSICS

THIRD SERIES, VOLUME 53, NUMBER 3 MARCH 1996

RAPID COMMUNICATIONS

The Rapid Communications section is intended for the accelerated publication of important new results. Since manuscripts submitted to this section are given priority treatment both in the editorial office and in production, authors should explain in their submittal letter why the work justifies this special handling. A Rapid Communication should be no longer than 4 printed pages and must be accompanied by an abstract. Page proofs are sent to authors.

Dirac's contour representation in thermofield dynamics

A. Vourdas

Department of Electrical Engineering and Electronics, University of Liverpool, Brownlow Hill, Liverpool L69 3BX, United Kingdom

R. F. Bishop

Department of Physics, University of Manchester Institute of Science and Technology (UMIST), P.O. Box 88, Manchester M60 1QD, United Kingdom

(Received 5 July 1995)

The Dirac contour representation and its properties are studied. It provides an elegant formalism for an extension of the harmonic-oscillator Hilbert space into a larger space that is suitable for the description of oscillator systems at both positive and negative temperatures. The analytic continuation of various physical quantities into the negative temperature region is examined in detail, and several interesting connections are revealed.

PACS number(s): 03.65.Ca, 05.70.−a, 42.50.Ar

Analytic representations play an important role in the study of various aspects of quantum physics. Examples include the Bargmann (or holomorphic) representation [1], other analytic representations used in the theory of coherent states [2–4] and quantum many-body–field theory [5], and several recent developments in conformal field theory. In all such cases the powerful theory of analytic functions is used in a quantum-mechanical context.

In this Rapid Communication we extend the previous Dirac contour representation [6] in order to introduce an enlarged Hilbert space that is suitable for a coherent theory of harmonic oscillators at negative temperatures. The formalism both incorporates earlier ideas about negative temperatures (see, e.g., Ref. [7]) and extends our own earlier work [8] on thermal coherent states and their properties. It is potentially 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 [9], although the mathematical details are different. The formalism is also useful in any generalized thermodynamics context that includes negative temperatures; in black hole physics, etc. We note that even when limited to positive temperature the formalism is valuable in practical quantum optics applications, as has been demonstrated elsewhere [4].

We label with the index p (for positive temperatures) the Hilbert space $\mathscr{H}_p$, and all the states and operators contained within it, which are associated with the harmonic oscillator, specified in terms of the usual creation and annihilation operators, $a_p^\dagger$ and a_p, respectively. We shall show that the Dirac contour representation within $\mathscr{H}_p$ can naturally be extended into another Hilbert space $\mathscr{H}_n$, similarly labeled with the index n (for negative temperatures). The formalism in $\mathscr{H}_n$ alone is very similar to the formalism in $\mathscr{H}_p$ alone. However, we show that by considering the enlarged Hilbert space $\mathscr{H}_p \oplus \mathscr{H}_n$, the space $\mathscr{H}_n$ can be interpreted as a Hilbert space of the harmonic oscillator at negative temperatures.

In the Dirac contour representation [5] of $\mathscr{H}_p$, the normalized eigenbras and eigenkets of the number operator $a_p^\dagger a_p$ are represented as

$$\langle N;p| \rightarrow (N!)^{\frac{1}{2}} z^{-N-1}, \quad |N;p\rangle \rightarrow (N!)^{-\frac{1}{2}} z^n, \tag{1}$$

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

$$|f;p\rangle = \sum_N f_N |N;p\rangle, \quad \langle f;p| = \sum_N f_N^* \langle N;p|, \tag{2}$$

where, here and henceforth, all sums on N (and M) run from zero to infinity, are represented as

$$|f;p\rangle \rightarrow \sum_N f_N (N!)^{-\frac{1}{2}} z^N \equiv f_k^p(z), \tag{3}$$

$$\langle f;p| \rightarrow \sum_N f_N^* (N!)^{\frac{1}{2}} z^{-N-1} \equiv f_b^p(z), \tag{4}$$

where the indices k and b refer to ket and bra, respectively. When $\Sigma_N |f_N|^2 = 1$, the normalized function $f_k^p(z)$ is a holomorphic function in the complex plane $z \in \mathbf{C}$, whereas $f_b^p(z)$ is clearly nonanalytic.

By making use of the simple relation,

$$\oint_{C'} \frac{dz}{2\pi i} \frac{\exp(\zeta^* z)}{z^{N+1}} = \frac{(\zeta^*)^N}{N!}, \tag{5}$$

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

$$\oint_C \frac{dz}{2\pi i} f_b^p(z) \exp(\zeta^* z) = [f_k^p(\zeta)]^*, \tag{6}$$

under conditions of convergence that need to be specified on an individual basis, but that generally amount to the anticlockwise contour C enclosing the singularities of $f_b^p(z)$. The scalar product of two states may similarly be represented as

$$\langle f;p|g;p\rangle = \oint_C \frac{dz}{2\pi i} f_b^p(z) g_k^p(z) = \sum_{N=0}^{\infty} f_N^* g_N. \tag{7}$$

A simple example of the Dirac contour representation in $\mathscr{H}_p$ is provided by the standard Glauber coherent state $|A;p\rangle$ for which

$$|A;p\rangle \rightarrow \exp(-\tfrac{1}{2}|A|^2 + Az), \tag{8}$$

$$\langle A;p| \rightarrow \exp(-\tfrac{1}{2}|A|^2)(z - A^*)^{-1}, \quad |z| > |A|. \tag{9}$$

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 Eqs. (6) and (7), the point A must lie inside the contour C.

At this point it is interesting to consider the relationship between the Dirac contour representation and the more familiar Bargmann (or holomorphic) representation [1], in which the normalizable ket state $|f;p\rangle$ of Eq. (2) is also represented by the holomorphic function $f_k^p(z)$ of Eq. (3), but where its corresponding adjoint bra state $\langle f;p|$ is represented by the complex conjugate function $[f_k^p(z)]^*$. By inserting into Eq. (7) the relation

$$g_k^p(z) = \int \frac{d^2\zeta}{\pi} \exp(\zeta^* z - |\zeta|^2) g_k^p(\zeta), \tag{10}$$

which is valid for all holomorphic functions $g_k^p(z)$, and by making use of Eq. (6), we readily derive the alternative relation

$$\langle f;p|g;p\rangle = \int \frac{d^2\zeta}{\pi} e^{-|\zeta|^2} [f_k^p(\zeta)]^* g_k^p(\zeta), \tag{11}$$

which is the usual relation for the inner product in the Bargmann representation of $\mathscr{H}_p$.

An arbitrary operator Θ_p in $\mathscr{H}_p$,

$$\Theta_p \equiv \sum_{M,N=0}^{\infty} \Theta_{MN} |M;p\rangle\langle N;p|, \tag{12}$$

has the Dirac contour representation,

$$\Theta_p(z_1,z_2) = \sum_{M,N=0}^{\infty} \Theta_{MN} \left(\frac{N!}{M!}\right)^{\frac{1}{2}} \frac{z_1^M}{z_2^{N+1}}. \tag{13}$$

Its trace is given by the elegant formula

$$\begin{aligned} \mathrm{Tr}\Theta_p &\equiv \sum_N \Theta_{NN} = \sum_N \oint_{C_1} \oint_{C_2} \frac{dz_1 dz_2}{(2\pi i)^2} \Theta_p(z_1,z_2) \frac{z_2^N}{z_1^{N+1}} \\ &= -\frac{1}{4\pi^2} \oint_{C_1} \oint_{C_2} \frac{dz_1 dz_2}{z_1 - z_2} \Theta_p(z_1,z_2), \\ &\qquad C_2 < C_1, \end{aligned} \tag{14}$$

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

$$\Theta_p|g;p\rangle \rightarrow \oint_C \frac{dz'}{2\pi i} \Theta_p(z,z') g_k^p(z'), \tag{15}$$

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

$$\langle f;p|\Theta_p \rightarrow \oint_C \frac{dz'}{2\pi i} f_b^p(z') \Theta_p(z',z). \tag{16}$$

Similarly, if $\Theta_{1;p}$ and $\Theta_{2;p}$ are two operators in $\mathscr{H}_p$ 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

$$\Theta_{1;p}\Theta_{2;p} \rightarrow \oint_C \frac{dz}{2\pi i} \Theta_{1;p}(z_1,z) \Theta_{2;p}(z,z_2). \tag{17}$$

As illustrative examples we now consider the Dirac contour representations of the operators 1_p, a_p, $a_p^\dagger$, and $a_p^\dagger a_p$. For the unit operator 1_p, $\Theta_{MN} = \delta_{M,N}$, and Eq. (13) 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 Eq. (15) lies outside the contour C, and hence that the result is zero. In this sense we are, therefore, justified in saying that for $|z_1|>|z_2|$, the Dirac contour representation of 1_p is zero. We write accordingly,

$$1_p \rightarrow (z_2-z_1)^{-1}\theta(|z_2|-|z_1|), \tag{18}$$

where $\theta(x)$ is the unit step function; $\theta(x)\equiv 1$ for $x>0$, and $\theta(x)\equiv 0$ for $x\leqslant 0$. We may likewise show

$$a_p \rightarrow (z_2-z_1)^{-2}\theta(|z_2|-|z_1|), \tag{19}$$

$$a_p^\dagger \rightarrow z_1(z_2-z_1)^{-1}\theta(|z_2|-|z_1|), \tag{20}$$

$$a_p^\dagger a_p \rightarrow z_1(z_2-z_1)^{-2}\theta(|z_2|-|z_1|). \tag{21}$$

We may also show more generally that the following representations hold for arbitrary (integral) powers of the basic creation and destruction operators,

$$(a_p^\dagger)^M \rightarrow z_1^M(z_2-z_1)^{-1}\theta(|z_2|-|z_1|), \tag{22}$$

$$(a_p)^N \rightarrow N!(z_2-z_1)^{-N-1}\theta(|z_2|-|z_1|). \tag{23}$$

Use of Eq. (17) also yields the relations for normal-ordered and antinormal-ordered products,

$$(a_p^\dagger)^M(a_p)^N \rightarrow N! z_1^M(z_2-z_1)^{-N-1}\theta(|z_2|-|z_1|), \tag{24}$$

$$(a_p)^N(a_p^\dagger)^M \rightarrow \left[\left(\frac{d}{dz_1}\right)^N \frac{z_1^M}{z_2-z_1}\right]\theta(|z_2|-|z_1|). \tag{25}$$

The further use of Eq. (15) then also shows that

$$(a_p^\dagger)^M(a_p)^N|g;p\rangle \rightarrow z^M\left(\frac{d}{dz}\right)^N g_k^p(z), \tag{26}$$

$$(a_p)^N(a_p^\dagger)^M|g;p\rangle \rightarrow \left(\frac{d}{dz}\right)^N z^M g_k^p(z). \tag{27}$$

We thus observe that the mode of action of the operators $a_p^\dagger$ and a_p on ket states $|g;p\rangle$ within $\mathscr{H}_p$ is equivalent to multiplication by z and differentiation with respect to z, respectively, of the holomorphic function $g_k^p(z)$, i.e., $a_p^\dagger \rightarrow z$, $a_p \rightarrow d/dz$, 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 *nonanalytic* functions $f_b^p(z)$ cannot be so simply expressed.

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

$$\rho_p^{\text{th}}(\beta) \equiv (1-e^{-\beta})\exp(-\beta a_p^\dagger a_p), \quad \beta \geqslant 0. \tag{28}$$

Its Dirac contour representation is simply constructed as

$$\rho_p^{\text{th}}(\beta;z_1,z_2) = \frac{1-e^{-\beta}}{z_2-e^{-\beta}z_1}\,\theta(|z_2|-e^{-\beta}|z_1|). \tag{29}$$

We turn next to the Hilbert space $\mathscr{H}_n$, for which the Dirac contour representation of the normalized eigenbras and eigenkets of the number operator $a_n^\dagger a_n$ is that of the corresponding eigenkets and eigenbras, respectively, of $\mathscr{H}_p$,

$$\langle N;n| \rightarrow (N!)^{-\frac{1}{2}} z^N, \quad |N;n\rangle \rightarrow (N!)^{\frac{1}{2}} z^{-N-1}. \tag{30}$$

Thus, the representations of bra and ket states are opposite in $\mathscr{H}_p$ and $\mathscr{H}_n$: this is their only difference. Arbitrary states $|f;n\rangle$ and $\langle f;n|$ in $\mathscr{H}_n$ have analogous expansions to that in Eq. (2) for $\mathscr{H}_p$, and have the corresponding Dirac contour representations,

$$|f;n\rangle \rightarrow \sum_N f_N(N!)^{\frac{1}{2}} z^{-N-1} \equiv f_k^n(z), \tag{31}$$

$$\langle f;n| \rightarrow \sum_N f_N^*(N!)^{-\frac{1}{2}} z^N \equiv f_b^n(z). \tag{32}$$

We note that the overlap of any state in $\mathscr{H}_n$ with any state in $\mathscr{H}_p$ is identically zero. Operators $\Theta_n \equiv \Sigma_{M,N}\Theta_{MN}|M;n\rangle\langle N;n|$ in $\mathscr{H}_n$, defined analogously to Eq. (12) in $\mathscr{H}_p$, are represented by the corresponding functions,

$$\Theta_n(z_1,z_2) = \sum_{M,N} \Theta_{MN}\left(\frac{M!}{N!}\right)^{\frac{1}{2}} \frac{z_2^N}{z_1^{M+1}}. \tag{33}$$

The analogs of Eqs. (18)–(21) are readily shown to be

$$1_n \rightarrow (z_1-z_2)^{-1}\theta(|z_1|-|z_2|), \tag{34}$$

$$a_n \rightarrow z_2(z_1-z_2)^{-1}\theta(|z_1|-|z_2|), \tag{35}$$

$$a_n^\dagger \rightarrow (z_1-z_2)^{-2}\theta(|z_1|-|z_2|), \tag{36}$$

$$a_n^\dagger a_n \rightarrow z_2(z_1-z_2)^{-2}\theta(|z_1|-|z_2|). \tag{37}$$

A comparison of Eqs. (18), (19), and (21) with Eqs. (34), (36), and (37) reveals the following relations:

$$1_p - 1_n \rightarrow (z_2-z_1)^{-1}, \tag{38}$$

$$a_p + a_n^\dagger \rightarrow (z_2-z_1)^{-2}, \tag{39}$$

$$a_p^\dagger a_p + a_n a_n^\dagger \rightarrow z_1(z_2-z_1)^{-2}. \tag{40}$$

In order to analytically continue the operator $a_p^\dagger$ of Eq. (20) with the operator a_n of Eq. (35) we need to introduce first an "extended" destruction operator $\tilde{a}_n$,

$$\tilde{a}_n \equiv a_n + |0;p\rangle\langle 0;n|. \tag{41}$$

We note that operators $\mathscr{L}$ that map states from $\mathscr{H}_p$ into $\mathscr{H}_n$ and vice versa, namely,

$$\mathscr{L} \equiv \sum_{M,N} (A_{MN}|M;p\rangle\langle N;n| + B_{MN}|M;n\rangle\langle N;p|), \tag{42}$$

have the Dirac contour representation,

$$\mathscr{L}(z_1,z_2) = \sum_{M,N} [A_{MN}(M!N!)^{-\frac{1}{2}} z_1^M z_2^N + B_{MN}(M!N!)^{\frac{1}{2}} z_1^{-M-1} z_2^{-N-1}]. \tag{43}$$

Equation (43) shows immediately that the Dirac contour representation of the operator $|0;p\rangle\langle 0;n|$ is 1. Thus, Eqs. (35) and (41) yield the mapping

$$\tilde{a}_n \rightarrow z_1(z_1-z_2)^{-1}\theta(|z_1|-|z_2|), \tag{44}$$

in the same sense as described previously, and hence

$$a_p^\dagger - \tilde{a}_n \rightarrow z_1(z_2-z_1)^{-1}. \quad (45)$$

Equations (39) and (45) show that as we cross the boundary $|z_1|=|z_2|$ [e.g., as the point z passes through the contour C in Eq. (15)], the transition $a_p \rightarrow a_n^\dagger$, $a_p^\dagger \rightarrow -\tilde{a}_n$ 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., $f(a_p, a_p^\dagger) \not\rightarrow f(a_n^\dagger, -\tilde{a}_n)$, as is already apparent from Eqs. (38) and (40).

The thermal density operator $\rho_n^{\rm th}(\beta)$ in $\mathscr{H}_n$, with $\beta \geqslant 0$, is defined exactly as in Eq. (28), but with $a_p \rightarrow a_n$. Use of Eq. (33) readily yields its Dirac contour representation,

$$\rho_n^{\rm th}(\beta; z_1, z_2) = \frac{1-e^\beta}{z_2 - e^\beta z_1}\, \theta(-|z_2| + e^\beta |z_1|). \quad (46)$$

We see clearly that Eq. (46) represents the analytic continuation of Eq. (29), defined in $\mathscr{H}_p$, into what in $\mathscr{H}_p$ is the *"forbidden region"* $\beta<0$ and $|z_2|<e^{-\beta}|z_1|$. Whereas the region $\beta<0$ is forbidden within either $\mathscr{H}_p$ or $\mathscr{H}_n$ alone, the enlarged space $\mathscr{H}_p \oplus \mathscr{H}_n$ allows a precise and meaningful framework for a description of negative temperatures. It is this result, together with a series of other results in the same general context, which we indicate below, that leads to the interpretation of $\mathscr{H}_n$ within this context as a negative temperature Hilbert space.

More precisely, we define the generalized thermal density operator $\rho^{\rm th}(\beta)$, for all real values of β,

$$\rho^{\rm th}(\beta) = \begin{cases} \rho_p^{\rm th}(\beta), & \beta>0 \\ \rho_n^{\rm th}(-\beta), & \beta<0, \end{cases} \quad (47)$$

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

$$\rho^{\rm th}(\beta) = \frac{1-e^{-\beta}}{z_2 - e^{-\beta} z_1}\, \theta[\beta(|z_2| - e^{-\beta}|z_1|)]. \quad (48)$$

Analogous results to those given above can also be proved for the entropy operator $\rho^{\rm th} \ln \rho^{\rm th}$, whose trace is proportional to the von Neumann entropy. Full details will be given elsewhere. Such results also strengthen our interpretation of $\mathscr{H}_n$ as a Hilbert space for the harmonic oscillator at negative temperatures.

In previous work [8] 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. The present work puts such observations onto a sounder footing, since we have now explicitly extended the original Hilbert space to accommodate the negative temperature states. Indeed, an alternative and simpler proof can now be given, which relies on the above mapping $a_p \leftrightarrow a_n^\dagger$, $a_p^\dagger \leftrightarrow -\tilde{a}_n$ between $\mathscr{H}_p$ and $\mathscr{H}_n$, and on the fact that the P and Q representations of a given operator are directly related, respectively, to its antinormal- and normal-ordered forms. Mathematical details will be given elsewhere.

In summary, we have shown that one of the prime features of the Dirac contour representation is that it accommodates easily and elegantly an extended Hilbert space suitable for the description of quantum physics at negative temperatures. Its close relationship with thermo-field-dynamics and its generalization is most easily discussed in terms of the thermal coherent states and their generalization to the displaced negative-binomial coherent mixed states, which we have investigated rather fully in previous work [8]. We intend to publish elsewhere a full account of the interrelationships between these new forms of coherent states and their various representations.

One of us (R.F.B.) gratefully acknowledges a research grant from the Engineering and Physical Sciences Research Council (EPSRC) of Great Britain.

[1] V. Bargmann, Commun. Pure Appl. Math. **14**, 180 (1961); **14**, 187 (1961); **20**, 1 (1967).

[2] F.A. Berezin, Math. USSR Izv. **8**, 1109 (1974); **9**, 341 (1975); Commun. Math. Phys. **40**, 153 (1975).

[3] A. Vourdas, Phys. Rev. A **45**, 1993 (1992); Phys. Scr. **T48**, 84 (1993); J. Math. Phys. **34**, 1223 (1993); **35**, 2687 (1994).

[4] P. Adam, J. Janszky, and A.V. Vinogradov, Opt. Commun. **80**, 155 (1990); J. Janszky, P. Adam, and A.V. Vinogradov, Phys. Rev. Lett. **68**, 3816 (1992); P. Domokos, P. Adam, and J. Janszky, Phys. Rev. A **50**, 4293 (1994).

[5] J.S. Arponen and R.F. Bishop, Ann. Phys. (N.Y.) **207**, 171 (1991); **227**, 275 (1993); **227**, 334 (1993).

[6] P.A.M. Dirac, Commun. Dublin Inst. Adv. Studies Ser. A **1**, 1 (1943); J. Schwinger, *Quantum Kinematics and Dynamics* (Benjamin, New York, 1970); H.Y. Fan, Z.W. Liu, and T.N. Ruan, Commun. Theor. Phys. (Beijing) **3**, 175 (1984); H.Y. Fan and J.R. Klauder, Mod. Phys. Lett. A **9**, 1291 (1994).

[7] N.F. Ramsey, Phys. Rev. **103**, 20 (1956).

[8] R.F. Bishop and A. Vourdas, J. Phys. A **20**, 3743 (1987); A. Vourdas and R.F. Bishop, Phys. Rev. A **50**, 3331 (1994); **51**, 2353 (1995).

[9] W. Wöger, H. King, R.J. Glauber, and J.W. Haus, Phys. Rev. A **34**, 4859 (1986).