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An operator method of evaluating the Bloch density matrix for an oscillator in a constant magnetic field

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Abstract. A new method is proposed in evaluating the Bloch density matrix for a three-dimensional charged harmonic oscillator placed in a constant magnetic field. The method first reduces the operator exp $(-\beta\hat{H})$ to a product of several factors of a simple nature by using the commutation relations among the Hamiltonian components and by performing some transformations on the Hamiltonian, and then calculates the matrix element. The method is especially efficient when the system has a rotational symmetry around the axis parallel to the magnetic field, but it is also useful in other cases. A generalised problem in which a uniform electric field coexists is also discussed.

To make the whole discussion consistent, the density matrix for a one-dimensional harmonic oscillator, which plays an essential role in the whole problem, is recalculated in the spirit of this method, and it is shown that the present method derives the well known form of the Bloch density matrix for this system in a quite elementary way, without reference to any advanced knowledge of eigenfunctions.

1. Introduction

Recently considerable interest has arisen in the evaluation of the Bloch density matrix $\langle \boldsymbol{r}|\exp(-\beta\hat{H})|\boldsymbol{r}'\rangle$ for a three-dimensional charged oscillator placed in a constant magnetic field (March and Tosi 1985, Manoyan 1986, Glasser 1987, Habeeb 1987) as well as of the propagator $\langle \boldsymbol{r}|\exp(-\mathrm{i}Ht/\hbar)|\boldsymbol{r}'\rangle$ for the same system (Chen 1984, Davies 1985, Kokiantonis and Castrigiano 1985, Urrutia and Manterola 1986), which may be regarded as an analytic continuation of the Bloch density matrix with a pure imaginary β.

Of these previous calculations, March and Tosi solved the Bloch equation, making some modifications on the procedure developed by Sondheimer and Wilson (1951). Habeeb utilised the canonical transformation studied previously by Glas *et al* (1978). Urrutia and Manterola used the Schwinger action principle and all the others utilised the path integral method.

It is true that all of these treatments have their own merits, but it is also undeniable that they rely on somewhat oversophisticated techniques and need more or less involved manipulations. In this paper, therefore, we develop an alternative method which is much simpler than any of the previous treatments, both in principle and in practice.

In this method we first focus our attention on the operator $\exp(-\beta\hat{H})$ and try to reduce it to a product of several operators of simple nature, carefully keeping the characteristic features of the Hamiltonian in mind. Once this factorisation of the operator $\exp(-\beta\hat{H})$ is achieved, the evaluation of its matrix elements is a rather simple matter. For a general potential such a simple reduction will not necessarily be possible and one has to be satisfied with an approximation based on some expansion theorems such as Kubo's (1952). In the present problem, however, the Hamiltonian is simple enough and one can in fact achieve a simple factorisation of the operator $\exp(-\beta\hat{H})$, either by utilising the commutation relations among the Hamiltonian components or by making simple transformations. In certain situations the factorisation is even trivial from the commutability among components of the Hamiltonian.

In the following sections we describe the actual procedures to evaluate the Bloch density matrix according to this programme. As a first step, in the next section we apply the method to the evaluation of the Bloch density matrix for a simple harmonic oscillator, which plays an essential role in the subsequent calculations. This will also serve as an illustration of the characteristic features of the present method. In § 3 we deal with a three-dimensional charged harmonic oscillator placed in a uniform magnetic field. There one will see how simply and efficiently the present method can lead to the results. Section 4 deals with a generalised problem in which a constant electric field coexists with the magnetic field. Finally, in § 5 we give concluding remarks.

2. The Bloch density matrix for a simple harmonic oscillator

As will be seen in subsequent sections, the Bloch density matrix for a three-dimensional charged harmonic oscillator placed in a constant magnetic field can eventually be reduced to a product of the density matrices for simple (one-dimensional) harmonic oscillators. As a preliminary, therefore, in this section we evaluate the Bloch density matrix for a simple harmonic oscillator by an operator factorisation method. The reason why we take up this well known problem here is threefold: firstly, we want to deal with the whole problem in a unified and consistent way. Secondly, the basic ideas of the present method are most clearly exemplified in the treatment of this simple system. Thirdly, to the author's knowledge, the procedure described here cannot be found in the literature. Although a similar treatment has independently be done by Wang (1987), he utilised an advanced procedure, i.e. the Baker-Campbell-Hausdorf relations for the Lie algebras of SU(1, 1) derived by Fisher *et al* (1984) and Truax (1985), so that the present method would still be worth recording for its very elementary and simple character.

Now, the Hamiltonian of the system is given by

$$\hat{H} = (1/2m)(\hat{p}^2 + m^2\omega^2\hat{x}^2). \tag{2.1}$$

First we notice that by an operator

$$\hat{S} = \exp(-m\omega\hat{x}^2/2\hbar) \tag{2.2}$$

and its inverse $\hat{S}^{-1}$ the Hamiltonian $\hat{H}$ can be transformed into the following form:

$$\begin{aligned}\hat{H}' &= \hat{S}^{-1}\hat{H}\hat{S} \\ &= \hat{a} + \hat{b}\end{aligned} \tag{2.3}$$

where

$$\hat{a} = (1/2m)\hat{p}^2 \tag{2.4a}$$

and

$$\hat{b} = \tfrac{1}{2}\mathrm{i}\omega(\hat{x}\hat{p} + \hat{p}\hat{x}). \tag{2.4b}$$

One of the simplest ways to get the right-hand side of (2.3) will be the use of the formula

$$\exp(\tau\hat{A})\hat{B}\exp(-\tau\hat{A}) = \sum_{n=0}^{\infty}\frac{\tau^n}{n!}\hat{C}_n \qquad (2.5a)$$

where

$$\hat{C}_0 = \hat{B} \qquad \hat{C}_n = [\hat{A}, \hat{C}_{n-1}] \qquad (n \geq 1) \qquad (2.5b)$$

(see, for example, Merzbacher 1970).

From (2.3) it immediately follows that

$$\begin{aligned}\exp(-\beta\hat{H}) &= \hat{S}\exp[-\beta(\hat{a}+\hat{b})]\hat{S}^{-1} \\ &= \exp(-m\omega\hat{x}^2/2\hbar)\exp[-\beta(\hat{a}+\hat{b})]\exp(m\omega\hat{x}^2/2\hbar). \qquad (2.6)\end{aligned}$$

A further factorisation is possible for $\exp[-\beta(\hat{a}+\hat{b})]$ as follows:

$$\exp[-\beta(\hat{a}+\hat{b})] = \exp(-\beta'\hat{a})\exp(-\beta\hat{b}) \qquad (2.7a)$$

where

$$\beta' = [\exp(2\beta\hbar\omega) - 1]/2\hbar\omega. \qquad (2.7b)$$

In fact, if we define $\hat{K}(\beta)$ by

$$\exp[-\beta(\hat{a}+\hat{b})] = \hat{K}(\beta)\exp(-\beta\hat{b}) \qquad (2.8)$$

and differentiate both sides of (2.8) with respect to β, we have

$$\begin{aligned}\mathrm{d}\hat{K}(\beta)/\mathrm{d}\beta &= -\hat{K}(\beta)\exp(-\beta\hat{b})\hat{a}\exp(\beta\hat{b}) \\ &= -\exp(2\beta\hbar\omega)\hat{K}(\beta)\hat{a}. \qquad (2.9)\end{aligned}$$

In deriving the last expression for the right-hand side of (2.9) the commutation relation between $\hat{a}$ and $\hat{b}$, i.e.

$$[\hat{a}, \hat{b}] = 2\hbar\omega\hat{a} \qquad (2.10)$$

as well as the formula (2.5a) are used. The solution of the differential equation (2.9) which fulfils the initial condition $\hat{K}(0) = 1$ is just the first factor of the right-hand side of (2.7a).

Thus, using (2.7a) and (2.7b), one obtains a full factorisation of $\exp(-\beta\hat{H})$ as

$$\exp(-\beta\hat{H}) = \exp(-m\omega\hat{x}^2/2\hbar)\exp(-\beta'\hat{p}^2/2m)\exp(-\beta\hat{b})\exp(m\omega\hat{x}^2/2\hbar). \qquad (2.11)$$

Now, the evaluation of the Bloch density matrix is quite straightforward:

$$\langle x|\exp(-\beta\hat{H})|x'\rangle = \exp[m\omega(x'^2 - x^2)/2\hbar]J \qquad (2.12a)$$

$$J = \int_{-\infty}^{\infty}\mathrm{d}p\langle x|\exp(-\beta'\hat{p}^2/2m)|p\rangle\langle p|\exp(-\beta\hat{b})|x'\rangle \qquad (2.12b)$$

where $|x\rangle$ and $|x'\rangle$ are the eigenkets of $\hat{x}$ belonging to eigenvalues x and x', respectively, while $|p\rangle$ is the eigenket of $\hat{p}$ belonging to the eigenvalue p. The integrand of (2.12b) can be written in a simple form if one notes that the operator $\exp(-\beta\hat{b})$ is a scale change operator with the following property (see (B.12) of Kirzhnits (1967)):

$$\exp(-\beta\hat{b})|x'\rangle = \exp(\beta\hbar\omega/2)|x''\rangle \qquad (\text{for any } |x'\rangle) \qquad (2.13a)$$

where $|x''\rangle$ is the normalised eigenket of $\hat{x}$ belonging to the eigenvalue x'' given by

$$x'' = \exp(\beta\hbar\omega)x'. \qquad (2.13b)$$

Using the relation (2.13b) the integral J becomes

$$J = \exp(\beta\hbar\omega/2) \int_{-\infty}^{\infty} \exp(-\beta' p^2/2m)\langle x|p\rangle\langle p|x''\rangle \, dp$$

$$= (2\pi\hbar)^{-1} \exp(\beta\hbar\omega/2) \int_{-\infty}^{\infty} \exp\{-(\beta'/2m)p^2$$

$$+ (i/\hbar)[x - x' \exp(\beta\hbar\omega)]p\} \, dp$$

$$= [m\omega/2\pi\hbar \sinh(\beta\hbar\omega)]^{1/2} \exp\{-m\omega[x - x' \exp(\beta\hbar\omega)]^2$$

$$\times \exp(-\beta\hbar\omega)/2\hbar \sinh(\beta\hbar\omega)\}. \tag{2.14}$$

Substituting this into (2.12a) we finally obtain

$$\langle x|\exp(-\beta\hat{H})|x'\rangle = A \exp\{-[c_1(x+x')^2 + c_2(x-x')^2]\} \tag{2.15a}$$

where

$$A = [m\omega/2\pi\hbar \sinh(\beta\hbar\omega)]^{1/2} \tag{2.15b}$$

$$c_1 = (m\omega/4\hbar) \tanh(\beta\hbar\omega/2) \tag{2.15c}$$

$$c_2 = (m\omega/4\hbar) \coth(\beta\hbar\omega/2). \tag{2.15d}$$

This is the familar form of the Bloch density matrix for a simple harmonic oscillator first given in the pioneering work of Husimi (1940). It is very characteristic of the present method that it can derive the above result using only commutator algebras and elementary integrations, without any explicit reference to the eigenfunctions of $\hat{H}$, in contrast to the conventional method.

3. The Bloch density matrix for a charged oscillator in a constant magnetic field

Consider a three-dimensional harmonic oscillator with an electric charge e placed in a constant magnetic field of strength $\mathcal{H}$. The direction of the magnetic field is assumed to be parallel to one of the principal axes of the oscillator, say the z axis, so that the vector potential may be taken as

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

The general cases in which the magnetic field is not necessarily parallel to one of the principal axes of the oscillator will be left for future work. With this choice of the vector potential, the Hamiltonian of the system may be written as

$$\hat{H} = (1/2m)(\hat{p} - e\hat{A}/c)^2 + \tfrac{1}{2}m(\omega_1^2\hat{x}^2 + \omega_2^2\hat{y}^2 + \omega_3^2\hat{z}^2)$$

$$= \hat{H}_t + \hat{H}_z \tag{3.2}$$

$$\hat{H}_t = \hat{H}_x + \hat{H}_y - \omega\hat{L}_z \tag{3.3}$$

$$\hat{H}_x = (1/2m)\hat{p}_x^2 + \tfrac{1}{2}m\omega_1'^2\hat{x}^2 \tag{3.4a}$$

$$\hat{H}_y = (1/2m)\hat{p}_y^2 + \tfrac{1}{2}m\omega_2'^2\hat{y}^2 \tag{3.4b}$$

$$\hat{H}_z = (1/2m)\hat{p}_z^2 + \tfrac{1}{2}m\omega_3^2\hat{z}^2 \tag{3.4c}$$

where

$$\omega = e\mathscr{H}/2mc \qquad \omega_i' = (\omega_i^2 + \omega^2)^{1/2} \qquad (i = 1, 2) \tag{3.5a}$$

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x. \tag{3.5b}$$

Clearly, $\hat{H}_z$ commutes with any one of $\hat{H}_x$, $\hat{H}_y$ and $\hat{L}_z$, so that we have

$$\exp(-\beta\hat{H}) = \exp(-\beta\hat{H}_t)\exp(-\beta\hat{H}_z). \tag{3.6}$$

For a further reduction of the right-hand side of (3.6) it will be convenient to divide the problem into two cases: case (a) in which $\omega_1 = \omega_2$ and case (b) in which $\omega_1 \neq \omega_2$.

3.1. Case (a): $\omega_1 = \omega_2 = \omega_0$

In this case the present method becomes particularly simple. Obviously

$$[\hat{H}_x, \hat{H}_y] = 0. \tag{3.7}$$

Also, since the harmonic oscillator potential has a rotational symmetry about the z axis,

$$[(\hat{H}_x + \hat{H}_y), \hat{L}_z] = 0. \tag{3.8}$$

Using these facts, one can immediately decompose $\exp(-\beta\hat{H}_t)$ as

$$\exp(-\beta\hat{H}_t) = \exp(-\beta\hat{H}_x)\exp(-\beta\hat{H}_y)\exp(\beta\omega\hat{L}_z) \tag{3.9}$$

which yields

$$\exp(-\beta\hat{H}) = \exp(-\beta\hat{H}_x)\exp(-\beta\hat{H}_y)\exp(-\beta\hat{H}_z)\exp(\beta\omega\hat{L}_z). \tag{3.10}$$

To evaluate the Bloch density matrix $\langle \boldsymbol{r}|\exp(-\beta\hat{H})|\boldsymbol{r}'\rangle$, recall that for a real parameter θ the operator $\exp(\mathrm{i}\theta\hat{L}_z/\hbar)$ represents a rotation around the z axis through an angle θ and has the following property:

$$\exp(\mathrm{i}\theta\hat{L}_z/\hbar)|\boldsymbol{r}\rangle = |\boldsymbol{r}''\rangle \qquad \text{for any } |\boldsymbol{r}\rangle = |x\rangle|y\rangle|z\rangle \tag{3.11a}$$

where

$$|\boldsymbol{r}''\rangle = |x''\rangle|y''\rangle|z''\rangle \tag{3.11b}$$

$$x'' = x\cos\theta + y\sin\theta \qquad y'' = -x\sin\theta + y\cos\theta \qquad z'' = z. \tag{3.11c}$$

Here the kets $|x''\rangle$, $|y''\rangle$ and $|z''\rangle$ as well as $|x\rangle$, $|y\rangle$ and $|z\rangle$ are normalised eigenvectors of $\hat{x}$, $\hat{y}$ and $\hat{z}$ belonging to the eigenvalues denoted in $|\ \rangle$. Note that the relation given by (3.11a)-(3.11c) hold even when θ becomes pure imaginary. Substituting $\theta = -\mathrm{i}\hbar\beta\omega$ into (3.11a)-(3.11c), we have

$$\exp(\beta\omega\hat{L}_z)|\boldsymbol{r}'\rangle = |\boldsymbol{r}''\rangle = |x''\rangle|y''\rangle|z''\rangle \tag{3.12a}$$

$$\begin{aligned} x'' &= x'\cosh(\beta\hbar\omega) - \mathrm{i}y'\sinh(\beta\hbar\omega) \\ y'' &= y'\cosh(\beta\hbar\omega) + \mathrm{i}x'\sinh(\beta\hbar\omega) \\ z'' &= z'. \end{aligned} \tag{3.12b}$$

With the help of (3.12a), we can obtain

$$\langle \boldsymbol{r}|\exp(-\beta\hat{H})|\boldsymbol{r}'\rangle = \langle x|\exp(-\beta\hat{H}_x)|x''\rangle\langle y|\exp(-\beta\hat{H}_y)|y''\rangle\langle z|\exp(-\beta\hat{H}_z|z''\rangle. \tag{3.13}$$

Clearly each factor of the right-hand side of (3.13) is the Bloch density matrix for a linear harmonic oscillator of the form of (2.15a). A straightforward calculation yields

$$\langle \boldsymbol{r}|\exp(-\beta\hat{H})|\boldsymbol{r}'\rangle = C_{12}(x, y; x', y'; \beta)C_3(z; z'; \beta) \tag{3.14}$$

where

$$\begin{aligned} C_{12}(x, y; x'y'; \beta) &= \langle x|\exp(-\beta\hat{H}_x)|x''\rangle\langle y|\exp(-\beta\hat{H}_y)|y''\rangle \\ &= [m\omega'/2\pi\hbar \sinh(\beta\hbar\omega')] \\ &\quad\times \exp\{-a_1[(x+x')^2+(y+y')^2] - a_2[(x-x')^2+(y-y')^2] - \mathrm{i}b(xy'-x'y)\} \end{aligned} \tag{3.15}$$

and

$$\begin{aligned} C_3(z, z'; \beta) &= \langle z|\exp(-\beta\hat{H}_z)|z'\rangle \\ &= [m\omega_3/2\pi\hbar \sinh(\beta\hbar\omega_3)]^{1/2}\exp\{-[c_1(z+z')^2 + c_2(z-z')^2]\}. \end{aligned} \tag{3.16}$$

The quantity ω' in (3.15) is defined as

$$\omega' = (\omega_0^2 + \omega^2)^{1/2} \tag{3.17}$$

and the coefficients in (3.15) and (3.16) are

$$a_1 = [m\omega'/4\hbar \sinh(\beta\hbar\omega')][\cosh(\beta\hbar\omega') - \cosh(\beta\hbar\omega)] \tag{3.18a}$$

$$a_2 = [m\omega'/4\hbar \sinh(\beta\hbar\omega')][\cosh(\beta\hbar\omega') + \cosh(\beta\hbar\omega)] \tag{3.18b}$$

$$b = m\omega' \sinh(\beta\hbar\omega)/\hbar \sinh(\beta\hbar\omega') \tag{3.18c}$$

$$c_1 = (m\omega_3/4\hbar)\tanh(\beta\hbar\omega_3/2) \tag{3.18d}$$

$$c_2 = (m\omega_3/4\hbar)\coth(\beta\hbar\omega_3/2). \tag{3.18e}$$

The expression (3.15) for $C_{12}(x, y; x'y'; \beta)$ exactly coincides with the result obtained by March and Tosi (1985). Also, if one rewrites (3.15) and (3.16) by using the cyclindrical coordinates and substitutes them into the expression (3.14), one will immediately be led to the result obtained by Manoyan (1986).

3.2. Case (b): $\omega_1 \neq \omega_2$

In this case the situation becomes somewhat complicated because $\hat{L}_z$ no longer commutes with $(\hat{H}_x + \hat{H}_y)$. But one can still reduce the operator $\exp(-\beta\hat{H}_t)$ into a product of simple factors by eliminating the $\hat{L}_z$ term included in $\hat{H}_t$ by an appropriate unitary transformation as below.

Let $\hat{U}_1(\theta_1)$, $\hat{U}_2(\theta_2)$ and $\hat{U}_A(\theta_1, \theta_2)$ be the operators defined by

$$\hat{U}_1(\theta_1) = \exp(-\mathrm{i}m\omega\theta_1\hat{x}\hat{y}/\hbar) \tag{3.19a}$$

$$\hat{U}_2(\theta_2) = \exp(-\mathrm{i}\theta_2\hat{p}_x\hat{p}_y/m\hbar\omega) \tag{3.19b}$$

$$\hat{U}_A(\theta_1, \theta_2) = \hat{U}_1(\theta_1)\hat{U}_2(\theta_2). \tag{3.19c}$$

The unitary operator $\hat{U}_A(\theta_1, \theta_2)$, together with its Hermitian conjugate $\hat{U}_A^\dagger(\theta_1, \theta_2)$, transforms $\hat{x}$, $\hat{y}$, $\hat{p}_x$ and $\hat{p}_y$ as

$$\hat{U}_A^\dagger \hat{x} \hat{U}_A = \hat{x} + (\theta_2/m\omega)\hat{p}_y \tag{3.20a}$$

$$\hat{U}_A^\dagger \hat{y} \hat{U}_A = \hat{y} + (\theta_2/m\omega)\hat{p}_x \tag{3.20b}$$

$$\hat{U}_A^\dagger \hat{p}_x \hat{U}_A = (1-\theta_1\theta_2)\hat{p}_x - m\omega\theta_1\hat{y} \tag{3.20c}$$

$$\hat{U}_A^\dagger \hat{p}_y \hat{U}_A = (1-\theta_1\theta_2)\hat{p}_y - m\omega\theta_1\hat{x}. \tag{3.20d}$$

With the choice of the values of θ_1 and θ_2 given by

$$\theta_1 = (\omega_2'^2 - \omega_1'^2 - S)/4\omega^2 \tag{3.21a}$$

$$\theta_2 = -2m\omega^2/S \tag{3.21b}$$

where S is defined as

$$S = \operatorname{sgn}(\omega_2'^2 - \omega_1'^2)[(\omega_2'^2 - \omega_1'^2)^2 + 8\omega^2(\omega_1'^2 + \omega_2'^2)]^{1/2} \tag{3.22}$$

it may readily be shown that $\hat{H}_t$ defined by (3.3a) can be transformed as

$$\hat{U}_A^\dagger \hat{H}_t \hat{U}_A = \hat{H}_1 + \hat{H}_2 \tag{3.23}$$

where

$$\hat{H}_1 = (1/2m_1)\hat{p}_x^2 + \tfrac{1}{2}m_1\Omega_1^2\hat{x}^2 \tag{3.24a}$$

$$m_1 = 2mS/[S + (\omega_2'^2 - \omega_1'^2) - 4\omega^2] \tag{3.24b}$$

$$\Omega_1^2 = \tfrac{1}{2}(\omega_1'^2 + \omega_2'^2 + 2\omega^2 - S) \tag{3.24c}$$

$$H_2 = (1/2m_2)\hat{p}_y^2 + \tfrac{1}{2}m_2\Omega_2^2\hat{y}^2 \tag{3.25a}$$

$$m_2 = 2mS/[S + (\omega_2'^2 - \omega_1'^2) + 4\omega^2] \tag{3.25b}$$

$$\Omega_2^2 = \tfrac{1}{2}(\omega_1'^2 + \omega_2'^2 + 2\omega^2 + S). \tag{3.25c}$$

Note that $\hat{H}_1$ and $\hat{H}_2$ commute with each other. Also, it can be shown that m_1, m_2, Ω_1^2 and Ω_2^2 are positive, provided that $\omega_1^2 = \omega_1'^2 - \omega^2 > 0$ and $\omega_2^2 = \omega_2'^2 - \omega^2 > 0$. If $\omega_i = 0$ ($i = 1, 2$), then $\Omega_i = 0$, but m_i remains positive. Thus, in an extended meaning, $\hat{H}_1$ and $\hat{H}_2$ are the Hamiltonians of two independent harmonic oscillators.

Clearly it follows from (3.23)-(3.25) that

$$\begin{aligned}\exp(-\beta\hat{H}_t) &= \hat{U}_A \exp[-\beta(\hat{H}_1 + \hat{H}_2)]\hat{U}_A^\dagger \\ &= \hat{U}_A \exp(-\beta\hat{H}_1)\exp(-\beta\hat{H}_2)\hat{U}_A^\dagger\end{aligned} \tag{3.26}$$

so that we have a full factorisation of $\exp(-\beta\hat{H})$ as

$$\exp(-\beta\hat{H}) = \hat{U}_A \exp(-\beta\hat{H}_1)\exp(-\beta\hat{H}_2)\hat{U}_A^\dagger \exp(-\beta\hat{H}_z). \tag{3.27}$$

The Bloch density matrix can now be written as

$$\langle \boldsymbol{r}|\exp(-\beta\hat{H})|\boldsymbol{r}'\rangle = C(x, y; x', y'; \beta)\langle z|\exp(-\beta\hat{H}_z)|z'\rangle \tag{3.28}$$

where

$$\begin{aligned}C(x, y; x', y'; \beta) &= \langle x|\langle y|\hat{U}_A \exp(-\beta\hat{H}_1)\exp(-\beta\hat{H}_2)\hat{U}_A^\dagger|x'\rangle|y'\rangle \\ &= \int\!\!\int\!\!\int\!\!\int_{-\infty}^{\infty} \mathrm{d}x_1\,\mathrm{d}y_1\,\mathrm{d}x_2\,\mathrm{d}y_2 \langle x, y|\hat{U}_A|x_1, y_1\rangle\langle x_1|\exp(-\beta\hat{H}_1)|x_2\rangle \\ &\quad \times \langle y_1|\exp(-\beta\hat{H}_2)|y_2\rangle\langle x_2, y_2|\hat{U}_A^\dagger|x', y'\rangle.\end{aligned} \tag{3.29}$$

The factors $\langle x_1|\exp(-\beta\hat{H}_1)|x_2\rangle$, $\langle y_1|\exp(-\beta\hat{H}_2)|y_2\rangle$ and $\langle z|\exp(-\beta\hat{H}_z)|z'\rangle$ on the right-hand side of (3.29) are again the density matrices for harmonic oscillators. The matrix elements of transformation operator can be evaluated as

$$\begin{aligned}\langle x, y|\hat{U}_A|x', y'\rangle &= \langle x|\langle y|\hat{U}_A|x'\rangle|y'\rangle \\ &= \exp(-\mathrm{i}m\omega\theta_1 xy/\hbar)\langle x, y|\exp(-\mathrm{i}\theta_2\hat{p}_x\hat{p}_y/m\hbar\omega)|x', y'\rangle \\ &= \exp(-\mathrm{i}m\omega\theta_1 xy/\hbar)\int_{-\infty}^{\infty}\int \mathrm{d}p_x\,\mathrm{d}p_y\,\exp(-\mathrm{i}\hbar\theta_2 p_x p_y/m\hbar\omega) \\ &\quad\times\langle x|p_x\rangle\langle y|p_y\rangle\langle p_x|x'\rangle\langle p_y|y'\rangle \\ &= (1/2\pi\hbar|B|)\exp[(-\mathrm{i}/\hbar B)(-Axy+xy'+x'y-x'y')] \end{aligned} \tag{3.30a}$$

where

$$A = 1-\theta_1\theta_2 \qquad B = -\theta_2/m\omega. \tag{3.30b}$$

Thus a straightforward calculation yields

$$\begin{aligned}\langle \boldsymbol{r}|\exp(-\beta\hat{H})|\boldsymbol{r}'\rangle &= C(x, y; x', y'; \beta)[m\omega_3/2\pi\hbar\sinh(\beta\hbar\omega_3)]^{1/2} \\ &\quad\times\exp\{-(m\omega_3/4\hbar)[\tanh(\beta\hbar\omega_3/2)(z+z')^2+\coth(\beta\hbar\omega_3/2)(z-z')^2]\}\end{aligned} \tag{3.31}$$

$$\begin{aligned}C(x, y; x'y'; \beta) &= M(\beta)\exp[-(\mathrm{i}A/\hbar B)(xy-x'y')]\exp[a(x+x')^2+a'(x-x')^2 \\ &\quad+b(y+y')^2+b'(y-y')^2+c(x+x')(y-y')+c'(x-x')(y+y')]\end{aligned} \tag{3.32}$$

where

$$M(\beta) = (2\pi\hbar m_1\Omega_1)^{-1}(m_1 m_2\Omega_1\Omega_2)^{1/2}[\gamma_1\gamma_1'\sinh(\beta\hbar\Omega_1)\sinh(\beta\hbar\Omega_2)]^{-1/2} \tag{3.33}$$

$$a = -(4\hbar\gamma_1)^{-1} \qquad a' = -(4\hbar\gamma_1')^{-1} \tag{3.34a}$$

$$b = -(4\hbar\gamma_2)^{-1} \qquad b' = -(4\hbar\gamma_2')^{-1} \tag{3.34b}$$

$$\begin{aligned}c &= \mathrm{i}\coth(\beta\hbar\Omega_1/2)/2m_1\Omega_1\hbar B\gamma_1 \\ c' &= \mathrm{i}\tanh(\beta\hbar\Omega_1/2)/2m_1\Omega_1\hbar B\gamma_1\end{aligned} \tag{3.34c}$$

$$\gamma_1 = \coth(\beta\hbar\Omega_1/2)/m_1\Omega_1 + m_2\Omega_2 B^2\coth(\beta\hbar\Omega_2) \tag{3.35a}$$

$$\gamma_1' = \tanh(\beta\hbar\Omega_1/2)/m_1\Omega_1 + m_2\Omega_2 B^2\tanh(\beta\hbar\Omega_2) \tag{3.35b}$$

$$\gamma_2 = \coth(\beta\hbar\Omega_2/2)/m_2\Omega_2 + m_1\Omega_1 B^2\coth(\beta\hbar\Omega_1) \tag{3.35c}$$

$$\gamma_2' = \tanh(\beta\hbar\Omega_2/2)/m_2\Omega_2 + m_1\Omega_1 B^2\tanh(\beta\hbar\Omega_1). \tag{3.35d}$$

To compare this result with those of previous studies, one may rewrite (3.32) in the following form:

$$\begin{aligned}C(x, y; x'y'; \beta) &= N(\beta)\exp\{(m/2\hbar D(\beta))[\alpha_1(x^2+x'^2)+\alpha_2(y^2+y'^2) \\ &\quad+\alpha_3 xx'+\alpha_4 yy'+\alpha_5(x'y-xy')+\alpha_6(xy-x'y')]\}.\end{aligned} \tag{3.36}$$

The calculated results for the coefficients α_1-α_6 as well as $N(\beta)$, $D(\beta)$ are in agreement with those obtained by Habeeb (1987) if one corrects unfortunate misprints found in his (24) and (25) by removing all the primes on ω_1' and ω_2' appearing there and by replacing $(\Omega_2^2-\Omega_1^2)$ in his expression for α_6 by $(\omega_1^2-\omega_2^2)$. Also, the coefficients correspond closely to those of the propagator obtained by Kokiantonis and Castrigiano (1985) and Urrutia and Manterola (1986).

In finishing this subsection it will be worth adding some comments. Essentially the same diagonalisation of $\hat{H}_t$ as given in (3.23) was achieved by Glas *et al* (1978) without explicit use of the transformation operators $\hat{U}_A$ and $\hat{U}_A^+$ (Habeeb (1987) utilised their result in his calculation of the density matrix). However, the use of the explicit form of the unitary transformation operators certainly makes the treatment of the problem easier and more transparent. The simplicity of the present method in the evaluation of the transformation function will suffice to see this (compare (3.30) with the derivation of (30) of Glas *et al* (1978)).

Also, it should be emphsasised that the above procedure for reducing $\exp(-\beta\hat{H})$ to a product of factors of a simple nature is not unique. For example, the same result can be attained by the use of $\hat{U}_B=\hat{U}_2\hat{U}_1$. There will be several other ways which lead to the equivalent result. Some of these will be reported elsewhere.

4. The case when a uniform electric field coexists

So far we have developed an operator method to evaluate the Bloch density matrix for an oscillator placed in a constant magnetic field. With a slight modification the same method can also be applicable to a generalised case in which a uniform electric field $\boldsymbol{E}(E_x, E_y, E_z)$ coexists.

The Hamiltonian now becomes

$$\hat{H}=\hat{H}_0(\hat{\boldsymbol{r}})+e\boldsymbol{E}\cdot\hat{\boldsymbol{r}} \tag{4.1a}$$

$\hat{H}_0(\hat{\boldsymbol{r}})$ being the Hamiltonian for zero electric field, i.e.

$$\hat{H}_0(\hat{\boldsymbol{r}})=(1/2m)[\hat{\boldsymbol{p}}-e\hat{\boldsymbol{A}}(\hat{\boldsymbol{r}})/c]^2+\tfrac{1}{2}m(\omega_1^2\hat{x}^2+\omega_2^2\hat{y}^2+\omega_3^2\hat{z}^2) \tag{4.1b}$$

and

$$\hat{\boldsymbol{A}}(\hat{\boldsymbol{r}})=(-\tfrac{1}{2}\mathcal{H}\hat{y},\tfrac{1}{2}\mathcal{H}\hat{x},0). \tag{4.1c}$$

If one defines a constant vector $\boldsymbol{r}_0$ by

$$\boldsymbol{r}_0=(x_0,y_0,z_0)=(-e/m)(E_x/\omega_1^2,E_y/\omega_2^2,E_z/\omega_3^2) \tag{4.2}$$

the Hamiltonian $\hat{H}$ may be rewritten as

$$\hat{H}=\hat{H}'-\tfrac{1}{2}m(\omega_1^2x_0^2+\omega_2^2y_0^2+\omega_3^2z_0^2) \tag{4.3}$$

where

$$\hat{H}'=(1/2m)[\hat{\boldsymbol{p}}-e\hat{\boldsymbol{A}}(\hat{\boldsymbol{r}})/c]^2+\tfrac{1}{2}m[\omega_1^2(\hat{x}-x_0)^2+\omega_2^2(\hat{y}-y_0)^2+\omega_3^2(\hat{z}-z_0)^2]. \tag{4.4}$$

Now it is easy to see that by a gauge transformation using the unitary operator $\hat{\Gamma}$ defined by

$$\hat{\Gamma}=\exp\left(-\mathrm{i}\frac{e\mathcal{H}}{2\hbar c}(y_0\hat{x}-x_0\hat{y})\right) \tag{4.5}$$

and its Hermitian conjugate $\hat{\Gamma}^{+}$, $\hat{H}'$ may be transformed as

$$\hat{\Gamma}^{+}\hat{H}'\hat{\Gamma} = (1/2m)[\hat{\boldsymbol{p}} - e\hat{\boldsymbol{A}}(\hat{\boldsymbol{r}} - \boldsymbol{r}_0)/c]^2 + \tfrac{1}{2}m[\omega_1^2(\hat{x} - x_0)^2 + \omega_2^2(\hat{y} - y_0)^2 + \omega_3^2(\hat{z} - z_0)^2]$$
$$= \hat{H}_0(\hat{\boldsymbol{r}} - \boldsymbol{r}_0). \tag{4.6}$$

Since $\hat{H}_0(\hat{\boldsymbol{r}} - \boldsymbol{r}_0)$ can be related to $\hat{H}_0(\hat{\boldsymbol{r}})$ by the displacement operator $\exp(\mathrm{i}\boldsymbol{r}_0 \cdot \hat{\boldsymbol{p}}/\hbar)$ as

$$\hat{H}_0(\hat{\boldsymbol{r}} - \boldsymbol{r}_0) = \exp(-\mathrm{i}\boldsymbol{r}_0 \cdot \hat{\boldsymbol{p}}/\hbar)\hat{H}_0(\hat{\boldsymbol{r}}) \exp(\mathrm{i}\boldsymbol{r}_0 \cdot \hat{\boldsymbol{p}}/\hbar) \tag{4.7}$$

it follows that

$$\hat{H} = \hat{\Gamma} \exp(-\mathrm{i}\boldsymbol{r}_0 \cdot \hat{\boldsymbol{p}}/\hbar)\hat{H}_0(\hat{\boldsymbol{r}}) \exp(\mathrm{i}\boldsymbol{r}_0 \cdot \hat{\boldsymbol{p}}/\hbar)\hat{\Gamma}^{+} + \tfrac{1}{2}m(\omega_1^2x_0^2 + \omega_2^2y_0^2 + \omega_3^2z_0^2). \tag{4.8}$$

Accordingly

$$\exp(-\beta\hat{H}) = \exp[-\beta m(\omega_1^2x_0^2 + \omega_2^2y_0^2 + \omega_3^2z_0^2)/2]$$
$$\times \hat{\Gamma} \exp(-\mathrm{i}\boldsymbol{r}_0 \cdot \hat{\boldsymbol{p}}/\hbar)\exp[-\beta\hat{H}_0(\hat{\boldsymbol{r}})]\exp(\mathrm{i}\boldsymbol{r}_0 \cdot \hat{\boldsymbol{p}}/\hbar)\hat{\Gamma}^{+} \tag{4.9}$$

which immediately leads to

$$\langle \boldsymbol{r}|\exp(-\beta\hat{H})|\boldsymbol{r}'\rangle$$
$$= \exp[-\beta m(\omega_1^2x_0^2 + \omega_2^2y_0^2 + \omega_3^2z_0^2)/2]$$
$$\times \exp\{-\mathrm{i}(m\omega/\hbar)[y_0(x - x') - x_0(y - y')]\}$$
$$\times \langle \boldsymbol{r} - \boldsymbol{r}_0|\exp[-\beta\hat{H}_0(\hat{\boldsymbol{r}})]|\boldsymbol{r}' - \boldsymbol{r}_0\rangle. \tag{4.10}$$

In deriving (4.10) use is made of the relation

$$\exp(\mathrm{i}\boldsymbol{r}_0 . \hat{\boldsymbol{p}}/\hbar)|\boldsymbol{r}\rangle = |\boldsymbol{r} - \boldsymbol{r}_0\rangle. \tag{4.11}$$

Since $\hat{H}_0(\hat{\boldsymbol{r}})$ is nothing other than the Hamiltonian of an oscillator in a constant magnetic field discussed before, the last factor on the right-hand side of (4.10) can be obtained from the results obtained in the preceding sections by a simple replacement $(\boldsymbol{r}, \boldsymbol{r}') \to (\boldsymbol{r} - \boldsymbol{r}_0, \boldsymbol{r}' - \boldsymbol{r}_0)$.

For an isotropic oscillator, in particular, $\langle \boldsymbol{r}|\exp[-\beta\hat{H}_0(\hat{\boldsymbol{r}})]|\boldsymbol{r}'\rangle$ is equal to what is given in (3.16) with an obvious replacement of ω_3 by ω_0. In this simple case, therefore, one has

$$\langle \boldsymbol{r}|\exp(-\beta\hat{H})|\boldsymbol{r}'\rangle$$
$$= A \exp(-\beta m\omega_0^2\boldsymbol{r}_0^2/2) \exp\{-\mathrm{i}(m\omega/\hbar)[y_0(x - x') - x_0(y - y_0)]\}$$
$$\times \exp\{-a_1[(x + x' - 2x_0)^2 + (y + y' - 2y_0)^2] - a_2[(x - x')^2 + (y - y')^2]$$
$$- \mathrm{i}b[(x - x_0)(y' - y_0) - (x' - x_0)(y - y_0)] - [c_1(z + z' - 2z_0)^2 + c_2(z - z')^2]\} \tag{4.12a}$$

where

$$\boldsymbol{r}_0 = (x_0, y_0, z_0) = (-e/m\omega_0^2)(E_x, E_y, E_z) \tag{4.12b}$$

and the coefficients are those given in (3.18a)-(3.18e). If one puts $\boldsymbol{E} = (0, 0, E)$, as a special case of (4.12a), one obtains

$$\langle \boldsymbol{r}|\exp(-\beta\hat{H})|\boldsymbol{r}\rangle$$
$$= A \exp(-\beta m\omega_0^2\boldsymbol{r}_0^2/2) \exp\{-a_1[(x + x')^2 + (y + y')^2]$$
$$- a_2[(x - x')^2 + (y - y')^2] - \mathrm{i}b(xy' - x'y)$$
$$- c_1[(z + z' - 2z_0)^2 + c_2(z - z')^2]\} \qquad z_0 = -eE/m\omega_0^2 \tag{4.13}$$

which is in agreement with (2) of Glasser (1987), except for the spin term included in it.

Similarly if one puts $\boldsymbol{E} = (E, 0, 0)$, one obtains

$$\begin{aligned}\langle \boldsymbol{r}|\exp(-\beta\hat{H})|\boldsymbol{r}'\rangle \\ &= A\exp(-\beta m\omega_0^2 x_0^2/2)\exp[(\mathrm{i}m\omega/\hbar)x_0 y] \\ &\quad\times\exp\{-a_1[(x+x'-2x_0)^2+(y+y')^2]-a_2[(x-x')^2+(y-y')^2] \\ &\quad -c_1[(z+z')^2+c_2(z-z')^2]\} \qquad x_0=-eE/m\omega_0^2.\end{aligned} \tag{4.14}$$

The expression (4.14) will be useful in the study of the effect of the transverse electric field on various physical systems which can be approximated by an isotropic oscillator model.

5. Conclusions

In the preceding sections we have developed a new method of evaluating the Bloch density matrices for a charged oscillator placed in uniform magnetic, and electric, fields and have seen that the present method brings about a remarkable simplification in the calculation of this quantity. Some new results have also been presented. Since one may formally regard the propagator $\langle \boldsymbol{r}|\exp(-\mathrm{i}\hat{H}t/\hbar)|\boldsymbol{r}'\rangle$ as the Bloch density matrix for a pure imaginary β, one can also use the present method in the evaluation of the propagator.

Needless to say, the Bloch density matrix is a quantity of fundamental importance in describing the properties of an assembly of independent particles moving in an effective potential field. In fact, once it is known, both the Dirac density matrix and the partition function for the independent fermions can be evaluated straightforwardly as the inverse Laplace transforms of either the Bloch density matrix itself or some function including it (Sondheimer and Wilson 1951, March and Murray 1960). Thus a great many problems can be reduced to the evaluation of the Bloch density matrix.

Since there are many systems which are well approximated by an assembly of independent oscillators, the present method and its results will usefully be applied to a variety of problems in nuclear and condensed matter physics as well as in atomic physics.

Apart from its actual applications, the harmonic oscillator is one of the rare examples of exactly solvable problems in quantum mechanics. Also, it has provided us with much information about essential features from the very early stage of quantum mechanics to the present day. It will always be useful to study such a fundamental problem from various points of view. We hope that in this meaning, too, the present study would give some contribution in casting light on a certain aspect of the oscillator problem.

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