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Use of the coherent states in evaluating the canonical density matrix for a harmonic oscillator

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Abstract. An alternative method for evaluating the canonical density matrix $\langle x|\exp(-\beta\hat{H})|x'\rangle$ for a one-dimensional harmonic oscillator is proposed. The method uses the coherent states, i.e. the eigenstates of the annihilation operator $\hat{a}$, as the basis of the expansion of $\exp(-\beta\hat{H})|x'\rangle$ in place of the Hermite functions which are used in the conventional treatment. It is shown that the use of the coherent states makes it much easier to evaluate the density matrix than the other methods. As a direct extension of the method, the density matrix for a three-dimensional harmonic oscillator placed in a uniform magnetic field is recalculated in the creation-annihilation operator formalis. Some other uses of the coherent states in operator problems, such as the Wigner distribution function, are also discussed. Two alternative derivations of the Gaussian integral formula are also given, which plays an important role in the present problem as well as in various other problems in physics

1. Introduction

In a previous paper (Yonei 1989, referred to as I in this paper) we proposed a simple method of evaluating the canonical density matrix $\langle x|\exp(-\beta\hat{H})|x'\rangle$ for a one-dimensional harmonic oscillator as a basis of constructing the canonical density matrix for a three-dimensional charged oscillator placed in a uniform magnetic field. Although that method is simple enough, it deals with the problem by the direct use of the position and the momentum operators. It is commonly recognised, however, that most problems of the harmonic oscillators can be made easier by the use of the creation and annihilation operators. It would be natural, therefore, to ask whether this is also the case in the evaluation of the canonical density matrix. As far as one uses the eigenvectors $|n\rangle$ of the Hamiltonian $\hat{H}$ as the basis set to expand $\exp(-\beta\hat{H})|x'\rangle$, nothing new seems to arise in the evaluation of the canonical density matrix; one simply has

$$\langle x|\exp(-\beta\hat{H})|x'\rangle = \sum_{n=0}^{\infty} \exp[-\beta\hbar\omega(n+\tfrac{1}{2})]\langle x|n\rangle\langle n|x'\rangle \tag{1.1}$$

and in carrying out the summation one eventually has to rely on the Fourier integral representation of the Hermite polynomials, the same procedure as that used in the usual treatment of the problem (see Ishihara 1971, for example).

However, the situation seems to become quite different if one uses the eigenvectors of the annihilation operator $\hat{a}$, which are called the coherent states and play important roles in the problems of quantum optics, instead of $|n\rangle$. In fact, the use of the coherent states as a basic set of the representation certainly makes the problem simpler and

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easier; all that is required is to carry out the Gauss integrals, apart from some elementary knowledge about the properties of coherent states.

The purpose of this paper is to show the usefulness of the coherent states in the evaluation of $\langle x|\exp(-\beta\hat{H})|x'\rangle$ for the harmonic oscillator by describing the actual procedure of their use, as a supplement to the previous study I. In the next section we first give a brief summary of the basic properties of coherent states and then calculate $\langle x|\exp(-\beta\hat{H})|x'\rangle$ using them. As a direct extension of the same idea, in section 3 we reformulate the evaluation method of the density matrix for an oscillator placed in a constant magnetic field. Section 4 is devoted to a supplementary discussion of another use of the coherent states in the oscillator problem and in section 5 we give our conclusion. In the appendix we give two alternative methods for obtaining the Gauss integral because the same procedures may be applied to the evaluation of the other integrals and to the author's knowledge, they can not be found in the literature.

2. The coherent states and their use in the evaluation of the canonical density matrix for a harmonic oscillator

Before discussing the canonical density matrix for a harmonic oscillator, we give a brief summary of the properties of the coherent states. As to a detailed description of them one should refer to the literature (Glauber 1963, Klauder *et al* 1968, Louisell 1973).

The Hamiltonian $\hat{H}$ for a harmonic oscillator of mass m and angular frequency ω may be expressed as

$$\hat{H} = \hbar\omega(\hat{n}+\tfrac{1}{2}) \tag{2.1}$$

$$\hat{n} = \hat{a}^{\dagger}\hat{a} \tag{2.2}$$

where the annihilation operator $\hat{a}$ and the creation operator $\hat{a}^{\dagger}$ are defined by

$$\begin{cases} \hat{a} = (m\omega/2\hbar)^{1/2}\hat{x} + \mathrm{i}(2m\hbar\omega)^{-1/2}\hat{p} \\ \hat{a}^{\dagger} = (m\omega/2\hbar)^{1/2}\hat{x} - \mathrm{i}(2m\hbar\omega)^{-1/2}\hat{p}. \end{cases} \tag{2.3}$$

The coherent states $|\alpha\rangle$ are normalised eigenstates of the operator $\hat{a}$, i.e.,

$$\hat{a}|\alpha\rangle = \alpha|\alpha\rangle \qquad \langle\alpha|\alpha\rangle = 1 \tag{2.4}$$

and they can be expressed in terms of the eigenkets of $\hat{n}$, $|n\rangle$, as follows:

$$\begin{aligned} |\alpha\rangle &= \exp(-|\alpha|^2/2)\sum_{n=0}^{\infty}\alpha^n|n\rangle/(n!)^{1/2} \\ &= \exp(-|\alpha|^2/2)\exp(\alpha\hat{a}^{\dagger})|0\rangle \end{aligned} \tag{2.5}$$

$|0\rangle$ being the lowest eigenstate of $\hat{n}$.

It is easy to verify the following formulae:

$$(1/\pi)\iint \mathrm{d}^2\alpha|\alpha\rangle\langle\alpha| \equiv (1/\pi)\int_{-\infty}^{\infty}\mathrm{d}\sigma\int_{-\infty}^{\infty}\mathrm{d}\tau|\alpha\rangle\langle\alpha| = 1 \tag{2.6}$$

$$\sigma = \mathrm{Re}(\alpha) \qquad \tau = \mathrm{Im}(\alpha)$$

and

$$\langle x|\alpha\rangle = (m\omega/\pi\hbar)^{1/4}\exp(-\tau^2+\mathrm{i}\sigma\tau)\exp[-(cx-\alpha)^2] \tag{2.7a}$$

where

$$c = (m\omega/2\hbar)^{1/2}. \tag{2.7b}$$

In addition to these relationships the following formula plays a crucial role in the present application:

$$\exp(\lambda\hat{n})|\alpha\rangle = \exp[-(1-|\gamma|^2)|\alpha|^2/2]|\alpha'\rangle \tag{2.8a}$$

for an arbitrary number λ where

$$\gamma = \exp(\lambda) \qquad \text{and} \qquad \alpha' = \gamma\alpha. \tag{2.8b}$$

Now we turn our attention to the canonical density matrix, which can be written as

$$\langle x|\exp(-\beta\hat{H})|x'\rangle = \exp(-\beta\hbar\omega/2)\langle x|\exp(-\beta\hbar\omega\hat{n})|x'\rangle. \tag{2.9}$$

The second factor of the right-hand side of (2.9) can be calculated in the following manner.

$$\begin{aligned} A &= \langle x|\exp(-\beta\hbar\omega\hat{n})|x'\rangle \\ &= \langle x|\exp(-\beta\hbar\omega\hat{n}/2)\exp(-\beta\hbar\omega\hat{n}/2)|x'\rangle \\ &= (1/\pi)\int_{-\infty}^{\infty}\mathrm{d}\sigma\int_{-\infty}^{\infty}\mathrm{d}\tau\langle x|\exp(-\beta\hbar\omega\hat{n}/2)|\alpha\rangle\langle\alpha|\exp(-\beta\hbar\omega\hat{n}/2)|x'\rangle \\ &= (1/\pi)(m\omega/\pi\hbar)^{1/2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(\sigma,\tau)\,\mathrm{d}\sigma\,\mathrm{d}\tau \end{aligned} \tag{2.10a}$$

$$f(\sigma,\tau) = \exp[-(1-\gamma^2)|\alpha|^2]\langle x|\alpha'\rangle\langle\alpha'|x'\rangle \tag{2.10b}$$

where α and τ are again the real and imaginary parts of α, respectively, while

$$\gamma = \exp(-\beta\hbar\omega/2) \qquad \text{and} \qquad \alpha' = \gamma\alpha. \tag{2.11}$$

Recalling (2.7a, b) for $\langle x|\alpha\rangle$, we have

$$f(\sigma,\tau) = \exp[-g(\sigma,\tau)] \tag{2.12a}$$

$$g(\sigma,\tau) = (cx-\alpha)^2 + (cx'-\alpha^*)^2 + (1-\gamma^2)\sigma^2 + (1+\gamma^2)\tau^2. \tag{2.12b}$$

A straightforward calculation yields

$$\begin{aligned} g(\sigma,\tau) &= (1+\gamma^2)\{\sigma + [\gamma/(1+\gamma^2)]c(x+x')\}^2 \\ &\quad + (1-\gamma^2)\{\tau + [\gamma/(1-\gamma^2)]c(x-x')\}^2 \\ &\quad + (m\omega/4\hbar)[(1-\gamma^2)/(1+\gamma^2)](x+x')^2 \\ &\quad + (m\omega/4\hbar)[(1+\gamma^2)/(1-\gamma^2)](x-x')^2. \end{aligned} \tag{2.13}$$

Substituting (2.12a) and (2.13) into (2.10a), and carrying out the Gauss integrals, we have

$$\begin{aligned} A &= \langle x|\exp(-\beta\hbar\omega\hat{n}|x'\rangle \\ &= (m\omega/\pi\hbar)^{1/2}[(1+\gamma^2)(1-\gamma^2)]^{-1/2} \\ &\quad \times\exp\{-(m\omega/4\hbar)\{[(1-\gamma^2)/(1+\gamma^2)](x+x')^2 \\ &\quad + [(1+\gamma^2)/(1-\gamma^2)](x-x')^2\}\}. \end{aligned} \tag{2.14}$$

Recalling that $\gamma = \exp(-\beta\hbar\omega/2)$, one can write

$$(1-\gamma^2)(1+\gamma^2) = 2\sinh(\beta\hbar\omega)\exp(-\beta\hbar\omega) \tag{2.15a}$$

$$(1-\gamma^2)/(1+\gamma^2) = \tanh(\beta\hbar\omega/2) \tag{2.15b}$$

$$(1+\gamma^2)/(1-\gamma^2) = \coth(\beta\hbar\omega/2). \tag{2.15c}$$

A substitution of (2.14)-(2.15c) into (2.9) leads to the familiar expression

$$\begin{aligned}\langle x|\exp(-\beta\hat{H})|x'\rangle \\ &= [m\omega/2\pi\hbar\sinh(\beta\hbar\omega)]^{1/2} \\ &\quad\times\exp\{-(m\omega/4\hbar)[\tanh(\beta\hbar\omega/2)(x+x')^2+\coth(\beta\hbar\omega/2)(x-x')^2]\}.\end{aligned} \tag{2.16}$$

If one compares the above procedure with that of the conventional treatment of the problem, one will find that a considerable simplification is brought about by the use of the coherent states. It may be worthwhile mentioning that the coherent states can also be used to evaluate the density matrix for a free particle. In fact, in terms of the operators $\hat{a}$ and $\hat{a}^{+}$ defined in (2.1), the Hamiltonian $\hat{H} = (1/2m)\hat{p}^2$ can be expressed as

$$\hat{H} = \tfrac{1}{4}\hbar\omega(\hat{a}-\hat{a}^{+})^2. \tag{2.17}$$

It is easy to see that

$$\begin{aligned}\hat{H} &= \exp[\tfrac{1}{4}(\hat{a}^{+}+\hat{a})^2](\hbar\omega\hat{a})\exp[-\tfrac{1}{4}(\hat{a}^{+}+\hat{a})^2] \\ &= \exp(m\omega x^2/2\hbar)(\hbar\omega\hat{a})\exp(-m\omega x^2/2\hbar).\end{aligned} \tag{2.18}$$

Thus

$$\langle x|\exp(-\beta\hat{H})|x'\rangle = \exp[-\beta m\omega(x^2-x'^2)/2\hbar]\langle x|\exp(-\beta\hbar\omega\hat{a})|x'\rangle. \tag{2.19}$$

By the use of the coherent states the second factor of the right-hand side of (2.19) can easily be obtained, which leads to the familiar expression

$$\langle x|\exp(-\beta\hat{H})|x'\rangle = (m/2\pi\hbar^2\beta)^{1/2}\exp[-m(x-x')^2/2\hbar^2\beta]. \tag{2.20}$$

3. The canonical density matrix for an oscillator in a constant magnetic field

The method developed in the preceding section can immediately be extended to a more general problem, i.e. the evaluation of the canonical density matrix for an oscillator placed in a constant magnetic field of strength $\mathcal{H}$. The same problem was fully discussed in I using the usual expression of $\hat{H}$ by $\hat{r}$ and $\hat{p}$. However, it will be useful and instructive to reformulate the problem following the spirit of the method developed in section 2 because it brings about some new aspects to the problem. Here we restrict ourselves mainly to the case of an isotropic oscillator because this simplest case will be enough to exemplify the main features of the procedure.

The direction of the magnetic field is assumed to be parallel to the z axis, so that the vector potential may be taken as

$$\hat{\boldsymbol{A}} = (-\tfrac{1}{2}\mathcal{H}\hat{y}, \tfrac{1}{2}\mathcal{H}\hat{x}, 0). \tag{3.1}$$

With this choice of the vector potential, the Hamiltonian of an isotropic oscillator with electric charge e may be written as

$$\hat{H} = (1/2m)(\hat{\boldsymbol{p}} - e\hat{\boldsymbol{A}}/c)^2 + \tfrac{1}{2}m\omega_0^2\hat{\boldsymbol{r}}^2 = \hat{H}_t + \hat{H}_z \tag{3.2a}$$

$$\hat{H}_t = (1/2m)(\hat{p}_x^2 + \hat{p}_y^2) + \tfrac{1}{2}m\omega_0^2(\hat{x}^2 + \hat{y}^2) + \hat{H}_L \tag{3.2b}$$

$$\hat{H}_L = -\omega(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x) \tag{3.2c}$$

$$\hat{H}_z = (1/2m)\hat{p}_z^2 + \tfrac{1}{2}m\omega_0^2\hat{z}^2 \tag{3.2d}$$

where

$$\omega = e\mathscr{H}/2mc \qquad \text{and} \qquad \omega' = (\omega_0^2 + \omega^2)^{1/2}. \tag{3.2e}$$

If one defines the annihilation and creation operators by

$$\begin{cases} \hat{a}_i = (m\omega_i/2\hbar)^{1/2}\hat{x}_i + \mathrm{i}(2m\hbar\omega_i)^{-1/2}\hat{p}_i \\ \hat{a}_i^\dagger = (m\omega_i/2\hbar)^{1/2}\hat{x}_i - \mathrm{i}(2m\hbar\omega_i)^{-1/2}\hat{p}_i \qquad (i = 1, 2, 3) \end{cases} \tag{3.3}$$

where

$$(\hat{x}_1, \hat{x}_2, \hat{x}_3) = (\hat{x}, \hat{y}, \hat{z}), (\hat{p}_1, \hat{p}_2, \hat{p}_3) = (\hat{p}_x, \hat{p}_y, \hat{p}_z) \tag{3.4}$$

$$\omega_1 = \omega_2 = \omega' \qquad \omega_3 = \omega_0 \tag{3.5}$$

the expression (3.2b) may be expressed in terms of them as

$$\hat{H} = \hat{H}_t + \hat{H}_3 \tag{3.6a}$$

$$\hat{H}_t = \hat{H}_1 + \hat{H}_2 + \hat{H}_L \tag{3.6b}$$

$$\hat{H}_i = \hbar\omega_i(\hat{n}_i + \tfrac{1}{2}) = \hbar\omega_i(\hat{a}_i^\dagger\hat{a}_i + \tfrac{1}{2}) \qquad (i = 1, 2, 3) \tag{3.6c}$$

$$\hat{H}_L = \mathrm{i}\hbar\omega\hat{A} = \mathrm{i}\hbar\omega(\hat{a}_1^\dagger\hat{a}_2 - \hat{a}_1\hat{a}_2^\dagger). \tag{3.6d}$$

Since

$$[\hat{H}_1, \hat{H}_2] = [\hat{H}_2, \hat{H}_3] = [\hat{H}_3, \hat{H}_1] = [(\hat{H}_1 + \hat{H}_2), \hat{H}_L] = 0 \tag{3.7}$$

$$\begin{aligned} \exp(-\beta\hat{H}) &= \exp(-\beta\hat{H}_t)\exp(-\beta\hat{H}_3) \\ &= \exp(-\beta\hat{H}_1)\exp(-\beta\hat{H}_2)\exp(-\beta\hat{H}_L)\exp(-\beta\hat{H}_3) \end{aligned} \tag{3.8}$$

which in turn leads to

$$\begin{aligned} \langle \boldsymbol{r}|\exp(-\beta\hat{H})|\boldsymbol{r}'\rangle &= \langle x, y|\exp(-\beta\hat{H}_1)\exp(-\beta\hat{H}_2)\exp(-\beta\hat{H}_L)|x', y'\rangle \\ &\quad \times \langle z|\exp(-\beta\hat{H}_3)|z'\rangle. \end{aligned} \tag{3.9}$$

As pointed out in I, $\exp(-\beta\hat{H}_L)$ is a rotation operator about the z axis with a pure imaginary angle; in fact,

$$\exp(-\beta\hat{H}_L)|x', y'\rangle = |x'', y''\rangle \tag{3.10a}$$

$$\begin{cases} x'' = x'\cosh(\beta\hbar\omega) - \mathrm{i}y'\sinh(\beta\hbar\omega) \\ y'' = y'\cosh(\beta\hbar\omega) + \mathrm{i}x'\sinh(\beta\hbar\omega). \end{cases} \tag{3.10b}$$

Thus one has

$$\begin{aligned} \langle \boldsymbol{r}|\exp(-\beta\hat{H})|\boldsymbol{r}'\rangle &= \langle x|\exp[-\beta\hbar\omega'(\hat{n}_1 + \tfrac{1}{2})]|x''\rangle\langle y|\exp[-\beta h\omega'(\hat{n}_2 + \tfrac{1}{2})]|y''\rangle \\ &\quad \times \langle z|\exp[-\beta h\omega_0(\hat{n}_3 + \tfrac{1}{2})]|z'\rangle. \end{aligned} \tag{3.11}$$

Each factor of (3.11) is the density matrix of a simple harmonic oscillator of the form given in (2.16), so that a simple substitution of the expression (2.16) into the factors appearing in (3.11) leads to the final result, which is the same as that given in equations (3.14)-(3.18e) of I. Clearly the above procedure is essentially the same as that developed in I, except for the use of the creation and annihilation operators, and is probably one of the simplest ways to evaluate the density matrix for an isotropic oscillator in a constant magnetic field. However, the description of the problem by the creation and annihilation opertators also opens another possibilities to the way of the solution. In the following we outline two of such alternative procedures. Since $\langle z|\exp(-\beta\hat{H}_3)|z'\rangle$ can be factored out of $\langle \boldsymbol{r}|\exp(-\beta\hat{H})|\boldsymbol{r}'\rangle$, we focus our attention only on the matrix element $\langle x, y|\exp(-\beta\hat{H}_t)|x'y'\rangle$ hereafter.

Method 1. This method is based on the same factorisation of the density matrix as that given by (3.9). The matrix element $\langle x, y|\exp(-\beta\hat{H}_t)|x', y'\rangle$ may be expanded in terms of the coherent states as

$$\langle x, y|\exp(-\beta\hat{H}_t)|x', y'\rangle = \pi^{-2}\iiiint d^2\alpha_1\, d^2\alpha_2 \times \langle x, y|\exp(-\beta\hat{H}_1)\exp(-\beta\hat{H}_2)\exp(-\beta\hat{H}_L)|\alpha_1\alpha_2\rangle\langle\alpha_1\alpha_2|x', y'\rangle. \tag{3.12}$$

Here $|\alpha_1, \alpha_2\rangle$ is a simultaneous, normalised eigenket of $\hat{a}_1$ and $\hat{a}_2$:

$$\hat{a}_i|\alpha_1, \alpha_2\rangle = \alpha_i|\alpha_1, \alpha_2\rangle \qquad (i=1,2) \qquad \langle\alpha_1, \alpha_2|\alpha_1, \alpha_2\rangle = 1. \tag{3.13}$$

It may be readily verified that the operator $\exp(\theta\hat{A})$ again plays a role of the rotation operator in (α_1, α_2)-space with the following property:

$$\exp(\theta\hat{A})|\alpha_1, \alpha_2\rangle = B|\alpha_1', \alpha_2'\rangle \tag{3.14a}$$

$$\alpha_1' = \alpha_1\cos\theta + \alpha_2\sin\theta \qquad \alpha_2' = -\alpha_1\sin\theta + \alpha_2\cos\theta \tag{3.14b}$$

$$B = \exp[\tfrac{1}{2}(|\alpha_1'|^2 + |\alpha_2'|^2 - |\alpha_1|^2 - |\alpha_2|^2)]. \tag{3.14c}$$

Thus,

$$C_{12}(x, y; x'y'; \beta) = \langle x, y|\exp(-\beta\hat{H}_t)|x, 'y'\rangle = \pi^{-2}\exp(-\beta\hbar\omega')\iiiint F(\alpha_1, \alpha_2)\langle\alpha_1|x'\rangle\langle\alpha_2|y'\rangle\, d^2\alpha_1\, d^2\alpha_2 \tag{3.15a}$$

where

$$F(\alpha_1, \alpha_2) = \langle x, y|\exp(-\beta\hbar\omega'\hat{n}_1)\exp(-\beta\hbar\omega'\hat{n}_2)\exp(i\hbar\omega\hat{A})|\alpha_1, \alpha_2\rangle = B_1\langle x|\alpha_1'\rangle\langle y|\alpha_2'\rangle \tag{3.15b}$$

$$\alpha_1' = \alpha_1\cosh(\beta\hbar\omega) + i\alpha_2\sinh(\beta\hbar\omega) \qquad \alpha_2' = -i\alpha_1\sinh(\beta\hbar\omega) + \alpha_2\cosh(\beta\hbar\omega) \tag{3.15c}$$

$$B_1 = \exp[\tfrac{1}{2}(|\tilde{\gamma}\alpha_1|^2 + |\tilde{\gamma}\alpha_2|^2 - |\alpha_1|^2 - |\alpha_1|^2)] \tag{3.15d}$$

$$\tilde{\gamma} = \exp(-\beta\hbar\omega'). \tag{3.15e}$$

In the course of the above calculation the relation (2.8) is utilised. Carrying out the integration (3.15*a*), which is a repetition of the Gaussian integrals, one will easily be led to the same result as that given in equation (3.15) of I. One might think that the procedure would be somewhat tedious compared with the previous procedure (3.10*a*)-(3.11). Actually, however, the amount of trouble that one has to take is much the same in the both procedures. Also one should notice that the procedure described here directly leads to the result, without preliminary knowledge of the density matrix for the simple harmonic oscillator.

Method 2. This method is based on an alternative factorisation of $\exp(-\beta\hat{H})$ described below.

Let $\hat{T}$ be an operator defined by

$$\hat{T}=\exp(-\mathrm{i}\hat{a}_1\hat{a}_2^\dagger)\exp(-\tfrac{1}{2}\mathrm{i}\hat{a}_1^\dagger\hat{a}_2). \tag{3.16}$$

It can easily be verified that

$$\begin{aligned}\hat{T}^{-1}\hat{a}_1\hat{T}&=\hat{a}_1-\tfrac{1}{2}\mathrm{i}\hat{a}_2 \qquad & \hat{T}^{-1}\hat{a}_1^\dagger\hat{T}&=\tfrac{1}{2}\hat{a}_1^\dagger+\mathrm{i}\hat{a}_2^\dagger\\ \hat{T}^{-1}\hat{a}_2\hat{T}&=-\mathrm{i}\hat{a}_1+\tfrac{1}{2}\hat{a}_2 \qquad & \hat{T}^{-1}\hat{a}_2^\dagger\hat{T}&=\tfrac{1}{2}\mathrm{i}\hat{a}_1^\dagger+\hat{a}_2^\dagger.\end{aligned} \tag{3.17}$$

Thus the Hamiltonian $\hat{H}_\mathrm{t}$ can now be rewritten as

$$\hat{H}_\mathrm{t}=\hat{T}(\hat{H}_1'+\hat{H}_2')\hat{T}^{-1} \tag{3.18}$$

where

$$\hat{H}_i'=\hbar\Omega_i(\hat{n}_i+\tfrac{1}{2}) \qquad (i=1,2) \tag{3.19a}$$

$$\Omega_1=\omega'+\omega \qquad \Omega_2=\omega'-\omega. \tag{3.19b}$$

It immediately follows that

$$\exp(-\beta\hat{H}_\mathrm{t})=\hat{T}\exp(-\beta\hat{H}_1)\exp(-\beta\hat{H}_2)\hat{T}^{-1} \tag{3.20}$$

from which one can express $C_{12}(x,y;x'y';\beta)$ as

$$\begin{aligned}C_{12}(x,y;x'y';\beta)&\\ &=\langle x,y|\hat{T}\exp(-\beta\hat{H}_1)\exp(-\beta\hat{H}_2)\hat{T}^{-1}|x',y'\rangle\\ &=\pi^{-2}\exp(-\beta\hbar\omega')\iiiint \mathrm{d}^2\alpha_1\,\mathrm{d}^2\alpha_2\langle x,y|\Phi(\alpha_1,\alpha_2)\rangle\\ &\quad\times\langle\Phi'(\alpha_1,\alpha_2)|x',y'\rangle\end{aligned} \tag{3.21}$$

where

$$\begin{aligned}|\Phi(\alpha_1,\alpha_2)\rangle&=\hat{T}\exp(-\tfrac{1}{2}\beta\hbar\Omega_1\hat{n}_1)\exp(-\tfrac{1}{2}\beta\hbar\Omega_2\hat{n}_2)|\alpha_1,\alpha_2\rangle\\ &=\exp(b)|(\gamma_1\alpha_1-\tfrac{1}{2}\mathrm{i}\gamma_2\alpha_2),-\mathrm{i}(\gamma_1\alpha_1+\tfrac{1}{2}\mathrm{i}\gamma_2\alpha_2)\rangle\end{aligned} \tag{3.22a}$$

$$b=|\gamma_1\alpha_1|^2+\tfrac{1}{4}|\gamma_2\alpha_2|^2-\tfrac{1}{2}(|\alpha_1|^2+|\alpha_2|^2) \tag{3.22b}$$

$$\begin{aligned}|\Phi'(\alpha_1,\alpha_2)\rangle&=\hat{T}^{-1}\exp(-\tfrac{1}{2}\beta\hbar\Omega_1\hat{n}_1)\exp(-\tfrac{1}{2}\beta\hbar\Omega_2\hat{n}_2)|1,2\rangle\\ &=\exp(b')|(\tfrac{1}{2}\gamma_1\alpha_1-\mathrm{i}\gamma_2\alpha_2),-\mathrm{i}(\tfrac{1}{2}\gamma_1\alpha_1+\mathrm{i}\gamma_2\alpha_2)\rangle\end{aligned} \tag{3.23a}$$

$$b'=\tfrac{1}{4}|\gamma_1\alpha_1|^2+|\gamma_2\alpha_2|^2-\tfrac{1}{2}(|\alpha_1|^2+|\alpha_2|^2) \tag{3.23b}$$

$$\gamma_1=\exp(-\tfrac{1}{2}\beta\hbar\Omega_1) \qquad \gamma_2=\exp(-\tfrac{1}{2}\beta\hbar\Omega_2). \tag{3.24}$$

Here use is made of formula

$$\exp(\lambda\hat{a}_i^\dagger)|\alpha_i\rangle=\exp[\tfrac{1}{2}(|\alpha_i+\lambda|^2-|\alpha_i|^2)]|\alpha_i+\lambda\rangle \tag{3.25}$$

The integration appearing in (3.21) is again reduced to the Gaussian integrals and one eventually has the result which exactly coincides with equation (3.16) of I.

As far as the evaluation of the density matrix is concerned, method 2 seems to be less simple. However, method 2 has another merit. If $|n_1, n_2\rangle$ is an orthonormal eigenket of $H_1' + H_2'$ satisfying

$$(\hat{H}_1' + \hat{H}_2')|n_1, n_2\rangle = \hbar[\Omega_1(n_1+\tfrac{1}{2}) + \Omega_2(n_2+\tfrac{1}{2})]|n_1, n_2\rangle \tag{3.26}$$

one has from (3.18)

$$\hat{H}_t\hat{T}|n_1, n_2\rangle = \hbar[\Omega_1(n_1+\tfrac{1}{2}) + \Omega_2(n_2+\tfrac{1}{2})]\hat{T}|n_1, n_2\rangle. \tag{3.27}$$

Since the eigenkets $|n_1, n_2\rangle$ form a complete set, (3.27) clearly tells us that the eigenvalue of $\hat{H}_t$ is given by

$$E_{n_1,n_2} = \hbar[\Omega_1(n_1+\tfrac{1}{2}) + \Omega_2(n_2+\tfrac{1}{2})] \tag{3.28}$$

and the corresponding eigenkets can be expressed as

$$|\Psi_{n_1,n_2}\rangle = c_N\hat{T}|n_1, n_2\rangle \tag{3.29}$$

c_N being the normalisation constant which may again be determined using the coherent states.

As to the more general problem in which the oscillator is anisotropic, one can utilise the factorisation procedure of $\exp(-\beta\hat{H})$ developed in I. Its translation into the language of the creation and annihilation operators is easy if one uses various transformation properties of operators such as, for example,

$$\begin{aligned}\hat{x}_i &= (\hbar/2m\omega_i)^{1/2}(\hat{a}_i^\dagger + \hat{a}_i)\\ &= (\hbar/2m\omega_i)^{1/2}\exp(\hat{a}_i^2/2)\hat{a}_i^\dagger\exp(-\hat{a}_i^2/2)\end{aligned} \tag{3.30a}$$

$$\begin{aligned}\hat{p}_i &= \mathrm{i}(m\hbar\omega_i/2)^{1/2}(\hat{a}_i^\dagger - \hat{a}_i)\\ &= \mathrm{i}(m\hbar\omega_i/2)^{1/2}\exp(-\hat{a}_i^2/2)\hat{a}_i^\dagger\exp(\hat{a}_i^2/2).\end{aligned} \tag{3.30b}$$

After the factorisation is achieved, the calculation is similar to that of method 2 described above, except for some additional complexity coming from the anisotropic nature of the problem. The result, of course, coincides with that given in (3.31)-(3.35*d*) of I.

4. Supplementary remarks

An ingenious alternative way to evaluate the canonical density matrix for a simple harmonic oscillator has been proposed by Kubo (1955, 1964). According to Kubo the canonical density matrix can be evaluated in the following way:

$$\langle x+\tfrac{1}{2}\eta|\exp(-\beta\hat{H})|x-\tfrac{1}{2}\eta\rangle = (2\pi\hbar)^{-1}\int_{-\infty}^{\infty} G(\xi, \eta)\exp(-\mathrm{i}\xi x/\hbar)\,\mathrm{d}\xi \tag{4.1}$$

where

$$G(\xi, \eta) = \mathrm{Tr}\{\exp(-\beta\hat{H})\exp[\mathrm{i}(\xi\hat{x} + \eta\hat{p})/\hbar]\}. \tag{4.2}$$

The function $G(\xi, \eta)$ is closely related to the Wigner distribution function $W(x, p)$ (Wigner 1932, Moyal 1949) because the latter can be written as

$$W(x, p) = (2\pi\hbar)^{-2}\iint_{-\infty}^{\infty} G(\xi, \eta)\exp[-\mathrm{i}(\xi x + \eta p)/\hbar]\,\mathrm{d}\xi\,\mathrm{d}\eta. \tag{4.3}$$

Thus, the evaluation of $G(\xi, \eta)$ is important for obtaining the Wigner distribution function as well.

For the harmonic oscillator, (4.2) can be expressed in terms of the operators $\hat{a}$ and $\hat{a}^{+}$ as

$$G(\xi, \eta)=\exp[(|\lambda|^2-\beta\hbar\omega)/2]A(\xi, \eta) \tag{4.4a}$$

$$A(\xi, \eta)=\mathrm{Tr}[\exp(\mathrm{i}\lambda^*\hat{a}^{+})\exp(-\beta h\omega\hat{n})\exp(\mathrm{i}\lambda\hat{a})] \tag{4.4b}$$

where

$$\lambda=(2m\hbar\omega)^{-1/2}\xi-\mathrm{i}(m\omega/2\hbar)^{1/2}. \tag{4.4c}$$

In deriving (3.4a–c) use is made of the Glauber identity

$$\exp(\hat{A}+\hat{B})=\exp(\hat{A})\exp(-[\hat{A}, \hat{B}]/2) \tag{4.5}$$

which is valid for operators satisfying

$$[\hat{A}, [\hat{A}, \hat{B}]]=[\hat{B}, [\hat{A}, \hat{B}]]=0.$$

In Kubo's original treatment (Kubo 1955, 1964), the trace calculation of $A(\xi, \eta)$ is carried out on the basis of the eigenfunctions of $\hat{H}$. Naturally it includes an evaluation of the sum of a series, which needs some skill.

For the coherent states, on the other hand, the evaluation of the diagonal matrix elements of the quantity appearing in (3.4b) is a simple matter and the operation to get the trace is an integral calculation:

$$\mathrm{Tr}[\hat{F}]=(1/\pi)\iint\langle\alpha|\hat{F}|\alpha\rangle\,\mathrm{d}^2\alpha. \tag{4.6}$$

Accordingly, one can expect that the use of the coherent states makes the evaluation of the right-hand side of (4.4b) quite easy. In fact,

$$\begin{aligned}A(\xi, \eta)&=(1/\pi)\iint\langle\alpha|\exp(\mathrm{i}\lambda^*\hat{a}^{+})\exp(-\beta\hbar\omega\hat{n})\exp(\mathrm{i}\lambda\hat{a})|\alpha\rangle\,\mathrm{d}^2\alpha\\&=(1/\pi)\iint\exp[\mathrm{i}(\lambda\alpha+\lambda^*\alpha^*)]\langle\alpha|\exp(-\beta\hbar\omega\hat{n})|\alpha\rangle\,\mathrm{d}^2\alpha\\&=(1/\pi)\iint\exp[-(1-\gamma^2)|\alpha|^2+\mathrm{i}(\lambda\alpha+\lambda^*\alpha^*)]\,\mathrm{d}^2\alpha\end{aligned} \tag{4.7a}$$

where

$$\gamma=\exp(-\tfrac{1}{2}\beta\hbar\omega). \tag{4.7b}$$

If one expresses the last integral of (4.7a) in terms of the real and imaginary parts of α, it can be reduced to a product of two Gauss integrals, which immediately leads to the result

$$A(\xi, \eta)=(1-\gamma^2)^{-1}\exp[-|\lambda|^2/(1-\gamma^2)]. \tag{4.8}$$

As expected, the use of the coherent states certainly makes the calculation easy and elementary. A reason for the usefulness of coherent states in the quantum optics will surely be in the simplicity of this kind of calculation although physically their meaning as the states representing wavepackets with minimum uncertainty is more important.

Now, substituting (4.8) into (4.4a) and using relations (2.15a–c), one has

$$G(\xi, \eta)=[2\sinh(\beta\hbar\omega/2)]^{-1}\exp[-\coth(\beta\hbar\omega/2)(\xi^2+m^2\omega^2\eta^2)/(4m\hbar\omega)]. \tag{4.9}$$

The substitution of (4.9) into (4.1) again yields the same result as that given in (2.16). As a by-product one also obtains

$$W(x, p) = (\omega/\pi)C \exp[-(C/2m)(p^2 + m^2\omega^2x^2)] \tag{4.10a}$$

where

$$C = \tanh(\tfrac{1}{2}\beta\hbar\omega)/(\hbar\omega). \tag{4.10b}$$

5. Conclusion

In preceding sections we have developed an alternative method of evaluating the canonical density matrix for a simple harmonic oscillator and extended it to the same problem for an oscillator in a magnetic field, based on the creation and annihilation operator formalism.

Needless to say, the canonical density matrix is of fundamental importance in describing the properties of an assembly of independent particles moving in an effective potential field. One should also notice that once the canonical density matrix is given, one can immediately obtain the propagator simply by replacing β by a pure imaginary $\mathrm{i}t/\hbar$. On the other hand, it is virtually impossible to exhaust the examples of the systems which can exactly or approximately be described as an assembly of the harmonic oscillators. Thus, the evaluation of the canonical density matrix of the harmonic oscillator is an important basis of the quantum statistical mechanics.

In the author's view, it is always instructive to look at such a fundamental problem under various lights. It will particularly be true from the pedagogical point of view. For this reason, the present method will still deserve to be recorded although a number of ways have already been proposed (Kubo 1955, Feynman *et al* 1965, Wang 1987, Parisi 1988, Yonei 1989) to evaluate the canonical density matrix for the harmonic oscillator since the pioneer work by Husimi (Husimi 1940, see also Ishihara 1971 for a detailed calculation).

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Appendix. Alternative methods of evaluating the Gauss integral

In this appendix we give alternative ways to derive the formula of the Gauss integral,

$$A = \int_0^\infty \exp(-x^2)\,\mathrm{d}x = \tfrac{1}{2}\sqrt{\pi} \tag{A1}$$

which plays an important role in the evaluation of the canonical density matrix of a harmonic oscillator as well as other problems in mathematical physics.

(i) It is easy to see that

$$\int_0^\infty \exp[-(1+\alpha^2)t]\,\mathrm{d}t = (1+\alpha^2)^{-1} \tag{A2}$$

from which it immediately follows that

$$I=\int_0^\infty \mathrm{d}\alpha \int_0^\infty \exp[-(1+\alpha^2)t]\,\mathrm{d}t=\int_0^\infty (1+\alpha^2)^{-1}\,\mathrm{d}\alpha=\pi/2. \tag{A3}$$

Changing the order of integration in (A3), one has

$$I=\int_0^\infty \exp(-t)\,\mathrm{d}t \int_0^\infty \exp(-t\alpha^2)\,\mathrm{d}\alpha=\pi/2. \tag{A4}$$

Since

$$\int_0^\infty \exp(-t\alpha^2)\,\mathrm{d}\alpha=t^{-1/2}A \tag{A5}$$

one has

$$I=A\int_0^\infty t^{-1/2}\exp(-t)\,\mathrm{d}t=2A\int_0^\infty \exp(-s^2)\,\mathrm{d}s=2A^2 \tag{A6}$$

which immediately leads to the result (A1).

(ii) Consider the following integral:

$$J=\int_{-\infty}^{\infty} \exp(-x^2-\mathrm{i}xt)\,\mathrm{d}x$$

$$=\exp(-t^2/4)\int_{-\infty}^{\infty} \exp[-(x+\mathrm{i}t/2)^2]\,\mathrm{d}x=2A\exp(-t^2/4) \tag{A7}$$

where x and t being real variables.

Integrating each side with respect to t, one has

$$K=\int_{-\infty}^{\infty} \mathrm{d}t \int_{-\infty}^{\infty} \exp(-x^2-\mathrm{i}xt)\,\mathrm{d}x=8A^2. \tag{A8}$$

The change of the integration order yields

$$K=\int_{-\infty}^{\infty} \exp(-x^2)\,\mathrm{d}x \int_{-\infty}^{\infty} \exp(-\mathrm{i}xt)\,\mathrm{d}t=2\pi\int_{-\infty}^{\infty} \exp(-x^2)\delta(x)\,\mathrm{d}x=2\pi. \tag{A9}$$

From (A8) and (A9) one immediately obtains the result (A1).

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